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Contents

Five-day Workshop Reports

Chapter 1

Mathematics and physics of polymer entanglement: Emerging concepts and biomedical applications (10w5100)

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Introduction

This workshop focused on the mathematics associated with an array of cutting edge problems at the interface between the mathematical, physical, and biological sciences. In particular, the researchers targeted questions from work arising from molecular biology studies of DNA and other biopolymers for which an interdisciplinary approach could yield unique insights.

In the last decade or so, tremendous advances in the understanding of DNA behavior, including the effects of (i) storage (in viral capsids, eukaryotic nuclei, or bacterial cells), (ii) entanglement (knots and links), (iii) replication, (iv) transcription into RNA, and (v) repair and recombination (including site-specific and general), have been made at the hands of researchers working at the interface of mathematics, biology, and physics. Not only has the understanding of DNA as a biopolymer advanced rapidly, but emerging concepts have reached beyond the scope of DNA to a general understanding of the previously little-explored basic relationship between the local geometry of chain juxtaposition and global topology in polymer chains. Numerical simulations of lattice models as well as continuum freely-jointed and wormlike chain models demonstrated convincingly that the degree of 'hookedness' of an observed local juxtaposition correlates well with global topological complexity and the likelihood that a topoisomerase-like segment passage at the given juxtaposition would disentangle. This is a new paradigm opening up many avenues of computational and experimental research.

Moreover, these novel numerical results also serve to suggest a wealth of questions and conjectures that may be fruitfully addressed by field theory arguments from physics and by rigorous mathematics. Indeed, during the same time, we have noted a drastic increase in the precision in the language of biologists, with their incorporation of such important concepts as 'conjecture', 'hypothesis', and 'theory' following the traditional mathematical usage. An improved understanding of the languages of each of the three disciplines improves the communication, and as such, the understanding of each other. Increasing the awareness of mathematicians to (i) the complexity of the biological problems, as well as (ii) the cutting edge research results, even before they are published, facilitates an increased understanding of biopolymers, a primary goal of this workshop.

In the past, there have been efforts (such as the 2007 BIRS workshop 07w5095, The Mathematics of Knotting and Linking in Polymer Physics and Molecular Biology) to bring together researchers in these areas. Our goal was to include more Biologists/Experimentalists than before. As a result, this was the first opportunity for many of the invitees from different disciplines to meet each other. Thus the workshop enabled the advancement of existing collaborations at the interface between Biology, Mathematics and Physics and encouraged the development of new ones. The conference was timely for an additional important reason. Research funding for the pure mathematical and physical sciences has decreased recently. However, together with this troubling trend, there is an increase in funding opportunities for mathematicians and physicists working at the interface of the biological sciences, perhaps particularly in regard to medically relevant research.

Rich in important problems only answerable with an interdisciplinary approach, the study of DNA polymer science has had extraordinary successes quite recently, with the vast majority of these occurring at the interface of disciplines. Bringing a cadre of researchers working at the interface of polymer science to the Banff International Research Station for Mathematical Innovation and Discovery provided the opportunity to bridge these fields.

Presentations

A total of 35 researchers from Biology (12), Chemistry (1), Physics (7), Computer Science (1), and Mathematics (14) attended the meeting. This group was quite diverse. The participants had a mixture of experience, from grad students through senior professors; came from a wide-variety of institutions, from teaching colleges to research-intensive universities, medical schools, and government research institutes; and represented eight different countries.

The workshop had 28 presentations representing a wide body of interdisciplinary research on the DNA polymer. These can be categorized into roughly five areas: 1) linking number and supercoiling in DNA; 2) modeling polymers and entanglement; 3) confinement effects; 4) length effects; and 5) DNA sequence-specific effects and DNA replication factories. We introduce each of these topics and then discuss the presentations

Linking number and supercoiling in DNA

Recent emerging results have been made in all atom simulations of DNA. Whereas coarse-grained models have been extremely useful for understanding polymer behavior (for example, knotting, linking, and in general how they are packed into small spaces), the next series of questions must begin to include the surprising way that the change in linking number, Lk, is manifested in DNA. The observed bimodal response of DNA to Lk shows complete collapse of the DNA helix in sequence-dependent localized regions of the biopolymer with a concomitant relaxation back to B-form DNA in the rest of the biopolymer. At the same time, for the overwound helix, elastic polymer rod models work perfectly well. Mathematically and physically, this means, at least in the helix unwinding direction, that the assumptions of elastic rod theory are wrong and suggests that perhaps an asymmetric torsional potential would be physically more appropriate.

The workshop contained five talks on this subject.

Jonathan Fogg (Baylor College of Medicine, USA) spoke on *Supercoiling in DNA minicircles: To get the big picture, think small*. DNA supercoiling has a dramatic effect on its function. Indeed, for many biological processes a distinct threshold of supercoiling must be reached before the reaction can occur. Although the global conformational changes that occur as a result of supercoiling are reasonably well understood, relatively little is known about the consequences of DNA supercoiling on the local level. These sequence-specific conformational changes must surely dictate how proteins recognize and metabolize DNA. Even the largest DNA binding proteins are very small relative to chromosomal or plasmid DNA and are, therefore, unable to sense global DNA topology. Fogg, with his research group, developed and utilized a protocol to produce milligram quantities of supercoiled minicircle DNA, as small as 250 base pairs (bp). Individual topoisomers were isolated ranging from $\sigma = +0.08$ to -0.19. Their supercoiled minicircle substrates provide a unique insight into the local DNA structure of supercoiled DNA and how this is recognized and manipulated by enzymes. Several unexpected aspects of supercoiled DNA were revealed from their studies of DNA minicircles. They discovered that the addition or subtraction of three base pairs has a profound effect on the gel electrophoretic mobility of small DNA circles. The topoisomers of a 336 bp minicircle display a very regular pattern of electrophoretic mobility. When they generated topoisomers of 333 bp and 339 bp minicircles, however, several of these minicircles show unexpected electrophoretic behavior. They also discovered a topoisomer that appears to flip between open and writhed conformations, akin to the "frustrated" minicircles detected in their computational simulations. Notably, they found that positively supercoiled minicircles have a much higher propensity to writhe than negatively supercoiled minicircles, even in the absence of added divalent metal ions. In contrast, limited writhe was observed for negatively supercoiled minicircles in the absence of added divalent metal ions, demonstrating the importance of electrostatic effects on DNA structure. Many models of DNA elasticity incorrectly assume that positively supercoiled DNA is equal and opposite to negatively supercoiled DNA. Their findings prove there is a distinct asymmetry.

Sarah Harris (University of Leeds, England) spoke on *Computer Simulations of DNA Supercoiling at the Atomic Level*. The discovery of the structure of duplex DNA revealed how cells store genetic information. However, researchers are far from understanding the more complex biological question of how this information is regulated and processed by the cell. DNA topology and supercoiling is known to affect DNA transcription as changes in topology affect DNA conformation, and can thereby modify the interaction between regulatory DNA-binding proteins and their target sites. Small DNA circles offer a controllable model system for the systematic exploration of the dependence of DNA structure on supercoiling. Harris's research group uses computer simulation to explore the supercoiling-dependent conformation of small DNA circles, in particular their writhe, and how this is affected by supercoiling, salt concentration, DNA sequence and the size of the circles. The calculations use atomistic molecular dynamics simulation, and employ both implicit and explicit solvent models. They have been systematically testing their computational models against experimental data for small circles of between 65 and 214 bp. They have also been investigating the supercoiling-dependent binding of a 3rd DNA strand (triplex formation) to a target site within a writhed DNA circle for comparison with experimental data. These preliminary calculations are designed to explore the thermodynamics of supercoiling-dependent binding, and use triplex formation as a model system for exploring the importance of supercoiling in DNA recognition in general.

Steve Levene (University of Texas at Dallas, USA) spoke on *Loop-mediated regulation by lac repressor: does DNA supercoiling play a role?* Interactions of *E. coli* lac repressor (LacI) with a pair of operator sites on the same DNA molecule can lead to the formation of looped nucleoprotein complexes both *in vitro* and *in vivo*. The lac system is a major paradigm for loop-mediated gene regulation in prokaryotic cells; however, the complex interplay between DNA topology, modulation of chromosome topology by architectural-DNA binding proteins, and loop-mediated regulation remain poorly understood. Levene discussed the effects of DNA supercoiling on LacI mediated looping *in vitro* investigated by a combination of fluorescence resonance energy transfer studies, semi-analytical DNA elasticity calculations, and Monte Carlo simulation.

David Levens (Center for Cancer Research NIH, USA) spoke on *Genome-wide functional correlation between transcription, DNA conformation and topology*. His group is investigating the role of dynamic supercoiling in the regulation of gene expression and DNA structure *in vivo* and *in vitro*. They have developed a method to map unpaired bases across the genome using potassium permanganate. Besides the expected signature of transcription bubbles at promoters, other sites of non-B-DNA occurring outside of genes were often sensitive to transcription inhibition, suggesting a long-distance coupling between transcription and DNA conformation via transmission of mechanical stress (dynamic supercoils). Such stress is generated as DNA is threaded through the RNA polymerase active site and propagated to remote sequences. Supercoil sensitive unusual DNA structures may contribute to the real-time self-regulation of many genes. Previously his group has demonstrated the existence and measured the magnitude of such dynamical supercoils *in vivo*. Now, they have developed an approach to build a genome-scale map of DNA supercoiling using psoralen intercalation as a probe. The map shows that negative supercoiling often propagates to or beyond 2 kilobase (kb) upstream of active promoters. This supercoiling contributes to the formation of a variety of non-B DNAs, including quadruplex and Z-DNA. These non-B DNA structures may be recognized by proteins and contribute to a variety of control mechanisms. Overlaying the maps of DNA supercoiling and conformation with the *in vivo* binding sites of structure-sensitive transcription factors as well as sites of topoisomerase I and II action may reveal new modes of transcriptional regulation on a global scale.

Lynn Zechiedrich (Baylor College of Medicine, USA) spoke on *Supercoiled minicircles as gene therapy vectors*. To study DNA supercoiling and DNA topoisomerases, Zechiedrich's group created a way to make milligram quantities of minicircle DNAs of a few hundred base pairs. These DNAs have been extremely useful for this purpose and Fogg also discussed this work. Zechiedrich presented data showing that supercoiled minicircles are superior vectors for delivering DNA into human cell types that no other DNA vector has been previously able to penetrate. In cells, DNA sequence is transcribed from these minicircles into small RNAs that regulate gene expression. Even small genes can be expressed from supercoiled minicircles. Supercoiled minicircles resist sheer forces associated with gene therapy delivery and are significantly less susceptible to the nucleases in human serum than normal plasmid DNA vectors of a few thousand base pairs. These data show that supercoiled minicircles are a promising new tool for gene delivery.

Modeling polymers and entanglement

Developing and analyzing models of polymer and biopolymer entanglements is a multistage and interdisciplinary process. In order to be able to make direct quantitative comparisons with experiment, often polymer models must be highly complex and studied primarily by computer simulation. Such models are less likely to be mathematically tractable, however, and hence it is also often useful to investigate simplified polymer models with the goal of making qualitative comparisons with experiment. At the same time, defining and characterizing the nature of "entanglements" can raise questions of a purely mathematical nature. Thus to understand polymers such as DNA, a combination of efforts is necessary. As examples, researchers study individual polymers moving seemingly at random, such as wormlike rods and freely jointed chains, and collections of polymers, as in the case of chromosome territories (seen in the confinement section). These models provide a convenient framework for studying problems like the effect of local strand passages and the clasp conjecture for topoisomerase (i.e. that topoisomerase II acts preferentially at clasps). For example, one might use lattice polygons to study changes in knotting resulting from strand passage in certain configurations or pass to more topological methods using a tangle model. While researchers agree on what a knot is, there are subtleties concerning knot types such as chirality and orientation reversability, which become more problematic when one studies compositions of knots. The knot tables only tell part of the story, disregarding many of the properties of the actual configurations which become quite important in the physical world. These configurations hold other secrets as well, properties shared by all knotted configurations, such as quadrisecants, which can be studied using a combination of geometric and topological methods.

The workshop contained six talks on this subject.

Yitzhak Rabin (Bar-Ilan University, Israel) spoke on *Coupling of Twist and Writhe in Short DNA Rings*. While bending and twist can be treated as independent degrees of freedom for linear DNA molecules, the loop closure constraint introduces a coupling between these variables in circular DNA. Rabin performed Monte Carlo simulations of worm-like rods with both bending and twist rigidity, in order to study the coupling between the writhe and twist distributions for various DNA lengths. He found that for sufficiently short DNA, the writhe distribution differs significantly from that of a model with bending energy only and showed that the factorization approximation introduced by previous researchers coincides, within numerical accuracy, with his simulation results. Rabin concluded that the closure constraint is fully accounted for by the White-Fuller relation.

Hue Sun Chan (University of Toronto, Canada) spoke on *Selective Segment Passages at Hooked and Twisted Juxtapositions Consistently Rationalize the Decatenating, Unknotting and Supercoil-Tightening Actions of Type-2 Topoisomerases*. The mathematical basis of the hypothesis that type-2 topoisomerases recognize and act at specific DNA juxtapositions has been investigated by coarse-grained lattice polymer models, showing that selective segment passages at "hooked" juxtapositions can result in dramatic reductions in catenane and knot populations. The lattice modeling approach is now extended to account for the hallmark narrowing of variance of linking number (Lk) of DNA circles by type-2 topoisomerases. In general, the steady-state variance of Lk resulting from selective segment passages at a specific juxtaposition geometry j is inversely proportional to the average linking number, $\langle Lk \rangle_j$, of circles with the given juxtaposition. Based on this formulation, Chan demonstrated that selective segment passages at 'hooked' and 'twisted' juxtapositions reduces the variance of Lk. The dependence of this effect on model DNA circle size is remarkably similar to that observed experimentally for type-2 topoisomerases, which appear to be less capable in narrowing Lk variance for small DNA circles than for larger DNA circles. This behavior is rationalized by a substantial cancellation of writhe in small circles with hook-like juxtapositions. For an extended set of juxtapositions in their model, Chan's research group detects a significant correlation between the juxtapositions' supercoil simplification potential and their logarithmic decatenating potential as well as their logarithmic unknotting potential, a trend reminiscent of scaling relations between corresponding experimental measurements on type-2 topoisomerases from a variety of organisms. The consistent agreements between theory and experiment their group achieved argue strongly for type-2 topoisomerase action at hook- or twist-like DNA juxtapositions.

Michael Szafron (University of Saskatchewan, Canada) spoke on *Knotting Probabilities Resulting from a Local Strand Passage in a Knot-type K SAP.* Also motivated by understanding the action of type-2 topoisomerases on DNA, Szafron and Soteros have developed a self-avoiding polygon (SAP) lattice model to investigate the effect of random local strand passages on the knot-type of a ring polymer. For increasing SAP sizes, the limiting knot transition probability estimates obtained from Monte Carlo data for this model were presented. Evidence was provided that these limiting knot transition probabilities depend on the local juxtaposition at the strand passage site. This evidence provides further support for the hypothesis (mentioned above in the work of Chan's group) that selective segment passages according to the local juxtaposition geometry can reduce knot populations.

Dorothy Buck (Imperial College, England) spoke on *Topological Analysis of DNA Knotting and Unknotting*, joint work with Ken Baker and Andrew Lobb. Many protein-DNA interactions, such as site-specific recombination and (type II) topoisomerase-mediated unknotting and unlinking, act by cutting and resealing (double-stranded) DNA segments in a localized way. These enzymatic reactions can be modelled in terms of tangles, 3-dimensional balls with two properly embedded arcs, each representing a segment of DNA. The action of the protein can be thought of as removing one tangle and replacing it with another, e.g. a topoisomerase-initiated crossing change as replacing a (+1) tangle with a (-1) tangle, leaving the rest of the DNA unchanged. This replacement can be straightforward (as in the topoisomerase example above) or quite complex. Because of the plectonemic supercoiling of DNA, 'rational tangles' (formed by an alternating series of horizontal and vertical twists) are the most biologically relevant. Buck classified all possible rational tangles that can replace, in any prescribed manner, a given rational tangle, thus elucidating all possible protein mediated localized changes of DNA.

Jason Cantarella (University of Georgia, USA) spoke on *Intrinsic Symmetries of Knots and Links*. Given a link composed of several circular strands of DNA, each component is oriented and uniquely labeled by its sequence of base pairs. Can these components be reoriented? Can they switch places? The group of transformations of this type which can be realized by an isotopy of the link is called the "intrinsic" symmetry group of the link. Cantarella presented the first computations of the intrinsic symmetry groups of links with 8 and fewer crossings. The traditional definition of the symmetry group of a link is the mapping class group $MCG(S^3, L)$ of the pair S^3, L. The symmetry groups are the images of the traditional symmetry groups of links under the natural homomorphism from $MCG(S^3, L)$ onto $MCG(S^3) \times MCG(L)$.

Teresita Ramirez-Rosas (Grand Valley State University, USA) spoke on *Looking for a lower bound for the number of quadrisecants*. Ramirez-Rosas has been interested in finding a lower bound for the number of quadrisecants for a polygonal knot in general position in terms of its crossing number. Her immediate goal is to show the following:

Conjecture: A knot K with crossing number, $cr(K)$, has at least $\frac{1}{2}\left(\frac{2cr(K)+1}{3}\right)^2$ quadrisecants.

Ramirez-Rosas discussed some ideas that might lead us to find a lower bound for the number of quadrisecants. In particular, she talked about one of her results that can help us to solve this conjecture: given $x \in K$ the number of trisecants with starting or ending point at x is at least $\frac{2cr(K)+1}{3}$.

Confinement effects

In many practical situations of interest, macromolecules do not have full configurational freedom due to the constraints of geometric confinement, for example, when polymers are confined between two parallel planes as in models of steric stabilization of dispersions or DNA molecules contained in a capsid. Macromolecules so confined exhibit significantly different average and individual structure in comparison with those in free environments. Also, effective confining arises in the case of macromolecules that have specific hydrophobic and hydrophilic regions or when regions have restricted flexibility or torsion. While, in general, one might believe that great progress has occurred in understanding the storing, knotting, and winding of polymers, in fact rather little is known rigorously and many fundamental questions seem just beyond our grasp, both theoretically or via numerical studies. Further effort is clearly needed and promising steps are being taken in these areas.

The workshop contained five talks on this subject.

Javier Arsuaga (San Francisco State University, USA) spoke on *Modeling of Chromosome Intermingling by Partially Overlapping Uniform Random Polygons*, joint work with Yuanan Diao and Rob Scharein. During the early phase of the cell cycle the eukaryotic genome is organized into chromosome territories. The geometry of the interface between any two chromosomes remains a matter of debate and may have important functional consequences. The Interchromosomal Network model (introduced by Branco and Pombo) proposes that territories intermingle along their periphery. In order to partially quantify this concept Arsuaga's group investigated the probability that two chromosomes form an unsplittable link. They used the uniform random polygon (URP) as a crude model for chromosome territories and modeled the interchromosomal network as the common spatial region of two overlapping uniform random polygons. This simple model allows one to derive some rigorous mathematical results as well as to perform computer simulations easily. They found that the probability that a uniform random polygon of length n partially overlaps a fixed polygon is bounded below by $1 - O(1/\sqrt{n})$. Arsuaga's group used numerical simulations to estimate the dependence of the linking probability of two uniform random polygons on the amount of overlapping. They propose that this dependence relation may be modeled as $\frac{1-ae+b(1-e)}{e\sqrt{mn}+b(1-e)}$ where $e > 0$. They used these results to model the data published by Branco and Pombo and observed that for the amount of overlapping observed experimentally the URPs have a non-zero probability of forming an unsplittable link.

Rob Scharein (Hypnagogic Software, Canada) spoke on *Bounds for the minimum step number of knots in the simple cubic lattice*, joint work with K. Ishihara, J. Arsuaga, Y. Diao, K. Shimokawa and M. Vazquez. Knots are found in DNA as well as in proteins, and they have been shown to be good tools for structural analysis of these molecules. An important parameter to consider in the artificial construction of these molecules is the minimum number of monomers needed to make a knot. Scharein addressed this problem by characterizing, both analytically and numerically, the minimum length (also called minimum step number) needed to form a particular knot in the simple cubic lattice. His group's analytical work is based on improvement of a method introduced by Diao to enumerate conformations of a given knot type for a fixed length. This method allows one to extend the previously known result on the minimum step number of the trefoil knot 3_1 (which is 24) to the knots 4_1 and 5_1 and show that the minimum step numbers for the 4_1 and 5_1 knots are 30 and 34, respectively. Using an independent method based on the BFACF algorithm, Scharein provided a complete list of numerical estimates (upper bounds) of the minimum step numbers for prime knots up to ten crossings, which are improvements over current published numerical results. They enumerated all minimum lattice knots of a given type and partitioned them into classes defined by BFACF type-0 moves.

Michael Schmid (Baylor College of Medicine, USA) spoke on *How can DNA get in and out of a virus capsid?* Double stranded DNA phages and viruses encapsidate their genome into a preformed capsid shell through one icosahedral vertex, which contains a portal protein complex. ATP is consumed, and the DNA is inserted, probably involving twisting. Extrusion of the DNA during cell or bacterial infection is accomplished through the same vertex. Schmid's lab (National Center for Macromolecular Imaging, Baylor College of Medicine) has determined the structure of several phages and viruses by cryoelectron microscopy (cryoEM). This technique aligns and averages thousands of individual 2D projection images in random orientations to produce a 3D reconstruction of the virus. Recently his lab has been able to perform this reconstruction without applying icosahedral symmetry, thus are able to see the unique vertex and the other non-icosahedral features. Clues as to the packing of the DNA include: 1) concentric shells of DNA spooled around the axis defined by the unique vertex, 2) a roughly hexagonal packing of the DNA helices against each other, 3) the terminus (last in) of the DNA runs up the axis toward the portal, among others. Many questions remain.

Cristian Micheletti (International School for Advanced Studies, Italy) spoke on *Coarse-grained simulations of DNA in confined geometries*. The packing of DNA inside bacteriophages arguably yields the simplest example of genome organisation in living organisms. An indirect indication of how DNA is packaged is provided by the detected spectrum of knots formed by DNA that is circularised inside the P4 viral capsid. The experimental results on the knot spectrum of the P4 DNA can be compared to results of coarse-grained simulation of DNA knotting in confined volumes. Micheletti started by considering a standard coarse-grained model for DNA which is known to be capable of reproducing the salient physical aspects of free (unconstrained) DNA. Specifically the model accounts for DNA bending rigidity and excluded volume interactions. By subjecting the model DNA molecules to spatial confinement it was found that confinement favours chiral knots over achiral ones, as found in the P4 experiments. However, no significant bias of torus over twist knots was found, contrary to what was found in P4 experiments. A good consistency with experiment can be found, instead, upon introducing an additional interaction potential accounting for the tendency of contacting DNA strands to order as in cholesteric liquid crystals. The degree of localization of the obtained knots was discussed in connection with the process of genome ejection out of the phage.

Alexander Grosberg (New York University, USA) spoke on *Large scale organization of DNA in chromosomes*. Recent experiments confirmed an old theoretical prediction that human genome (and presumably that of other eukaryotes) on the large scale (above the nucleosome size) is organized in the form of a crumpled fractal globule stabilized by the topological effects. Grosberg analyzed the application of the globule structure as a model for chromosome territories.

Length effects

The typical length of DNA in a cell ranges from thousands of base pairs in a virus, ~ 4 megabase pairs in bacteria, to ~ 3 billion base pairs in mammals or equivalently ~ 10 to 10 million Kuhn lengths. How does the length of DNA influence its topological and geometric properties such as knotting, linking and supercoiling? Is an organism's natural length of DNA optimal in terms of minimizing the possibility of topological obstructions to vital cellular processes such as replication and transcription while maximizing the amount of information that can be stored? In order to address this kind of question, theorists investigate the length dependence of the topological and geometric properties of model polymers. For lattice models of polymers, one can obtain mathematical proofs for the limiting behavior of, for example, knotting and linking probabilities as polymer length goes to infinity. Well established statistical mechanics and field theory arguments can also be used to predict the finite length scaling behavior of polymer properties such as the knotting probability or the average squared radius of gyration. Determining the length scale for which this scaling behavior is relevant, however, requires computer simulations and comparison to experiments. In general, much work remains on both the theory and experimental side in order to further bridge the gap. The mathematical facet of this work brings together topologists, geometers, statisticians, and computational scientists.

The workshop contained six talks on this subject.

Tetsuo Deguchi (Ochanomizu University, Japan) spoke on *Effective scaling approximations for knotting probability, topological swelling and the distance distribution of random knots*. Deguchi discussed various scaling approximations for the probability of random knotting and the mean square radius of gyration for random knots as functions of the number of segments. He also introduced an effective scaling formula for the distribution of the distances between two segments of polygon. For an illustration, consider knotting probability. For off-lattice models Deguchi numerically evaluated the probability of random knotting as a function of the number of nodes. He then found that two types of fitting formulas are quite effective, one for describing asymptotic behavior and another one for describing finite-size random knotting probability. Although the latter formula should be valid for a limited range of the number of nodes, it has a nice factorization property by which one can predict the probability of composite knots from those of the constituent prime knots. Deguchi's scaling approximations are particularly effective for finite-size random knots and should be fundamental in application to real ring polymers since all ring polymers have some finite number of segments. These results can be compared to experiments in the near future.

Bertrand Duplantier (Centre Energie Automique/Saclay, France) spoke on *Partition Function of a Freely-Jointed Chain in Half-Space*, joint work with Olivier Bernardi and Philippe Nadeau. When lecturing about the Physics of Biological Polymers in 2007 at EPFL (Lausanne), Duplantier was asked by Andrzej Stasiak about the statistics of a discrete freely-jointed chain anchored at a plane in three space, and under traction by a force. This problem is relevant to the description of DNA under traction and of proteins in translocation across a membrane. Surprisingly, the calculation of the canonical partition function is non-trivial, and must be done via a functional recursion over the number of monomers. The enumeration of configurations also involves specific combinatorial aspects, which bring in cell decompositions, Motzkin paths and bijections to trees, a long way from the original biological question!

Stu Whittington (University of Toronto, Canada) spoke on *Pattern theorems: What we know and what we wish we knew*. Pattern theorems are a way to show that certain events occur with high probability, and were used to show that lattice polygons (a model of ring polymers) are knotted with high probability when the polygon is large. Over the last twenty years new ways to prove pattern theorems have emerged and pattern theorems have been proved for new situations. Whittington's talk reviewed the idea behind pattern theorems and showed how they can be used to prove results about topological and geometrical entanglement complexity. In spite of the progress made recently there are still many areas where a pattern theorem would be useful or where a sharper form of a pattern theorem would give improved results. Some of these open questions were discussed.

Mahshid Atapour (York University, Canada) spoke on *Exponential Growth of the Number of n-edge Linked Clusters in $\mathbb{Z}^3$ and the Consequences in Entanglement Percolation*. An animal in the simple cubic lattice is a finite connected subgraph of $\mathbb{Z}^3$. Let a_n be the number (up to translation) of n-edge animals in $\mathbb{Z}^3$. In 1967, Klarner proved that a_n grows exponentially. Let e_n be the number (up to translation) of all n-edge linked clusters, i.e. subgraphs of $\mathbb{Z}^3$ in which the connected components (animals) are (topologically) non-splittable. Atapour explained how it can be proved that e_n also has a finite exponential growth rate. She also mentioned some of the important consequences of this result in entanglement percolation.

Andrew Rechnitzer (University of British Columbia, Canada) spoke on *Counting knotted polygons (nearly)*. The Rosenbluth method of simulating self-avoiding walks has become one of the standard methods for studying polymer statistics. The algorithm was originally developed in the 1950s by Hammersley & Morton and Rosenbluth & Rosenbluth, but suffered from poor convergence. This changed in the mid 90s with Grassberger's development of a pruned and enriched implementation called PERM. It was soon followed by multicanonical and flat-histogram implementations which have become indispensable tools for exploring the critical behaviour of polymer systems. Combinatorially, one can think of the Rosenbluth method as a technique of 'approximate enumeration' which produces precise estimates of the number of conformations of a particular size and energy. This same method can then be applied to many other combinatorial problems provided there is a unique and unambiguous way of constructing the underlying objects. Unfortunately, self-avoiding polygons (SAPs) are not such a system. Rechnitzer discussed this history and described two recent extensions of the original Rosenbluth algorithm which allow the approximate enumeration of two-dimensional SAPs and SAPs of fixed knot type in three dimensions in joint work with Buks van Rensburg.

Buks Janse Van Rensburg (York University, Canada) *Statistics of knotted lattice polygons*. Polygons in the cubic lattice are simple closed curves in three space and have well-defined knot types. The number of lattice polygons of length n and knot type K in the cubic lattice is $p_n(K)$, where we consider two polygons to be equivalent under translations in the lattice. For example, if K is the unknot $\emptyset$, then $p_4(\emptyset) = 3$, $p_6(\emptyset) = 22$, $p_8(\emptyset) = 207$ and so on. Determining $p_n(K)$ for arbitrary n and knot types K is a difficult numerical problem, but the GAS-algorithm can be used for approximate enumeration of $p_n(K)$. Janse van Rensburg presented the results of simulations resulting from collaborations with Rechnitzer to estimate the approximate values of $p_n(K)$ for some knot types K. The scaling of $p_n(K)$ was discussed, and evidence presented that $p_n(K) \sim A_K n^{\alpha-2+N_K} \mu_\emptyset^n$; where N_K is the number of prime components in the knot type K and $\mu_\emptyset^n$ is the growth constant for unknotted polygons. The relative frequencies of knot types in lattice polygons were also discussed.

DNA sequence effects and replication factories

The so-called "base-pair step parameters" provide remarkable predictive powers with regards to the conformation of a DNA polymer. Next approaches should start to include not only nearest neighbor effects, but even next nearest neighbor effects. How to model this mathematically and computationally is an enormous yet exciting new challenge. The DNA sequence, of course, dictates both the structural deformations that occur as a consequence of underwinding and overwinding DNA, as well as the electrostatics. In addition, the DNA sequence, as well as Lk, counterions, and water, all come into play in the formation of the so-called "alternative secondary structure of DNA". Researchers have made great inroads into the understanding of these structures and how important they are for DNA. Medically, the structures that result can cause human suffering and account for the cause of several important and fairly common human diseases.

Instead of free, unconstrained DNA filling up space in a cell, in fact the proteins that replicate and transcribe DNA are "fixed" in the cell in what biologists have named "factories". During replication, for example, this means that the DNA moves, at a rate of 100-1000 base pairs/second. In front of the factories, the DNA will have to be transiently overwound and this overwinding is unlikely to be allowed to adopt the geometric configuration of writhe. White's adaptation to DNA of $Lk = Tw + Wr$, therefore, must be now modeled to limit writhe and mathematical considerations of variations in twist and writhe should aid in the understanding of this important biological phenomenon. The single double helix train track in front of the factory, during replication has, behind the factory, split into two train tracks with partial gaps on one side and a nick on the other. The topological interplay between linking number and catenation is likely to be governed by mathematical and physical principals. Thus replicating DNA involves extraordinary structures with tremendous topological complications, and this is a mechanism desperately in need for improved mathematical modeling. At the same time, it is the long-established concepts in DNA topology and knot theory that have helped guide the understanding of this remarkable biopolymer. The mathematics involved includes tangle, braid, knot, link, and polymer modeling. The study of the characteristics of both equilibrium as well as kinetic aspects of DNA now include geometric, spatial, and topological facets that may be implicated in these mechanisms as well as the characteristics of polymers under a variety of solvent conditions. While these studies require advances in computational methods to fully illuminate the equilibrium properties, sufficient information appears already to be available to inform an understanding of experimental observations.

The workshop contained six talks on this subject.

Wilma Olson (Rutgers University, USA) spoke on *Protein-mediated DNA looping and gene expression*. Making sense of gene regulation in living systems requires understanding of the looping properties of DNA in crowded, multi-component systems. The presence of non-specific binding proteins that introduce sharp bends, localized untwisting, and/or dislocation of the DNA double-helical axis, stabilizes functional repression loops ranging from as few as 65 base pairs to as many as tens of thousands of base pairs. As a first step in the analysis of such looping, Olson's group investigated the effects of various proteins on the configurational properties of fragments of DNA, treating the DNA at the level of base-pair steps and incorporating the known effects of various proteins on DNA double-helical structure. The presentation highlighted some of the new models and computational techniques that her group has developed to generate the three-dimensional configurations of protein-mediated DNA loops and illustrate new insights gained from their work about the effects of various proteins on DNA topology and the apparent contributions of the non-specific binding proteins to gene expression.

Phoebe Rice (University of Chicago, USA) spoke on *Structural model for how Sin recombinase exploits topology*. Sin is a DNA recombinase belonging to the serine resolvase family. For various biological reasons, these enzymes convert one large DNA circle into two smaller ones. To prevent other recombination products, the system is regulated by a 'topological filter' - it is only enzymatically active when the two partner sites are brought together in a synaptic complex containing three interdomainal supercoiling nodes. Using crystal structures of individual components, Rice's group constructed a 3-dimensional model for this synaptic complex. They also used biochemical assays to address the details of how this catalytic regulation is enforced. Rice presented preliminary data showing that a different serine resolvase, Tn3, uses different protein-DNA interactions to construct a regulatory complex with the same DNA topology.

Georgi Muskhelishivili (Jacobs University, Germany) spoke on *General organisational principles of the transcriptional regulation system: a tree or a circle?* The fundamental problem in attempting a holistic description of the transcriptional regulation system is of a methodological nature and lies in the necessity of integrating the systemic and structural-molecular views. Recent advances of systemic approaches to gene expression provide unforeseen opportunities for relating extensive datasets describing the transcriptional regulation system as a whole. However, due to the multifaceted nature of the phenomenon, these datasets often contain logically distinct types of information determined by the underlying approach and adopted methodology of data analysis. Consequently, to integrate the datasets comprising information on the states of chromatin structure, transcriptional regulatory network and cellular metabolism, a novel methodology enabling interconversion of logically distinct types of information is required. Muskhelishivili provided a holistic conceptual framework for the analysis of the global transcriptional regulation as a system coordinated by the structural coupling between the transcription machinery and DNA topology, acting as interdependent sensors and determinants of metabolic functions. In this operationally closed system any transition in physiological state represents an emergent property determined by shifts in structural coupling, whereas genetic regulation acts as a genuine device converting one logical type of information into the other.

Jue D. Wang (Baylor College of Medicine, USA) spoke on *Co-orientation of Replication and Transcription Preserves Genome Integrity*. In many bacteria, there is a genome-wide bias towards co-orientation of replication and transcription, with essential and/or highly expressed genes further enriched co-directionally. Wang's group previously found that reversing this bias in the bacterium Bacillus subtilis slows replication elongation, and proposed that this effect contributes to the evolutionary pressure selecting the transcription-replication co-orientation bias. This selection might have been based purely on selection for speedy replication; alternatively, the slowed replication might actually represent an average of individual replication-disruption events, each of which is counter-selected independently because genome integrity is selected. To differentiate these possibilities and define the precise forces driving this aspect of genome organization, Wang's group generated new strains with inversions either over 1/4 of the chromosome or at ribosomal RNA (rRNA) operons. Applying mathematical analysis to genomic microarray snapshots, they found that replication rates vary dramatically within the inverted genome. Replication is moderately impeded throughout the inverted region, which results in small but significant competitive disadvantage in minimal medium. Importantly, replication is strongly obstructed at inverted rRNA loci in rich medium. This obstruction results in disruption of DNA replication, activation of DNA damage response, loss of genomic integrity and cell death. Wang's results strongly suggest that preservation of genome integrity drives the evolution of co-orientation of replication and transcription, a conserved feature of genome organization.

Tim Hughes (University of Toronto, Canada) spoke on *High nucleosome occupancy is encoded at human regulatory sequences*. Active eukaryotic regulatory sites are characterized by open chromatin, and yeast promoters and transcription factor binding sites (TFBSs) typically have low intrinsic nucleosome occupancy, i.e. these sequences are disfavored when naked DNA and histone octamers are assembled *in vitro*. Hughes showed that in contrast to yeast, DNA at human promoters, enhancers, and TFBSs generally encodes high intrinsic nucleosome occupancy. In most cases his group examined, these elements also have high experimentally measured nucleosome occupancy *in vivo*. These regions typically have high G+C content, which correlates positively with intrinsic nucleosome occupancy, presumably due to high bend, twist, tip etc. parameters, as well as reduced probability of rigid, nucleosome-excluding polyA-like sequences. Hughes proposed that high nucleosome affinity is directly encoded at regulatory sequences in the human genome to restrict access to regulatory information that will ultimately be utilized in only a subset of differentiated cells. He also proposed that nucleosomes may play direct roles in the function of active enhancers. Their findings also present a functional consequence of variation in base content that is observed at diverse scales in eukaryotic genomes.

Wei Yang (NIH, USA) spoke on *Lessons learnt from a DNA helicase UvrD*. How do molecular motors convert chemical energy to mechanical work? Helicases and nucleic acids offer simple motor systems for extensive biochemical and biophysical analyses. Atomic resolution structures of UvrD-like helicases complexed with DNA in the presence of AMPPNP, ADPPi, and Pi reveal several salient points that aid understanding mechano-chemical coupling. Each ATPase cycle causes two motor-domains to rotationally close and open. At a minimum, two motor-track contact points of alternating tight and loose attachment convert domain rotations to uni-directional movement. A motor is poised for action only when fully in contact with its track and, if applicable, working against a load. The orientation of domain rotation relative to the track determines whether the movement is linear, spiral or circular. Motors powered by ATPases likely deliver each power stroke in two parts, before and after ATP hydrolysis.

Conclusion

The workshop was designed to intentionally maximize relaxed interactions among the diverse participants. On the last day of the workshop, we held a short meeting to get feedback on the format and the participants were asked what they liked, what they might change, whether or not they learned anything new, and whether they will start new collaborations from the meeting.

Some of the comments about the meeting included:

"I talked to several biologists in a more detailed way than at many meetings."

"I have attended quite a few conferences covering material that lies at the interface between mathematics and other sciences; this conference was far and away the one with the most communication between fields. The talks were very accessible and it was clear that ideas were genuinely flowing between disciplines."

"I think it was very successful in general and inspired me personally to think about applications of maths to genetic regulation."

"The meeting had the right balance between the various communities and, in my view, all speakers were able to communicate effectively their research to an audience with a very mixed background."

In the weeks that have followed since our meeting, we the organizers continue to receive notice of one of our speakers visiting the country or laboratory of another, interactions that might never have taken place without the extraordinary opportunity afforded by BIRS.

Participants

Arsuaga, Javier (San Francisco State University)
Atapour, Mahshid (York University)
Buck, Dorothy (Imperial College)
Cantarella, Jason (University of Georgia)
Chan, Hue Sun (University of Toronto)
Darcy, Isabel (University of Iowa)
Deguchi, Tetsuo (Ochanomizu University)
Diao, Yuanan (University of North Carolina)
Duplantier, Bertrand (Centre Energie Automique / Saclay)
Ernst, Claus (Western Kentucky University)
Fogg, Jonathan (Baylor College of Medicine)
Grosberg, Alexander (New York University)
Harris, Sarah (University of Leeds)
Hughes, Tim (University of Toronto)
Janse van Rensburg, Esaias J (York University)
Levene, Stephen (University of Texas at Dallas)
Levens, David (Center for Cancer Research NIH)
Mastin, Matt (University of Georgia)
Micheletti, Cristian (International School for Advanced Studies)
Muskhelishivili, Georgi (Jacobs University)
Olson, Wilma (Rutgers University)
Rabin, Yitzhak (Bar-Ilan University)
Ramirez-Rosas, Teresita (University of California)
Rawdon, Eric (University of Saint Thomas)
Rechnitzer, Andrew (University of British Columbia)
Rice, Phoebe (University of Chicago)
Scharein, Rob (Hypnagogic Software)
Schmid, Michael (Baylor College of Medicine)
Simon, Jonathan (University of Iowa)
Soteros, Christine (University of Saskatchewan)
Szafron, Michael (University of Saskatchewan)
Wang, Jade (Baylor College of Medicine)
Whittington, Stuart (University of Toronto)
Yang, Wei (NIH)
Zechiedrich, Lynn (Baylor College of Medicine)

Chapter 2

Multi-scale Stochastic Modeling of Cell Dynamics (10w5058)

Jan 17 - Jan 22, 2010

Organizer(s): Lea Popovic (Concordia University), Brian Ingalls (University of Waterloo), Jonathan Mattingly (Duke University), Peter Swain (University of Edinburgh)

Overview of the Field

A cellular network can be modelled mathematically using principles of chemical kinetics. These are particularly useful for studying the dynamic aspects of cells such as gene transcription, translation, regulation, and protein-protein interactions. Due to a large number of parameters, variables and constraints in cellular networks, numerical and computational techniques are often necessary. The development of computational approaches and analytical results to understand these dynamic processes is essential for the elucidation of cellular mechanisms. An increasing number of scientists are working to improve these approaches and to create, refine and test dynamical models in order to accurately reflect observations, and acquire predictive explanatory power.

At the cellular level, chemical dynamics are often dominated by the action of regulatory molecules present at levels of only a few copies per cell. Intrinsic noise due to random fluctuations of these components appears to have significant consequences: the observed large variation in morphology, rates of development, physiological responses in a cell often lead to a randomization of phenotypic outcomes and non-genetic population heterogeneity. Hence, stochastic modeling of the molecular dynamics within a cell is necessary in order to fully describe a set of expected outcomes. In many cases of biological interest some of the chemical species in the network are present in much lower abundance than others and the reaction rate constants can vary over several orders of magnitude. This implies that standard concentration scaling of stochastic models in assessing chemical dynamics does not provide a good representation of the behavior of the system, and that development of stochastic models on multiple scales is necessary.

Recent Developments and Open Problems

Cellular pathways involve many different molecular species, which are interconnected by an even larger number of chemical reactions, which poses a complex analytical problem. For prediction and simulation purposes, it is essential to reduce both the modeling and computational complexity of the problem, while still capturing all the essential characteristics and behavior of such a network. This has recently stimulated the development and analysis of stochastic models for biochemical networks and dynamics with multiple scales. A rigorous approach to this problem poses many interesting and challenging mathematical questions. Mathematical approaches can contribute directly to solve some of these problems in the following ways:

a. Numerous simulation algorithms are currently being developed for stochastic reaction systems on different time scales. The error of such simulations has not yet been fully explored, nor have the results from stochastic theory for systems on multiple scales been fully utilized to improve the development of such computational efforts.

b. Experimentalists are exploring the effect of stochastic mechanisms on the stability and robustness of components of these complex pathways. They are hoping to observe the effects that the dynamical properties of the system have on noise transmission, its amplification or damping, as well as whether some molecular systems may have evolved to use the stochasticity to its advantage. Fluctuation methods and stochastic dynamics may be combined to yield analytical answers to some of these questions.

c. Recent advances in single cell measurement techniques have yielded a wealth of new data which are being mined for important biological content. The temporal data are observations from stochastic dynamical systems, and statistical methods for stochastic processes can help extract some relevant parameters and make predictions for the behavior of the system.

Presentation Highlights

Presentations covered a wide range of mathematical, theoretical and computational issues in systems biology modeling, focusing in particular on stochastic and multiscale issues. In order of discussion -

Des Higham: Discrete versus Continuous in Simple Gene Regulation Models

Markov jump processes can provide accurate models in many applications, notably chemical and biochemical kinetics, and population dynamics. Stochastic differential equations offer a computationally effcient way to approximate these processes. It is therefore of interest to establish results that shed light on the extent to which the jump and diffusion models agree. This talk focused on mean hitting time behaviour in a thermodynamic limit, with examples of three simple types of reaction where analytical results can be derived, and where we found that the match between mean hitting time behavior of the two models is vastly different in each case. Furthermore, we stress that in many examples there is no guarantee that the diffusion model stays non-negative.Thus, care must be exercised when using diffusion models for reaction systems. ([1])

Jin Wang: Potential and Flux Landscape Framework for Understanding Stability and Robustness of Cellular Network

Studying the cell cycle process is crucial for understanding cell growth, proliferation, development, and death. We uncovered some key factors in determining the global robustness and function of the budding yeast cell cycle by exploring the underlying landscape and flux of this nonequilibrium network. The dynamics of the system is determined by both the landscape which attracts the system down to the oscillation orbit and the curl flux which drives the periodic motion on the ring. This global structure of landscape is crucial for the coherent cell cycle dynamics and function. The topography of the underlying landscape, specifically the barrier height separating basins of attractions, characterizes the capability of changing from one part of the system to another. This quantifies the stability and robustness of the system. We studied how barrier height is influenced by environmental fluctuations and perturbations on specific wirings of the cell cycle network. When the fluctuations increase, the barrier height decreases and the period and amplitude of cell cycle oscillation is more dispersed and less coherent. The corresponding dissipation of the system quantitatively measured by the entropy production rate increases. This implies that the system is less stable under fluctuations. In this talk we identify some key structural elements for wirings of the cell cycle network responsible for the change of the barrier height and therefore the global stability of the system through the sensitivity analysis. We show results are in agreement with recent experiments and also provide new predictions. ([2])

Ted Perkins: Trajectory inference for stochastic chemical kinetic models

Continuous-time Markov chains are used to model systems in which transitions between states as well as the time the system spends in each state are random. Many computational problems related to such chains have been solved, including determining state distributions as a function of time, parameter estimation, and control. However, the problem of inferring most likely trajectories, where a trajectory is a sequence of states as well as the amount of time spent in each state, appears unsolved. We studied three versions of this problem: (i) an initial value problem, in which an initial state is given and we seek the most likely trajectory until a given final time, (ii) a boundary value problem, in which initial and final states and times are given, and we seek the most likely trajectory connecting them, and (iii) trajectory inference under partial observability, analogous to finding maximum likelihood trajectories for hidden Markov models. In this talk we show that maximum likelihood trajectories are not always well-defined, and describe a polynomial time test for well-definedness. When well-definedness holds, we show that each of the three problems can be solved in polynomial time, and we develop efficient dynamic programming algorithms for doing so. ([3])

Ruth Williams: Coupled enzymatic degradation of proteins

A major challenge for systems biology is to deduce the molecular interactions that underly correlations observed between concentrations of different intracellular molecules. While direct explanations such as coupled transcription/translation or direct protein-protein interactions are often considered, potential indirect sources of coupling have received much less attention. In this talk, I will report on an investigation involving both theory and experiment of how correlations can arise generically from a post-translational coupling mechanism involving the processing of multiple protein species by a common enzyme. In this talk we show how the model can be posed in framework of multiclass queueing systems, and how we obtained the correlation of the stationary distribution for the protein species.

Samuel Kou: Multi-resolution inference of stochastic models from partially observed data

Inferring parameter values for diffusion models from data is often complicated by the fact that the underlying stochastic process is only partially observed. Likelihood based inference faces the difficulty that likelihood is usually not available even numerically. Conventional approach discretizes the stochastic model to approximate the likelihood. In order to have desirable accuracy, one has to use highly dense discretization. However, this usually imposes unbearable computation burden. In this talk we will introduce the framework of Bayesian multi-resolution inference to address this difficulty. By working on different resolution (discretization) levels simultaneously and by letting the resolutions talk to each other, we improve not only the computational efficiency, but also estimation accuracy. We illustrate our approach by examples.

Matthew Scott: Modeling intrinsic noise in continuous systems

In this talk I will consider systems that involve both reactions and spatial transport, treating chemical species at different locations as different species types. I will discuss recent work using an analytic approximation method to derive moments and spatiotemporal correlations in systems modeled using a reaction transport master equation. Our approach obtains moments via Van Kampen expansion, and uses a Fourier transform of factorial cumulants in order to obtain spatial correlation spectrum.

Di Liu: Numerical methods for stochastic bio-chemical reacting networks with multiple time scales

Multiscale and stochastic approaches play a crucial role in faithfully capturing the dynamical features and making insightful predictions of cellular reacting systems involving gene expression. Despite their accuracy, the standard stochastic simulation algorithms are necessarily inefficient for most of the realistic problems with a multiscale nature characterized by multiple time scales induced by widely disparate reactions rates. In this talk, I will discuss some recent progress on using asymptotic techniques for probability theory to simplify the complex networks and help to design efficient numerical schemes. We compare Nested SSA, multiscale SSA, and the slow-scale SSA algorithms, and we discuss methods of dynamic adaptation (re-evaluation of fast/slow classification) in multiscale algorithms. ([4])

Darren Wilkinson: Bayesian inference for stochastic networks

In this talk l give an overview of statistical methods for parameter inference for stochastic kinetic models, with emphasis on Bayesian approaches and sequential likelihood free MCMC, and discuss software. I will show an example application to stochastic kinetic modelling of p53/Mdm2 oscillations. ([5])

Moises Santillan: Evolution of the distributions for stochastic gene expression subject to negative feedback regulation

In this talk we discuss a simplification of the master equation (via an adiabatic approximation) and the numerical solution of the reduced master equation. The accuracy of this procedure is tested by comparing its results with analytic solutions (when available) and with Gillespie stochastic simulations. We employ our approach to study the stochastic expression of a simple gene network, which is subject to negative feedback regulation at the transcriptional level. We consider the influence of negative feedback on the amplitude of intrinsic noise, and the relaxation rate of the system probability distribution function to the steady solution. Our results suggest the existence of an optimal feedback strength that maximizes this relaxation rate. ([6])

Paul Tupper: An Apparent Paradox of State-Dependent Diffusion

We consider an experiment of molecular diffusion on a two-dimensional rectangular lattice periodic boundary conditions. This rectangular lattice is partitioned into panels of equal size that alternate between two diffusion coefficients, one being twice the value of the other. Two contrary theoretical predictions of the motion of the diffusing particle are available. The first prediction (from stochastic calculus) observes that the diffusion coefficient influences how much time is spent on each side of the lattice. The second prediction (from statistical mechanics) states that the particle should spend the same amount of time on both sides of the partition. In this talk we discuss how these predictions depend on our interpretation of the diffusion coefficient as we take the limit of discrete systems.

Sayan Mukherjee: Multiscale factor models for molecular networks

In this talk a factor modeling framework is developed that is both predictive of phenotypic or response variation and the inferred factors offer insight with respect to underlying physical or biological processes. The method is general and can be applied to a variety of scientific problems. We focus on modeling complex disease phenotypes (etiology of cancer) as a motivating example. In this setting, the factors capture gene or protein interaction networks at different scales – breadth of the interaction network. The method integrates multiscale analysis on graphs and manifolds developed in applied harmonic analysis with sparse factor models, a mainstay of applied statistics. ([7])

Rachel Kuske: Model choice for mixed mode oscillations: coherence resonance and delay bifurcations

Many neuronal systems and models display a certain class of mixed mode oscillations (MMOs) consisting of periods of small amplitude oscillations interspersed with spikes. Various models with different underlying mechanisms have been proposed to generate this type of behavior. Stochastic versions of these models can produce similarly looking time series, often with noise-driven mechanisms different from those of the deterministic models. We present a suite of measures which, when applied to the time series, serves to distinguish models and classify routes to producing MMOs, such as noise-induced oscillations or delay bifurcation. By focusing on the subthreshold oscillations, we analyze the interspike interval density, trends in the amplitude and a coherence measure. We develop these measures on a biophysical model for stellate cells and a phenomenological FitzHugh-Nagumo-type model and apply them on related models. The analysis highlights the influence of model parameters and reset and return mechanisms in the context of a novel approach using noise level to distinguish model types and MMO mechanisms. Ultimately, we indicate how the suite of measures can be applied to experimental time series to reveal the underlying dynamical structure, while exploiting either the intrinsic noise of the system or tunable extrinsic noise. ([8])

David Anderson: Simulation methods for stochastically modeled population processes

While exact simulation methods exist for discrete-stochastic models of biochemical reaction networks, they are often times too inefficient for use because the number of computations scales linearly with the number of reaction events; thus, approximate algorithms have been developed. However, stochastically modeled reaction networks often have ”natural scales” and it is crucial that these be accounted for when developing and analyzing numerical approximation methods. I will show that conducting such a non-standard error analysis leads to fundamentally different conclusions than previous analyses. Another option for approximating discrete-stochastic models of chemical reaction networks is to use a diffusion approximation. However, even in the regimes where such an approximation is preferable to the discrete numerical approximation methods, it is now necessary to approximate the diffusion process. In the second portion of my talk I will show how the special structure of chemical reaction networks can be utilized to develop an efficient and easy to implement method that is second order accurate in the weak sense for such diffusion processes. ([9],[10])

Eldon Emberly: A mechanism for polar protein localization in bacteria

We discuss a model for the cell cycle in the asymmetrically dividing bacteria Caulobacter Crescentus. We are interested in how polar localization of PopZ protein influences the biochemical calculations that bacteria need to perform cell differentiation.

John Fricks: Modeling Neck Linker Extension in Kinesin Molecular Motors

The kinesin molecular motor family takes a single 8 nanometer step forward for each ATP hydrolyzed except in rare cases. Recent experiments have demonstrated multiple steps including frequent back steps may be possible if the necklinker connecting the heads of the kinesin are extended. In this talk I will present a detailed intra-step model of kinesin stepping which allows for multiple steps and show that asymptotic quantities can be calculated usinga combination of limit theorems for semi-Markov processes and matrix analytic techniques for Markov chains. ([11])

Hye-Won Kang: The optimal size for space discretization for chemical reaction-diffusion networks

In this talk, I will discuss how to discretize space for the stochastic spatially-discrete model for chemical reaction-diffusion networks. A system with reaction and diffusion is modeled using a continuous time Markov jump process. Diffusion is described as a jump to the neighboring compartments with proper spatial discretization. Considering stationary mean and variance of each species in each compartment, the optimal size for spatial discretization will be suggested. I will show conditions for the exponential convergence to the uniform solution in the corresponding deterministic spatially-continuous model for chemical reaction-diffusion networks. Conditions obtained from the deterministic model approximate criteria for the optimal size for space discretization from the stochastic model well.

Peter Pfaffelhuber: Spatial aspects of multiscale chemical reaction networks

In modeling interactions between different types of molecular species in a population one often makes the assumption that the system is ”well mixed”. This is reflected in the fact that the rate at which reactions between species occur is proportional the overall number of each of the species types that are needed as inputs for the reaction. Intuitively this assumption is correct if molecular transport is ”much faster” than the interactions. When molecular transport is not fast enough to insure spatial homogeneity of the system, one needs to address the role of space in the evolution of the total amount of each species in the system. In this talk we will present a model for a spatially inhomogeneous system. By making different assumptions on how fast the molecular transport is relative to the interactions, we will derive results for the evolution of the total amount of each species in the system, and discuss how they differ from results in a homogeneous system.

Mads Kaern: A framework for stochastic simulations of gene expression within evolving heterogeneous cell populations

The stochastic dynamics of individual cells typically take place within larger populations that are heterogeneous with respect to each individual and evolve with their own intricate dynamics. Noticeably, phenotypic heterogeneity associated with intrinsic or extrinsic noise in single cells may greatly impact population-level dynamics. Such couplings can be demonstrated experimentally using engineered gene regulatory networks, and is expected to have implications in numerous areas ranging from stem cell differentiation and development to drug-resistance within microbial or cancer cell populations. To facilitate the study of such multi-scale dynamical problems, we have developed an algorithm that combines an exact method to simulate molecular-level fluctations in single cells and a constant-number Monte Carlo method to simulate time-dependent statistical characteristics of growing cell populations. To benchmark performance, we compare simulation results with steady-state and time-dependent analytical solutions for several scenarios, including steady-state and time-dependent gene expression and the effects of cell growth, division, and DNA replication. This comparison demonstrates that the algorithm provides an efficient and accurate approach to model the effects of complex biological features on gene expression dynamics. Additionally, we show that the algorithm can quantitatively reproduce expression dynamics within bet-hedging cell populations during their adaption to environmental stress, indicating that it provides the framework suitable for simulating and analyzing realistic models of heterogeneous population dynamics combining molecular-level stochastic reaction kinetics, relevant physiological details and phenotypic variability. ([12])

Hans Othmer: A Multi-Scale Analysis of Reacting Systems

We discuss theoretical and experimental approaches to three distinct developmental systems that illustrate how theory can influence experimental work and vice-versa. The chosen systems - Drosophila melanogaster, bacterial pattern formation, and pigmentation patterns - illustrate the fundamental physical processes of signaling, growth and cell division, and cell movement involved in pattern formation and development. These systems exemplify the current state of theoretical and experimental understanding of how these processes produce the observed patterns, and illustrate how theoretical and experimental approaches can interact to lead to a better understanding of development. We use multiscale analysis of the chemical reaction systems to obtain analytic approximations for amounts of different chemical species. ([13])

Greg Rempala: Statistical and Algebraic Methods for Analyzing Stochastic Mass Action Kinetics

With the development of new sequencing technologies of modern molecular biology, it is increasingly common to collect time-series data on the abundance of molecular species encoded within the genomes. This presentation shall illustrate how such data may be used to infer the parameters as well as the structure of the biochemical network under mass-action kinetics. We use algebraic methods as an alternative to conventional hierarchical statistical methods, and carry out network inference by deciding which rate constants are significantly different from zero. ([14])

David McMillen: Bacterial gene expression: modelling and (some) experiments

Plasmid-borne gene expression systems have found wide application in the emerging fields of systems biology and synthetic biology, where plasmids are used to implement simple network architectures, either to test systems biology hypotheses about issues such as gene expression noise or as a means of exerting artificial control over a cell's dynamics. In both these cases, fluorescent proteins are commonly applied as a means of monitoring the expression of genes in the living cell, and efforts have been made to quantify protein expression levels through fluorescence intensity calibration and by monitoring the partitioning of proteins among the two daughter cells after division; such quantification is important in formulating the predictive models desired in systems and synthetic biology research. A potential pitfall of using plasmid-based gene expression systems is that the high protein levels associated with expression from plasmids can lead to the formation of inclusion bodies, insoluble aggregates of misfolded, nonfunctional proteins that will not generate fluorescence output; proteins caught in these inclusion bodies are thus dark to fluorescence-based detection methods. Our results suggest that computational models using protein numbers derived from fluorescence measurements should take these into account, especially when working with rapidly growing cells. ([15])

Peter Swain: Modelling stochasticity in gene expression

Gene expression is a stochastic, or noisy, process. This noise comes about in two ways. The inherent stochasticity of biochemical processes such as transcription and translation generates intrinsic noise. In addition, uctuations in the amounts or states of other cellular components lead indirectly to variation in the expression of a particular gene and thus represent extrinsic noise. We show that simultaneous measurement of two identical genes per cell enables discrimination of these two types of noise. Although the intrinsic stochasticity inherent in biochemistry is relatively well understood, cellular variation, or 'noise', is predominantly generated by interactions of the system of interest with other stochastic systems in the cell or its environment. Such extrinsic fluctuations are nonspecific, affecting many system components, and have a substantial lifetime, comparable to the cell cycle (they are 'colored'). Here, we extend the standard stochastic simulation algorithm to include extrinsic fluctuations. On a model that involves all the major steps for transcription and translation, we show that these fluctuations affect mean protein numbers and intrinsic noise, can speed up typical network response times, and can explain trends in high-throughput measurements of variation. If extrinsic fluctuations in two components of the network are correlated, they may combine constructively (amplifying each other) or destructively (attenuating each other). Our results demonstrate that both the timescales of extrinsic fluctuations and their nonspecificity affect the function and performance of biochemical networks. ([16], [17])

Konstantin Mischaikow: Developing a Database for the global dynamics of multiparameter systems

My most recent work has been on developing topological methods for the analysis of the global dynamics of multiparameter nonlinear systems. I will discuss new computational tools based on topological methods that extracts coarse, but rigorous, combinatorial descriptions of global dynamics of multiparameter nonlinear systems. These techniques are motivated by several observations: 1) In many applications there are models for the dynamics, but specific parameters are unknown or not directly computable. To identify the parameters one needs to be able to match dynamics produced by the model against that which is observed experimentally; 2) It is well established that nonlinear dynamical systems can produce extremely complicated dynamics, e.g. chaos, that is not structurally stable. However experimental measurements are often too crude to identify such fine structure in the dynamics or to establish the parameter values to sufficient precision even at points that are structurally stable; 3) Often the models themselves are based on heuristics as opposed to being derived from first principles and thus the fine structure of the dynamics produced by the models may be of little interest for the applications in mind. To make the above mentioned comments concrete I will use a simple model arising in population biology. I am very interested in combining these methods with stochastic dynamics. ([18])

Qian, Hong: Nonequilibrium phase transition Emerging landscape, time scales, and the chemical basis for epigenetic-inheritance

We consider a small driven biochemical network, the phosphorylation-dephosphorylation cycle (or GTPase) with a positive feedback. We investigate its bistability, with fluctuations, in terms of a nonequilibrium phase transition based on ideas from large-deviation theory. We show that the nonequilibrium phase transition has many of the characteristics of classic equilibrium phase transition: Maxwell construction, discontinuous first-derivative of the "free energy function", Lee-Yang's zero for the generating function, and a tricritical point that matches the cusp in nonlinear bifurcation theory. As for the biochemical system, we establish mathematically an emergent "landscape" for the system. The landscape suggests three different time scales in the dynamics: (i) molecular signaling, (ii) biochemical network dynamics, and (iii) cellular evolution. For finite mesoscopic systems such as a cell, motions associated with (i) and (iii) are stochastic while that with (ii) is deterministic. We suggest that the mesoscopic signature of the nonequilibrium phase transition is the biochemical basis of epigenetic inheritance. ([19])

Lev Tsimring: Dynamics and synchronization of synthetic gene oscillators

We designed and constructed a novel two-component gene oscillator in bacteria E. coli, based on principles observed to be critical for the core of many circadian clock networks. The design of the oscillator was based on a common motif of two inter-connecting positive and negative feedback loops. A small transcriptional delay in the negative feedback loop leads to stochastic relaxation oscillations which are further amplified and stabilized by the positive feedback loop. We use computational modeling to develop design criteria for achieving oscillations in this system. Drawing on analogy to integrate-and-fire dynamics in neuroscience, we have coined the term degradeand fire oscillations to describe the essence of the dynamics. In our subsequent work, we engineered gene network with global intercellular coupling that is capable of generating synchronized oscillations in a growing population of cells. Using microfluidic devices tailored for cellular populations at differing length scales, we investigated the collective synchronization properties along with spatiotemporal waves occurring at millimetre scales. ([20])

Tom Kurtz: Diffusion Approximation for Multiscale Reaction Network Models

Ćlassical stochastic models for chemical reaction networks are given by continuous time Markov chains. Methods for characterizing these models will be reviewed focusing primarily on obtaining the models as solutions of stochastic equations. The primary focus of the talk will be on employing stochastic analytic methods for these equations to understand the multiscale nature of complex networks and to exploit the multiscale properties to simplify the network models. A diffusion approximation will be described for the slow changing components of a multi-scale system. ([21])

Katharina Best: Is anybody out there? Modelling spatial scaling in quorum sensing

Intercellular communication by means of small signal molecules synchronizes gene expression and coordinates functions among bacteria. This population density-dependent regulation is known as quorum sensing. Quorum sensing is frequently mediated by N-acylhomoserine lactone autoinducers. We investigate the molecular mechanism and regulation of quorum sensing in order to establish a predictive mathematical model of autoinducer signalling in this organism. To this end, we describe the dynamical system of the reactions responsible for the autoinducing behaviour within the bacterial cell and extend it to include coupling via a common environment. In a further step, we investigate the spatial organisation of the communicating cells.

Tomas Gedeon: Somitogenesis clock-wave initiation requires differential decay and multiple binding sites for clock protein

Somitogenesis is a process common to all vertebrate embroys in which repeated blocks of cells arise from presomatic mesoderm (PSM) to lay the foundational pattern for trunk and tail development. Somites form in the wake of passing waves of periodic gene expression that originate in the tailbud and sweep posteriorly across the PSM. Previous work has suggested that the waves result from a spatiotemporally graded control protein that affects the oscillation rate of the clock-gene expression. With a minimally constructed mathematical model, we study the contribution of two control mechanisms to the formation of this gene-expression wave. We test four biologically motivated model scenarios with either one or two clock protein transcription binding sites, and with or without differential decay rates for clock protein monomers and dimers. We examine the sensitivity of wave formation with respect to multiple model parameters and robustness to heterogeneity in cell population. We find that only a model with both multiple binding sites and differential decay rates is able to reproduce experimentally observed waveforms. The wave formation is robust to heterogeneous parameters in the cell population. Our results show that the experimentally observed characteristics of somitogenesis wave initiation constrain the underlying genetic control mechanisms.

David Cottrell: Incorporating diffusion in stochastic models of gene expression

A natural subject to explore in the study of biomolecular reaction networks, is the effect of spatial diffusion and molecular motility on the quantitative and qualitative properties of the biological systems. When there are no bimolecular reactions present, as in the case of the standard model of gene expression, the evolution equations are linear, and an analytical treatment becomes feasible. Our aim is to consider a simple branching-process model for gene expression and extend this to a branching-diffusion model where molecules diffuse in free-space. We derive differential equations related to several statistics and analytically compute a number of quantities related to the spatial correlations of the system.The mathematical approach that we take relies on the fact that the system can be modeled by a branching process, i.e. a process for which there is no interaction between the particles. Branching processes permit a useful decomposition due to the linearity of the process with respect to the initial condition. We take advantage of this property by considering a system of moment generating functions with xed initial conditions and construct the corresponding evolution equations. ([23])

Scientific Progress Made

The workshop explored new research directions and the ways in which researchers in stochastic dynamics, statistics and systems biology can join efforts in advancing our understanding of complex networks and stochastic dynamics in cells. Presentations stimulated many productive conversations between participants, resulting in a number of new project ideas. In particular, as a result of meeting for the first time at the workshop, Hong Qian (University of Washington) and Matthew Scott (Waterloo) have started up a collaboration to analyze nonlinear effects in fluorescence correlation spectroscopy. Also, David Anderson (University of Wisconsin), Des Higham (Strathclyde, Glasgow) and Ruth Williams (UC San Diego) spent some time at BIRS discussing possible diffusion approximations to biochemical reaction network models that capture the natural positivity constraints on concentrations. This has led to a nice joint collaboration that they are currently working on. In both cases the groups did not really know each other before and this BIRS workshop was fundamental to bringing members of the groups together. Inspired by the talk of Mads Kaern (Ottawa), Jonathan Mattingly (Duke), Lea Popovic (Concordia) and postdoc John McSweeney (SAMSI) started a project on the effect that randomness from cell division plays in intracellular chemical reaction systems. A number of other projects between workshop participants previously begun reached significant progress during the workshop. Specifically Paul Tupper (Simon Fraser) finished a paper with Peter Swain (Edinburgh) and made significant progress on a project with Jonathan Mattingly (Duke). Likewise, Tom Kurtz (University of Wisconsin) and Lea Popovic (Concordia) finished a paper on diffusion approximations for reaction networks on multiple scales. Many workshop attendees stressed that the excellent facilities at BIRS (in particular the smaller rooms with lots of board space) were really helpful for their in depth discussions.

Outcome of the Meeting

The workshop brought together mathematical scientists working in disparate scientific communities: probability, stochastic analysis, stochastic numerics, applied mathematics, statistics, bioinformatics, bioengineering. There was also a significant presence of young researchers: 2 graduate students, 3 postdocs, 5 assistant professors. Important problems for future research directions were identified and discussed, starting a number of new collaborations in the process.

Participants

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Chapter 3

Theory and Applications of Matrices Described by Patterns (10w5024)

Jan 31 - Feb 05, 2010

Organizer(s): Pauline van den Driessche (University of Victoria), Richard Brualdi (University of Wisconsin-Madison), Shaun Fallat (University of Regina), Leslie Hogben (Iowa State University), Bryan Shader (University of Wyoming)

Overview of the Field

Over the past several decades, linear algebra, combinatorics, and graph theory have grown into substantial and central disciplines in mathematics. These areas not only blend a range of mathematical tools, but also enrich the vitality of mathematics by connecting many branches of mathematics to various significant applications. Furthermore, the interaction between linear algebra, graph theory, and combinatorics has developed into a true discipline "combinatorial matrix theory" that continues to attract bright young people. Pattern classes of matrices represent an important focused subset of this discipline. Examples of applications that fall within this focus are models of problems in economics, mathematical biology (especially ecological food webs), statistical mechanics, and communication complexity, where the signs rather than the magnitudes of interactions are known.

The problems discussed at the workshop are related to determining, for three types of patterns, what spectra are allowed by a given pattern. Using $*$ to denote a nonzero real number, the three types of patterns are:

- symmetric $(0, *)$ patterns (corresponding to graphs) describing symmetric real matrices;
- general $(0, *)$ patterns (corresponding to digraphs or to bipartite graphs) describing real matrices; and
- $(+, -, 0)$ patterns (corresponding to signed digraphs or to signed bipartite graphs) describing real matrices.

Specific problems that are relevant to all three types of patterns include minimum rank problems, identification of spectrally and inertially arbitrary patterns, pattern-nonsingular matrices, and concepts and questions related to specific matrices associated with the pattern.

Problems related to a general $(0, *)$ pattern include the nonnegative inverse eigenvalue problem for a given pattern; minimum rank of a (rational) nonnegative matrix for a given pattern; and real (or rational) nonnegative factorizations based on the $(0, *)$ patterns of the factors. An open problem related to $(+, -, 0)$ patterns is potential stability, which has important applications in dynamical systems.

Two main objectives of the workshop were:

1. To bring together researchers with differing perspectives, including those in other areas of the mathematical and computational sciences that use the concepts of pattern matrices, but often with differing terminology.

2. To simultaneously examine several specific problems from the perspective of the three pattern types and to cross-apply techniques from one type of pattern to others.

These objectives were accomplished as follows. The workshop provided a single forum in which recent important results and applications were disseminated, and from which new collaborations have emerged. In addition, the workshop enabled researchers in combinatorial matrix theory to keep abreast of developments central to their own interests and exposed them to the array of recent activity and new applications taking place in this important and emerging area. It also enabled researchers in applied areas (e.g., communication complexity) to become familiar with theoretical results that have application.

Recently connections have been identified between minimum rank results and communication complexity, where minimum rank is called sign-rank or dimension complexity. While researchers in this field have recognized the importance of linear algebra, many are unaware of recent results on the minimum rank problem; analogously, researchers working on minimum rank are often unaware of recent developments involving sign-rank in communication complexity. The workshop devoted substantial time and effort to the goal of bridging this gap, and there is no doubt that new collaborations and lines of communication were created. It is of course too early to tell what will come from these collaborations.

Although many researchers on minimum rank problems are aware of the strategies used to attack the problem for each type of pattern, group discussion of the similarities and differences in the approaches to the minimum rank problem across the three types of patterns was initiated leading to a more unified approach.

Participants at this workshop also studied the eigenvalues of certain matrices associated with a graph, including the adjacency matrix and the Laplacian matrix (and a newly introduced skew-adjacency matrix of a graph), with an emphasis on obtaining information to determine (or assess the likelihood) that two graphs are non-isomorphic.

This BIRS workshop on matrices described by patterns was the first workshop devoted to this subject since the very successful "Spectra of families of matrices described by graphs, digraphs, and sign patterns" workshop held at the American Institute of Mathematics (AIM) Oct. 23-27, 2006, which led to ten publications. The focus of both this BIRS workshop and the AIM workshop were inspired by the emergence of pattern matrices as a dominant theme in the successful 2-day workshop "Directions in Combinatorial Matrix Theory" held at BIRS May 6-8, 2004. This is an area of substantial and growing interest. This BIRS workshop provided an opportunity to build on these activities and brought together a more scientifically diverse group. It is expected to be a significant catalyst for continued progress and development of the area. In addition, it may provide an impetus for the organization of future special sessions dedicated to this subject.

As evidenced by the detailed program of the workshop, it welcomed participation from junior researchers, and facilitated the building of collaborations between junior and senior researchers by actively involving them in collaborative research through the use of focused research groups. The organizers promoted an informal atmosphere to the proceedings, with time for casual discussions and research collaborations. The day plan was designed to promote the sharing of information, identification of open problems, and active research on a small number of such problems as selected by the group.

Structure of the workshop

This workshop used a focused collaborative research group structure that is designed to build new mathematical collaboration around specific mathematical goals. While a typical workshop may offer some free time for existing collaborators to work, the use of research groups organized at the workshop fosters new collaborations and full inclusion of junior/less well-known participants. The design used also allows more time for research and has fewer talks than a typical workshop, and is scheduled dynamically, that is, in response to developments during the workshop. The schedule as it actually occurred can be found at `http://www.public.iastate.edu/~lhogben/BIRSschedule.html#sched`. Here we give an overview and explain the purpose of the workshop structure and schedule.

The goal for much of the workshop (Monday, Tuesday, Thursday, part of Friday) was to identify specific problems related to the two themes of minimum rank/communication complexity and spectral graph theory, form small research groups to attack specific problems, and actually begin work on the problems chosen. Monday was devoted to minimum rank of matrices described by a pattern and connections to communication complexity; overview talks were given on these topics in the morning and early afternoon. Although the original intent had been to have all the talks in the morning and select problems in the afternoon, the morning was rather full, and we realized that splitting into small groups so early might split researchers by background, contrary to the intent to bring different perspectives together. Furthermore, forming minimum rank/communication complexity research groups on Monday would complicate forming research groups for problems in spectral graph theory on Tuesday. Thus (scheduling dynamically), the lunch break was taken before the last talk on communication complexity, and the remainder of the afternoon was spent in discussion trying to bridge minimum rank and communication complexity.

On Tuesday morning there were overview talks on two areas of spectral graph theory. With all this background in place, Tuesday afternoon began with the creation of a list of open problems on these two themes; that list appears in Section 3. Having participants create such a list is integral in forming research groups. After generating the list, the participants selected problems and began work in three groups, each containing a mix of junior and senior researchers and participants with varying mathematical perspectives. The three groups continued their work on Thursday, and presented reports on progress on Friday morning. These reports appear in Section 3. Note that each group in fact explored more than one of the questions as new ideas emerged. It is expected the groups will continue their work via e-mail, visits, and at meetings that several members attend.

Wednesday morning was devoted to a talk by Dale Olesky surveying the current state of work on potential stability. The talk was followed by a discussion of promising approaches. Wednesday afternoon was left free, and Wednesday evening was used to showcase junior researchers in the field. The speakers, titles, and abstracts are listed in Section 3.

In preparation for the workshop, a bibliography focussing on the specific topics of our workshop was compiled and circulated to participants. The bibliography grew throughout the workshop, and the final bibliography is now available to all the participants.

Presentation Highlights

In keeping with our twin goals (1) to engage both established and junior researchers, and (2) to encourage discussion, interaction, and collaboration between researchers with diverse scientific perspective, there were two types of talks:

1. Talks giving an overview of current developments in the field by established researchers.

2. Research reports by junior researchers.

Overview talks

The intent of the overview talks was to bring people with different perspectives on the problem together and to facilitate collaboration. These talks were held primarily on the mornings of the first three days, and fell into three groups.

On Monday, L. Hogben and B. Shader spoke on the minimum rank matrices described by a graph, digraph, or sign pattern, and V. Srinivasan and J. Forster on communication complexity and the role of matrix theory and sign patterns in its development.

On Tuesday, problems in spectral graph theory were introduced by W. Haemers, speaking on graphs determined by their spectra, and V. Nikiforov speaking on spectral properties of Hermitian matrices with applications to matrix patterns.

On Wednesday, D. D. Olesky surveyed potential stability of sign patterns. Slides of Olesky's talk are available at `http://www.public.iastate.edu/~lhogben/PotentialStability.pdf` and a video is at `http://www.birs.ca/birspages.php?task=eventvideos&event_id=10w5024`.

Minimum rank and communication complexity

A graph, digraph, or signed digraph describes the zero-nonzero or sign pattern of a family of matrices. The matrices may be symmetric, positive semidefinite, or not necessarily symmetric, and the diagonal entries may be free or constrained, depending on the type of (di)graph or pattern. A minimum rank problem is to determine the minimum among the ranks of the matrices in one of these families; the determination of maximum nullity is equivalent. Considerable progress has been made on the minimum rank problem for the family of symmetric matrices described by a simple graph (free diagonal), although the problem is far from solved. The techniques for the symmetric minimum rank problem were surveyed, and extensions to digraphs and sign patterns were discussed. The minimum rank problem has been completely solved for all types of tree patterns.

The sign-rank of a pattern is defined to be the minimum rank of a real matrix with that sign pattern. The sign-rank of a matrix is a measure of the robustness of the rank of a matrix with that sign pattern under sign preserving perturbations. Techniques were presented for constructing $(+,-)$ patterns of low sign-rank, including the use of Vandemonde matrices, and the following related facts:

$$\text{If the } m\times n\ (+,-) \text{ pattern } P \text{ has at most } k \text{ sign changes per row, then sign-rank } P \le k+1. \tag{3.1}$$

$$\text{If the } m\times n\ (+,-) \text{ pattern } P \text{ has at least } k \text{ sign changes per row, then sign-rank } P \le n-k. \tag{3.2}$$

For a function $f : X \times Y \to \{\pm 1\}$, the communication complexity of f is the minimum number of bits that needs to be exchanged by two parties, Alice and Bob, to compute f when Alice is given an input $x \in X$ and Bob is given an input $y \in Y$ respectively. Communication complexity is a central area of research in theoretical computer science with many interesting applications. Formal definitions of various notions of communication complexity were presented and some techniques used to prove lower bounds results in this area were surveyed. Of particular interest in the context of this workshop is unbounded error randomized communication complexity, as it is is known to be bounded below by $\log_2(\text{sign-rank}(A))$ where $A = [a_{ij}]$ is the matrix whose (x, y) entry is $\text{sgn}(f(x, y))$.

J. Forster's bound for an $m \times n$ $(+,-)$ pattern P is

$$\text{sign-rank}(P) \ge \frac{\sqrt{mn}}{\|M\|}$$

where M is the $(1,-1)$ matrix with sign pattern P, and $\|M\|$ is the spectral norm. Forster's bound gives

$$\text{sign-rank}(\text{sgn}(H)) \ge \frac{\sqrt{n\cdot n}}{\|H\|} = \frac{n}{\sqrt{n}} = \sqrt{n}$$

where H is an $n \times n$ Hadamard matrix and $\text{sgn}(H)$ is its sign pattern. An outline of the proof and extensions of these results were presented.

Spectral graph theory

Willem Haemers' talk dealt with the question: "Which graphs are determined by their spectrum?". For various kind of matrices associated with a graph (e.g., the adjacency matrix and the Laplacian matrix), this is a difficult but intriguing question. It is conjectured that the answer is that almost all graphs are spectrally determined (for the adjacency and the Laplacian matrix), but it has only been proved in a very few cases. On the other hand, there are many graphs that are known to not be determined by their spectrum. The talk surveyed some history, recent developments, and interesting open problems concerning the above question.

Vladimir Nikiforov spoke on the spectra of Hermitian matrix properties, where a *Hermitian matrix property* is a class of Hermitian matrices closed under permutations of the index set. His talk presented two types of Hermitian matrix properties and discussed some general theorems about their spectra.

First, a Hermitian matrix property $\mathcal{P}$ is called *hereditary* if $A \in \mathcal{P}$ implies that every principal submatrix of A is in $\mathcal{P}$. Many natural classes of Hermitian matrices are in fact hereditary, e.g., the positive definite matrices, or all Hermitian matrices with least eigenvalue exceeding -2010. Second, a Hermitian matrix property $\mathcal{P}$ is called *multiplicative* if $A \in \mathcal{P}$ implies that $A \otimes J_p \in \mathcal{P}$, where p can be any positive integer, J_p

stands for the all ones $p \times p$ matrix and $\otimes$ denotes the Kronecker product. Note that "positive semidefinite" is a multiplicative property, but "positive definite" is not.

When a hereditary or multiplicative property consists of matrices with bounded entries, some fairly general theorems about their extremal eigenvalues can be proved. The motivation for this approach comes from graph theory and computer science.

Potential stability

A *sign pattern* $\mathcal{S} = [s_{ij}]$ is a matrix with entries in $\{+, -, 0\}$ and its associated *sign pattern class* is

$$Q(\mathcal{S}) \ = \ \{A = [a_{ij}] : a_{ij} \in \mathbb{R} \text{ and } \operatorname{sgn} a_{ij} = s_{ij} \text{ for all } i, j\}.$$

An $n \times n$ sign pattern $\mathcal{S}$ is *potentially stable* if $\mathcal{S}$ allows (negative) stability; i.e., if there exists a real matrix $A \in Q(\mathcal{S})$ for which each eigenvalue of A has negative real part. The problem of specifying necessary and sufficient conditions for potential stability has remained unsolved for over forty years, and this talk summarized progress by many researchers, including recent developments. Conditions were given that are either necessary or sufficient for potential stability for general sign patterns. In addition, necessary and sufficient conditions were given for potential stability for some sign patterns having a directed graph that is a tree, including those for which the directed graph is a star. Complete lists of all potentially stable tree sign patterns are known for $n = 2, 3, 4$. Techniques for constructing potentially stable sign patterns were described, and open problems concerning potential stability were given.

Research reports

On Wednesday evening a session of short talks was held to showcase young researchers in both linear algebra and communication complexity (followed by a modest reception hosted by the organizers in the Corbett Hall Lounge to encourage and honor these young people). The titles and abstracts of these reports follow.

Louis Deaett, University of Victoria, The rank of a matrix and the girth of its graph

In the case of a positive semidefinite matrix, a result of Moshe Rosenfeld provides a lower bound on the rank when the graph of the matrix is triangle-free. We'll show a new proof of this bound. We also consider the possibility of generalizing the bound under a stronger condition on the girth of the graph.

Jason Grout, Drake University, Computing bounds for minimum rank with Sage

I will explain and give examples of a suite of functions in Sage that use a number of bounds from the literature to compute minimum rank bounds in Sage. The suite also includes a lookup table of minimum ranks for all graphs with fewer than 8 vertices. This program is currently being formatted for inclusion in Sage, and will then be in every copy of Sage, enhancing Sage's comprehensive graph functionality. These functions are a collaborative work between Laura DeLoss, Tracy Hall, Josh Lagrange, Tracy McKay, Jason Smith, Geoff Tims, and myself, and were initially developed in Leslie Hogben's early graduate research class at Iowa State University. For an earlier version of the program, see `http://arxiv.org/abs/0812.1616`.

Alexander Sherstov, Microsoft Research (New England), Sign-Rank and the Polynomial Hierarchy in Communication Complexity

The *sign-rank* of a matrix $A = [A_{ij}]$ with ± 1 entries is the least rank of a real matrix $B = [B_{ij}]$ with $A_{ij}B_{ij} > 0$ for all i, j. We obtain the first exponential lower bound on the sign-rank of a matrix computable by the polynomial hierarchy in communication complexity. Namely, let $f(x, y) = \bigwedge_{i=1}^{m} \bigvee_{j=1}^{m^2} (x_{ij} \wedge y_{ij})$. We show that the matrix $[f(x, y)]_{x,y}$ has sign-rank $\exp(\Omega(m))$. This in particular implies that $\Sigma_2^{cc} \not\subseteq \mathsf{UPP}^{cc}$, which solves an open problem in communication complexity posed by Babai, Frankl, and Simon (1986).

Our result additionally implies a lower bound in learning theory. Specifically, let $\phi_1, \ldots, \phi_r : \{0, 1\}^n \to \mathbb{R}$ be functions such that every DNF formula $f : \{0, 1\}^n \to \{-1, +1\}$ of polynomial size has the representation $f \equiv \operatorname{sgn}(a_1\phi_1 + \cdots + a_r\phi_r)$ for some reals $a_1, \ldots, a_r$. We prove that then $r \geq \exp(\Omega(n^{1/3}))$, which essentially matches an upper bound of $\exp(\tilde{O}(n^{1/3}))$ due to Klivans and Servedio (2001).

Finally, our work yields the first exponential lower bound on the size of *threshold-of-majority* circuits computing a function in AC^0. This generalizes and strengthens the results of Krause and Pudlák (1997). Joint work with Alexander Razborov (University of Chicago).

Sebastian Cioabă, University of Delaware, On decompositions of complete hypergraphs

In this talk, I will study the minimum number of complete r-partite r-uniform hypergraphs needed to partition the edges of the complete r-uniform hypergraph on n vertices. This problem is the hypergraph extension of the classical Graham-Pollak theorem.

Michael Cavers, University of Regina, On the energy of graphs

The concept of the energy of a graph was defined by Ivan Gutman in 1978 and originates from theoretical chemistry. To determine the energy of a graph, we essentially add up the eigenvalues (in absolute value) of the adjacency matrix of a graph. Recently, the Laplacian energy, distance energy, incidence energy, signless Laplacian energy and normalized Laplacian energy has received much interest. We will look at these different types of energies and see how they are affected by the structure of a graph. In the past ten years, there have been more than 150 papers published on graph energy, and it continues to be a highly researched topic by pure mathematicians and theoretical chemists alike.

In-Jae Kim, Minnesota State University, On eventual positivity

An $n \times n$ real matrix A is said to be eventually positive if there exists a positive integer k_0 such that $A^k > 0$ (entrywise positive) for all positive integers $k \geq k_0$. An $n \times n$ sign pattern $\mathcal{A}$ is potentially eventually positive (PEP) if $\mathcal{A}$ has a realization that is eventually positive. In this talk, some necessary or sufficient conditions for a sign pattern to be PEP are given. In addition, it is shown that the minimum number of positive entries in a PEP sign pattern is $n+1$. Joint work with A. Berman, M. Catral, L. M. DeAlba, A. Elhashash, F. J. Hall, L. Hogben, D. D. Olesky, P. Tarazaga, M. J. Tsatsomeros, P. van den Driessche.

Open problems

On Tuesday afternoon the whole group discussed open questions in minimum rank and communication complexity (related to connections between the fields) and spectral graph theory (related to the co-spectral graphs and classes of Hermitian matrices). A subset of problems was selected, groups were formed, and work began that afternoon. On Wednesday, following Olesky's talk on potential stability, the whole group brainstormed open questions in potential stability related to the recent developments that had been surveyed. Lists of questions generated in the problem session and questions from the overview talks on minimum rank and communication complexity, and on spectral graph theory are given below.

Open questions in minimum rank and communication complexity

1. Is there a Forster-type bound for $(0,+)$ patterns? For information on Forster's bound, see Section 3. More generally, can one use sign-rank techniques for $(+,-)$ patterns on $(0,+)$ patterns? Note that it is easy to transform a $(0,1)$ matrix M to a $(1,-1)$ matrix M' via a rank one perturbation, but this does not immediately give information of the relationship between the sign-rank/minimum rank of sgn(M) and sign-rank/minimum rank of sgn(M').

2. Is there a Forster-type bound for $(0,+,-)$ patterns? More generally, can one use sign-rank techniques for $(+,-)$ patterns on $(0,+,-)$ patterns?

3. For a symmetric $(+,-)$ pattern, if we consider only symmetric matrices having the given pattern, is there a (higher) Forster-type bound?

4. Can we find a family with significantly higher symmetric minimum rank/sign-rank than the Hadamard patterns?

5. For a symmetric $(+,-)$ pattern, if we consider only symmetric matrices having the given pattern, is there an analog of (3.1) (see Section 3)?

6. What can be said about minimum rank and sign-rank of $(+, -, ?)$ patterns where ? denotes $+$, $-$, or 0?

7. It is known that the minimum rank of a simple graph, mr(G) satisfies

$$\text{mr}(G) \leq |G| - \kappa(G)$$

where $\kappa(G)$ is the vertex connectivity of G, and in fact a positive semidefinite matrix can be found to realize the upper bound. Is there an analog of this result for $(+, -)$ patterns?

8. Find $(+, -)$ patterns of large sign rank.

9. The rigidity function $R_A(r)$ of a real $n \times n$ matrix A is the minimum number of entries needed to be changed in order to bring the rank down to r (i.e. the Hamming distance to a rank r matrix). Hadamard matrices seem to have large rigidity. Can one constuct an explicit family of matrices A such that $R_A(r) \geq (n-r)^2$?

10. What can be said about sign-rank of $(0, +, -)$ patterns with other properties such as allowing orthogonality, allowing eventual positivity, allowing eventual nonnegativity, allowing nilpotence, spectrally arbitrary patterns?

11. (The δ-conjecture) Let $\delta(G)$ and $\kappa(G)$ denote the minimum degree and vertex connectivity of a graph G with n vertices. It is known that the minimum rank of G is at most $2(n-\delta(G))$ and at most $n-\kappa(G)$. It is conjectured that the minimum rank of G is at most $n - \delta(G)$.

12. Construct a "large" family of "dense" graphs G having minimum rank greater than $\frac{1}{7}|G|$ (for $|G|$ large, almost all graphs have minimum rank greater than $\frac{1}{7}|G|$).

Open questions on spectral graph theory

1. Given a graph G with adjacency matrix A, can non-isomorphic graphs be distinguished by examining the spectra of the family of skew adjacency matrices obtained by signing the nonzero entries of A so as to produce skew symmetric matrices, in all possible ways? This was answered negatively by Group 3.

2. Find additional *interesting* families of connected graphs that are determined by their spectra.

3. (Inverse Eigenvalue Problem for Adjacency Matrix) What are the possible eigenvalues of the adjacency matrix of a graph? What if extra zeros can be added to the spectrum? Consider a small number of nonzero eigenvalues as a special case.

4. (Inverse Eigenvalue Problem for Laplacian) What are the possible eigenvalues of the Laplacian matrix of a graph? What if extra zeros can be added to the spectrum? Consider a small number of nonzero eigenvalues as a special case.

5. What are the possible inertias of the adjacency matrix of a graph?

6. What are the possible inertias of the Laplacian matrix of a graph.

7. Investigate the maximum absolute value of an eigenvalue $\lambda \neq \pm d$ of a d-regular graph.

Group reports

Group 1

Group members: Richard Brualdi, Jürgen Forster, Jason Grout, Leslie Hogben, Ryan Martin, Bryan Shader, Sasha Sherstov, Venkatesh Srinivasan and Pauline van den Driessche.

This group's work was motivated by the following problem:

> Given an $m \times n$ $(+,-,?)$-pattern $P = [p_{ij}]$, determine the smallest k such that there exist vectors $u_1, u_2, \ldots, u_k \in \mathbb{R}^m$ and $v_1, \ldots, v_k \in \mathbb{R}^n$ with sgn$(u_i^T v_j) = p_{ij}$ whenever $p_{ij} \neq ?$.

In communication terms, one can view P as describing a "partial problem", $f : S \to \{+.-\}$, where $S = \{(i,j) : p_{ij} \neq ?\}$. Thus, Alice and Bob know a priori that they only need to be able to determine $f((i,j))$ for $(i,j) \in S$. In matrix completion terms, we are asking for the smallest sign-rank of a $(0,+,-)$ pattern obtained from P by allowing the ?s to be $+$ or $-$, or even $+$, $-$, or 0.

This led the group to the problem of characterizing $(+.-)$ sign-patterns that have small or large minimum rank, where some observations and initial results were obtained. It is a standard result from qualitative matrix theory that the $m \times n$ $(+,-)$ sign-pattern P has minimum rank m if and only if it contains a matrix that is sign-equivalent to Λ_m, where Λ_m is the $m \times 2^{m-1}$ matrix whose columns are all the $m \times 1$ vectors with entries $+$ or $-$ and whose first coordinate is $+$. It is easy to characterize $(+,-)$ sign-patterns with minimum rank 1, both in terms of the sign changes in a column (P has minimum rank 1 if and only if it is sign-scalable to the matrix of all $+$s) and in terms of a forbidden configuration (P has minimum rank 1 if and only if A does not contain a matrix that is sign-equivalent to Λ_2). A more difficult task is to characterize $(+,-)$ sign-patterns of minimum rank at most 2. The group was able to establish both a characterization in terms of sign-changes, and a forbidden configuration characterization involving Λ_3. Characterizing $(+,-)$ sign-patterns with minimum rank at most 3 was recognized as a daunting task as a result of Peter Shor implies that this problem is NP-complete. However, the group began the process of relating $(+,-)$ sign-patterns of minimum rank at most 3 to realizable rank 3 oriented matroids. The Pappus configuration was used to construct a sign-pattern of minimum rank 4 and not containing any matrix sign-equivalent to Λ_4. Further research along these lines is on-going with the goal of classifying the $(+,-)$ sign-patterns of minimum rank 3 and "small" order, and will involve the study of pseudo-line configurations from the theory of oriented matroids.

The discussions led to the development of several algorithms for studying the minimum rank of $(+,-)$ patterns. These algorithms have been implemented in Sage and will be made available to the mathematical community.

In addition, the group worked, and continues to work, on using probabilistic methods (e.g., the Regularity Lemma) to aid in the study of $(+,-)$ sign-patterns with certain forbidden configurations (e.g., Λ_k).

The group also plans to work on the following questions:

- Is there a combinatorial interpretation of Forster's theorem?
  Or is there a weaker result than Forster's theorem that gives a combinatorial reason for a $(+,-)$ sign-pattern to have large minimum rank?
- Can one characterize the $m \times n$ $(+,-)$ sign-patterns of minimum rank $m-1$, or $m-2$?

Group 2

Group members: Louis Deaett, In-Jae Kim, Vladimir Nikiforov, Dale Olesky, Kevin Vander Meulen,

The meeting introduced us to a result of Jürgen Forster that provides a lower bound of $\sqrt{n}$ on the sign-rank of an $n \times n$ Hadamard matrix. This result led to the first linear lower bound on the unbounded-error probabilistic communication complexity of a natural family of Boolean functions. We have begun investigating new avenues for establishing upper and lower bounds on the sign-rank of Hadamard matrices and of other $\pm$ patterns in general. We have already managed to improve a known upper bound on the sign-rank of large Hadamard matrices. We expect that by refining our construction we will be able to improve this upper bound further. Other upper bound techniques involve analysis of the extreme numbers of "sign changes" occurring within rows of the matrix. In the context of Hadamard matrices we have discovered provable limits on the power of this method. On the lower bound side, beyond the analytic methods of Forster few other techniques are known, and these seem limited to combinatorial arguments based on the presence of large L-matrices. A simple counting argument shows that even for a Hadamard matrix of order as small as 64, the lower bound provided by these L-matrices cannot match the lower bound of Forster. Hence, no combinatorial technique of reasonable power seems to be known, and the combinatorial behavior of sign-rank in general seems wide open for investigation. Such a combinatorial understanding could lead to new techniques for proving upper and lower bounds. Our group includes researchers at different levels of experience who have not previously collaborated. We have begun to explore how new combinatorial tools could lead to new techniques for improving upper and lower bounds related to sign-rank and communication complexity. We intend to continue this fruitful collaboration.

Group 3

Group members: Michael Cavers, Sebastian Cioabă, Shaun Fallat, David Gregory, Willem Haemers, Steve Kirkland, Judi McDonald, Michael Tsatsomeros

The group's work centered on eigenvalues for graphs. We began with an investigation of the following inverse eigenvalue question for graphs: given a collection of real numbers, how can it be determined whether or not it is the non-zero part of the adjacency spectrum of some graph. It was noted that without the caveat of looking for the non-zero part of the spectrum, that question is quite difficult, since for example, a resolution of that problem would settle the existence question for certain projective planes. However, being given the freedom to add zeros to a candidate spectrum provides considerable leeway. After some consideration of the solution of the corresponding inverse eigenvalue problem for nonnegative integer matrices, the group decided to move in another direction.

Motivated by an interest in trying to find ways to distinguish between graphs that have cospectral adjacency matrices, the group considered the following family of skew adjacency matrices: given a graph G with adjacency matrix A, the family of skew adjacency matrices for G is formed by signing the nonzero entries of A so as to produce skew symmetric matrices, in all possible ways. It was thought possible that perhaps a pair of adjacency cospectral graphs might be distinguished by looking at the spectra of the corresponding skew adjacency matrices. This possibility was quickly refuted, when the group observed that any pair of adjacency cospectral trees must also share the same skew spectrum.

This last observation led the group to address the problem of characterizing the graphs for which all members of the family of skew adjacency matrices have a common spectrum. A conjecture was formulated on that problem, and work on the resolution of that conjecture is ongoing.

Outcomes of the Meeting

We thank BIRS for supporting this workshop, which all participants found valuable and stimulating.

It is expected that the three working groups or subsets thereof will continue their collaborations on the problems identified, which will likely lead to publications.

Such papers may be submitted to the *Linear Algebra and its Applications* Special Issue on the occasion of the Workshop at the Banff International Research Station titled: "Theory and Applications of Matrices described by Patterns." (January 31 - February 5, 2010). Papers within the scope of the Workshop are solicited from all interested whether or not a participant in the Workshop. The deadline for submission of papers is October 1, 2010. Papers for submission should be sent to one of the four special editors, Shaun Fallat, Leslie Hogben, Bryan Shader, or Pauline van den Driessche. They will be subject to normal refereeing procedures according to *LAA* standards. The editor-in-chief responsible for this special issue is Richard A. Brualdi.

Several surveys introducing the themes of the workshop are also planned. Shaun Fallat and Leslie Hogben will update and broaden their 2007 survey on the problem of minimum rank of a graph to digraphs, sign patterns, and positive semidefinite minimum rank. Venkatesh Srinivasan will survey linear algebraic methods and problems in communication complexity with an emphasis on minimum rank/sign-rank problems.

A webpage associated with the workshop, including the schedule, abstracts, and the slides of D. D. Olesky's Potential Stability talk, is available at `http://www.public.iastate.edu/~lhogben/BIRSschedule.html`.

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Chapter 4

Branching random walks and searching in trees (10w5085)

Jan 31 - Feb 05, 2010

Organizer(s): Louigi Addario-Berry (Universite de Montreal), Nicolas Broutin (INRIA Rocquencourt), Luc Devroye (McGill University), Colin McDiarmid (Oxford University)

Overview of the subject

A branching random walk is a Galton-Watson tree T to which the individuals have been assigned spatial positions (in $\mathbb{R}$, say), in the following manner. The root r is placed at the origin. Each child c of the root is independently given a random position P_c; the distribution of each such displacement is given by some real random variable X. More generally, when an individual u has a child v, v appears at position $P_v = P_u + X_v$, where X_v is an independent copy of X. This yields a natural, though idealized, discrete model of how a population may diffuse over time.

Branching random walks are a natural and basic object of study in probability, and are far from being fully understood. Furthermore, branching random walks turn out to have strong connections in other parts of mathematics and theoretical computer science. To highlight a particularly notable example, consider the problem of understanding the *minimum (most negative) position* of any individual in the n'th generation of T, which we denote M_n. An understanding of this random variable ends up being fundamental for analyzing the expected worst-case behavior of a host of data structures of great interest to the theoretical computer science community. The behavior of the expected value $\mathbb{E}M_n$ also turns out to be intimately connected to the uniqueness of "travelling-wave" solutions to a reaction-diffusion equation called the Kolmogorov–Petrovskii–Piskounov equation, given by $\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} + f(u)$, taking solutions $u(x,t) : \mathbb{R} \times \mathbb{R}^+ \to [0,1]$. This equation has received much attention using both probabilistic and analytical techniques.

The second part of the workshop title refers to the closely related problem of *finding* individuals, or paths, in a tree T, that have particular, desirable properties. Though we may know via probabilistic arguments that with very high probability, M_n is at least x, it may be impractical to actually find an individual with displacement x. For example, if we are searching in a branching random walk tree whose branching distribution B satisfies $\mathbb{E}B > 1$, then the expected number of individuals in generation n grows exponentially in n. If there is only one v in generation n with displacement $P_v \leq x$, then to find this individual may take exponential time. There are several known approaches for finding individuals that come close to attaining the minimal displacement while using limited resources; however, a general understanding of optimal strategies for finding good approximations has yet to be developed.

Very recently, Bramson and Zeitouni (2007,2008+), Addario-Berry and Reed (2009), and Hu and Shi (2008+) have all proved related results on the position of the minimum M_n and on its concentration around its mean; these results build on existing work by Biggins, Devroye, and McDiarmid, among others. It is now clear that for a wide range of branching random walks, there are constants $\alpha \in \mathbb{R}$ and $\beta > 0$ such that M_n is roughly $\alpha n + \beta \log n$ in expectation and in probability (though, as established by Hu and Shi, *not* almost surely). Furthermore, $\mathbf{P}\{M_n - \mathbf{E}M_n > x\}$ decays exponentially quickly in x.

These recent results are established using very different techniques. Bramson and Zeitouni prove their concentration result by connecting the BRW to a family of recursive equations and then studying a related Lyapunov function; Addario-Berry and Reed use a rather combinatorial argument based on the second moment method; and Hu and Shi proceed by connecting a certain exponential martingale with a distinguished path called the "spine" of the tree. There are some intriguing links between the three methods, and a deeper understanding of these links has the potential to lead to a common strengthening of all three results.

From the algorithmic point of view, it is natural to ask whether we can efficiently *find* an individual in the n'th generation who attains or comes close to attaining the minimum position M_n. One extremely natural technique for doing finding an individual with small displacement is the following: given all the individuals seen thus far, consider the individual with the minimum displacement and explore its children. We refer to this approach as the *greedy algorithm*. Aldous (1992) first analyzed this procedure, in the context of binary trees, and gave sufficient conditions for the greedy algorithm to find a path approximating the path to M_n up to a fixed error ϵn in the slope. Aldous further made the (very natural) conjecture that the greedy algorithm stochastically optimizes the minimum position seen up to time t. Surprisingly, this conjecture turns out to be false, as was shown by Stacey (1999); however, Stacey also showed that the greedy algorithm is optimal in a much weaker sense than that proposed by Aldous, and posed multiple intriguing questions about the strongest sense in which some form of optimality holds. (It is worth mentioning the work of Karp and Pearl (1983) and McDiarmid (1992), who studied the behavior of "bounded backtracking" algorithms for finding individuals with small displacement, also using the connection with branching random walks.)

More recently, Pemantle (2008+) has proposed a new algorithm, also of a "greedy" variety for finding individuals whose displacement is close to M_n; the algorithm applies in the case that the displacements are Bernoulli. Pemantle has proved (for certain "subcritical" choices of the Bernoulli parameter) that the running time of this algorithm is with high probability best possible up to $o(n)$ terms. A key step that will be required for the analysis of the remaining cases of this algorithm is to understand branching random walks in which all particles whose displacement exceeds a fixed slope are "killed" and no longer reproduce. Pemantle has also made an intriguing conjecture about the *class* of algorithms in which optimal algorithms must lie.

When using results on branching random walk to analyze (usually tree-based) data structures, one of the primary obstacles is the fact that branching random walks are usually limit objects for the data structures in question. To apply results for BRW to the data structures themselves, one must somehow "pass from infinite to finite", and it is usually far from clear how to proceed. For example, the expected worst-case query time is essentially determined by the finitization of the minimum displacement M_n. Using this fact, it is rather straightforward to bound the first-order asymptotics of the expected worst-case query time (i.e. to "finitize" the fact that $M_n = (1 + o(1))\alpha n$), but understanding lower order terms can be extremely difficult. For the case of binary search trees, the link with (binary branching, exponential displacement) branching random walks has been known since work of Biggins, Devroye, and Pittel in the 1980's. However, pinning down the lower-order behavior of worst-case query time was only accomplished (by Reed and, later, Drmota) in 2003. A substantial part of the technical challenge in Reed's approach was dealing with the finitization, and his solution made heavy use of binary branching. Chauvin and Drmota (have had some success at extending Drmota's approach to more general search trees; however, a general strategy for handling this finitization remains elusive.

Finally, one may consider a generalization of the branching random walk model, where the displacements are given by a Markov chain (displacements along distinct edges remain independent), or where the random displacements depend on the initial position. In this case much less is known about the behavior of the system. The first-order asymptotics can be derived without much more difficulty than in branching random walks, but lower order behavior seems much harder to handle. A common approach is to renormalize so that the first order term vanishes (i.e. so that $M_n = o(n)$) by subtracting a fixed constant from each displacement. Once this is done, even the question of recurrence or transience is rather difficult; though at this point it is rather well understood due to work of Comets, Menshikov and Popov (1998), Machado and Popov (2000,2001,2003), Gantert and Müller (2006) and Müller (2008+).

Overview of the workshop

During the week of the workshop there was a strong emphasis on direct contact and collaboration; as such, we limited talks to the mornings of the workshop, and spent the afternoons discussing and working in groups. For the first two afternoons we had problem sessions, to help motivate future discussions. What follows is a summary of some of the substantial open problems that were presented during the workshop.

Overview of some of the open problems arising from or presented at the workshop.

ARCSINE TYPE LAW IN A BRANCHING RANDOM WALK?
Yueyun Hu

Let $(V(x),\ x \in \mathbb{T})$ be a branching random walk on the real line. The positions of the particles in the n-th generation are denoted by $(V(x),\ |x| = n)$. Let $[\![\emptyset,\ x]\!] = \{x_0, x_1, ..., x_n\}$ be the set of vertices on the shortest path connecting the origin $\emptyset$ to x such that $|x_i| = i$ for $i = 0, ..., n$. Define $\overline{V}(x) := \max_{y \in [\![\emptyset,\, x]\!]} V(y)$, for $x \in \mathbb{T}$. It has been shown in Hu and Shi (2007, Ann. Prob.) that $\min_{|x|=n} \overline{V}(x)$ plays an important role in the study of random walk in random environment on the tree $\mathbb{T}$. Recently, Fang and Zeitouni (2009, Arxiv) and Faraud, Hu and Shi (2010, preprint) have independently obtained the asymptotic behaviors of the min-max $\min_{|x|=n} \overline{V}(x)$. Let $x^{*,n}$ be a vertex in nth generation satisfying $\overline{V}(x^{*,n}) = \min_{|x|=n} \overline{V}(x)$. We are interested in

$$\tau_n := \min\{j \leq n : V(x_j^{*,n}) = \overline{V}(x^{*,n})\}.$$

Question: Does $\frac{\tau_n}{n}$ converge as $n \to \infty$? If yes, what is the limiting distribution?

RECONSTRUCTING SCENERY FROM A MARKED GENEALOGICAL TREE
Serguei Popov

Let us put 0s and 1s to the sites of $\mathbb{Z}^d$, $d \geq 2$, at random (e.g., independently and with equal probabilities). This "coloring" of $\mathbb{Z}^d$ is referred to as *scenery*. Then, consider a branching random walk starting from one particle at the origin: the transition probabilities are those of the simple random walk, and each particle is substituted by two on each step. Then, to each vertex of the genealogical tree of the BRW (which is a rooted binary tree in this case), we put 0 or 1 according to the color the corresponding particle observes. The problem is: having only this genealogical tree with marks, obtain an algoritheorem that a.s. reconstructs the original scenery (up to shift/reflection).

FROGS
Nina Gantert

The frog model can be described as follows. Let G be a graph and take one vertex to be the origin. Initially there is a number of sleeping particles ("frogs") at each site of the graph G except at the origin. The origin contains one active frog. The active frog then starts a discrete-time simple random walk on the vertices of G. Each time an active frog visits a site with sleeping frogs the latter become active and start moving according to the same random walk as the active frogs, independently from everything else. An interpretation of the model is the distribution of information: Active frogs hold some information and share them with sleeping frogs as soon as they meet. The sleeping frogs become active and start helping in the process of spreading the information (cf. [21]). The frog model can also be interpreted as a "once-branching" random walk, i.e. a branching random walk where branching takes only place in a site which is visited for the first time.
We denote by η_x the number of sleeping frogs initially in x. One is interested in recurrence and transience, i.e. whether the probability of having infinitely many visits to the origin is 1 or strictly less than 1.

For a symmetric random walk on $\mathbb{Z}^d$, the frog model (starting with one frog at each site) is known to be recurrent, cf. [19] and [20]. There are variants of the model where the frogs have random lifetimes, and one is interested in survival/extinction of the process (and its dependence on the parameters), see [21]. Another question which has been investigated for the model is the existence of shape theorems.

Open problems

(1) Consider the frog model with simple random walk. Not even for transitive graphs, starting with one frog everywhere, recurrence and transience are settled: an example of a graph where this question is open is the binary tree.
(2) A natural conjecture is the following: Assume that the graph G is transitive, the underlying random walk is homogeneous and the initial configuration η is i.i.d. Then we have either

$$P_\eta \left[\text{the origin is visited infinitely often}\right] = 0 \qquad \mu\text{-a.s.}$$

or

$$P_\eta \left[\text{the origin is visited infinitely often}\right] = 1 \qquad \mu\text{-a.s.}$$

For background on the model and further open problems, we refer to [21] and [18].

SURVIVAL OF BRANCHING RANDOM WALKS ON GRAPHS
Sebastien Mueller

A branching random walk (BRW) on a graph G is defined as follows: start the process with one particle in the origin, then inductively each particle dies at rate 1 and gives birth to new particles at each neighboring vertex at rate λ independently of the rest of the process. There exists some $\lambda_c = \lambda_c(G)$ such that the process dies out a.s. if $\lambda < \lambda_c$ and survives with positive probability if $\lambda > \lambda_c$.

Open question 1: What is λ_c?

One may start with the following:

Open question 1a: Let the underlying graph be a realization $\mathcal{T}$ of a Galton–Watson tree. What is $\lambda_c(\mathcal{T})$?

Open question 2: What happens in the critical case, i.e., $\lambda = \lambda_c$?
Background
The branching random walk (BRW) on a locally finite graph $G = (V, E)$ is a continuous-time Markov process whose state space is a suitable subset of $\mathbb{N}^V$. The BRW with parameter λ is described through the number $\eta(t, v)$ of particles at vertex v at time t and evolves according the following rules: for each $v \in V$

$$\begin{aligned} \eta(t,v) &\rightarrow \eta(t,v) - 1 \text{ at rate } \eta(t,v) \\ \eta(t,v) &\rightarrow \eta(t,v) + 1 \text{ at rate } \lambda \sum_{u: uv \in E} \eta(t,u). \end{aligned}$$

Let $o \in V$ be some distinguished vertex of G and denote $\mathbb{P}_o$ the probability measure of the process started with one particle at o at time 0. Define $Z(t) = \sum_v \eta(t, v)$ the number of particles at time t. One says the BRW survives (with positive probability) if

$$\mathbb{P}_o \left(Z(t) > 0 \text{ for all } t \geq 0 \right) > 0.$$

Define the *first moment matrix* $M = (m(x, y))_{x,y \in V}$: $m(u, v) := \lambda$ if $uv \in E$ and $m(u, v) := 0$ otherwise. In other words: $M = \lambda \cdot A$, where A is the adjacency matrix of the graph $G = (V, E)$. Survival of a branching processes is connected to the (expected) growth rate. It turns out that the following definition is very useful:

$$\lambda(M) := \inf\{\lambda > 0 : \exists 0 < f \in L_\infty : \ \lambda M f \geq f\}$$

Bertacchi and Zucca [22] answered Question 1 in the following way:

Theorem 1 $\lambda_c = \lambda(M)$

Despite the latter theorem there are no known *non-trivial* examples where one can really calculate or describe explicitly the critical value λ_c. Observe that for all Cayley graphs, transitive graphs or even quasi-transitive graphs one does have a good description of λ_c, see [22] or earlier work [25], [31]. Furthermore, for percolation clusters on graphs with bounded degree it turns out that $\lambda_c = 1$.

A natural candidate for a non-trivial example is the BRW on a Galton–Watson tree. This model was studied in Pemantle and Stacey [24]. While they obtained a partial description of λ_c, Question 1a is open in the sense that no general formula for λ_c in terms of the offspring distribution of the Galton–Watson process is known.

The method used in [22] does not seem to carry over to the critical case. In [22], they also give an example (in a more general setting) that survival may also occur in the critical case. This example does not apply for graphs with bounded degrees, so that one might conjecture that in our setting the BRW always dies out in the critical case.

Searching in random trees
COLIN MCDIARMID

Consider an infinite complete binary tree, with iid edge-lengths X_e. For each node v let its ‘position’ or ‘birth time’ $S(v)$ be the sum of the edge-lengths along the path to it from the root. Let M_n denote the first birth time of a node in generation n (at depth n). How quickly can we find a node v in generation n with $S(v)$ equal to M_n or nearly so?

The setting is a little too special for some algoritheoremic questions since there are no dead-ends, so let us generalise to a Galton-Watson tree with bounded family size and mean family size $m > 1$, conditioned on survival.

Suppose that the edge-lengths are Bernouilli. The problem is easy if $m\,\mathbb{P}(X_e = 0) > 1$, as the first birth times M_n stay bounded, and it is easy to find an optimal node; and further, in the case $m\,\mathbb{P}(X_e = 0) = 1$ the first birth times grow only like $\log\log n$ and again it is easy to find an optimal node, see [31, 32].

Let us suppose then that $m\,\mathbb{P}(X_e = 0) < 1$. It has been known since the work of Hammersley, Kingman and Biggins in the mid 70s that, conditional on survival, there is a constant $\gamma > 0$ such that $M_n/n \to \gamma$ a.s. (and we may specify γ). Further, for any $\epsilon > 0$ there is a polynomial time algoritheorem, which, with high probability conditional on survival, finds a node v in generation n with $S(v) < (1+\epsilon)\gamma n$, see [31, 32]. Here ‘time’ refers to number of edge-lengths examined.

This seemed a satisfactory algoritheoremic result: the optimal value was known up to an error term $o(n)$, and we could quickly find a node with birth time at most a similar distance from the optimum. But now we know the optimum value very precisely. Following limited earlier steps in [33], it is shown by Addario-Berry and Reed in [26] that M_n has expected value $\gamma n + \alpha\log n + O(1)$ for a given constant α, and M_n is strongly concentrated around this value.

Thus now it seems natural to seek a node v with $S(v)$ closer to the optimum value, and not settle for a birth time which is ϵn too big. There have been recent results suggesting that we can restrict a search to ‘small’ parts of the tree and still come close to an optimal solution, see [30, 29]. Also, see [27, 28, 35] for related work with a different algoritheoremic target (what is the best node you cacn find at any depth within n steps?)

Thus we ask how close to the optimum we can come in polynomial time? In other words, what is the smallest ‘accuracy term’ $\delta(n)$ for which there is a polynomial time algoritheorem which, with high probability conditional on survival, finds a node v in generation n with $S(v) \le B(n)+\delta(n)$? The ‘staged’ back-tracking algoritheorem from [31, 32] will handle $\delta(n) = n\log\log n/\log n$, but what about say $\delta(n) = n^{\frac{1}{2}}$? Also, we could also abandon polynomial time, and ask say whether in time $O(2^{n^{\frac{1}{3}}})$ we can come within $n^{\frac{1}{3}}$ of the optimum value?

BRANCHING POINT PROCESSES
Louigi Addario-Berry

Let $\mathcal{U}$ be the *Ulam–Harris tree*, which has vertex set $\bigcup_{n=0}^{\infty} \mathbb{N}^n$ (we take $\mathbb{N}^0 = \emptyset$ by convention), is rooted at $\emptyset$, and in which a node $u_1u_2\ldots u_k$ has parent $u_1u_2\ldots u_{k-1}$ and children $\{u_1u_2\ldots u_kv, v \in \mathbb{N}\}$.

Let P be a point process on $\mathbb{R}$. We assume that P is such that almost surely, P has a (random) least element $p_0 > -\infty$ and that P almost surely has no accumulation points, so that it is possible to list the elements of P in increasing order as $\{p_i\}_{i\in\mathbb{N}}$. (If P has only finitely many elements, then we let $p_i = +\infty$ for all $i > |P|$.) We may then form a branching random walk with reproduction-diffusion mechanism P by associating to each node $v \in \mathcal{U}$ an independent copy P^v of $\mathcal{P}$. For a child vi of node v, we then view p_i^v as the displacement from v to vi. For a node $v = u_1u_2\ldots u_k$, writing $v^0 = \emptyset$ and $v^i = u_1u_2\ldots u_i$ for $1 \le i \le k$, the *position* S_v of v is then $\sum_{i=0}^{k-1} p_{u_{i+1}}^{v^i}$, the sum of the displacements along the path from the root to v. Let M_n be the minimum position of any node in $\mathbb{N}^n$. By our assumptions on the point process, there is almost surely a node achieving this minimum value.

In a sequence of papers, each building on the results of the last, [36], [37] and [38] showed that under suitable conditions on the point process P, there is a finite constant γ such that, conditional on the survival of the branching process,

$$M_n/n \to \gamma \qquad \text{almost surely.}$$

When Hammersley initiated this research into the first-order behavior of M_n, he posed several questions to which complete answers remain unknown. In particular, he asked when more detailed information about $M_n - \gamma n$ than that given by the above law of large numbers can be found, about the expectation of M_n, and about whether the higher centralized moments of M_n are bounded. Thanks to the work of several researchers the answer to this question is now understood in great detail and in quite some generality *under the assumption that P is almost surely finite.* My question is about how easily this assumption can be removed.

Open question 1: Under what conditions on the point process P does $\mathbb{E}\{M_n\}$ have the form $an + b\log n + O(1)$, for some constants $a, b > 0$.

A technical difficulty to extending at least some of the techniques that work when P is almost surely finite, is the following. When P is almost surely finite, by randomly permuting the finite-displacement children of each node, it is possible to assume that in fact the finite displacements to the children of a node are identically distributed. This yields that the sequence of displacements down any non-backtracking path from the root using only finite-displacement edges, has precisely the behaviour of a random walk. Results on sample paths of random walks (a now-standard technique in analyzing branching random walks) can then be brought to bear on the problem. It turns out [**?**] that this technique can also be made to work when P is infinite if the inter-point spacings of P are independent and identically distributed. However, this only describes a relatively limited number of point processes. A potentially more powerful approach would be to extend existing results on sample paths of random walks to random-walk-like sequences of jumps where the jumps are not necessarily iid. As this is potentially a bit vague, here is a concrete open problem which could guide an attack via this sort of approach.

Open question 2: Let $(x_1,\ldots,x_n)$ be real numbers with $\sum_{i=1}^n x_i = s \le \sqrt{n}$. Find sufficient conditions on $(x_1,\ldots,x_n)$ to ensure that if $\sigma : [n] \to [n]$ is a uniformly random permutation, then

$$\mathbb{P}\left\{\sum_{j=1}^{i} x_j > 0,\ 0 < j < n\right\} = \Omega\left(\frac{k}{n}\right).$$

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Chapter 5

Small scale hydrodynamics: microfluidics and thin films (10w5035)

Feb 07 - Feb 12, 2010

Organizer(s): Richard Craster (Imperial College London) G. M. Homsy (University of British Columbia) Demetrios Papageorgiou (Imperial College London)

Context and Objectives

The meeting was organized from the point of view that a revolution is currently occurring in the miniaturization of fluid mechanical devices. Many developments are driven by medical, biochemical, bioanalytical, nanoliter scale chemical reaction engineering, and microfluidic "lab-on-a-chip" devices. Still others find their motivation in the development of advanced materials, such as superhydrophobic and patterned surfaces with unique wetting, electrical and material properties, self-assembled materials that acquire their structure as a result of non-hydrodynamic forces, and so-called 'complex fluids': colloids, polymer solutions, and particulate suspensions, that involve what is often counter-intuitive fluid mechanical behavior. Electromagnetic forces, surface tension and surface tension variations due to coupling with other fields, substrate variations, and complex rheology all become more efficient at the small scales involved and represent additional forces and degrees of freedom that can be used to manipulate flows in new ways. Theories and approaches appropriate for larger scale fluid mechanics are either not valid or need to be re-interpreted or extended. For instance, the devices feature fluid layers so thin that often gravity is irrelevant while other forces created by, say, minute temperature, chemical or wettability gradients become dominant. Microfluidic devices often feature small scale mechanical pumps, sensors, and strong coupling between thermal, chemical, electromagnetic and fluid velocity fields. The further advancement of such devices would greatly benefit from mathematical modelling and predictive analysis.

Scientists working on microfluidics, and thin films, often operate in disparate and disconnected communities. The lead journals and scientific meetings are often quite different and often have different foci. The sheer pace of progress means that many ideas and avenues are possibly being pursued in parallel. Additionally, there is the lost opportunity for interdisciplinary approaches that enable quantum leaps forward in understanding and development of both new devices and new mathematical approaches. There is no obvious venue where experimentalists, modellers, and applied mathematicians from the two communities are brought into contact with the specific aim of identifying areas ripe for synergistic advances. This workshop provided exactly this venue.

Hence, the main objective of this workshop was to bring together the leading researchers in microfluidics and thin films from across several disciplines in order to foster awareness and the cross-disciplinary transfer of ideas. The broad and interdisciplinary nature of the participants led to a lively workshop characterised by interaction and discussion.

Scientific Progress and Outcomes

Participants were all allocated 25 minute talks with time for questions and discussion built into the format. The talks were grouped into sessions that followed broad themes, there was deliberately no attempt to separate theory and experiment talks. The workshop allowed younger researchers and postdocs to present their recent results, while more experienced researchers tended to present more of an overview of their research and of their area. All presentations were of very high quality and stimulated discussion, some leading to new collaborations. The speakers, talk titles and abstracts are listed in alphabetical order in the following section, with the programme itself given at the end of the report. Notably the programme was organised around themes rather than methods allowing for maximal interaction and, as can be seen from the absracts, was strongly inter-disciplinary in nature.

By all measures, the workshop was a success. We were fully subscribed at 43 participants, the vast majority of whom stayed for the entire week. In terms of demographics, the speakers included 8 women ranging from very senior full professors to assistant professors, postdoctoral researchers and PhD students, all from major universities and highly-ranked departments. There was also an excellent mix of junior and senior participants. There were 16 junior level researchers, including 2-3 postdoctoral fellows, representing a full 40 percent of the total number of attendees.

The workshop was very broad in scope, and encompassed the leading experts in experimental, computational, and theoretical aspects of a wide range of phenomena. This was one of its strengths, but makes a concise summary of outcomes difficult. We include here the following testimonials received, which give a good representation of the success of the workshop.

“I really enjoyed the workshop, and I would like to thank you for giving me the opportunity to come and present my work. The organization was splendid, and it was a very nice group of people. Also, I find that 25 minutes is sort [of] the ideal talk length... Regarding suggestions for a future workshop, I think you should definitely do it (or whoever else takes over, let me know if you need some help by the way). The setup is ideal, both for talks and informal discussions. I would suggest maybe having a few more students come and give talks (possibly shorter), as I think they would benefit from mixing with the faculty. And, at least in my mind, the more experimental talks, the better!”

“Thank you very much for organizing this outstanding workshop in such a nice environment! I think it was useful for people working actively in the field and it would be a good idea to organize something similar in 2-3 years. I would suggest to enforce speakers to be on schedule and to leave a bit more freedom when to have dinner since some of us come from different time zones.”

“The meeting covered a wide variety of topics... with all papers at the forefront of the area. I enjoyed the single session with all talks in the same lecture theatre, meeting new people and catching up with old friends. The facilities, such as computing/printing etc including the hall of residence were great. Nice informal atmosphere with plenty of opportunity for discussions. On the plus side also the fact that all attendees stayed at the same hall. Overall a great experience, hope there is a follow-up meeting.”

“[The meeting] was one of the best if not the best meeting I have attended. The scientific program was excellent and the workshop provided a very good opportunity to hear what people are thinking about in microfluidics etc. Without a doubt, it will influence the things I work on next... The organization, facilities etc. were all first class. Clearly, it would be very good to hold a similar meeting again.”

“Thanks again for organizing such a wonderful meeting in Banff, and for inviting me to be a part of it. It was a rare joy to spend four days in such a beautiful and stimulating environment.”

“Great environment for a workshop – small, high quality participants, meals together, lounge, all contributed to a very interactive environment. I met many people I had not previously known, furthered one collaboration and potentially started at least one other. The range of topics was great – a bit of eclecticism is good in meetings like this but you don’t want too much. I think this workshop struck the balance really well. I would be excited to attend another in a couple years.”

“I particularly enjoyed the conference at BIRS. The format... allows for much greater interaction between participants. As everyone stays in the dorm and eats in the cafeteria, it is difficult not to form contacts. As a new worker, these sorts of contacts are invaluable to me. Work I had done impinged on two of the topics... making several directly relevant to my research. In two of these cases, the work discussed had not been published and came from fields that I wouldn’t normally read the literature from... The mix of disciplines meant that there were people I would not normally see talk. The mix of theory and experiment made the conference particularly fruitful.... The organization of the conference around the topic of microfluidics rather than a technique made this sort of interaction more likely, but credit is due to the organizers for building a program that was so well integrated."

"I had an excellent time and learned a great deal. The number of participants was just right—I had the chance to talk with everyone there. I also liked the length of the talks and the way there was usually a break after every 2 or 3 talks. Of course, the setting and facilities were superb. I would support having a similar workshop in the future, perhaps in 3 or 4 years... It would be good to bring in some new people so that there are fresh viewpoints. I think it worked very well the way you had a mix of junior and senior people, and people from a variety of disciplines and backgrounds."

"The workshop was very good: impeccably organized, top-notch scientific level, a spectacular location, and wonderful food! I was very impressed by the standard of the presentations: all speakers seemed genuinely concerned to put over their work in a clear and interesting way. I made several new contacts, and got ideas for problems to work on."

"It was really one of the best workshops that I have attended in a long time and did provide new collaborations and ideas, even in my own dept. It would be great to have another workshop."

"I am very honored to be invited to talk to such as distinguished audience at this point in my career. I learned a great deal in every talk and it was great to see what a wide range of problems and approaches people are studying in the small scale fluids world. A number of people had suggestions for future directions or directed me to relevant literature. I had an in depth discussion with one of the participants that will greatly help with some of the problems that have cropped up in the course of my experiments. The format was much better than a national meeting-type conference (my only other point of comparison). It really allowed for some in depth conversations to happen. A particular highlight for me was having meals with everyone else at the workshop. Not only was the food great, but it gave me a chance to meet people I probably would have never met at a national meeting in an informal environment."

Summary of Presentations

Shelley Anna: The Impact of Surfactant Sorption Kinetics on Microscale Tipstreaming In this talk, we examine the role of surfactant adsorption and desorption at the oil-water interface in the tipstreaming process, in which submicron sized droplets are synthesized via formation of a thin thread emitted from a larger parent drop.

Neil Balmforth: First contact in a viscous fluid A lubrication theory is presented for the effect of fluid compressibility and solid elasticity on the descent of a two-dimensional smooth object falling under gravity towards a plane wall through a viscous fluid. The final approach to contact, which takes infinite time in the absence of both effects, is determined by numerical and asymptotic methods. Compressibility can lead to contact in finite time either during inertially generated oscillations or if the viscosity decreases sufficiently quickly with increasing pressure. The approach to contact is invariably slowed by allowing the solids to deform elastically; specific results are presented for an underlying elastic wall modelled as a foundation, half-space, membrane or beam.

Michael Booty: Surfactant solubility effects We investigate the influence of surfactant, and in particular the influence of solubility of surfactant in the bulk flow, on the evolution of a prestretched inviscid bubble surrounded by a viscous fluid. Direct numerical simulations at low Reynolds number show that insoluble surfactant can cause the bubble to contract to form a quasisteady slender thread connecting parent bubbles, whereas in the absence of surfactant the bubble proceeds directly to pinch-off near a local minimum radius of the initial profile. Surfactant solubility effects in the diffusion-controlled regime are expressed by three parameters, and we present results on the influence of these on thread formation. The simulations are complemented by a long wave analysis for a capillary jet in the Stokes flow limit, which bears out the mechanisms described in the simulations. With soluble surfactant, a slender thread forms but can pinch-off later due to exchange of surfactant between the interface and exterior bulk flow. (Joint work with Yuan-Nan Young, Michael Siegel, and Jie Li.)

Richard Braun: Models for the Dynamics of the Human Tear Film Lubrication theory is used to describe the dynamics of models for the human tear film in one-dimensional moving domains and two-dimensional eye-shaped domains. In the latter, the boundary conditions and flow in the sub-millimeter menisci around the edge of the domain appear to be very important. Results for the two cases will be compared and contrasted. (This work is in collaboration with K.L. Maki, W.D. Henshaw, P.E King-Smith, L. P. Cook, T.A. Driscoll, and A. Heryudono)

Kenny Breuer: Droplet formation and contact line flows We look at a variety of problems motived by contact drop deposition - the generation of small drops on a hydrophobic substrate generated using a retracting needle. The resulting droplet size depends strongly on the complex interactions between the liquid bridge surface tension, governing droplet pinchoff, and the contact line motion which limits the liquid bridge retreat as a depositing needle is withdrawn from the substrate. We present theoretical results on the liquid bridge stability with a moving contact line, and explore the sensitivity of these results to the dynamic contact angle behavior. These predictions are compared with detailed experiments on the droplet size, free-surface shape and evolution and finally measurements, with sub-micrometer scale resolution, of the flow near the retreating contact line.

Joao Cabral: Spinodal Clustering of Nanoparticle-Polymer Mixture in Thin Films We report the spinodal clustering in polymer-nanoparticle mixtures in thin films of polystyrene (PS) and fullerenes C60. Supported PS-C60 blend fims annealed above Tg develop surface undulations with dominant wavelength lambda 1-10 micrometer, which depends on film thickness h (20-500 nm), molecular mass Mw, temperature T and time t. The initial wavelength scales with h and coarsen- ing kinetics follow $\lambda\ t^{\alpha}$. The morphology eventually pins at long times (t$\sim$72 h), while dewetting does not take place in this time frame. Power law exponents are found to be alpha=1/3 for large thick- nesses (h $\sim$ 170 nm) and to decrease effectively to zero as h $\rightarrow$ 20 nm. The spinodal morphology occurs for PS Mw $>$ 10 kg/mol while dewetting suppression and film stability is observed for lower Mw ($\sim$2 kg/mol). The emergence of a spinodal topography in high-Mw PS-C60 thin films results from the interplay between particle-particle and particle-substrate attraction.

Hsueh-Chia Chang: A Micro-Scale Electrokinetic Instability: Selection of the Over-Limiting Current We show experimentally and theoretically that the overlimiting DC current across a membrane or an electrode with a diffusion-limited electron-transfer reaction is determined by a hydrodynamic instability related to miscible fingering. An ion-depleted zone develops on one side of the membrane and propagates into the bulk as a diffusion front. However, the diffusion front destabilizes at a particular distance from the membrane, which is determined with a spectral theory specific to the self-similar diffusion front, and selects the depletion layer thickness to determine the ion flux density at the overlimiting current region.

Richard Craster: Rupture and interfacial deformation of electrokinetic thin films We investigate the evolution of an electrolyte film surrounding a second electrolyte core fluid inside a uniform cylindrical tube and in a core-annular arrangement, when electrostatic and electrokinetic effects are present. The limiting case when the core fluid electrolyte is a perfect conductor is examined. We analyse asymptotically the thin annulus limit to derive a nonlinear evolution equation for the interfacial position, that accounts for electrostatic and electrokinetic effects and is valid for small Debye lengths that scale with the film thickness, that is charge separation takes place over a distance that scales with the annular layer thickness. The equation is derived and studied in the Debye-Hückel limit (valid for small potentials) as well as the fully nonlinear Poisson-Boltzmann equation. These equations are characterised by an electric capillary number, a dimensionless scaled inverse Debye length and a ratio of interface to wall electrostatic potentials. We explore the effect of electrokinetics on the interfacial dynamics using a linear stability analysis and perform extensive numerical simulations of the initial value problem under periodic boundary conditions. Allied nonlinear analysis is carried out to investigate fully singular finite-time rupture events that can take place. Depending upon the parameter regime, the electrokinetics either stabilise or destabilise the film and, in the latter case, cause the film to rupture in finite time. In this case, the final film shape can have a ring or line-like rupture; the rupture dynamics are found to be self-similar. In contrast, in the absence of electrostatic effects, the film does not rupture in finite time but instead evolves to very long-lived quasi-static structures that are interrupted by an abrupt re-distribution of these very slowly evolving drops and lobes. The present study shows that electrokinetic effects can be tuned to rupture the film in finite time and the time to rupture can be controlled by varying the system parameters. Some intriguing and novel behaviour is also discovered in the limit of large scaled inverse Debye lengths, namely stable and smooth non-uniform steady state film shapes emerge as a result of a balance between destabilising capillary forces and stabilising electrokinetic forces.

Brian Duffy: Quasi-steady spreading of a thin ridge of fluid with temperature-dependent surface tension on a heated or cooled substrate We derive an implicit solution of the thin-film equations for the free-surface profile of the ridge, and use this (along with a Tanner law for the moving contact lines) to examine the possible forms that the ridge's evolution may take. In some cases we find that there may be three (qualitatively different) stable "stationary" states. This is joint work with G. J. Dunn, S. K. Wilson and D. Holland.

Jan Eijkel: The generation of sub-micrometer droplets in a microfluidic system and their self-organization into 3D lattices We generated O/W droplets at the interface between a nanochannel (100-900 nm high) and a microchannel (10 micrometer high). Droplets with a diameter downto 700 nm were produced. Under certain conditions the droplets spontaneously organized into a 3D lattice inside the microchannel. The droplet formation mechanism at the nanochannel/microchannel interface involves the formation of thinning oil filaments extending to the interface, and at present is not understood.

Eliot Fried: Derivation of a dynamical equation for the contact line of an evaporating sessile drop During the early 1950s, J.D. Eshelby developed a framework for the defective crystal lattices. Central to that framework is the notion of configurational force. Whereas Newtonian forces are linked to the motion of material particles, configurational forces are associated with defects that may move with respect to material particles. For crystals, examples of such objects include impurities, dislocations, cracks, and phase interfaces. Eshelbys approach involved a creative synthesis and extension of ideas appearing in J.L. Lagranges work on generalized coordinates and forces, J.W. Gibbs work on the equilibrium of heterogeneous substances, J. Larmors work on the luminiferous aether, and E. Noethers work on conservation laws arising from the invariance of functionals. In Eshelbys approach, the configurational force acting on a defect is determined by computing the variation of the total energy with respect to changes in the configuration of the defect. Eshelbys contributions set the stage for many important contributions to the study of defects in solids, perhaps the most celebrated of these being to fracture, where the relevant configurational force acts at the tip of a crack and is the J-integral derived independently, and without knowledge that Eshelby had done so previously, by G.P. Cherepanov and J.R. Rice.

Being variational, Eshelbys approach is predicated on the provision of constitutive relations. Further, it allows for at most infinitesimal departures from equilibrium and accounts only artificially for dissipative mechanisms which generally accompany the motion of defects. Beginning in the early 1990s, M.E. Gurtin constructed a theory that frees Eshelbys framework of these restrictions. This approach distinguishes carefully between basic laws, which hold for large classes of materials, and constitutive relations, which distinguish between different classes of materials. Configurational forces are treated as primitive and are assumed to obey a balance distinct from the conventional balances of linear and angular momentum. Further, power expenditures associated with the motion of defects are accounted for properly in the statement of the energy balance and the entropy imbalance is used to determine physically reasonable restrictions on constitutive relations. A major advantage of Gurtins theory is that objects such as the J-integral arise independent of constitutive assumptions and encompass not only to the standard elastic case but also to cases where inelastic effects are present.

Recently, Gurtin's approach has been used to develop a theory for evaporation and other fluid-fluid phase transformation, with focus on interfacial equations. In this talk, that theory is extended to yield a dynamical equation the contact line of an evaporating sessile drop. In addition to bulk and interfacial excess quantities, this equation accounts naturally for the energy of the contact line and for frictional terms that have previously been included on an ad hoc basis.

Michael Graham: Transport and collective dynamics in suspensions of swimming microorganisms A suspension of swimming organisms is an example of an active complex fluid. At the global scale, it has been suggested that swimming organisms such as krill can alter mixing in the oceans. At the laboratory scale, experiments with suspensions of swimming cells have revealed characteristic swirls and jets much larger than a single cell, as well as increased effective diffusivity of tracer particles. This enhanced diffusivity may have important consequences for how cells reach nutrients, as it indicates that the very act of swimming toward nutrients alters their distribution. The enhanced diffusivity has also been proposed as a scheme to improve transport in microuidic devices and might be exploited in microuidic cell culture of motile organisms or cells.

The feedback between the motion of swimming particles and the fluid flow generated by that motion is thus very important, but is as yet poorly understood. In this presentation we describe theory and simulations of hydrodynamically interacting microorganisms that shed some light on the observations. In the dilute limit, simple arguments reveal the dependence of swimmer and tracer velocities and diffusivities on concentration. As concentration increases, we show that cases exist in which the swimming motion generates dramatically enhanced transport in the fluid. This transport is coupled to the existence of long-range correlations of the fluid motion. Furthermore, the mode of swimming matters in a qualitative way: microorganisms pushed from behind by their flagella are predicted to exhibit enhanced transport and long-range correlations, while those pulled from the front are not. A physical argument supported by a mean eld theory sheds light on the origin of these effects. These results imply that different types of swimmers have very different effects on the transport of nutrients or chemoattractants in their environment; this observation may be related to the evolution of different modes of swimming.

Michael Gratton: Suppressing van der Waals driven rupture through shear. An ultra-thin viscous film on a substrate is susceptible to rupture instabilities driven by van der Waals (London dispersion) attractions. When a unidirectional "wind" shear τ is applied to the free surface, the rupture of instabilities in two dimensions is suppressed for τ greater than a critical value τ_c and is replaced by a new, permanent, finite amplitude structure, a Dispersion-Capillary Wave that travels at approximately the speed of the surface. If three-dimensional disturbances are allowed, the shear is decoupled from disturbances perpendicular to the flow, and line rupture would occur. In this case, replacing the unidirectional shear with a new shear whose direction rotates with angular speed $\hat{\omega}$ suppresses the rupture if $\tau >\sim 2\tau_c$. For the maximizing wave number, $\tau_c \approx 10^{-2}\,\mathrm{dyn\,cm^{-2}}$ at $\hat{\omega} \approx 1\,\mathrm{rad\,s^{-1}}$ for a film with physical properties similar to water at a thickness of $100\,\mathrm{nm}$.

Anette Hosoi: Low temperature solvent annealing of organic thin films These are films made of organic materials for use in electronics and LCD panels. In order to increase mobility, it is necessary to convert the amorphous state to a crystalline one. I will discuss both experimental results and models describing the annealing process.

Serafim Kalliadasis: Influence of spatial heterogeneities on contact line dynamics We consider contact line motion over spatially heterogeneous substrates by using a two-dimensional droplet of a partially wetting fluid spreading over such substrates as a model system. The spreading dynamics is modelled under the assumption of small contact angles where the long-wave expansion in the Stokes-flow regime can be employed to derive a single equation for the evolution of the droplet thickness. Through a singular perturbation approach, the flow in the vicinity of the contact line is matched asymptotically with the flow in the bulk of the droplet to yield a set of two coupled differential equations for the spreading rates of the two droplet fronts. Analysis of these equations for deterministic substrates reveals a number of intriguing features that are not present when the substrate is flat. In particular, we demonstrate the existence of multiple equilibrium states whichallows for a hysteresis-like effect on the apparent contact line. Further, we demonstrate a stick-slip-type behaviour of the contact line as it moves along the local variations of the substrate shape and the interesting possibility of a relatively brief recession of one of the contact lines. Finally, our formalism is used to investigate droplet equilibria in the presence of small-scale, random substrate variations. Using an appropriate stochastic representation for such substrates, we provide a rational definition of ”substrate roughness” and we assess the statistics of droplet equilibria and dynamics of droplet spreading via a perturbation approach.

R. Krechetnikov: On Marangoni-driven interfacial singularities and their resolution In this talk I will discuss the origin and physical mechanisms of Marangoni-driven singularities at fluid interfaces, in particular in the context of tip-streaming problems, and the development of a mathematical theory aimed at their resolution.

Satish Kumar: Stretching and Slipping of Liquid Bridges near Plates and Cavities The dynamics of liquid bridges are relevant to a wide variety of applications including high-speed printing, extensional rheometry, and floating-zone crystallization. Although many studies assume that the contact lines of a bridge are pinned, this is not the case for printing processes such as gravure, lithography, and microcontacting. To address this issue, we use the Galerkin/finite element method to study the stretching of a finite volume of Newtonian liquid subject to contact line slip and confined between (i) two flat plates, one of which is stationary and the other moving, and (ii), one moving flat plate and a stationary cavity.

Eric Lauga: Small-scale swimming: Physical and mathematical constraints Fluid mechanics plays a crucial role in many cellular processes. One example is the external fluid mechanics of motile cells such as bacteria, spermatozoa, and essentially half of the microorganisms on earth. In this talk we discuss the basic fluid mechanics processes relevant for cell locomotion.

Charles Maldarelli: The Self-Propulsion of a Droplet in a Two-Dimensional Microchannel Driven by a Gradient in the Superhydrophobicity of the Channel Walls Methods for the propulsion of aqueous droplets through a network of microfluidic channels is central to the development of lab-on-chip technologies for chemical analysis. These technologies use the coordinated trafficking and combination of droplets moving through the microfluidic network to execute the fundamental steps of dilution, reaction and separation which are involved in a chemical study. The dominance of capillary forces on the microfluidic length scale suggests their use in devising mechanisms for the droplet motion that would be self-propelling, and would therefore not require off-chip sources of power to actuate the motion. This study examines the hydrodynamics of contact angle propulsion of droplets in microfluidic channels. We consider the propulsion of a single droplet which occludes a two dimensional channel filled with air. The arcs representing the interfaces (menisci) of the droplet intersect the inside surface of the channel at finite contact angles with the magnitude of the angle and hence the curvature of the arcs determined by the surface energy of the walls. In contact angle propulsion, the capillary pressure in the liquid under the menisci on either end of the droplet is used to propel the droplet down the channel. If the channel walls are modified so that the contact angle of an aqueous phase in contact with the channel wall changes with position down the channel, a drop situated in this gradient will experience a difference in the curvatures and capillary pressures between its two ends which can propel the droplet. We consider the case in which gradients in the contact angle are generated on a microtextured surface. Aqueous droplets in contact with hydrophobic, microtextured surfaces trap air in the gaps between the solid parts of the texture creating very large (super hydrophobic) contact angles (Cassie-Baxter wetting) relative to the plane of the wall. A gradient in contact angle along a channel wall created by a gradient in microtexture is ideal for propelling droplets because the droplet liquid moves with reduced friction over the cushions of trapped air, and the larger contact angles allow drops to roll, which prevents liquid from being left behind a moving drop. A simple model of a surface embedded with a uniform microtexture is constructed consisting of contiguous half disks of a given radius and surface energy with the disk centers arranged in a straight line parallel to the plane of the wall. Low Reynolds number solutions for the pressure driven movement of a semi-infinite slug through the channel are obtained to identify the conditions for Casie-Baxter wetting. Gradients in the microstructure are also constructed to study propulsion. Microtexture gradients are obtained by increasing the radius of the disks in the direction down the channel while keeping the height of the disks relative to the plane of the wall constant. Solutions are obtained for the velocity of droplets along these surfaces as a function of the microtexture parameters and surface hydrophobicity.

Omar Matar: Interfacial flows in the presence of additives The presence of additives, which may or may not be surface active, can have a dramatic influence on interfacial flows. The presence of surfactants alters the interfacial tension and drives Marangoni flow that leads to fingering instabilities in drops spreading on ultra-thin films. Surfactants also play a major role in coating flows, foam drainage, jet breakup and may be responsible for the so-called “super-spreading” of drops on hydrophobic substrates. The addition of surface-inactive nano-particles to thin films and drops also influences the interfacial dynamics and has recently been shown to accelerate spreading and to modify the boiling characteristics of nanofluids. These findings have been attributed to the structural component of the disjoining pressure resulting from the ordered layering of nanoparticles in the region near the contact line. In this talk, we present a collection of results which demonstrate that the above-mentioned effects of surfactants and nano-particles can be captured using long-wave models.

M.J. Miksis: Dynamics of Lipid Bilayer Vesicles in Viscous Flow The dynamics of a lipid bilayer vesicle in a Stokes flow is studied. The model accounts for the bending resistance of the membrane, the transport of lipids along the monolayers, and the slip between the monolayers. Small amplitude perturbations from a spherical vesicle are considered and at leading order, a nonlinear system of equations for the dynamics of the interface and the mean lipid density is found and studied.

Sushanta Mitra: Capillary Flow for Microfluidic Applications Capillary flow is often used in various microfluidic devices like Lab-on-a-Chip (LOC) to transport biomolecules, chemicals, and analytes from the inlet reservoir to different locations within the device. The talk will discuss the mechanism of capillary transport in microchannels in presence of a finite reservoir volume. The influence of microbead suspension on the capillary flow will also be discussed. Often electrical fields are also used in a LOC to manipulate analytes of interest. A mathematical framework to investigate the combined electroosmotic and capillary flow will be presented. The talk will end with an application of capillary transport through a microfluidic device with integrated pillars.

Susan J. Muller: Experiments in microfluidic stagnation point flows: opportunities for trapping, deforming, and analyzing DNA, vesicles & other microscale objects We have designed and fabricated a series of microdevices that create stagnation points at which microscale objects may be trapped and subjected to flow forces. In the simplest of these, the cross-slot, microscale objects such as DNA may be trapped and stretched to a steady-state extension that is determined by the flow strength, as demonstrated by the pioneering work of Chu and co-workers (Science, 276, 1997). We will present three extensions of this idea: 1) the design and use of more complex devices to allow the systematic variation of flow type as well as flow strength near the stagnation point (the microfluidic four-roll mill) , 2) the use of stagnation point flows for single molecule studies of enzyme binding kinetics and sequence detection in DNA, and 3) the use of stagnation point flows for studies of the dynamics of vesicles.

A. Pascall: Induced charge electrokinetics over controllably contaminated electrodes Experimental data on induced charge electro-osmosis (ICEO) and related phenomena have shown that the standard theory consistently overpredicts slip velocities by up to a factor of 1000. Here we present experiments in which we controllably ‘contaminate’ the metallic surface with a thin dielectric film or Au-thiol self assembled monolayer, and derive a theory for ICEO that incorporates both dielectric effects and surface chemistry, which both act to decrease the slip velocity relative to a ‘clean’ metal. Data for over a thousand combinations of electric field strength and frequency, electrolyte composition, dielectric thickness and surface chemistry show essentially unprecedented quantitative agreement with our theory.

D.T. Papageorgiou: Electrostatically induced instabilities in interfacial flows. Several problems will be discussed where electric fields are used to either enhance or reduce interfacial instabilities found in a wide class of viscous flows. For example, electric fields can destabilise two-layer shear flows or falling film flows at small Reynolds numbers, and can increase the deformation of viscous drops suspended in a Couette device. In the case of axisymmetric liquid jets, we predict a stabilisation of the capillary pinching event accompanied with the formation of liquid microthreads. We use a combination of asymptotically derived evolution equations and direct numerical simulations in order to analyse such probelms.

Sumita Pennathur: Fundamental transport of electrolyte solutions in nanofluidic channels with finite wall charge In this talk, I would like to present both theoretical and experimental results pertaining to electrolyte flow in nanofludic channels. This will include channels of different heights, electric double layer thicknesses, and surface wall charge composition, as well as different electrolyte fluids. Both pressure-driven and electroomostic flow will be investigated.

Nikos Savva: Three-phase contact line at small scale We investigate the area around an equilibrium three-phase contact line at a small scale by using a density functional approach. A typical system is made of a planar wall in contact with a Lennard-Jones gas below the critical temperature. The wall exerts an attractive force on the fluid molecules so that a thin film can usually form between the wall and the gas. We focus on two cases. When the chemical potential is smaller than its coexistence value and the system presents a phase transition with respect to the film thickness, we examine the area between the two equilibrium film thicknesses. It appears to be smooth and several molecular diameters long. When the chemical potential is at its coexistence value, computations of the equilibrium density profiles show a well formed contact angle whose value follows closely the Young equation. A deviation from this equation is observed in the immediate vicinity of the contact line.

Eric S.G. Shaqfeh: The Microfluidics of NonSpherical Colloidal Particles and Vesicles with Application to Blood Additives Many dispersions of colloidal particles with application in materials processing, biological assays, or medicine, contain elongated particles (e.g. ellipsoidal disks, rods, etc.) Recently these particles have been used in drug delivery applications because of the inability of leukocytes to easily rid them from the circulation. Moreover such particles are useful at the nanoscale for application in cancer therapies, either for detection of tumor vasculature or for the delivery of anti-cancer agents to tumor endothelial cells. Thus, the study of anisotropic particulate flows with adhesion in microchannels especially in mixtures with vesicle flows (i.e. red blood cells) has taken on a particularly important set of engineering applications. We will review our computer simulations of these processes with a view toward virtual prototyping and engineering these therapies.

Amy Shen: Complex fluids under confinement and flow The flow of complex fluids in confined geometries produces rich and new phenomena due to the interaction between the intrinsic length-scales of the fluid and the geometric length-scales of the device. In this talk, I will choose two model systems to illustrate the idea. First, I will focus on a micellar solution system that yields a novel route to synthesizing bio-compatible nanoporous sol-gels. Through a combination of experiment and modeling I will show how self-assembly, confinement, and flow can be utilized to control fluid microstructure and system phase transitions, and thus to enhance the controlled synthesis of bio-compatible new materials. Second, I will illustrate how confinement and flow can modify the self-assembly of supramolecular hydrogels and their subsequent thermal properties.

Mike Siegel: A hybrid numerical method for fluid interfaces with soluble surfactant

We address a significant difficulty in the numerical computation of fluid interfaces with soluble surfactant that occurs in the practically important limit of large bulk Peclet number Pe. At thigh values of Pe in typical fluid-surfactant systems, there is a transition layer near the interface in which the surfactant concentration varies rapidly. Accurately resolving this layer is a challenge for traditional numerical methods but is essential to evaluate the exchange of surfactant between the interface and bulk flow. We present recent work that uses the slenderness of the layer to develop a fast and accurate 'hybrid' numerical method that incorporates a separate analysis of the dynamics in the transition layer into a full numerical solution of the interfacial free boundary problem.

Todd Squires: Microrheology of phospholipid monolayers: direct visualization of stretching, flowing, yielding and healing While the static properties of fluid-fluid interfaces have long been studied – and continue to be – the dynamic properties of interfaces have proven more elusive. I will describe a new technique we have developed to measure the interfacial rheology – the viscous and elastic properties – of fluid-fluid interfaces, typically laden with some surface-active species (molecular surfactants, copolymers, colloids, etc.). Using microfabrication techniques, we make ferromagnetic, amphiphilic microdisk probes that are ideally suited for active interfacial microrheology. By applying an oscillatory torque using electromagnets, and measuring the resulting (oscillatory) displacement, we create a small-scale Couette interfacial rheometer that is exceedingly sensitive to the rheology of the interface. A novel feature is our ability to directly visualize the interface during the measurement, which allows us to directly correlate the microstructural deformation with the measured response. In particular, we explore the linear and nonlinear rheology of a monolayer of the phospholipid DPPC in the liquid-condensed phase, which our experiments reveal to have a far richer dynamical response than has been previously reported. In particular, we demonstrate viscoelasticity, history-dependence, yielding, aging and a surprisingly long-lived recoil, which we relate directly to deformation and cooperative motion of individual LC domains.

Kathleen Stebe: Orientation and Assembly of anisotropic particles by capillary interactions There is significant scientific and technological potential if reliable means are developed to assemble anisotropic particles into ordered structures. Capillary attraction holds promise as a means of orienting, assembling and positioning particles. Capillary interactions arise spontaneously between partially wet particles at fluid interfaces. Particles at interfaces deform the interface to satisfy their wetting boundary conditions. The deformations expand the area of the interface relative to a planar case. The product of this excess area and the surface tension is an excess energy associated with the particle. Capillary attractions arise when deformation fields from neighboring particles overlap; the excess area created by the particles decreases as the particles approach each other. Capillary interactions are remarkably large; the surface tension of an aqueous-air interface is 72 mN/m or 18 kT/nm2, so the elimination of even 1 nm2 of surface area translates into significant energy reduction in particle assembly. Here, particles with shape anisotropy create undulations with excess area that can be locally elevated at certain locations around the particle. The local elevation of excess area (and therefore excess energy) makes these sites locations for preferred assembly, causing particles to orient and aggregate in preferred orientations. We present means to dictate object orientation, alignment, and the sites for preferred assembly, including means of promoting registry of features on particles. We also demonstrate that particle deformation fields interact with background interface shape to assume preferred alignments. These ideas are developed for the example of a right circular cylinder using analysis, experiment and numerics. A series of other shapes are then studied to illustrate the generality of the concepts developed.

Paul Steen: Vibrations of a constrained cylindrical interface Pinning a cylindrical liquid/gas interface along an axial line stabilizes the Plateau-Rayleigh instability, as is well-known. We generalize this kind of constraint to include partial contact of the liquid with a conforming solid support, and study the stability limits and the inviscid capillary oscillations of the interface, as both depend on the extent of constraint.

Jean-Luc Thiffeault: Nonlinear dynamics of phase separation in thin films We present a long-wavelength approximation to the Navier-Stokes Cahn-Hilliard equations to describe phase separation in thin films. The equations we derive underscore the coupled behaviour of free-surface variations and phase separation. We introduce a repulsive substrate-film interaction potential and analyse the resulting fourth-order equations by constructing a Lyapunov functional, which, combined with the regularizing repulsive potential, gives rise to a positive lower bound for the free-surface height. The value of this lower bound depends on the parameters of the problem, a result which we compare with numerical simulations. While the theoretical lower bound is an obstacle to the rupture of a film that initially is everywhere of finite height, it is not sufficiently sharp to represent accurately the parametric dependence of the observed dips or ‘valleys’ in free-surface height. We observe these valleys across zones where the concentration of the binary mixture changes sharply, indicating the formation of bubbles. Finally, we carry out numerical simulations without the repulsive interaction, and find that the film ruptures in finite time, while the gradient of the Cahn–Hilliard concentration develops a singularity.

Dmitri Tseluiko: Electrified liquid films When applied, an electric field affects the stability of a liquid film and can either reduce or promote irregularities in the film surface, both of which can be desirable for applications. I will consider various situations when an electric field acts of liquid films flowing down flat plates or over topographical features.

Jean-Marc Vanden-Broeck: The influence of electric fields on nonlinear free surface flows Nonlinear free surface flows in the presence of electric fields are studied. Both inviscid and viscous fluids are considered. The mathematical problem involves solving the fluid mechanics equations coupled with the Maxwell equations. Fully nonlinear solutions are obtained by boundary integral equation methods and asymptotic solutions are derived for thin films.

Thomas Ward: Droplet production in a microfluidic flow focusing device via interfacial saponification chemical reaction Microfluidic flow-focusing technology will be used to investigate the production of a surfactant via an interfacial chemical reaction. In the absence of a chemical reactions the drop shapes remain constant from the time of break up at the flow-focusing nozzle until they exit the channel. In the presence of the chemical reaction there is modification of the shape depending on the reactant concentrations. These values are measured for a variety of flow conditions with observable trends that seem to depend on the reaction rate, suggesting that the Damköhler number may be the most suitable parameter for characterizing these types of flows.

Stephen Wilson: Theoretical and Experimental Studies of Droplet Evaporation Combined programme of physical experiments and mathemtical theory has cast new light on the ubiquitous problem of droplet evaporation, in particular the key role the substrate and the atmosphere play in this physically important problem. In this talk I’ll review our recent work in this area and highlight directions for future study.

Leslie Yeo: Peculiar Interfacial Phenomena Driven by Surface Acoustic Waves The fluid-structural coupling arising from the large substrate accelerations, typically up to 10 million g’s, associated with surface acoustic waves give rise to peculiar microscale colloidal and interfacial phenomena. Interesting free surface colloidal patterning dynamics are observed at the low power spectrum whereas interfacial destabilization leading toward long slender jets and even drop atomization is observed at the high power spectrum. These unique phenomena provide ample opportunities for further investigation, particularly with regards to the fundamental physicochemical mechanisms governing the poorly understood behaviour and their application for ultrafast microfluidic actuation and manipulation.

Hong Zhao: Direct numerical simulation of vesicle dynamics in shear flow and generalized linear flows The dynamics of vesicle in shear flow and generalized linear flows is of intense research interest. Besides the tank treading and tumbling motions that are predicted by the classic Keller–Skalak theory, the vesicle can undergo a third “trembling” motion as observed in experiment. There have been several perturbation theories for explaining the phenomena and predicting the boundaries of flow regime transition. We herein perform high–fidelity direct numerical simulations that are based on Stokes–flow boundary integral equations, where the vesicle is modeled as a bending–resisting two-dimensional incompressible fluid that is commonly accepted and used in perturbation theories. The tank-treading angles obtained numerically agree well with experiments. Under different flow parameters, all three motion patterns (tank–treading, tumbling and trembling) are obtained unambiguously from our deterministic simulations. The transition boundaries between flow regimes are determined for vesicles of several reduced volumes, and are compared with both experiments and perturbation theories.

Partcicpants

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Braun, Richard (University of Delaware)
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Wilson, Stephen (University of Strathclyde)
Yeo, Leslie (Monash University)
Zhao, Hong (Stanford University)

Chapter 6

Convex Algebraic Geometry (10w5007)

Feb 14 - Feb 19, 2010

Organizer(s): Markus Schweighofer (Universitat Konstanz) Bernd Sturmfels (University of California at Berkeley) Rekha Thomas (University of Washington)

An emerging field

Many geometric objects arising naturally in science and technology possess two desirable properties. They are *convex* and *semialgebraic*. *Convex sets* have the property that one can move between any two of its points along a straight line without leaving the set. *Semialgebraic sets* can be described by combining polynomial inequalities by simple logical operations. The areas of mathematics primarily investigating these objects are *Convex Analysis* and *Real Algebraic Geometry*, respectively. Algorithmically, the property of being convex and a semialgebraic description of a set can both be exploited each on its own. However, at the moment, these methods are totally different and disjoint with huge limitations.

Convexity can lead to very fast numerical algorithms for navigating a geometric object. However, for these algorithms to work, one needs additional structure such as an easily computable self-concordant barrier function on the interior of the set [17]. For semialgebraic sets, very general symbolic algorithms are known to investigate and handle them [4]. However, these algorithms are often not efficient enough for practical purposes.

In spite of their ubiquity, the investigation of the special features of convex semialgebraic sets have been neglected for a long time. Only in recent years have new results and methods come up that have resulted in these geometric objects receiving attention from a wide range of areas including Classical Algebraic Geometry, Complexity Theory, Control Theory, Convex Geometry, Functional Analysis, Optimization Theory and Real Algebraic Geometry [22, 13, 15, 24, 1, 27]. Starting less than a decade ago, there have been more and more meetings where people from some of these areas have come together, with convex semialgebraic sets serving as a central tool of common interest.

The motivation behind organizing this meeting was the realization that it is now time for the emergence of an area of research where convex semialgebraic sets are the central objects of study rather than supporting tools. We call this area *Convex Algebraic Geometry* and it is devoted to the systematic study of convex semialgebraic sets.

The objects of study

Our objects of study live most of the the time in an n-dimensional Euclidean space, i.e., a space spanned by n axes, any two of which are perpendicular. One-dimensional space consists just of one axis, and its convex subsets are intervals (which also happen to be semialgebraic).

The first non-trivial, but still very special case, is that of two-dimensional space. This is a plane spanned by two axes which meet in an *origin*. Figures in this plane can often be nicely visualized by drawing them on a sheet of paper. Examples of convex semialgebraic subsets of the plane include single points, line segments, open and closed discs (more generally, an open disc together with a *finite* number of connected subsets of its boundary), the closed or open area circumscribed by a triangle, a trapezoid or an octagon (or more generally, a convex polygon). It is also possible to round the corners of such shapes. As another example, the set of all points (x, y) with $y \geq x^2$ (the area above a parabola) is a convex semialgebraic set, but we cannot replace x^2 by $\exp(x)$ here since then we no longer have a semialgebraic set.

Though each of our eyes sees only a two-dimensional picture of our environment, we are used to thinking in three dimensions since three-dimensional space is locally a good model for the space in which we live. Examples of convex semialgebraic subsets of three-dimensional space include balls, cones, pyramids, cylinders and platonic solids like a tetrahedron, a cube, an octrahedron, a dodecahedron, an icosahedron, the small rhombicosidodecahedron or the deltoidal hexecontahedron. Idealized pie slices and houses are also convex and semialgebraic. Again one can round the corners. In reality, an egg is not convex since one can discover little hills on the eggshell by looking at it under a microscope. Also its surface is unlikely to be semialgebraic since it is the result of a biological process. But for all practical purposes we can think of an egg as being convex and semialgebraic. This is also true for the shape of many, but not all, potatoes.

Mathematicians are used to investigating spaces with more than three dimensions. In fact, they carry over almost all geometric notions at least to arbitrary finite dimension. One of the many reasons for this is that our brain has a strong capacity to think in geometric terms, and we want to use this capacity to also understand phenomena which cannot be described by three coordinates only. The most prominent example of this is to think of time as an additional space coordinate. For example, to analyze an ice hockey game, it might be sufficient to think of the positions of the players and the puck at any given time as differently colored points in two dimensional space. Using the third coordinate for time, these positions move along differently colored curves in three-dimensional space which can be seen as a braid. For a football game, it might be more appropriate to start already with three dimensions and add time as a fourth dimension.

By means of analogy (passing from three to four dimensions is much like passing from two to three dimensions) and formal logic, mathematicians manage to extend their geometric intuition to higher dimensions. It is a daily routine for them to think geometrically in high-dimensional spaces. For example, the space of possible states of an engine could consist of many coordinates describing such parameters as the position and speed of the cylinders as well as temperature and pressure inside them. Thinking of it as a geometric object helps in understanding how to steer it from one state to another.

Convexity is highly desirable for many purposes [26, 2, 3]. It is one of the most useful features for navigating a geometric object. The class of semialgebraic sets, on the other hand, is perhaps the most obvious class of nonlinear geometric objects that should, in principle, be amenable to algorithms. Thus convex semialgebraic sets in an arbitrary finite-dimensional space are interesting objects of study especially since techniques which make use of both convexity and the semialgebraic property are ill-developed at present.

Spectrahedra and linear matrix inequalities

Symbolic computation with semialgebraic sets is a classical subject. Extensive work has been done on such problems such as, effective real quantifier elimination, computing the connected components of the set, polynomial system solving, and computing the dimension [4]. In the presence of convexity, it should however be possible to solve many of these algorithmic issues in a much more effective way.

Traditionally there are also a lot of techniques, mainly in numerical computation (and here in Convex Optimization [17]) that take advantage of convexity. Perhaps the most prominent example is Linear Programming (LP) which is used in a lot of real world applications.

Until recently, there were very few techniques combining the convex and the semialgebraic points of view. A very interesting new line of research tries to exploit Semidefinite Programming (SDP) for handling convex semialgebraic sets. SDP is an increasingly well-known generalization of LP which still has nice theory and for which good software packages exist. Whereas LP is optimization of a linear function on a polyhedron (i.e., a solution set of a system of linear inequalities), SDP is optimization of a linear function on a *spectrahedron*, i.e., a solution set of a *linear matrix inequality* (LMI). An LMI is an inequality of the form

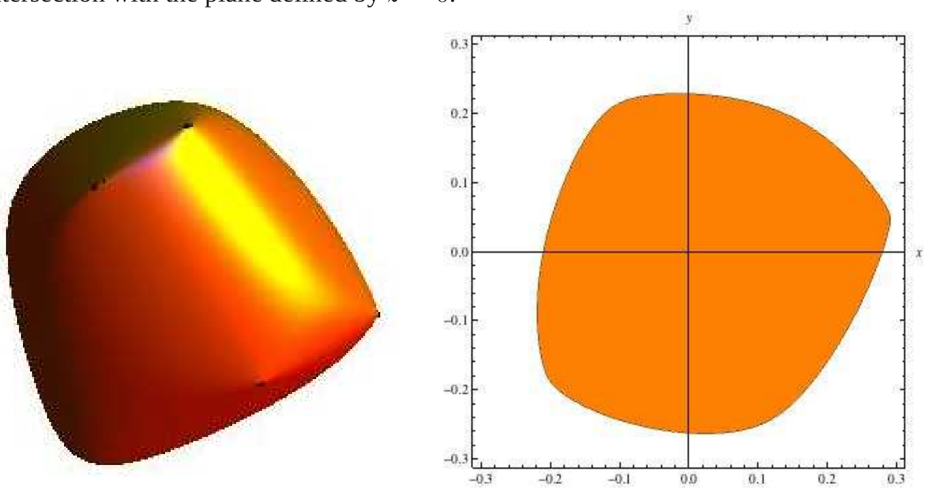
$$L(x) \succeq 0 \qquad (x \in \mathbb{R}^n) \tag{6.1}$$

where L is a symmetric linear matrix polynomial, i.e.,

$$L = A_0 + X_1 A_1 + \cdots + X_n A_n$$

where each A_i is a symmetric $s \times s$-matrix, the X_i are variables and $\succeq 0$ means positive semidefinite (i.e., all eigenvalues are nonnegative). When one restricts the A_i to be diagonal matrices, then (6.1) is just a linear system of inequalities. In some vague sense, spectrahedra and SDP generalize polyhedra and LP in much of the same way that symmetric matrices generalize diagonal matrices. Because symmetric matrices can be diagonalized, much of the theory of LP (such as interior point methods, see [17]) goes through for SDP. On the other hand, SDP is much more expressive than LP as can be seen in Figure 1.

Figure 6.1: A spectrahedron defined by the linear matrix inequality $I + xA + yB + zC \succeq 0 \quad (x, y, z \in \mathbb{R}^3)$ with 10×10 matrices A, B and C whose entries were uniformly and independently chosen among -1, 0 and 1, and its intersection with the plane defined by $z = 0$.



An LMI is likely to be a good representation of a convex semialgebraic set. It makes convexity an obvious feature of the set whereas in a semialgebraic description (a logical formula involving polynomial inequalities) the convexity is usually hidden. One of the current core questions in Convex Algebraic Geometry is which convex semialgebraic sets are defined by an LMI, i.e., are spectrahedra, see Section 6. Another extremely important question is what can be modeled by SDP using slack variables, i.e., which sets are projections (or equivalently, linear images) of spectrahedra, see Section 6.

Rigidly convex sets and real zero polynomials

For trivial reasons not every convex semialgebraic set is a spectrahedron. An important question is what makes a convex semialgebraic set a spectrahedron? For example spectrahedra are always closed. It is also known that spectrahedra share other special properties with polyhedra (e.g., they are basic closed and all their faces are exposed). All properties of spectrahedra known at the moment are subsumed by a crucial notion introduced by Helton and Vinnikov called *rigid convexity* [11]. To explain this notion, we need to introduce the notion of real zero (RZ) polynomials.

A polynomial p is a real zero polynomial at $a \in \mathbb{R}^n$ (is RZ at a, for short) if $p(a) > 0$ and all complex zeros of the univariate polynomial obtained by restricting p to a straight line passing through a are real. In other words, a polynomial of degree d is RZ at a point a if it has d real zeros counted with multiplicity on each generic line through a. It can be shown that a polynomial that is RZ at a is also RZ at any point in a small neighborhood of a. We refer to this by saying that the RZ property *spreads out*.

A subset $C \subseteq \mathbb{R}^n$ is called *rigidly convex* if there is a point $a \in \mathbb{R}^n$ and a polynomial p with the real zero property at a such that C equals the closure of the connected component of $\{x \in \mathbb{R}^n \mid p(x) > 0\}$ at a. Note that being convex is not part of the definition of "rigidly convex". However, it can be shown in an elementary way that each rigidly convex set is indeed convex (cf. [25]).

Each spectrahedron is rigidly convex inside its affine hull (i.e., identifying its affine hull with $\mathbb{R}^d$ where d is the dimension of the spectrahedron). To see this, we suppose that we are given a full-dimensional spectrahedron in $\mathbb{R}^n$. Then it can be seen easily that it can be written as $\{x \in \mathbb{R}^n \mid L(x) \succeq 0\}$ for a symmetric linear matrix polynomial L having the additional property that there is $a \in \mathbb{R}^n$ with $L(a) \succ 0$. Here $\succ 0$ stand for *positive definite*, i.e., all eigenvalues are (strictly) positive. Now the determinant of L is easily seen to be RZ at a (essentially because symmetric matrices have all its eigenvalues real) and the given spectrahedron is the closure of the connected component at a of the positivity set of this determinant.

Rigidly convex sets share all of the currently known properties of spectrahedra [25, 20]. In particular, they are semialgebraic sets which are *basic closed*, i.e., can be described by a finite system of weak polynomial inequalities (by means of the so-called *Renegar derivatives* which were the subject of many discussions during the workshop). Also they are convex sets all of whose faces are exposed. Rigid convexity is the strongest property of spectrahedra known so far. If one wants to show that some basic closed semialgebraic set with exposed faces is not a spectrahedron, then at the current state of the art, *the* thing to do, is to show that it is not rigidly convex.

To this end, it is useful to introduce another slight reformulation of rigid convexity based on the notions of algebraic interiors and their minimal polynomials, going back to Helton and Vinnikov as well. An *algebraic interior* in $\mathbb{R}^n$ is the closure of a connected component of the positivity set $\{x \in \mathbb{R}^n \mid p(x) > 0\}$ of a polynomial p (note that it is always closed, and despite the word "interior", never open except if it is the whole space). By definition, rigidly convex sets (and in particular spectrahedra) are algebraic interiors. Such a polynomial p of smallest possible degree is uniquely defined up to a positive constant factor and we call it the *minimal polynomial* of this algebraic interior. A crucial observation is that the minimal polynomial is a factor of every other such polynomial p.

It follows that an algebraic interior is rigidly convex if and only if its minimal polynomial is a real zero polynomial at some of its interior points, or equivalently at *any* of its interior points (since the RZ property spreads out as mentioned above). For example, the television screen like set $\{(x_1, x_2) \in \mathbb{R}^2 \mid x_1^4 + x_2^4 \leq 1\}$ is an algebraic interior with minimal polynomial $1 - X_1^4 - X_2^4$. This polynomial is not RZ at the origin. Hence the television screen is a convex basic closed semialgebraic set with only exposed faces which is not rigidly convex and therefore not a spectrahedron. On the other hand, the disc $\{(x_1, x_2) \in \mathbb{R}^2 \mid x_1^2 + x_2^2 \leq 1\}$ is an algebraic interior whose minimal polynomial $1 - X_1^2 - X_2^2$ is RZ at the origin. Therefore the disc is rigidly convex. In fact, it is even a spectrahedron since

$$\{(x_1, x_2) \in \mathbb{R}^2 \mid x_1^2 + x_2^2 \leq 1\} = \left\{(x_1, x_2) \in \mathbb{R}^2 \mid \begin{pmatrix} 1 & x_1 & x_2 \\ x_1 & 1 & 0 \\ x_2 & 0 & 1 \end{pmatrix} \succeq 0 \right\}.$$

Starting from spectrahedra which are intrinsically *real* objects, we defined rigidly convex sets and see now that the Zariski closure of their boundaries, seen as a *complex* algebraic varieties are important. This is only one of the many points where classical complex algebraic geometry comes into play. To visualize this thread of thinking, we ask the reader to look again at Figure 6.1 above and then compare it with the derived Figures 6.2, 6.3 and 6.4 below. Topologically, what you see is a set of nested ovals (which might touch), the innermost of them being the boundary of the convex set we started with.

Helton and Vinnikov showed in their seminal article [11] that each rigidly convex set of dimension at most two is a spectrahedron. As a quite trivial example, we remark that this is a way of seeing that the disc mentioned above is a spectrahedron without explicitly writing down an LMI defining it. Their result relies on the theory of *determinantal representations*. In fact, they even showed that each RZ polynomial, say RZ at the origin, in two variables has a *positive determinantal representation*, i.e. is the determinant of a linear symmetric matrix polynomial $L = A_0 + X_1A_1 + \cdots + X_nA_n$ where each A_i is a real matrix and A_0 is *positive definite* (in our case $n = 2$). Then the associated rigidly convex set, namely the closure of the connected component of $\{x \in \mathbb{R}^n \mid p(x) > 0\}$ at the origin, equals $\{x \in \mathbb{R}^n \mid L(x) \succeq 0\}$ and therefore is a spectrahedron. This result of Helton and Vinnikov on positive determinantal representation of

Figure 6.2: The real zero set of the minimal polynomial of the spectrahedron from Figure 6.1 intersected with the cube $[-1,1]^3$, and its intersection with the plane defined by $z = 0$.

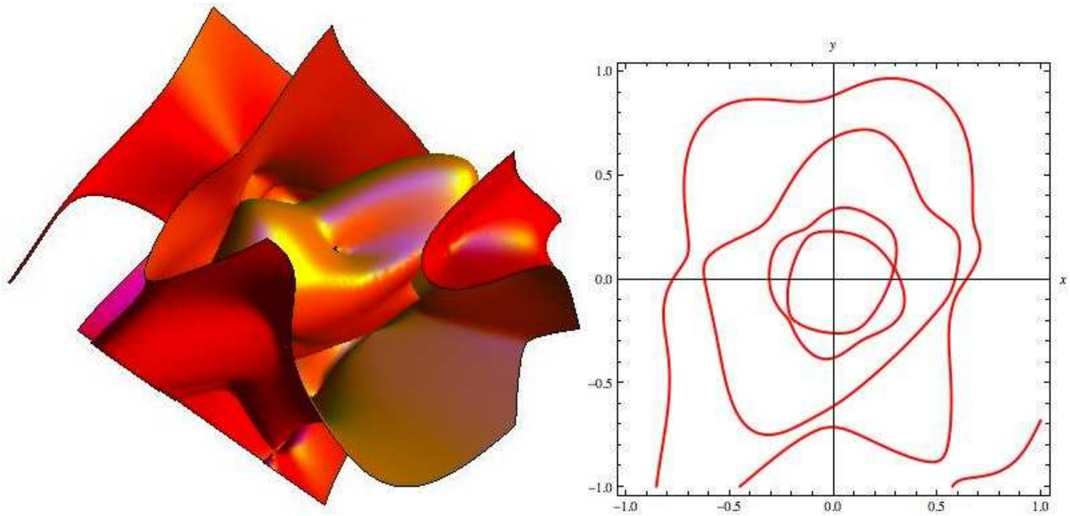
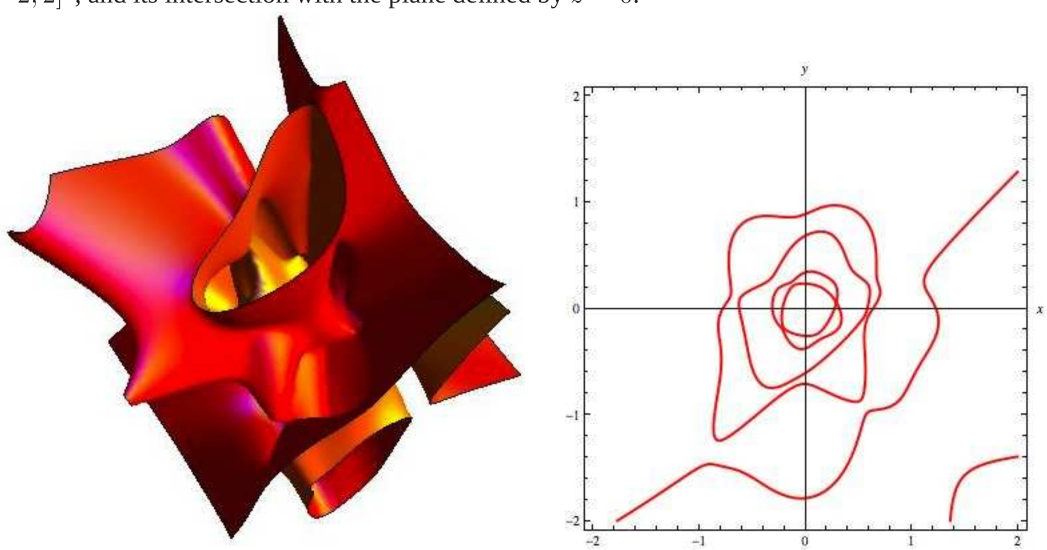


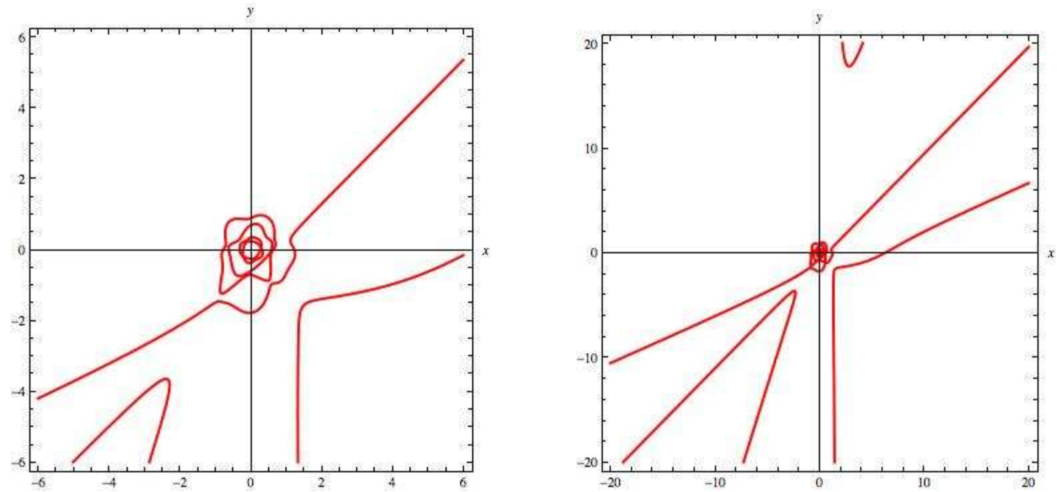
Figure 6.3: The real zero set of the minimal polynomial of the spectrahedron from Figure 6.1 intersected with the cube $[-2,2]^3$, and its intersection with the plane defined by $z = 0$.



RZ polynomials in two variables is equivalent to an old conjecture of Peter Lax (who was awarded the Abel Prize in 2005) originally formulated for homogeneous polynomials in three variables, see [14].

One of the most prominent open problems in Convex Algebraic Geometry, subject to many discussions at the workshop, is whether the results of Helton and Vinnikov can be extended to more than two variables. In fact, Helton and Vinnikov conjectured that each rigidly convex set (of any dimension) is a spectrahedron. This very important conjecture is still open. Furthermore, Helton and Vinnikov even conjectured that each RZ polynomial (in any number of variables) has a positive determinantal representation though their proof which uses deep Algebraic Geometry clearly could not be extended to more than two variables. After some discussion among workshop participants, Petter Brändén (Royal Institute of Technology, Stockholm) was able to solve this major problem in the negative during the workshop. This gave rise to an extra talk that Petter Brändén gave on Thursday morning in addition to his regular talk on Wednesday. This special talk

Figure 6.4: The real zero set of the minimal polynomial of the spectrahedron from Figure 6.1 intersected with $[-6, 6] \times [-6, 6] \times \{0\}$ and $[-20, 20] \times [-20, 20] \times \{0\}$, respectively.



was one of the highlights of the workshop since he even gave an extremely sophisticated argument, based on matroid theory, that even a weaker conjecture is false, namely that *some power* of each RZ polynomial has a positive determinantal representation (which would also imply the characterization of spectrahedra by rigid convexity). See [5] for these results, the proof for the stronger conjecture has been simplified since by Tim Netzer [19] who also attended the workshop.

However, there remain many open questions concerning the existence of positive determinantal representations. Some of these would still imply a full characterization of spectrahedra via rigid convexity. Others would work towards it. For example, it is known that the Renegar derivatives [25, 20] of RZ polynomials are again RZ at the same point. The real zero set of the Renegar derivative of a polynomial interlaces the real zero set of the polynomial. More precisely, between any of the two ovals (cf. Figures 6.2 to 6.4) and outside of the outermost oval of the real zero set of the RZ polynomial there is an oval of the Renegar derivative. If you draw the ovals of a polynomial and of its Renegar derivative, then the two innermost ovals are boundaries of convex sets, the innermost coming from the polynomial and the second innermost one from its Renegar derivative. Now define the Renegar derivative of a spectrahedron as the rigidly convex set defined by the Renegar derivative of its minimal polynomial. Even the following very special case of the conjecture of Helton and Vinnikov is open: Is the Renegar derivative of a spectrahedron (or at least of a polyhedron) again a spectrahedron?

Also largely open is the question of how to decide whether positive determinantal representations of RZ polynomials exist and how to produce them in an effective way. See [8] for a recent related result and for an overview of what has been done in this direction.

Projections of spectrahedra and semidefinite representations

As discussed above, perhaps the most natural class of convex sets going beyond polyhedra that is accessible to effective manipulation consists of spectrahedra. However, many convex semialgebraic sets one would like to deal with in an effective way are not spectrahedra. Whereas the projection (or linear image) of a polyhedron remains a polyhedron, the class of spectrahedra is not closed under projections. As a trivial example, the open half line $\mathbb{R}_{>0}$ of positive real numbers can be written as

$$\mathbb{R}_{>0} = \left\{ x \in \mathbb{R} \mid \exists y \in \mathbb{R} : \begin{pmatrix} x & 1 \\ 1 & y \end{pmatrix} \succeq 0 \right\}$$

but it is not a spectrahedron since it is not closed. During the workshop several propositions were made for naming projections of spectrahedra, including *spectrahedral shadow* and *umbrahedron* (from *umbra*, the latin word for shadow). Here we call projections of a spectrahedron *semidefinitely representable*. A set $S \subseteq \mathbb{R}^n$ obviously is semidefinitely representable if and only if there is a symmetric linear matrix polynomial L in the original variables $X_1, \dots, X_n$ and finitely many additional variables $Y_1, \dots, Y_m$ such that

$$S = \{x \in \mathbb{R}^n \mid \exists y \in \mathbb{R}^m : L(x, y) \succeq 0\}.$$

We call such an L a *semidefinite representation* of S (in the literature it is sometimes also called a "lifted LMI representation").

Having a semidefinite representation of a convex semialgebraic set is very advantageous [16]. For instance, it allows you to optimize a linear function on the set via SDP by using the Y_i as slack variables. Also it turns out that more and more operations on semialgebraic convex sets (like the taking the interior for example) can be done in a very efficient way by using semidefinite representations, see for instance [19].

Large classes of convex semialgebraic sets are known to be semidefinitely representable [28, 7, 6, 23, 29]. In their seminal articles [9, 10], Helton and Nie conjecture that *each* convex semialgebraic set is semidefinitely representable. Note that the converse is clear since the properties of being convex and of being semialgebraic are preserved under projections (for trivial reasons and because of Tarski's real quantifier elimination, respectively). The conjecture of Helton and Nie is still open and is certainly one of the main questions in Convex Algebraic Geometry. More and more results seem to work in its favor.

First, there are results showing that a lot of basic closed semialgebraic sets are semidefinitely representable. The basic method for obtaining these results go back to Lasserre [12] and links semidefinitely representable sets to sums of squares representations of positive polynomials. The main idea is as follows. Start with a finite system of weak polynomial inequalities. The idea is to *linearize* it. Very naively, one could try to replace each monomial which is a product of at least two variables by a new variable Y_i. One would end up with a finite system of linear inequalities. The projection of its solution set on the X-space would clearly contain the solution set of the original system of inequalities. On the other hand this projection would be a polyhedron and therefore in general cannot be equal to the original solution set and not even to its convex hull. Lasserre's idea was to generate a whole infinite family of inequalities which are obviously redundant before the linearization but add valuable information after linearization. The infinite family is chosen in a way such that it becomes an LMI after linearization. As an example, the inequality $-X_1^4 + 2X^2 - X + 1 \geq 0$ could give rise to the family of additional redundant inequalities $(aX_1 + bX_2 + c)^2(-X_1^4 + 2X^2 - X + 1) \geq 0$ where $a, b, c \in \mathbb{R}$ are parameters. This family can now be rewritten as

$$\begin{pmatrix} a & b & c \end{pmatrix} \begin{pmatrix} 1-X_1-X_1^4+2X_2^2 & X_1-X_1^2-X_1^5+2X_1X_2^2 & X_2-X_1X_2-X_1^4X_2+2X_2^3 \\ X_1-X_1^2-X_1^5+2X_1X_2^2 & X_1^2-X_1^3-X_1^6+2X_1^2X_2^2 & X_1X_2-X_1^2X_2-X_1^5X_2+2X_1X_2^3 \\ X_2-X_1X_2-X_1^4X_2+2X_2^3 & X_1X_2-X_1^2X_2-X_1^5X_2+2X_1X_2^3 & X_2^2-X_1X_2^2-X_1^4X_2^2+2X_2^4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} =$$

$$(-X_1^4 + 2X_2^2 - X_1 + 1) \begin{pmatrix} a & b & c \end{pmatrix} \begin{pmatrix} 1 \\ X_1 \\ X_2 \end{pmatrix} \begin{pmatrix} 1 & X_1 & X_2 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \geq 0$$

where $a, b, c \in \mathbb{R}$. After linearization this becomes the LMI

$$\begin{pmatrix} 1 - X_1 - Y_1 + 2Y_2 & X_1 - Y_3 - Y_4 + 2Y_5 & X_2 - Y_6 - Y_7 + 2Y_8 \\ X_1 - Y_3 - Y_4 + 2Y_5 & Y_3 - Y_9 - Y_{10} + 2Y_{11} & Y_6 - Y_{12} - Y_{13} + 2Y_{14} \\ X_2 - Y_6 - Y_7 + 2Y_8 & Y_6 - Y_{12} - Y_{13} + 2Y_{14} & Y_2 - Y_5 - Y_{15} + 2Y_{16} \end{pmatrix} \succeq 0.$$

Now in this example the set of all $(x_1, x_2) \in \mathbb{R}^2$ such that there are $y_1, \dots, y_{16} \in \mathbb{R}$ satisfying this inequality clearly is all of $\mathbb{R}^2$ since it contains the solution set of the original solution set of the original inequality $-X_1^4 + 2X^2 - X + 1 \geq 0$ whose convex hull is $\mathbb{R}^2$.

Lasserre showed that using a procedure that systematizes this approach leads to LMI relaxations whose solution sets give arbitrarily good approximations to the convex hull of the solution set of the original system of polynomial inequalities in the case that the latter is compact. This uses machinery from Real Algebraic Geometry.

Using much more machinery, Helton and Nie showed that in a lot of cases you get under the same compactness assumption that a sufficiently high relaxation gives exactly the convex hull. See [9, 10] for their celebrated results. Some of their results use just Lasserre's construction together with an ingenious proof bounding the degree of certain sums of squares representations. Their strongest results, which make very few assumptions apart from compactness, use the Lasserre construction locally and glue together the “local” LMIs. This glueing approach is not completely constructive yet.

Netzer and others (see [19]) gave several constructions of how to obtain new semdefinitely representable sets from old ones. These constructions are explicit and can easily be implemented.

Using all these results, one can show that surprisingly many convex semialgebraic sets are semidefinitely representable. For example, the television screen from Section 6 has a semidefinite representation

$$\begin{aligned}\{(x_1,x_2)\in\mathbb{R}^2 \mid x_1^4+x_2^4\le 1\} &= \{(x_1,x_2)\in\mathbb{R}^2 \mid \exists y_1,y_2\in\mathbb{R} : 1-y_1^2-y_2^2\ge 0 \,\&\, y_1\ge x_1^2 \,\&\, y_2\ge x_2^2\}\\ &= \left\{(x_1,x_2)\in\mathbb{R}^2 \mid \exists y_1,y_2\in\mathbb{R} : \left(\begin{smallmatrix}1+y_1 & y_2\\ y_2 & 1-y_1\end{smallmatrix}\right)\succeq 0 \,\&\, \left(\begin{smallmatrix}y_1 & x_1\\ x_1 & 1\end{smallmatrix}\right)\succeq 0 \,\&\, \left(\begin{smallmatrix}y_2 & x_2\\ x_2 & 1\end{smallmatrix}\right)\succeq 0\right\}.\end{aligned}$$

Are all semialgebraic convex sets semidefinitely representable? Before one tries to show this, one might try to work out more examples. For example, the cone of copositive matrices of fixed size is clearly a semialgebraic convex set in the vector space of symmetric matrices. Except for small sizes, it seems to be a hard problem to find a semidefinite representation for it [18].

Talks

During this workshop, stimulated by discussions among the workshop participants after his talk, Petter Brändén (Royal Institute of Technology, Stockholm) found sophisticated counterexamples [5] to one of the most outstanding generalizations of the famous Lax Conjecture (proved by Helton and Vinnikov in [11], see [14]) on hyperbolic polynomials. This affects in a direct way one of the mainstreams in current research on semidefinite representability (see Section 6 above). His “bränd-new” result was presented in his spontaneously given second talk. See [5], cf. also [21].

In his video-taped talk, Victor Vinnikov made very accessible the basic ideas behind constructing LMI representations of spectrahedra. He also referred to Petter Brändén’s counterexample (presented in a spontaneous special talk the same morning) and showed that there is some hope for other generalizations of the Lax conjecture to hold (still having the desired consequences). Here is a complete list of talks.

1. **Basu, Saugata** Toda's theorem – real and complex (joint work with Thierry Zell)
2. **Blekherman, Greg** Convex forms and faces of the cone of sums of squares
3. **Brändén, Petter** Tropicalization of hyperbolic polynomials
4. **Brändén, Petter** A counterexample to the generalized Lax conjecture
5. **Derksen, Harm** (Poly)Matroid Polytopes
6. **Hauenstein, Jonathan** Numerical algebraic geometry
7. **Henk, Martin** Representing Polyhedra by Few Polynomials
8. **Kaltofen, Erich** Certifying the radius of positive semidefiniteness via our ArtinProver package (joint work with Sharon Hutton and Lihong Zhi)
9. **Labs, Oliver** Towards visualization tools for convex algebraic geometry
10. **Laurent, Monique** Error and degree bounds for positivity certificates on the hypercube
11. **Marshall, Murray** Lower bounds for a polynomial in terms of its coefficients
12. **Netzer, Tim** Spectrahedra and their projections
13. **Parrilo, Pablo** Nuclear norm minimization
14. **Plaumann, Daniel** Exposed faces and projections of spectrahedra
15. **Putinar, Mihai** Optimization of non-polynomial functions and applications
16. **Ranestad, Kristian** The convex hull of a space curve
17. **Renegar, Jim** Optimization over hyperbolicity cones
18. **Reznick, Bruce** The cones of real convex forms
19. **Rostalski, Philipp** SDP Relaxations for the Grassmann orbitope
20. **Scheiderer, Claus** Bounded polynomials and stability of preorderings
21. **Smith, Gregory** Determinantal equations
22. **Sottile, Frank** Orbitopes
23. **Theobald, Thorsten** Amoebas of genus at most 1
24. **Vallentin, Frank** Approximation algorithms for SDPs with rank constraints
25. **Vinnikov, Victor** Positive determinantal representations (joint work with Dmitry Kerner)
26. **Vinzant, Cynthia** Faces of the Barvinok-Novik orbitope

Acknowledgments

This workshop was a very productive week for the participants. All this happened in the great environment of the Rockies allowing for long walks and deep thoughts without the usual daily constraints preventing a researcher from concentrating on the real problems. Not to forget a lot of other things like the possibility for exercising and swimming, the very good and very easy to use internet access by cable, the helpfulness of the staff and the good food with incredibly many choices. Thanks a lot to the BIRS and its sponsors for the possibility to organize this meeting!

List of participants

Ahmadi, Amir Ali (MIT)
Basu, Saugata (Purdue University)
Blekherman, Greg (Virginia Bioinformatics Institute)
Braenden, Petter (Royal Institute of Technology)
Conversano, Annalisa (Universitaet Konstanz)
Derksen, Harm (Michigan)
Di Rocco, Sandra (KTH Stockholm)
Gouveia, Joao (University of Washington)
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Helton, Bill (University of California, San Diego)
Henk, Martin (University of Magdeburg)
Huisman, Johannes (Universite de Brest)
Kaltofen, Erich (North Carolina State University)
Klep, Igor (Univerza v Ljubljani)

Kuhlmann, Salma (Universität Konstanz)
Kurdyka, Krzysztof (Universite de Savoie)
Labs, Oliver (Universitaet des Saarlandes)
Lasserre, Jean-Bernard (LAAS-CNRS 7, Toulouse)
Laurent, Monique (Centrum Wiskunde & Informatica (CWI) and Tilburg University)
Marshall, Murray (University of Saskatchewan)
Netzer, Tim (Universität Leipzig)
Parrilo, Pablo (Massachusetts Institute of Technology)
Pasechnik, Dmitrii (Dima) (Nanyang Technological University)
Pena, Javier (Carnegie Mellon University)
Plaumann, Daniel (University of Konstanz)
Powers, Victoria (Emory University)
Putinar, Mihai (University of California, Santa Barbara)
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Chapter 7

Randomization, Relaxation, and Complexity (10w5119)

Feb 28 - Mar 05, 2010

Organizer(s): J. Maurice Rojas (Texas A&M University), Leonid Gurvits (Los Alamos National Laboratories), Pablo Parrilo (Massachusetts Institute of Technology)

Overview of Polynomial System Solving

Systems of polynomial equations arise naturally in applications ranging from the study of chemical reactions to coding theory to geometry and number theory. Furthermore, the complexity of the equations we wish to solve continues to rise: while engineers in ancient Egypt needed to solve quadratic equations in one variable, today we have applications in satellite orbit design and combustive fluid flow hinging on the solution of systems of polynomial equations involving dozens or even thousands of variables.
For example, the left-hand illustration above shows an instance of the orbit transfer problem, while the right-hand illustration above shows a level set for a reactive fluid flow. More precisely, in the first problem, one wants to use N blasts of a rocket to transfer a satellite from an initial orbit to a desired final orbit, using as little fuel as possible. The optimal rocket timings and directions can then be reformulated as the real solutions of a system of $45N$ sparse polynomial equations in $45N$ variables, thanks to recent work of Avendano and Mortari [1]. For reactive fluid flow, a standard technique is to decimate the space into small cubes and obtain an approximation to some parameter function (such as vorticity or temperature) via an expansion into polynomial basis functions. Asking for regions where a certain parameter lies in a certain interval then reduces to solving **millions** of polynomial systems — the precise number depending on the region and size of the cubes.

Far from laying the subject to rest, modern hardware and software has led us to even deeper unsolved problems concerning the hardness of solving. These questions traverse not only algebraic geometry but also number theory, algorithmic complexity, numerical analysis, and probability theory. The need to look beyond computational algebra for new algorithms is thus one of the main motivations behind this workshop.

Historical Highlights

In the 1980s and 1990s, work in computational algebra culminated in singly exponential complexity bounds for many fundamental problems involving polynomial equations. Highlights include: reducing arbitrary systems to an encoding involving a polynomial in a single variable (a.k.a. rational univariate reduction [31]), bounding Betti numbers of semi-algebraic sets [3], and computing geometric decompositions for complex algebraic sets [17]. 19th century techniques (such as resultants) and more recent techniques (such as Gröbner bases) began to receive increasingly reliable and efficient software implementations, and the limits of computational algebra began to emerge: all of the aforementioned problems, in their decision form, are $\mathbf{NP}$-hard. Furthermore, it also emerged that the classical techniques of computational algebra largely ignore the special structure of **real** solutions. So any new speed-ups must come from new mathematical ideas and/or relaxing the statement of the problem. We now review some more recent advances, in 3 settings: detecting, counting, and approximating solutions.

Detecting Solutions. Thanks to work of Koiran in the 1990s [23], it is now known that the truth of the Generalized Riemann Hypothesis (GRH) implies that deciding the existence of solutions over the complex numbers is doable in polynomial time if and only if $\mathbf{P} = \mathbf{NP}$. This intersection of algebraic complexity with two of the biggest unsolved problems in mathematics attests to the depth of polynomial system solving. One can expand this study of complexity by looking for more special kinds of solutions. For example, deciding the existence of **integral** solutions leads us to even higher complexity classes: The famous negative solution to Hilbert's Tenth Problem in 1970 [28] is a proof of the algorithmic impossibility of deciding the existence of integer solutions to (completely general) systems of polynomial equations.

Caught between $\mathbf{NP}$-hardness and complete intractability, one then clearly hopes that detecting real solutions lies closer to $\mathbf{NP}$, particularly since most applications require just the real solutions of systems of polynomial equations. That detecting real solutions is at least theoretically tractable was proved in the early twentieth century by Tarski [39]. More recently, various results have hinted at the possibility of polynomial-time algorithms in special settings, e.g., real feasibility for quadratic polynomials [2] and certain sparse polynomials [6]. These new algorithms take us farther and farther away from traditional commutative algebra.

Counting Solutions. Work of Bernstein, Khovanski, and Kushnirenko in the 1970s [5, 33] showed that counting the number of complex solutions of a system of sparse polynomials is (with high probability) the same as computing a mixed volume of polytopes. Later, in the 1990s, Dyer and other authors determined the algorithmic complexity of computing volumes and mixed volumes of polytopes [14, 15]. One thus began to see signs that counting complex solutions is close to being a $\#\mathbf{P}$-complete problem. Gurvits then made major advances by finding efficient approximation algorithms for mixed volumes, also unifying earlier quantitative results in convexity via the framework of hyperbolic polynomials [19, 18].

Once viewed from the point of view of toric geometry, the connections between convex geometry and complex algebraic geometry are more natural than surprising. In a more topological vein, there has been much recent progress on understanding the complexity of counting connected (and even irreducible) components of algebraic sets over the complex numbers [10]: one sees new complexity classes, including some from the more recent BSS model of computation [8].

Similar progress was made over the real numbers (see, e.g., [9]), but precise complexity bounds remain more elusive over the real numbers than over the complex numbers. In particular, it was discovered in the 1980s that the number of real solutions for systems of **sparse** polynomials could be dramatically smaller than the number of complex solutions [22]. Taking full advantage of sparsity (or other types of structure) when counting real roots remains a challenging problem in algorithmic complexity.

In a different direction, using toric geometric methods, Huber and Sturmfels presented an algorithm for computing mixed volume, thus counting exactly the number of complex solutions for certain sparse polynomial systems [20]. Even better, their methods also yielded a new numerical method for approximating complex solutions: polyhedral homotopy.

Approximating Solutions. The complexity of numerical solving presents new difficulties not present in the more discrete problems of detecting and counting solutions. In this setting, ideas from numerical linear algebra have entered algebraic geometry via the notion of the **condition number**.

The condition number is an invariant one can now associate to families of semi-algebraic sets [12] to extract important information about the complexity of numerical optimization questions, just as Betti numbers extract important topological information. And while condition numbers are about as difficult to compute as numerical solutions themselves, they admit useful expectation bounds when considered as random variables attached to families of random algebraic sets [37, 27, 11]. This has led to average case complexity bounds for polynomial system solving. Recasting traditional algebraic complexity results to incorporate the condition number is now a lively subarea of algorithmic algebraic geometry. So far, only classical homotopy algorithms have fully benefited from this point of view, so condition number analysis is still an open problem for many other algorithms. For instance, even polyhedral homotopy still lacks rigourous complexity bounds.

Nevertheless, some very recent algorithms show great performance in practice. For instance, Parrilo's seminal work [30] blends 19th century ideas (sums of squares and Hilbert's 17th Problem) with 20th century optimization (semidefinite programming, a.k.a. **SDP**) to yield an efficient algorithm for solving certain relaxations of polynomial systems. Much recent effort in the optimization community has then focussed on quantifying how close these relaxations are to the original systems of equations (see, e.g., [24]).

Extending the idea of numerical conditioning, one can ask what is the most theoretically sound method to solve a numerically ill-posed problem. This leads one to the study of the **nearest** ill-posed problem, and major advances by Zeng and others [21, 40] have already yielded numerically reliable algorithms for problems that would have been impossible to solve with earlier software.

One can also study the geometry of zero sets of random polynomials, independent of numerical conditioning. This has lead to deep connections with several complex variables and mathematical physics [13, 36]. The behavior of real roots of random systems, particularly with respect to sparsity, has proven even more challenging [16, 32, 35].

Goals of the Workshop. The study of systems of polynomial equations has thus led us to a greater understanding of the complexity of detecting, counting, and numerically approximating solutions. However, for many structured systems of equations (e.g., those with few real solutions and many complex solutions), polynomial-time algorithms remain only a tantalizing possibility. Also, on a more fundamental level, many of the advances in polynomial system solving involve so many different techniques that refining them to specially structured systems is daunting. This workshop thus focusses on emerging methods to attain such speed-ups, and the resulting interactions between optimization, theoretical computer science, and algebraic geometry.

Emerging Directions

Much how probabilistic methods are just beginning to enter algebraic geometry [35, 29], randomized complexity bounds for polynomial system solving (and precise general estimates on numerical stability) were virtually unknown until recently. In particular, Smale's 17th Problem [38] beautifully captured what was sorely missing from computational algebra:

> "Can a solution of n complex polynomial equations in n unknowns be found approximately, on the average, in polynomial time with a uniform algorithm?"

Smale's statement elegantly highlights 3 issues in polynomial system solving: (1) average case complexity, (2) the notion of approximation for solutions, and (3) the possibility of a polynomial-time solution for a numerical problem known to be $\mathbf{NP}$-hard in its decision form. Indeed, observe how Smale's 17th Problem asks for just **one** complex root, since the number of complex solutions is exponential in the input size (here measured to be the number of monomial terms of the input polynomial system). Note also that Smale's introduction of randomization and approximation (to enable a polynomial-time solution) is very much in parallel to the idea of relaxation in optimization: simplify a seemingly intractable problem by softening the notion of a solution.

While the role of real solutions does not enter in Smale's statement, advances in the study of sparse systems of polynomial equations (a.k.a. **fewnomial systems**) over the real numbers also blossomed in the early 2000s: Li, Rojas, and Wang proved dramatically improved bounds (independent of the degree of the underlying polynomials) for the number of real roots of certain sparse polynomial systems [26]. This was the first significant evidence that the famous earlier bounds of Khovanski [22] could be significantly improved. Furthermore, completely general and explicit bounds over the p-adic rational numbers were initiated in 2004 by Rojas [34], following Lenstra's seminal results in one variable [25].

Smale's 17th Problem was, from a practical point of view, settled positively by Beltran and Pardo in 2008 [4].[1] Based on this advance, and progress in algorithmic fewnomial theory, Rojas began to form new conjectures on the complexity of solving real polynomial systems. (See Section 7 below.)

Other sources for new speed-ups have emerged recently: Pablo Parrilo discovered in his Ph.D. thesis that Semi-definite Programming (SDP) can sometimes be used to maximize multivariate polynomial much faster

[1] Strictly speaking, the problem is still open because Smale asked for a deterministic algorithm, and the solution from [4] is a randomized algorithm with a small, but controllable, failure probability.

than the classical methods of computational algebra [30]. Also, perhaps one of the earliest 20th century signs that real solving could go faster than complex solving comes from work of Barvinok: he showed that detecting real roots for homogeneous multivariate quadratic polynomials could be done in polynomial time, contrary to known methods for computational algebra at the time [2].

Presentation Highlights

A central activity in our workshop was 22 talks delivered by our diverse group of researchers. Full information (including abstracts, slides for almost all talks, and video for 2 talks) is available from the BIRS website. So we outline the talks below, from the point of view of their major themes. Afterward, we include some information **not** listed at the BIRS website: Details from the talks of Greg Blekherman, Mihai Putinar, Leonid Gurvits, and Victor Vinnikov. (These 4 talks were done on the blackboard without slides.) We then conclude with a condensed list of the talks.

Algebra of Polynomial System Solving

The talk of **Bernard Mourrain** focussed on moment matrices and border bases as a means of finding a canonical form (for more efficient solving) for certain polynomial systems. **Laura Matusevich** then described deep connections between monomial ideals (which are an important ingredient in Gröbner basis algorithms) and hypergeometric functions. On a related note, **Sue Margulies** spoke on the connection between algorithms for polynomial ideals and the resolution of certain conjectures in graph theory.

Closer to our next theme, **Martin Avendaño** presented an elegant new approach to Descartes' Rule of Signs that connects to an extension of a famous result of Polya: the number of real roots of a univariate polynomial f is **exactly** the number of sign alternations in the ordered coefficient sequence of $(1+x)^N f(x)$ for N sufficiently large.

Sums of Squares and Real Solving

Chris Hillar spoke on rational solutions to sums of squares certificates of positivity, raising many intriguing open problems. For instance, let $A_0, \ldots, A_n$ be rational $m \times m$ symmetric matrices and define a (rational) spectrahedron to be any set of the form $\{(x_1, ..., x_n) \in \mathbb{R}^n \mid A_0 + x_1 A_1 + \cdots + x_n A_n \geq 0\}$, where the inequality indicates positive semidefiniteness. Determine those real algebraic numbers that can be obtained as the coordinates of a finite spectrahedron. This question is open already for $n=1$!

Martin Harrison, a graduate student at UCSB, spoke on expressing certain non-commutative polynomials as a sum of a minimal number of squares. **Korben Rusek**, a graduate student at Texas A&M, presented a new class of fewnomial bounds which give dramatically sharper upper bounds on the number of real solutions of certain specially structured sparse polynomial systems.

Continuing the topic of fewnomials, **Dan Bates** spoke about a new homotopy algorithm that follows a remarkably small number of solution paths and finds all real solutions of any nondegenerate polynomial system. The number of paths followed is between a certain fewnomial bound recently derived by Bates and Sottile and the true number of real solutions. **Rojas** spoke on an alternative homotopy algorithm, based on a simple modification of polyhedral homotopy, that follows a number of paths that is **exactly** the number of real roots. Rojas' method works for any polynomial system lying outside of a particular discriminant amoeba, thus leading to interesting questions on real random polynomial systems.

Numerical Methods

Tien-Yien Li spoke about his most recent algorithm for computing the mixed volume of polytopes, and how it leads to one of the fastest current implementations of homotopy solving. **Andrew Sommese** spoke about his methods for homotopy solving. Thanks to his extensive use of parallelization, Sommese's implementation is currently the only software that can beat Li's implementation for certain massive polynomial systems.

Turning to more theoretical issues, **Zhonggang Zeng** lectured on how to reliably solve univariate polynomials that are known to be degenerate, and even how to find the degeneracy structure. **Anton Leykin** then spoke on how homotopy solving can be made completely rigourous (via exact arithmetic and the use of recent quantitative bounds of Shub and Smale), even demonstrating a preliminary implementation in `Macaulay2`.

Geometry and Complexity

Mounir Nisse, a graduate student from Paris 6, gave us highlights of the connections between complex amoebae and amoebae over non-Archimedean fields. (Amoebae are the images of algebraic sets under a valuation map: over the complex numbers, the valuation is the log-absolute value map.) In particular, Nisse presented very recent work on characterizing **co**-amoebae. Co-amoebae are the image of algebraic sets under the phase map, and are a vital ingredient to a deeper understanding of the geometry of complex algebraic sets. The impact of co-amoebae for algorithmic algebraic geometry will be at least as great as that of amoeba theory.

Pascal Koiran gave an enlightening talk on Valiant's version of the $\mathbf{P}$ versus $\mathbf{NP}$ problem and the derandomization of polynomial identity testing. It turns out that circuit complexity provides a useful link between both problems, and a deeper study leads to the study of shallow circuits with high powered inputs. In particular, one is led to study the number of real roots of polynomials that are sums of products of sparse polynomials. Such polynomials are just beyond the current reach of fewnomial theory, and thus yield fascinating new directions in fewnomial theory.

Optimization and Beyond

Levant Tuncel gave a timely survey on the state of the art of interior point methods in conic programming. His talk helped clarify some misconceptions behind the complexity of semidefinite programming, and focussed on barrier functions and locally quadratic convergence. **Brendan Ames**, a graduate student at the University of Waterloo, spoke on SDP relaxations for compressive sensing and maximum clique problems via the nuclear norm (sum of singular values) of a matrix.

Jim Renegar gave a stimulating evening talk on the frontiers of optimization. In particular, he spoke about optimizing over hyperbolic cones (a problem which includes SDP as a very special case) and how variations of Smale's α-Theory allow new convergence bounds.

4 Talks Without Slides

Greg Blekherman: Blekherman considered criteria for determining when a real n-variate homogeneous polynomial of degree $2d$ is convex. (For homogeneous polynomials, convexity clearly implies nonnegativity, and thus convexity is a stronger restriction.) He showed how recent advances on quantifying how often nonnegative forms are sums of squares have analogues in the setting of convexity. In particular, Blekherman proved that there are convex forms that are **not** sums of squares. However, unlike the classical examples of Motzkin and others, not a single convex form is known that is **not** a sum of squares! Blekherman went on to give an elegant sufficient condition for convexity in terms of tight clustering of the values of a form, and then developed some of the quantitative bounds necessary for his existence proof.

Mihai Putinar: Putinar developed a beautiful analytic framework starting from the following basic problem: How does one determine if n given disks are non-overlapping? Putinar related this problem to positive semidefinite matrices and then proceeded to explore connections with orthogonal polynomials and tomography. Via some delicate estimates, he proceeded to prove new growth estimates of complex orthogonal polynomials with respect to certain area measures.

Leonid Gurvits: Gurvits' evening talk was an entertaining tour through hyperbolicity, convex geometry, and physics. First, Gurvits showed how the volume of a scaled Minkowski sum of convex bodies is a hyperbolic polynomial. He then proceeded to an elegant proof of the $\#\mathbf{P}$-hardness of computing the mixed volume of parllelograms. Gurvits then continued by giving a deterministic polynomial-time algorithm for $(1+\sqrt{2})^n$-factor approximation of the mixed volume of any n convex bodies, given access to a weak membership oracle. He then concluded with a fascinating account of the connections between quantum linear optics and the permanents of unitary matrices.

Victor Vinnikov: Vinnikov gave a fascinating talk on constructing determinantal representations of polynomials via noncommutative algebra. These results give deep insights into representations of convex sets as the feasible sets for linear matrix inequalities, i.e., spectrahedra. Such representations have deep implications for optimization as they are behind the question of how much more general hyperbolic programming is than SDP.

A Condensed List of the Talks (in order of presentation)

March 1, 2010 (monday)
J. Maurice Rojas (Texas A&M): Simple Homotopies for Just Real Roots
Tien-Yien Li (Michigan State): The mixed volume computation: MixedVol-2.0 vs. DEMiCs
Zhonggang Zeng (U Illinois, Carbondale): Solving Ill-posed Algebraic Problems: A Geometric Perspective
Pascal Koiran (ENS Lyons): Shallow circuits with high-powered inputs
Mounir Nisse (Institut de Mathématiques de Jussieu): Complex and Non-Archimedean (Co)Amoebas, and Phase Limit Sets

March 2, 2010 (tuesday)
Chris Hillar (UC Berkeley): Do rational certificates always exists for sum of squares problems?
Greg Blekherman (VBI): Volume of the Cone of Convex Forms and new Faces of the Cone of Sums of Squares
Levant Tuncel (Waterloo): Local Quadratic Convergence of Polynomial-Time Interior-Point Methods for Nonlinear Convex Optimization Problems
Mihai Putinar (UCSB): Discretization of Shapes via Orthogonal Polynomials
Martin Harrison (UCSB): Minimal Sums of Squares in a Free-* Algebra
Susan Margulies (Rice): Vizing's Conjecture and Techniques from Computer Algebra
Brendan Ames (Waterloo): Convex relaxation for the clique, biclique and clustering problems
Leonard Gurvits (Los Alamos National Labs): Mixed Volumes of Parallelograms and Other Cool Things

March 3, 2010 (wednesday)
Bernard Mourrain (INRIA Sophia-Antipolis): Moment matrices and border basis
Laura Matusevich (Texas A&M): Monomial ideals and hypergeometric equations
Jim Renegar (Cornell): Optimizing Over Hyperbolicity Cones By Using Their Derivative Relaxations

March 4, 2010 (thursday)
Dan Bates (Colorado State): Khovanskii-Rolle continuation for finding real solutions of polynomial systems
Andrew Sommese (Notre Dame): Recent work in Numerical Algebraic Geometry
Anton Leykin (Georgia Tech): Certified numerical homotopy continuation
Software Demos (by Dan Bates and Anton Leykin)
Martin Avendaño (Texas A&M): Descartes' Rule of Signs is exact!
Korben Rusek (Texas A&M): On Certain Structured Fewnomials
Victor Vinnikov (Ben-Gurion): Constructing determinantal representations via noncommutative techniques

March 5, 2010 (friday)
Impromptu Problem Session (featuring Leonid Gurvits, Pascal Koiran, and J. Maurice Rojas)

Scientific Progress Made

The best part of our workshop was the opportunity for experts who rarely see each other to speak freely about their work in a comfortable environment. An important aspect of these discussions was an impromptu open problem session.

At our problem session, Leonid Gurvits raised intriguing open questions on the approximability of mixed volume: should the best current factor for polynomial-time approximability really be so large? Gurvits also pointed out unusual parallels between polyhedral lifting and recent approaches to Boolean satisfiability.

The questions Pascal Koiran raised revealed that certain advances in fewnomial bounds over the real numbers would enable an attack on a constant-free version of Valiant's Problem, i.e., a variant of the $\mathbf{VP} \stackrel{?}{=}$

$\mathbf{VNP}$ problem. Koiran also pointed out a fascinating recent paper of Aaronson showing that if quantum linear optics is efficiently simulable, then the polynomial hierarchy collapses.

Finally, Rojas pointed out some unusual parallels between real algorithmic fewnomial theory and p-adic algorithmic fewnomial theory. In particular, at a coarse level, the complexity of detecting roots for sparse polynomials has similar complexity in both settings. However, sporadic differences occur already for univariate trinomials: detecting real roots is doable in polynomial-time but detecting p-adic rational roots is only known to be in $\mathbf{NP}$.

To obtain some additional perspective on the advances made during our workshop, it will be useful to return to Smale's 17th Problem (as described in Section 7) and see how the ideas arising from our workshop helped extend this question in a new direction.

DEFINITION 1 *We call an* $f \in \mathbb{R}[x_1, \ldots, x_n]$ *(with* $f(x) = \sum_{i=1}^{n+k} c_i x^{a_i}$, $c_i \neq 0$ *and* $x^{a_i} = x_1^{a_{1,i}} \cdots x_n^{a_{n,i}}$ *for all* i*, and the* a_i *distinct) an* $\boldsymbol{n}$**-variate** $(\boldsymbol{n}+\boldsymbol{k})$**-nomial**. *We also define* $\mathrm{supp}(f) := \{a_1, \ldots, a_{n+k}\}$ *to be the* **support** *of* f*. The collection of* n*-variate* $(n+k)$*-nomials in* $\mathbb{R}[x_1, \ldots, x_n]$ *is denoted* $\mathcal{F}_{n,n+k}$*. Also, if* $F := (f_1, \ldots, f_n)$ *with* $f_i \in \mathcal{F}_{n,n+k}$ *and* $\mathrm{supp}(f_i) = \{a_1, \ldots, a_{n+k}\}$ *for all* i *then we call* F *an* $(\boldsymbol{n}+\boldsymbol{k})$**-sparse** $\boldsymbol{n} \times \boldsymbol{n}$ **polynomial system (over** $\mathbb{R}$**)**. $\diamond$

DEFINITION 2 *Let* $\Omega(n, k)$ *denote the maximal number of non-degenerate roots, with all coordinates positive, of any* $(n+k)$*-sparse* $n \times n$ *polynomial system over* $\mathbb{R}$. $\diamond$

CONJECTURE 1. (OPTIMAL REAL FEWNOMIAL BOUNDS) *There are absolute constants* $C_2 \geq C_1 > 0$ *such that, for all* $n, k \geq 2$*, we have* $(n+k)^{C_1 \min\{k-1,n\}} \leq \Omega(n, k) \leq (n+k)^{C_2 \min\{k-1,n\}}$.

CONJECTURE 2. (SPARSE REAL ANALOGUE OF SMALE'S 17TH PROBLEM) *Suppose we fix either* n *or* k*, and we consider random systems* $(n+k)$*-sparse* $n \times n$ *systems* F *over* $\mathbb{R}$*. Then there are uniform algorithms that:*

A: compute a positive integer in polynomial-time that, with high probability, is exactly the number of roots of F *in the positive orthant.*

B: approximate a single solution of F *in* $\mathbb{R}^n$*, on the average, in polynomial time.*

The intuition that the complexity of finding just the real roots of polynomial systems depends only weakly on the number complex roots, for systems of equations with few real roots and many complex roots, is captured in a rigourous way by these last 2 conjectures. Note also how we progress from bounding the number of positive roots, to computing the exact number of positive roots with high probability, to approximating a single positive root efficiently.

Progress toward these conjectures has been made from different points of view. For instance, Rojas' bound over the p-adic numbers, and a more recent bound over the real numbers of Bihan and Sottile [7], provided evidence toward Conjecture 1. Conjecture 2 is heavily based on [6] and recent Chamber Cone methods, the latter covered in the first talk at this workshop.

Final Notes

Rojas proposed an AMS Contemporary Mathematics proceedings volume for this workshop which has now been provisionally approved. The editors will be Philippe Pébay, J. Maurice Rojas, and David C. Thompson. As of this writing, we have submissions from the following sets of authors:

Dan Bates & Andrew Sommese
Carlos Beltran & Luis-Miguel Pardo
Anton Leykin
Tien-Yien Li
Zhonggang Zeng

We also have commitments for papers from:

Martin Avedano & Ashraf Ibrahim
Saugata Basu
O. Bastani, C. Hillar, D. Popov, & J. M. Rojas
Bernard Shiffman & Steve Zelditch

All editors and authors are either attendees of our workshop or invitees who were unable to attend.

In closing, we would like to extend our humble thanks for the wonderful facilities and magnificent setting. BIRS is truly a treasure, and it was a privilege to hold our workshop here.

Participants

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Chapter 8

(0,2) Mirror Symmetry and Heterotic Gromov-Witten Invariants (10w5047)

Mar 07 - Mar 12, 2010

Organizer(s): Ilarion Melnikov (Max Planck Institute for Gravitational Physics (Albert Einstein Institute)), Jacques Distler (University of Texas), Ron Donagi (University of Pennsylvania), Savdeep Sethi (University of Chicago), Eric Sharpe (Virginia Tech)

Overview of the Field

Shortly after the construction of the ten-dimensional heterotic string theories, it was realized that a compactification of these theories on Calabi-Yau manifolds could yield four-dimensional supersymmetric Poincaré-invariant vacua with the massless spectrum consisting of minimal supergravity coupled to a chiral non-abelian gauge theory. This was a remarkable development in theoretical physics, as it connected a heterotic string theory—believed to be a consistent theory of quantum gravity—to a chiral gauge theory remarkably similar to the Standard Model.

Despite this beautiful relation, it was understood that a number of issues remained to be addressed. For example, it was difficult to produce either the Standard Model gauge group or a grand unified model with couplings that would lead to the Standard Model. Moreover, the construction was perturbative in two senses: the results required small string coupling and the large radius limit, the former being a statement about string perturbation theory, while the latter requiring the compactification geometry to be a smooth manifold with volume large compared to the string length. Both of these issues are intimately tied to the existence of moduli—parameters introduced by the compactification, such as Kähler and complex structures on the Calabi-Yau manifold. What is the structure of this moduli space? How do physical quantities depend on the moduli? Are there heterotic compactifications without a large radius limit? Can one obtain a Standard Model gauge group or a favorable grand unified theory? Does an understanding of these issues teach us something about non-perturbative effects in the heterotic string?

The answers to these questions inevitably lead to new mathematical structures. Broadly speaking, the purpose of the workshop was to bring together researchers who are developing the mathematical structures and applying them to the physical questions. Major themes of the workshop were:

- a generalization of the notion of mirror symmetry to heterotic theories;
- new constructions of four-dimensional vacua from the heterotic string.

In what follows, we will review these areas in a little more detail.

Generalizations of mirror symmetry

Mirror symmetry—a proven ground for rich and mutually beneficial interactions between mathematicians and physicists [1]— is an isomorphism of two superconformal field theories (SCFTs) defined on a genus g Riemann surface, with one theory associated to a Calabi-Yau manifold M, and the other to its mirror W. Already at genus zero, the isomorphism yields a precise relation between generating functions of genus zero Gromov-Witten invariants of M and "classical" algebro-geometric period computations on W. The study of mirror symmetry led to physically and mathematically significant insights into geometry, including the clarification of the moduli spaces of the SCFTs and the Calabi-Yau manifolds, the notion of quantum cohomology, computations of Gromov-Witten invariants, an explicit combinatoric construction of mirror pairs as complete intersections in toric varieties, and the homological mirror symmetry conjectures.

The SCFTs typically considered in mirror symmetry possess $(2, 2)$ world-sheet supersymmetry, a property with a number of important ramifications:

- in the case of $(2, 2)$ SCFTs associated to Calabi-Yau manifolds, the moduli space has a familiar local structure, splitting into the moduli space of the complexified Kähler form and the moduli space of complex structures;
- a $(2, 2)$ SCFT has a chiral ring—a set of local operators with a well-defined product;
- correlators of chiral operators are independent of world-sheet metric and are computed by a Topological Field Theory (TFT).

The correlators transform as sections of certain bundles over the moduli space and may be determined by working with a topologically twisted (2,2) non-linear sigma model—a field theory of maps from a Riemann surface to the Calabi-Yau manifold. The correlators of the resulting TFT provide a path integral representation for the Gromov-Witten generating functions. The twisting procedure may be refined in an important way when M is a hypersurface in a toric variety V [2]. The result is a "quantum restriction formula" that relates correlators in the M SCFT to correlators in a vastly simpler TFT associated to V, known as the gauged linear sigma model (GLSM) [2, 3]. Together with the mirror map—an isomorphism between the complexified Kähler moduli space of M and the complex structure moduli space of W—these completely determine the correlators.

Despite these remarkable features, the moduli space of $(2, 2)$ SCFTs typically constitute a surprisingly unremarkable locus in a larger moduli space of SCFTs preserving $(0, 2)$ supersymmetry [4, 5, 6, 7, 8]. This larger moduli space has a geometric interpretation: the defining data of a (torsion-free) $(0, 2)$ non-linear sigma model is a Calabi-Yau manifold M and a stable holomorphic vector bundle $E \to M$, with

$$c_1(E) = 0 \text{ and } \mathrm{ch}_2(E) = \mathrm{ch}_2(TM).$$

A $(2, 2)$ point corresponds to $E = TM$. For example, the familiar $(2, 2)$ SCFT associated to a quintic hypersurface in $\mathbb{C}P^4$ has 224 deformations that only preserve $(0, 2)$ supersymmetry, and all of the familiar quantities like the moduli space metric, Yukawa couplings, and quantum cohomology are expected to vary smoothly across the $(2, 2)$ locus. In addition, there are $(0, 2)$ theories without a $(2, 2)$ point in the moduli space. From the physical point of view, these $(0, 2)$ SCFTs provide the basic building blocks for a large class of phenomenologically interesting compactifications of the heterotic string.

Recent developments

Topological rings and quantum cohomology. A revival of interest in world-sheet (0,2) models came with the observation [9] that (0,2) theories seemed to have a ground ring akin to the chiral ring of (2,2) models. This was first observed by an application of Hori-Vafa duality, and then was confirmed by direct computations [10]. In [11] a proof was given that such structures indeed exist for all theories based on a holomorphic bundle of rank less than 8 over a Calabi-Yau manifold. It was also shown that massive theories, such as those defined by a bundle over a toric variety possess the ring structure. Techniques were developed for computing these "topological heterotic rings" for (0,2) models constructed by deforming the tangent bundle over compact Kähler toric varieties [12, 13], for (0,2) Landau-Ginzburg models [14, 15], as well as for Calabi-Yau hypersurfaces in toric varieties via quantum restriction [16]. These developments were presented in the talks of Sharpe, Guffin, and McOrist.

The results of these computations are interesting from mathematical and physical perspectives alike. On the physics side, they encode non-trivial information about a strongly-coupled (0,2) quantum field theory and lead to (un-normalized) Yukawa couplings of space-time fields. Mathematically they lead to a deformation of the usual quantum cohomology, as well as a notion of a "quantum sheaf"—an object whose properties depend on both the complex structure and Kähler moduli of the underlying manifold.

A (0,2) mirror map. The concrete computations motivated a search for a generalization of the mirror map. On physical grounds, it is clear that since the (2,2) SCFTs associated to a mirror pair M and W are isomorphic, there must be a map of parameters for the deformations of TM to a bundle $E \to M$ to the deformations of TW to a bundle $F \to W$. Given a (2,2) GLSM for M inside a toric variety V, certain deformation are naturally realized as holomorphic parameters of the GLSM. Experience with (2,2) mirror symmetry suggested the hypothesis that a (0,2) mirror map should exchange the holomorphic parameters of the GLSM for $E \to M$ with those of the GLSM for $F \to M$. However, a counting of holomorphic parameters in mirror pairs showed that for most hypersurfaces $M \subset V$ this is not the case [17]. A priori this does not constitute a failure of mirror symmetry, as some of the deformations may be realized by more complicated operators, but it does make it difficult to find an explicit mirror map. Nevertheless, as reported in the lecture by Plesser, for a special class of GLSMs, corresponding to "reflexively plain polytopes" [17], where the number of GLSM parameters match on the two sides of the mirror, an explicit (0,2) map can be constructed [18]. It was shown that the proposed isomorphism exchanged the singular loci of the mirror theories—sub-varieties in the moduli space where the topological heterotic rings become singular. This constitutes a simple test of the proposal.

Towards higher genus results. The world-sheet methods described above are all, in one way or another, tied to the gauged linear sigma model. The relation between (2,2) gauged linear sigma model correlators and Gromov-Witten invariants at genus zero has been understood for some time; however, an extension beyond genus zero remained elusive. In his talk Diaconescu described a recently developed mathematical construction [19, 20]. If it is possible to generalize this to (0,2) models, it would provide a higher genus version of (0,2)-deformed Gromov-Witten theory.

Special geometry and Kähler potentials. While many aspects of the moduli space of (2,2) theories and (2,2) mirror symmetry have a straightforward (0,2) generalization, at least in the case where the bundle is a deformation of the tangent bundle, there are some notable exceptions. First, there is no longer a correspondence between the moduli fields and matter charged under the unbroken gauge group. More importantly, the moduli space of a (2,2) theory is constrained to be a special Kähler manifold. This is most straightforward to see in the context of type II string theory, where this follows from the requirements of $N = 2$ space-time supersymmetry, but it may also be determined directly in the heterotic string [21] by using Ward identities of the underlying (2,2) SCFT.

This is a remarkably powerful constraint, since it means that the Kähler potential, a real function of the moduli, is determined in terms of a holomorphic prepotential. The various techniques available to compute exact quantities as functions of the moduli are typically powerful enough to determine holomorphic quantities, such as superpotential couplings and prepotentials, but extending the methods to compute real quantities seems difficult, if not impossible.

A generic (0,2) compactification preserves $N = 1$ space-time supersymmetry. This requires the moduli space to be a Kähler Hodge manifold (i.e. a manifold X with a Kähler form with integral class in $H^2(X)$.), but does not impose more stringent conditions. At the same time, lacking the additional Ward identities of (2,2) SCFT, there are no other "obvious" constraints on the moduli space geometry. Thus, with the current state of affairs, the available computational techniques are seemingly not powerful enough to determine the Kähler potential, and hence the moduli space geometry.

The moduli space metric is an important lacuna in the understanding of heterotic string theory. For instance, it is needed to compute properly normalized physical couplings in the effective four-dimensional theory. In addition, a knowledge of the metric is needed to determine which (possibly singular) points in the moduli space are a finite distance away, and which correspond to infinite distance "de-compactification" limits.

Despite such a gloomy perspective from $N = 1$ supergravity, there is some reason to be optimistic. The key idea is that an $N = 1$ supergravity theory that arises from a string compactification may not be generic, and thus may have additional properties such as some notion of special geometry. Evidence for this has been found in the context of type II compactifications involving D-branes. It was shown some time ago in [22] that such a theory, although it possesses only $N = 1$ space-time supersymmetry, does seem to have a preferred set of holomorphic coordinates. While originally this was developed for D-branes on non-compact Calabi-Yau manifolds, the results have since been extended to F-theory and heterotic compactifications [23, 24, 25]. This work, presented by Jockers, offers a hope that the extra structure does give additional control on four-dimensional physics. In particular, a concrete proposal is made for the Kähler potential involving certain complex structure and bundle moduli.

Another perspective on this was offered by Quigley, who reported on ongoing work in collaboration with Anguelova and Sethi. The idea was to explicitly evaluate certain perturbative corrections to the Kähler potential for the complex moduli. They too found encouraging signs suggesting a decoupling between the different moduli beyond leading order results. It would be very interesting if this could be strengthened into a full non-renormalization theorem for the Kähler potential of complex and bundle moduli.

Open problems

The structure of (0,2) theories and their moduli spaces has been elucidated by a number of new results presented and discussed during the workshop. However, many exciting and crucial problems remain. A very incomplete list might be:

1. What is the mathematical framework appropriate to describe the quantum bundles and deformed quantum cohomology? Can recent results mathematical results on higher genus GLSM invariants be generalized to the (0,2) setting?

2. There is a proposed mirror map for models where the bundle is a deformation of TM. Can it be shown to exchange topological heterotic rings? Can the proposal be extended to other examples, say with bundles of rank 4 or 5? Does it relate the (0,2) mirror pairs found in [26, 27]?

3. Can the results be extended to the class of deformations that are not readily identified with holomorphic parameters of the GLSM? For instance, are such additional (0,2) deformations obstructed by world-sheet instantons?

4. Is there an $N = 1$ special geometry structure intrinsic to (0,2) half-twisted theories? F-theory/heterotic duality suggest that the answer is likely yes, but it would be instructive to find this structure directly.

5. Are there non-renormalization theorems for the Kähler potential? Can it be determined in terms of some holomorphic quantities?

New heterotic constructions

The preceding section dealt with the world-sheet properties of heterotic theories constructed in a rather standard fashion: the base manifold is a Calabi-Yau three-fold, and the bundle is a deformation of the tangent bundle. As already mentioned, such a construction has been known for some time, and while it may teach us some general lessons about (0,2) theories and their moduli spaces, it would be nice to get a handle on more generic theories. However, before one tackles issues of moduli spaces and stringy geometry of these more generic theories, it is necessary to produce the examples themselves.

At the level of perturbative heterotic string, in order to build a string vacuum with four-dimensional Poincaré invariance and minimal supersymmetry, we must choose a modular-invariant (0,2) SCFT with central charges $(c, \bar{c}) = (22, 9)$ and a supersymmetric GSO projection. Unfortunately, a classification of such objects is well out of the reach of current technology, and we must be content with a more specific constructions. Some of these, such as asymmetric orbifolds, have the advantage of being exactly solvable theories, while others have a closer connection to geometry.

The geometric models are defined by some anomaly-free (0,2) NLSM corresponding to a compactification geometry $E \to M$ as described above. Supersymmetry and anomaly cancellation require that M is a complex manifold with $c_1(TM) = 0$, while the bundle satisfies the topological conditions $c_1(E) = 0$

$\mod 2$ and $\text{ch}_2(E) = \text{ch}_2(TM)$. There are, however, additional requirements in order for the NLSM to be a superconformal theory at the quantum level. At leading order in the NLSM coupling α', these require E to admit a Hermitian Yang-Mills connection. In addition, the Hermitian form ω and the non-vanishing holomorphic three-form Ω defined on M must satisfy [28, 29]

$$4i\partial\bar{\partial}\omega = \alpha'(\text{Tr}R \wedge R - \text{Tr}F \wedge F), \qquad d(||\Omega||\omega \wedge \omega) = 0,$$

where R is the Ricci form and F is the curvature of the bundle E.

In general these are complicated equations, and the existence of solutions for general $E \to M$ satisfying the topological requirements is difficult to establish by a direct analysis. One standard approach is to consider solutions that have a large radius limit. In this limit the Hermitian form is closed, so that M is a Calabi-Yau manifold. As long as E is chosen to be a stable bundle, the Donaldson-Uhlenbeck-Yau theorem guarantees existence of a Hermitian Yang-Mills connection. This limit can be used a starting point for constructing a moduli space of solutions; moreover in the limit many properties of the effective four-dimensional theory can be determined by the algebraic geometry underlying $E \to M$.

A more ambitious approach is to look for a more general class of solutions, for instance on M that does not admit a Kähler structure, and thus cannot possess a large radius limit. This is the realm of heterotic flux compactifications. A priori, the resulting NLSMs must be taken with a large grain of salt, since the quantum corrections are large, and it is not obvious what the corrected string equations are, nor that a solution to the system above implies a solution to the full equations. Remarkably, duality arguments show that such theories do exist as bona fide heterotic vacua [30].

Recent developments

Bundles over Calabi-Yau manifolds. Heterotic compactifications over Calabi-Yau manifolds have been studied for almost the entire history of the heterotic string itself. In principle, many of the physical quantities are determined by specific algebraic geometry computations. For instance, the massless spectrum is determined by certain Dolbeault cohomology groups valued in the bundle and related sheaves. Similarly, Yukawa couplings of the matter theory may be computed by studying a holomorphic Chern-Simons theory on M.

These computations are, however, quite difficult in practice, and the technology is still being developed. In the workshop Donagi reviewed the spectral cover methods for constructing explicit bundles, computing spectra and Yukawa couplings. These techniques [31], based on Atiyah's construction of the moduli space of vector bundles over an elliptic curve, allow an explicit construction of phenomenologically interesting stable holomorphic bundles over elliptically fibered Calabi-Yau manifolds. These techniques have led to a heterotic construction of a theory with the charged matter spectrum of the minimal supersymmetric extension of the Standard Model [32], as well as explicit computations of certain Yukawa couplings, e.g. [33, 34].

In addition to the bundle data, there is also the choice of a base Calabi-Yau manifold. New manifolds are still being found, some with quite desirable (from a phenomenological point of view) properties. Candelas described one such construction, where a Calabi-Yau manifold with Euler number -6 is constructed as a quotient of a complete intersection in $(CP^2)^4$ by a freely acting group of order 12.

Heterotic flux backgrounds. Substantial progress has also been made in the study of compactifications where M does not admit a Kähler structure. It was shown in [35] that a class of M constructed as a non-trivial T^2 principal bundle over $K3$ does not admit a Kähler structure. This was just the sort of compactification identified by the duality argument of [30]. It was proven in [36] that such an M admits a solution to the NLSM equations of motion.

A substantial generalization of this construction [37] was discussed by Becker, who showed that there exists a much larger class of flux backgrounds. A particularly interesting technical point that arose in that investigation is a choice of preferred connection in defining the Chern-Simons terms appearing in the heterotic H-field. This choice is natural from the point of view of space-time supersymmetry and may substantially simplify a direct analysis of the existence of solutions.

Another important generalization, presented in Sethi's talk, concerns "non-geometric" compactifications of the heterotic string. The construction discussed the class of backgrounds obtained by fibering the heterotic string on a T^2 over some non-trivial base manifold. Such a compactification will be non-geometric provided that the Kähler and complex structure of the T^2 both undergo monodromies over the base space [38]. By using F-theory/heterotic duality it is possible to show that under certain conditions such a non-geometric compactification should be a consistent string vacuum.

There has also been progress on constructing a gauged linear sigma model for heterotic flux backgrounds [39, 40]. As discussed in Lapan's talk, the current constructions can only accommodate the rather special compactifications preserving $N = 2$ space-time supersymmetry. However, they do allow computations of exact spectra at Landau-Ginzburg points, and it is to be hoped that a further exploration of their properties will help to describe the moduli space of heterotic flux backgrounds, perhaps even leading to further generalizations of mirror symmetry and stringy geometry.

Open problems

Much remains to be understood in these large classes of backgrounds. We list just a few of the outstanding issues.

1. Are there world-sheet instanton corrections to the DUY stability conditions?
2. Can the methods based on half-twisted theories be applied to the phenomenologically promising compactifications?
3. Currently, there are few techniques for exploring the moduli space of heterotic flux backgrounds. Can we at least have a method for counting the moduli?
4. What are the topological heterotic rings in the linear sigma model for flux vacua?
5. Is there a world-sheet description of at least some of the non-geometric heterotic vacua?

Outcome of the meeting

The workshop brought together mathematicians and physicists who have been pursuing several quite distinct approaches to the heterotic string. The atmosphere created by BIRS—with simple organization, wonderfully efficient staff, excellent facilities, and of course incredible views—helped us to learn about the progress made, the technical issues, and the problems that remain in these different research directions. The small size of the workshop allowed the lectures to be fairly informal, often leading to an extended discussion with the speaker. These conversations would continue in the cozy atmosphere of Corbett Hall or while enjoying the great food in the dining hall. The workshop brought together several collaborations, allowing the members to work together, sometimes by grabbing a non-member for a consultation. A number of the problems defined at the workshop are now under active investigation, and we are sure that the collaborations either continued or begun at the workshop will open many new directions for progress. Several participants have voiced the opinion that the workshop was "one of the most useful I have ever attended," and we are sure this is sentiment that would be seconded by most, if not all of the attendees.

It is a pleasure to thank BIRS for this wonderful opportunity!

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Chapter 9

Quasi-isometric rigidity in low dimensional topology (10w5051)

Mar 07 - Mar 12, 2010

Organizer(s): Jason Behrstock (Lehman College, CUNY), Walter Neumann (Columbia University), Michael Kapovich (UC Davis)

Overview of the field and recent developments

The early work of Mostow, Margulis and Prasad on rigidity of arithmetic lattices has evolved into a broad use of quasi-isometry techniques in group theory and low dimensional topology. The word metric on a finitely generated group makes it into a metric space which is uniquely determined up to the geometric relation called quasi-isometry, despite the fact that the metric depends on the choice of generating set. As for lattices in suitable Lie groups, where quasi-isometry of lattices implies commensurability, the general quasi-isometric study of groups aims to understand the remarkable extent to which this completely geometric notion often captures algebraic properties of the group.

The Milnor-Schwarz Lemma provides an equivalence between the geometry of the word metric on the fundamental group of a compact Riemannian manifold (or metric complex) with the geometry of its universal cover. So the quasi-isometry study of groups also returns information about the spaces. This relationship has proved particularly productive in low dimensional geometry/topology.

There are currently a large variety of groups whose quasi-isometric geometry is actively being studied by geometric group theorists. Many of these groups have close relations to objects studied by low dimensional topologists. Examples of these include automorphism groups of free groups, mapping class groups (Hamenstädt, Behrstock-Kleiner-Minsky-Mosher), 3-manifold groups (Gromov-Sullivan, Cannon-Cooper, Eskin-Fisher-Whyte, Kapovich-Leeb, Rieffel, Schwartz, Behrstock-Neumann), solvable Lie groups (Eskin-Fisher-Whyte, Dymarz; the 3-dimensional group Solv had long been the holdout in understanding geometric 3-manifold groups), Artin groups (Bestvina-Kleiner-Sageev, Behrstock-Neumann), relatively hyperbolic groups (Drutu-Sapir, Osin), and others.

The study of many of these groups had been completely out of reach until the flurry of activity which has occurred in recent years, bringing many of these groups within grasp.

An old theorem of Stallings, the Ends Theorem, can be reinterpreted as quasi-isometric invariance of splitting over a finite group. Quasi-isometric rigidity of group splittings has remained an active area of research (Papasoglou, Mosher-Sageev-Whyte, etc.).

Questions of quasi-isometric rigidity and classification are studied using a range of techniques. Indeed, Gromov's Polynomial Growth Theorem, which was one of the seeds of the modern study of quasi-isometric rigidity since it implies that virtual nilpotence is quasi-isometrically rigid, already employed a large number of tools: representation theory, differential geometry, Montgomery–Zippen's proof of Hilbert's 5th problem, etc. Since then a number of other tools have also come into use, including quasi-conformal analysis, asymptotic cones, $CAT(0)$ geometry, logic, etc. Several recent proofs of outstanding problems have added new tools, including coarse differentiation used to answer questions about solvable Lie groups (Eskin-Fisher-Whyte), applications of the Continuum Hypothesis to resolve non-uniqueness questions about asymptotic cones (Kramer, Thomas, Tent, Shalah), harmonic analysis in Kleiner's new proof of Gromov's theorem, representation theory in the work of Shalom, etc.

Despite recent major advances, very significant problems remain. For example, little is known about the outer automorphism group of the free group, one of the central groups in the intersection of low dimensional topology and geometric group theory. There have been several inroads into quasi-isometry for Artin groups, but the general case remains wide open. Despite the fact that nilpotent groups were the first to be shown to be quasi-isometrically rigid, their quasi-isometric classification remains a well-known difficult question. Similarly classification of hyperbolic and relatively hyperbolic groups remains open although rigidity is known (Gromov, Drutu). And there are several other areas of active study.

This conference brought together a range of specialists whose expertise in order to educate each other in the broad spectrum of techniques and problems in quasi-isometric rigidity. A number of graduate students actively participated in the conference as well.

Program

Monday **March 8, 2010**

9:15–10:15 Mladen Bestvina, *The asymptotic dimension of mapping class groups is finite*
10:45–11:45 Christopher Cashen, *Line Patterns in Free Groups*
14:00–15:00 Jason Behrstock, *Quasi-isometric classification of right angled Artin groups*
15:30–16:30 Walter Neumann, *Quasi-isometry of 3-manifold groups*

Tuesday **March 9, 2010**

9:00–10:00 Linus Kramer, *Coarse rigidity of euclidean buildings*
10:30–11:30 Anne Thomas, *Lattices in complete Kac-Moody groups*
14:00–15:00 Michael Kapovich, *Ends of groups and harmonic functions*
15:30–16:30 Mark Hagen, *LERF after Dani Wise*

Wednesday **March 10, 2010**

9:00–10:00 Mark Sapir, *Dehn functions of groups and asymptotic cones*
10:30–11:30 Kevin Wortman, *Non-nonpositive curvature of some non-cocompact arithmetic lattices*

Thursday **March 11, 2010**

9:00–10:00 Xiangdong Xie, *Quasiisometries Łof some negatively curved solvable Lie groups*
10:30–11:30 Tullia Dymarz, *Bilipschitz equivalence vs. quasi-isometric equivalence*
14:00–15:00 Eduardo Martinez-Pedroza, *Separation of Quasiconvex Subgroups in Relatively Hyperbolic Groups*
15:30–16:30 Genevieve Walsh, *Quasi-Isometry classes of hyperbolic knot complements*

Presentations

Jason Behrstock (Lehman College, CUNY)
"QI classification of right-angled Artin groups"

This was the first of a two part talk involving joint work with Walter Neumann. This talk was on results from the papers [2] and [4], the second part was given by Walter Neumann and focused on the work in [3].

A *graph manifold* is an irreducible, non-geometric 3–manifold (possibly with boundary) for which every geometric piece is Seifert fibered. In the first half of the talk we discussed:

Theorem 2 (Behrstock–Neumann; [2]) *Let M, M' be graph manifolds (possibly with boundary). The following are equivalent:*

1. *$\widetilde{M}$ and $\widetilde{M}'$ are bilipschitz homeomorphic, here $\widetilde{M}$ denotes the universal cover.*
2. *$\pi_1(M)$ and $\pi_1(M')$ are quasi-isometric.*
3. *$BS(M)$ and $BS(M')$ are isomorphic as 2-colored trees, here $BS(M)$ is the Bass–Serre tree corresponding to the graph of groups decomposition of $\pi_1(M)$.*
4. *The minimal 2-colored graphs in the* bisimiliarity *classes of the colored decomposition graphs $\Gamma(M)$ and $\Gamma(M')$ are isomorphic.*

During this period we introduced the notion of *bisimiliarity* and gave a number of explicit examples. We sketched the proof of the above theorem, via a special case; showing that if M and M' are closed then their universal covers are bilipschitz homeomorphic, this answered an conjecture of Kapovich–Leeb from the early 90's.

Next we turned to applications of bisimilarity to the quasi-isometric classification of right-angled Artin groups. We introduced a family of such groups, n–tree groups which are the right-angled Artin groups associated to a family of n–dimensional simplicial complexes, namely the smallest family containing the n–simplex and with the property that the union of any two complexes in this class along a co-dimension one simplex is also in this class. For instance, for $n = 1$ this is the class of finite trees.

We then discussed:

Theorem 3 (Behrstock–Neumann; [2]) *Any two irreducible right angled 1–tree groups are quasi-isometric.*

N–tree groups admit an analogue of the geometric decomposition for 3–manifold groups, accordingly, some of the information in this geometric decomposition can be described via a finite bipartite colored graph, which we called $\Gamma(K)$, where K is the defining simplicial complex.

Theorem 4 (Behrstock–Januszkiewicz–Neumann; [4]) *Given two simplicial complexes K, K which yield n–tree groups. The groups A_K and $A_{K'}$ are quasi-isometric if and only if $\Gamma(K)$ and $\Gamma(K')$ are bisimilar after possibly reordering one of the color sets by an element of the symmetric group on $n+1$ elements.*

Mladen Bestvina (University of Utah)
"Asymptotic dimension of the mapping class group"

I started the talk with an introduction to asymptotic dimension. In particular, I recalled Gromov's proof that hyperbolic groups have finite asymptotic dimension and the Bell-Fujiwara argument that curve complexes associated to compact surfaces have finite asymptotic dimension.

Then I outlined a proof of the following theorem, joint with Bromberg and Fujiwara.

Theorem 5 *Mapping class groups have finite asymptotic dimension.*

The proof proceeds in three steps. The overall goal is to produce an action of a given mapping class group on the finite product $X_1 \times \cdots \times X_k$ with each X_i hyperbolic and of finite asymptotic dimension, such that an orbit map is a quasi-isometric embedding. Each X_i is obtained from a quasi-tree T_i by "blowing up" each vertex to the curve complex of a subsurface. The key step is the construction of T_i. This can be done "axiomatically", that is, whenever a group Γ acts on a set $\mathbb{Y}$ satisfying certain axioms, there is an induced action of Γ on a quasi-tree. A prototypical situation is that of a Kleinian group Γ acting on $\mathbb{H}^3$ with $\mathbb{Y}$ an orbit of axes of loxodromic elements. In our application, $\mathbb{Y}$ is a certain collection of isotopy classes of connected incompressible subsurfaces of the given surface Σ.

Christopher Cashen (University of Utah)
"Line patterns in free groups"

Take a word w in a free group F of rank at least 2. Consider a tree T quasi-isometric to F. The cosets of $\langle w \rangle$ in F correspond to a pattern of lines in T. We study a space called the *decomposition space*, which is a quotient of the boundary of T related to the line pattern. We use the cut set structure of this space to prove quasi-isometric rigidity results for line patterns. In particular, we would like to determine when the group of quasi-isometries of the free group that preserves the line pattern is conjugate into an isometry group of some "nice" space.

We show that this is never true if the decomposition space is disconnected, has cut points or has cut pairs. We conjecture that these are the only cases that the line pattern fails to be rigid. With some hypotheses on the complexity of the line pattern, we show that the pattern is rigid and furthermore that we can take the "nice" space to be a finite valence tree.

These results have applications to quasi-isometric classifications for graphs of free groups, including mapping tori of some free group automorphisms.

This is joint work with Natasa Macura.

Tullia Dymarz (Yale University)
"Bilipschitz equivalence is not equivalent to quasi-isometric equivalence for finitely generated groups"

A *quasi-isometric equivalence* between metric spaces is a map $f : X \to Y$ such that for some $K, C > 0$

$$-C + \frac{1}{K} d(x, y) \leq d(f(x), f(y)) \leq K d(x, y) + C$$

for all $x, y \in X$ and such that $nbhd_C(f(X)) = Y$. This is a generalization of the more common notion of a *bilipschitz equivalence*: a bijection between metric spaces that satisfies for some K

$$\frac{1}{K} d(x, y) \leq d(f(x), f(y)) \leq K d(x, y).$$

A natural question to ask is for which classes of metric spaces are these two notions equivalent. Burago-Kleiner and McMullen gave examples of a separated nets in $\mathbb{R}^2$ that are not bilipschitz equivalent to the integer lattice (but all nets are quasi-isometric). Our interest is in the class of finitely generated groups equipped with word metrics. For a finitely generated group Γ a choice of generating set S determines a Cayley graph Γ_S with metric d_S. The metric d_S depends on S but for any given group all Cayley graphs are bilipschitz equivalent. The examples of Burago-Kleiner and McMullen are not Cayley graphs of finitely generated groups. We prove the following Theorem:

Theorem 6 *Let F and G be finite groups with $|F| = n$ and $|G| = n^k$ where $k > 1$. Then there does not exist a bijective quasi-isometry between the lamplighter groups $G \wr \mathbb{Z}$ and $F \wr \mathbb{Z}$ if k is not a product of prime factors appearing in n.*

Mark Hagen (McGill University)
"LERF after Dani Wise"

We discuss recent work of Dani Wise on fundamental groups of special cube complexes, focusing on applications to the subgroup separability and virtual fibering of closed hyperbolic Haken 3-manifolds. A *special cube complex* is a cube complex whose immersed hyperplanes do not exhibit certain pathologies; equivalently, a cube complex is special if it admits a local isometry to the cube complex associated to a right-angled Artin group. Special cube complexes generalize graphs in the sense that cubical local isometries to special cube complexes are virtual retracts, as is the case for immersions of graphs. This is used to prove that quasiconvex subgroups of virtually special groups are separable (QCERF). Moreover, the right-angled Artin group characterization of special cube complexes shows that virtually special groups are "residually finite rational solvable" (RFRS).

A *quasiconvex hierarchy* for a group G is a way of constructing G from a (finite) collection of trivial groups by a finite sequence of iterated HNN extensions and amalgams in such a way that the edge groups are all quasiconvex in G. Wise showed that groups admitting a *quasiconvex hierarchy* are virtually fundamental groups of special cube complexes, and thus enjoy the QCERF and LERF properties. In particular, the Haken hierarchy for a closed hyperbolic 3-manifold M with a geometrically finite incompressible surface yields a quasiconvex hierarchy for $\pi_1 M$. That $\pi_1 M$ is subgroup separable is immediate from local quasiconvexity and QCERF. Virtual fibering follows from RFRS, by a result of Agol.

Michael Kapovich (University of California, Davis)
"Energy of harmonic functions and Gromov's proof of Stallings' theorem"

In his essay [9, Pages 228–230], Gromov gave a proof of the Stallings' theorem [26] on groups with infinitely many ends using harmonic functions:

Theorem 7 (Stallings) *Let G be a finitely-generated group with infinitely many ends. Then G splits nontrivially as an amalgam $G = G_1 *_{G_3} G_2$ or HNN extension $G_1 *_{G_3}$ with a finite edge group G_3.*

The goal of this talk is to provide the details for Gromov's arguments.

Let M be a complete Riemannian manifold of bounded geometry, which has infinitely many ends. Suppose that there exists a number R such that every point in M belongs to an R*–neck*, i.e., an R-ball which separates M into at least three unbounded components. (This property is immediate if M admits a cocompact isometric group action.)

Let $\bar{M} := M \cup Ends(M)$ denote the compactification of M by its space of ends. Given a continuous function $\chi : Ends(M) \to \{0, 1\}$, let

$$h = h_\chi : \bar{M} \to [0, 1]$$

denote the continuous extension of χ, so that $h|M$ is harmonic. The uniqueness of h easily follows from the maximum principle, while the existence of h is nontrivial was independently established in [12] and [18].

Let $H(M)$ denote the space of harmonic functions

$$\{h = h_\chi, \chi : Ends(M) \to \{0, 1\} \text{ is nonconstant}\}.$$

We give $H(M)$ the topology of uniform convergence on compacts in M. Let $E : H(M) \to \mathbb{R}_+ = [0, \infty)$ denote the energy functional.

Definition 9.0.0.1 *Given the manifold M, define its* energy gap $e(M)$ *as*

$$e(M) := \inf\{E(h) : h \in H(M)\}.$$

If M admits an isometric group action $G \curvearrowright M$, then G acts on $H(M)$ preserving the functional E. Therefore E projects to a lower semi-continuous functional $E : H(M)/G \to \mathbb{R}_+$, where we give $H(M)/G$ the quotient topology. Our main technical result is

Theorem 8 *1. $e(M) \geq \mu > 0$, where μ depends only on R, $\lambda_1(M)$ and geometry of M.*

2. If M admits a cocompact isometric group action, then $E : H(M)/G \to \mathbb{R}_+$ is proper in the sense that

$$E^{-1}([0, T])$$

is compact for every $T \in \mathbb{R}_+$.

Actually, it was observed by Bruce Kleiner that 1 easily implies 2.

We now sketch our proof of the Stallings' theorem. Since E is semicontinuous and proper mod G, E attains it minimum $e(M)$. Let $h \in H(M)$ be an energy-minimizing harmonic function. We then verify that the set $\Sigma := \{h(x) = \frac{1}{2}\}$ is *precisely-invariant* with respect to the action of G, i.e.. $g\Sigma \cap \Sigma \neq \emptyset$ iff $g\Sigma = \Sigma$. By choosing t sufficiently close to $\frac{1}{2}$ we obtain a smooth hypersurface $S = \{h(x) = t\}$ which is precisely-invariant under G and separates the ends of M. We then define *walls* if M to be the hypersurfaces $S_f = \{f = t\}, f = g^*(h)$ for some $g \in G$. We say that a hypersurface S_f *separates* points $x, y \in M$ if $f(x) < t$ while $f(y) > t$. We then define a graph T dual to the collection of walls in M: The edges of T are the walls, while the vertices of T are the "indecomposable" subsets of $M \setminus G \cdot S$, i.e., subsets which cannot be separated by one wall. We then verify that T is a tree. Clearly, G acts on T and the edge-stabilizers are finite since S is compact. Therefore, G splits over a finite group.

Linus Kramer (Universität Münster)
"Coarse rigidity of Euclidean buildings"

In my talk I presented the following results. We prove coarse (i.e. quasi-isometric) rigidity results for trees (simplicial trees and $\mathbb{R}$-trees) and, more generally, for discrete and nondiscrete Euclidean buildings. For trees, a key ingredient is a certain equivariance condition. Our main results are as follows.

Theorem 9 *Let G be a group acting isometrically on two metrically complete leafless trees T_1, T_2. Assume that there is a coarse equivalence $f : T_1 \to T_2$, that T_1 has at least 3 ends and that the induced map $\partial f : \partial T_1 \to \partial T_2$ between the ends of the trees is G-equivariant. If the G-action on ∂T_1 is 2-transitive, then (after rescaling the metric on T_2) there is a G-equivariant isometry $\bar{f} : T_1 \to T_2$ with $\partial f = \partial \bar{f}$. If T_1 has at least two branch points, then $\bar{f}$ is unique and has finite distance from f.*

Theorem 10 *Let X_1 and X_2 be metrically complete nondiscrete Euclidean buildings whose spherical buildings at infinity $\partial_{cpl} X_1$ and $\partial_{cpl} X_2$ are thick. Let $f : X_1 \times \mathbb{R}^{m_1} \to X_2 \times \mathbb{R}^{m_2}$ be a coarse equivalence. Then $m_1 = m_2$ and there is a combinatorial isomorphism $f_* : \partial_{cpl} X_1 \to \partial_{cpl} X_2$ between the spherical buildings at infinity which is characterized by the fact that the f-image of an affine apartment $A \subseteq X_1$ has finite Hausdorff distance from the f_*-image of A.*

We remark that the boundary map f_* is constructed in a combinatorial way from f. In general, a coarse equivalence between CAT(0)-spaces will not induce a map between the respective Tits boundaries.

Theorem 11 *Let $f : X_1 \times \mathbb{R}^{m_1} \to X_2 \times \mathbb{R}^{m_2}$ be as in Theorem 10 and assume in addition that X_1 has no tree factors. Then there is (after rescaling the metrics on the irreducible factors of X_2) an isometry $\bar{f} : X_1 \to X_2$ with boundary map $\bar{f}_* = f_*$. Put $f(x \times y) = f_1(x \times y) \times f_2(x \times y)$. If none of the de Rham factors of X_1 is a Euclidean cone over its boundary, then $\bar{f}$ is unique and $d(f_1(x \times y), \bar{f}(x))$ is bounded as a function of $x \in X_1$.*

For a more general statement see our preprint [16]. Theorem 10 and Theorem 11 were proved by Kleiner and Leeb under the additional assumptions that the Euclidean buildings are thick (i.e. that the thick points are cobounded) and that the spherical buildings at infinity are Moufang [13, 1.1.3] or compact [17, 1.3]. (These results extended, in turn, Mostow-Prasad rigidity [23].) By Tits' extension theorem every thick irreducible spherical building of rank at least 3 is automatically Moufang. The spherical building at infinity of an irreducible 2-dimensional Euclidean building, on the other hand, need not be either Moufang or compact; see, for example, [5]. In contrast to [13], we construct the combinatorial boundary map f_* of Theorem 10 first and then use it to obtain a simpler approach to Theorem 11.

This is a joint work with Richard M. Weiss

Eduardo Martínez-Pedroza (McMaster University) "Separation of Quasiconvex Subgroups in Relatively Hyperbolic Groups"

A subgroup H of a group G is *separable* if for any $g \in G - H$ there is a homomorphism π onto a finite group such that $\pi(g) \notin \pi(H)$. A group is *residually finite* if the trivial subgroup is separable, is *LERF* if every finitely generated subgroup is separable, and is *slender* if every subgroup is finitely generated. For example, finitely generated abelian groups are LERF and slender.

Given a relatively hyperbolic group with peripheral structure consisting of LERF and slender subgroups, we study separability of relatively quasiconvex subgroups. This is connected to residual finiteness of hyperbolic groups. It is not known whether all hyperbolic groups are residually finite. In particular, the main result of [1] is the following.

Theorem 12 *[1] If all hyperbolic groups are residually finite, then every quasiconvex subgroup of a hyperbolic group is separable.*

We extended this result, answering a question in [1], as follows:

Theorem 13 *[19] Suppose that all hyperbolic groups are residually finite. If G is a relatively hyperbolic group with peripheral structure consisting of subgroups which are LERF and slender, then any relatively quasiconvex subgroup of G is separable.*

This extension together with deep results in 3-manifolds have some interesting corollaries.

Corollary 9.0.0.2 *[19] If all hyperbolic groups are residually finite, then all finitely generated Kleinian groups are LERF.*

Corollary 9.0.0.3 *[19] If all fundamental groups of compact hyperbolic 3–manifolds are LERF, then all fundamental groups of finite volume hyperbolic 3–orbifolds are LERF.*

Theorem 13 is proved by combining one of combination theorems for quasiconvex subgroups in [20] with Theorem 12 and the Dehn filling technique of [10, 21].

The main technical result is stated below.

Definition 9.0.0.4 *A relatively quasiconvex subgroup H of G is called* fully quasiconvex *if for any subgroup $P \in \mathcal{P}$ and any $f \in G$, either $H \cap P^f$ is finite or $H \cap P^f$ is a finite index subgroup of P^f. (Here $P^f = fPf^{-1}$.)*

Theorem 14 *Let G be hyperbolic relative to a collection of slender and LERF subgroups. For any relatively quasiconvex subgroup Q and any $g \in G - Q$, there is a fully quasiconvex subgroup H, and a surjective homomorphism $\pi : G \longrightarrow \bar{G}$ such that*

1. *$Q < H$,*
2. *$\bar{G}$ is a word-hyperbolic group,*
3. *$\pi(H)$ is a quasiconvex subgroup of $\bar{G}$,*
4. *$\pi(g) \notin \pi(H)$.*

Theorem 13 is proved by combining one of combination theorems for quasiconvex subgroups in [20] with Theorem 12 and the Dehn filling technique of [10, 21]. The main technical result is stated below.

Definition 9.0.0.5 *A relatively quasiconvex subgroup H of G is called* fully quasiconvex *if for any subgroup $P \in \mathcal{P}$ and any $f \in G$, either $H \cap P^f$ is finite or $H \cap P^f$ is a finite index subgroup of P^f. (Here $P^f = fPf^{-1}$.)*

Theorem 15 *Let G be a torsion free group hyperbolic relative to a collection of slender and LERF subgroups. For any relatively quasiconvex subgroup Q of G and any element $g \in G$ such that $g \notin Q$, there is a fully quasiconvex subgroup H of G, and a surjective homomorphism $\pi : G \longrightarrow \bar{G}$ such that*

1. $Q < H$,
2. $\bar{G}$ *is a word-hyperbolic group,*
3. $\pi(H)$ *is a quasiconvex subgroup of* $\bar{G}$,
4. $\pi(g) \notin \pi(H)$.

We can prove Theorem 13 from Theorem 15 as follows: [Proof of Theorem 13] Let $Q < G$ be relatively quasiconvex, and let $g \in G \setminus Q$. By Theorem 15 there is a fully quasiconvex $H < G$ containing Q but not g, and a quotient $\pi : G \to K$ so that $\pi(g) \notin \pi(H)$, K is hyperbolic, and $\pi(K)$ is quasiconvex.

Assuming all hyperbolic groups are residually finite, Theorem 12 implies that there is a finite group F and a quotient $\phi : K \to F$ so that $\phi(\pi(g)) \notin \phi(\pi(H))$. Since $\phi(\pi(H))$ contains $\phi(\pi(Q))$, the map $\phi \circ \pi$ serves to separate g from Q.

This is a joint work with Jason Manning.

Walter Neumann (Columbia University)
"Quasi-isometries of 3-manifold groups"

The remaining case to be resolved for quasi-isometric classification of fundamental groups of compact 3–manifolds (allowing torus boundary components) is the case of irreducible 3-manifolds with non-trivial geometric decomposition in the sense of Thurston and Perelman.

The classification for non-geometric 3-manifolds with no hyperbolic pieces in their geometric decompositions was described in Jason Behrstock's talk (see subsection 9 and [2]). The general non-geometric case (also joint work with Behrstock, see [3]) is a combination of this case and the case when all pieces are hyperbolic, so my talk restricted to the all-hyperbolic case for simplicity. However, we assume that at least one piece is non-arithmetic, since if all pieces are arithmetic, then the manifold has very "arithmetic" behaviour, and the theory in this case is not yet fully worked out.

A non-geometric 3–manifold whose geometric decomposition decomposes it into hyperbolic pieces, at least one of which is non-arithmetic, is called an *NAH-manifold*.

The classification for graph-manifolds (no hyperbolic pieces) described in Behrstock's talk (subsection 9) was in terms of finite labelled graphs; the labelling consisted of a color black or white on each vertex and the classifying objects are such two-colored graphs which are minimal under a relation called *bisimilarity*. For NAH–manifolds the classification is again in terms of finite labelled graphs, and the the classifying objects are again given by labelled graphs which are minimal in a similar sense. The labelling is more complex: each vertex is labelled by the isomorphism type of a hyperbolic orbifold and each edge is labelled by a linear isomorphism between certain 2-dimensional $\mathbb{Q}$–vectorspaces. We call these graphs *NAH–graphs*. There is a natural morphism concept for such graphs, and the equivalence relation generated by existence of morphisms turns out to have a unique minimal object in each equivalence class. The main results are:

1. *These* minimal *NAH–graphs classify fundamental groups of NAH-manifolds up to quasi-isometry.*
2. *A minimal NAH–graph arises as the classifying graph for a quasi-isometry class of 3-manifold groups if and only if it is* balanced *(the product of determinants of the linear maps labelling edges along any closed path in the graph should be* ± 1*).*
3. *If the minimal NAH–graph is a tree and the vertex labels have no orbifold cusps then any two manifolds in the corresponding quasi-isometry class are commensurable.*

The third of these theorems and the "if" in the second are currently proved only under the assumption that the *Cusp Covering Conjecture* (CCC below) is true in dimension 3. They must therefore still be considered to be conjectural, although CCC is used in part for simplicity, and much less should be needed to prove these results.

CCC: *Any hyperbolic manifold* M *has a finite index subgroup of each of its cusp fundamental groups such that, for any choice of a smaller finite index subgroup* P_i *of each cusp fundamental group, there is a finite cover* $\bar{M} \to M$ *which restricts on each cusp of* $\bar{M}$ *to the covering given by the corresponding* P_i.

CCC (in all dimensions) is implied by the well known conjecture that any word-hyperbolic group is residually finite (RFCH). However the truth of RFCH is considered to be rather doubtful, while the Cusp Covering Conjecture is much more plausible.

Mark Sapir (Vanderbilt University)
"On Dehn functions of groups"

I formulated and proved Gromov's theorem that a group with all asymptotic cones simply connected has polynomial Dehn function and linear isodiametric function. A partial converse was proved by Papasoglu: groups with quadratic Dehn functions have simply connected asymptotic cones. There are many different types of examples of groups with quadratic Dehn functions. Nevertheless they all seem to satisfy some strong algorithmic properties. In particular I formulated a conjecture due to Rips that all these groups have solvable conjugacy problem. I presented a quasi-proof of this conjecture (due to Olshanskii and myself). It is not known if this proof works for all groups with quadratic Dehn function It does work for multiple HNN extensions of free groups. In particular, this and the result of Bridson and Groves imply that free-by-cyclic groups have solvable conjugacy problem. Finally I formulated the main new result obtained jointly with A. Olshanskii

Theorem 16 *There exists a finitely presented group with undecidablde word problem and almost quadratic Dehn function (that is the Dehn function is smaller than Cn^2 on arbitrary long intervals).*

Anne Thomas (Oxford University)
"Lattices in complete Kac–Moody groups"

Let G be a complete Kac–Moody group of rank 2 with symmetric Cartan matrix, defined over a finite field. An example is the "affine case" $G = SL_2(\mathbb{F}_q((t)))$, which is over $\mathbb{F}_q$. Such a group G is a totally disconnected locally compact group, which, apart from the affine case, is non-linear. The group G is obtained by completing a minimal or incomplete Kac–Moody group Λ with respect to some topology. For example, in the affine case $\Lambda = SL_2(\mathbb{F}_q[t, t^{-1}])$.

The group G acts on its Bruhat–Tits building X, a $(q + 1)$–regular tree, with quotient a single edge. We classify the cocompact lattices in G which act transitively on the edges of X. These lattices are given as graphs of groups, together with an embedding of the fundamental group of the graph of groups into G. Using this classification, we prove our main result:

Theorem 17 *Let G be a topological Kac–Moody group of rank 2 defined over the finite field $\mathbb{F}_q$, with symmetric generalised Cartan matrix $\begin{pmatrix} 2 & -m \\ -m & 2 \end{pmatrix}$, $m \geq 2$. Then for $q \geq 540$*

$$\min\{\mu(\Gamma\backslash G) \mid \Gamma \text{ a cocompact lattice in } G\} = \frac{2}{(q+1)|Z(G)|\delta}$$

where $\delta \in \{1, 2, 4\}$ (depending upon the particular group G). Moreover, we construct a cocompact lattice $\Gamma_0 < G$ realising this minimum.

Here, $Z(G)$ is the centre of G, which is a finite group and is the kernel of the G–action on X. For q even or $q \equiv 3 \mod 4$ we find the minimum covolume among cocompact lattices in G by proving that the lattice which realises this minimum is edge-transitive. For $q \equiv 1 \mod 4$, there are in general no edge-transitive lattices in G, and Γ_0 in this statement has two orbits of edges on X.

A result of independent interest is the following analogue of the fact that lattices in semisimple Lie groups do not contain unipotent elements:

Proposition 9.0.0.6 *Let G be as in Theorem 17 above. If Γ is a cocompact lattice in G, then Γ does not contain p–elements.*

This is proved using the dynamics of the G–action on X. Our proofs also use covering theory for graphs of groups, the Levi decomposition for the parahoric subgroups of G and finite group theory.

Genevieve Walsh (Tufts University)
"Quasi-isometry of hyperbolic knot complements"

A result due to R. Schwartz says that cusped hyperbolic 3-manifolds are rigid: they are quasi-isometric exactly when they are commensurable. Thus for hyperbolic knot complements, we have rigidity, and the remaining problem is to classify such knot complements up to commensurability. This is the goal of this work. An easier question is to understand how many knot complements are in a commensurability class. We say that $K \sim K'$ if the 3-manifolds $S^3 \setminus K$ and $S^3 \setminus K'$ are commensurable. Let $C(K) = \{K' | K \sim K'\}$. The following conjecture was made in [19].

Conjecture 9.0.0.7 *(Reid, Walsh) If $S^3 \setminus K$ is hyperbolic $|C(K)| \leq 3$.*

The following is substantial evidence for this conjecture.

Theorem 18 *(Boileau, Boyer, Walsh) Let K be a hyperbolic knot without hidden symmetries. Then $|C(K)| \leq 3$.*

For a Kleinian group Γ the commensurator $C^+(\Gamma)$ is the group of those elements g of $PSL(2, \mathbb{C})$ such that $\Gamma \cap g\Gamma g^{-1}$ is finite index in Γ and in $g\Gamma g^{-1}$. A hyperbolic knot admits hidden symmetries if the commensurator of Γ is strictly larger than the normalizer of Γ where $S^3 \setminus K = \mathbf{H}^3/\Gamma$. There are only two knots up to 12 crossings known to have hidden symmetries. In addition, there are restrictions on the shape on the cusp of a knot which has hidden symmetries. Thus we argue that not having hidden symmetries is a generic condition for knot complements. As a partial answer to the classification of hyperbolic knots up to commensurability, the proof yields that hyperbolic knot complements which do not admit hidden symmetries are commensurable exactly when they are cyclically commensurable. By this we mean that they admit a common cyclic cover. A more concrete classification is the following.

Theorem 19 *(Boileau, Boyer, Walsh) Let K by a periodic hyperbolic knot without hidden symmetries such that $|C(K)| > 1$. Then K is an unwrapped Berge-Gabai knot.*

Kevin Wortman (University of Utah)
"Non-nonpositive curvature of some non-cocompact arithmetic lattices"

We show that irreducible non-cocompact arithmetic groups of type A_n, B_n, C_n, D_n, E_6 and E_7 have an isoperimetric inequality in some dimension that is bounded below by an exponential function. Consequently, such groups do not satisfy any reasonable definition of nonpositive curvature, including for example, combability or $CAT(0)$.

The proof proceeds by constructing an infinite family of cycles in a neighborhood of an orbit of the arithmetic group acting on its associated symmetric space. The volumes of the cycles grow polynomially.

The volumes of any family of chains filling the cycles that are contained in the same neighborhood of the orbit grows exponentially, even though there exist fillings of polynomial volume in the symmetric space.

The proof is a generalization of the proof of Thurston-Epstein that $SL_n(\mathbb{Z})$ is not combable if $n \geq 3$. The cycles we construct are contained on a "horosphere", and their most efficient fillings extend into a horoball that is disjoint from the orbit neighborhood of the arithmetic group.

The type restriction from the statement of the result ensures the existence of a maximal proper parabolic subgroup whose unipotent radical is abelian. It is this parabolic group that determines the horosphere mentioned above, and the unipotent radical being abelian simplifies computations.

Xiangdong Xie (Georgia Southern University)
"Quasiisometries of some negatively curved solvable Lie groups"

Let A be an $n \times n$ matrix. Let $\mathbb{R}$ act on $\mathbb{R}^n$ by $(t, x) \to e^{tA}x$ ($t \in R$, $x \in \mathbb{R}^n$). Denote the corresponding semi-direct product by $G_A = \mathbb{R}^n \rtimes_A \mathbb{R}$. If the eigenvalues of A have positive real parts, then G_A admits left-invariant Riemannian metrics with negative curvature.

We classify all these G_A up to quasiisometry. We show that all quasiisometries between such manifolds (except when they are biLipschitz to the real hyperbolic spaces) are almost similarities and height-respecting.

Furthermore, we derive that such manifolds (except when they are biLipschitz to the real hyperbolic spaces) are not quasiisometric to any finitely generated groups.

Since two negatively curved spaces are quasiisometric if and only if their ideal boundaries are quasisymmetric, we prove these results by studying the quasisymmetric maps on the ideal boundary of these manifolds. We classify the ideal boundaries of negatively curved $G_A = \mathbb{R}^n \rtimes_A \mathbb{R}$ up to quasisymmetry, and show that every quasisymmetric map between the ideal boundaries (except when the solvable Lie groups are biLipschitz to the real hyperbolic spaces) are biLipschitz.

The results of Eskin-Fisher-Whyte, Dymarz and Peng yield quasiisometric classification and rigidity results for the class of groups $\{G_A\}$, where A has eigenvalues with positive real part and eigenvalues with negative real part, but has no eigenvalues with zero real part. Our results complement theirs. The proofs are also completely different.

Outcome of the Meeting

Due to late cancellations, the number of partipants was 17 instead of the planned 20, but there was a general consensus that the size of the group led to even closer interactions and more focussed discussion than is common at such meetings. Some progress was made on problems raised at the meeting, but it is too early to predict the full impact on new research and collaborations from the meeting. Suffice it to say that in conversations at the meeting and since, participants have described the meeting as having been unusually successful.

Participants

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Chapter 10

Geometric Scattering Theory and Applications (10w5106)

Mar 14 - Mar19, 2010

Organizer(s): Peter Perry (University of Kentucky), Peter Hislop (University of Kentucky), Rafe Mazzeo (Stanford University), Antonio Sa Barreto (Purdue University)

Overview of the Field

Classical scattering theory, by which we mean the scattering of acoustic and electromagnetic waves and quantum particles, is a very old discipline with roots in mathematical physics. It has also become an important part of the modern theory of linear partial differential equations. *Spectral geometry* is a slightly more recent subject, the goal of which is to understand the connections between the behavior of eigenvalues of the Laplace-Beltrami operator Δ_g on a compact Riemannian manifold (M, g) and various features of the geometry and topology of this manifold. *Geometric scattering theory* has developed over the past few decades as a unification and extension of these two fields, though certain aspects of the field go back much further. On the one hand, scattering theory is the natural replacement for the study of eigenvalues on complete, noncompact manifolds since the spectrum of the Laplace-Beltrami operator may often contain only continuous spectrum, whereas there is still a rich theory for some of the other objects in scattering theory described below. On the other hand, the study of scattering theory in the setting of Riemannian manifolds adds many new subtleties and problems over those encountered for traditional Schrödinger operators on Euclidean space by allowing for spaces with various more intricate types of asymptotic geometries. This broader perspective has turned out to be surprisingly revealing and to shed light on many of the classical problems in scattering on Euclidean spaces. This 'unification' of scattering theory and spectral geometry was proposed as a systematic area of study in a series of lectures given by R. Melrose at Stanford in 1994 [11]. Since that time the field has grown substantially, partly along some of the lines that Melrose had foreseen, but in many exciting and unexpected directions as well.

Geometric scattering theory encompasses the study, in the broadest sense, of the spectrum of the Laplace-Beltrami operator Δ_g and other natural elliptic operators on complete, noncompact Riemannian manifolds (M, g) with geometries which are 'asymptotically regular' at infinity. While there is no precise definition of this condition, it encompasses many natural settings and includes such cases as manifolds which are asymptotically Euclidean or conic, asymptotically cylindrical or periodic, asymptotically (either real or complex) hyperbolic, or modeled on other locally or globally symmetric spaces of noncompact type. The objects of study include the resolvent of the Laplace-Beltrami operator Δ_g given by

$$R(\lambda) = (\Delta_g - \lambda)^{-1},$$

which is a priori defined as a holomorphic family of L^2 bounded operators when λ is away from the spectrum. In many cases, the resolvent can be extended to act between other function spaces, and in that sense can be continued to a meromorphic operator-valued function. The poles of this meromorphic extension are called *resonances*. Resonances are the natural generalizations of L^2 eigenvalues. Another central object in geometric scattering theory is the *scattering operator*, which can be defined as follows. For manifolds which are (asymptotically) Euclidean, and endowed with a system of polar coordinates (r, θ) at infinity, a solution of $(\Delta_g - \lambda)u = 0$ has an asymptotic expansion of the form

$$u(r, \theta) \sim r^{\frac{1-n}{2}} \left(f(\theta) e^{ir\sqrt{\lambda}} + g(\theta) e^{-ir\sqrt{\lambda}} \right) + \mathcal{O}(r^{-\frac{1+n}{2}}),$$

where $n = \dim M$. It is known that (at least when λ is not an eigenvalue or a resonance), if f is any function on the sphere at infinity, then there is a uniquely associated 'generalized eigenfunction' u with eigenvalue λ having the above form. Hence, for for a function f on the sphere at infinity, there is a uniquely associated matching coefficient g. The scattering operator is the map

$$(S(\sqrt{\lambda})f)(\theta) = g(\theta).$$

For manifolds with other types of asymptotic geometry, there is a corresponding definition based on the fact that generalized eigenfunctions have an asymptotic expansion at infinity similar to the one above. Like the resolvent, the scattering operator also has a meromorphic extension in many situations, and its poles are (usually) the same as the set of resonances. The resolvent and scattering operator carry the same information, in principle, but both are very interesting objects of study in their own right. The scattering operator is traditionally studied in the physics literature because it is presumably the one which is actually observable.

The approach to scattering theory outlined so far is called stationary scattering theory since dynamics has played no explicit role. There are two different ways that dynamics can enter the picture. The first is that the long-term behavior of the geodesic flow on (M, g) has a profound affect on the scattering operator and resonances. One of the important and broad areas of investigation in this field is to determine the relationships between these various objects in scattering theory and the dynamical properties of geodesic flow. Questions here stretch from the field now called quantum chaos, which has deep connections with number theory, to the large area around the Selberg and Arthur trace formulæ and the many more general trace formulæ coming from the physics literature. The second way that scattering theory relates to dynamics is that all of stationary scattering theory can be recast in terms of behavior of solutions to the associated wave equation

$$\Box u := (\partial_t^2 - \Delta_g)u = 0.$$

The scattering operator, for example, can be understood as a means of comparing the long-time evolution of the Cauchy data, i.e. the map

$$\left(u|_{t=0} \, , \, \partial_t u|_{t=0} \right) \longmapsto \left(u|_{t=T} \, , \, \partial_t u|_{t=T} \right),$$

to the corresponding Cauchy data evolution for a 'free' operator, e.g. the wave operator on a space which contains only information about the asymptotic geometry of (M, g), but discards all the interior geometric and topological 'complexities' which cause the scattering. There are many relationships between these two notions of dynamics, of course, most centered around the fundamental principle that singularities of the solutions $u(t, z)$ of this wave equation are invariant under the Hamiltonian flow associated to the principle symbol of $\Box$ on $T^*(\mathbb{R} \times M)$, which is closely related to the geodesic flow on M.

Taking this broader perspective–i.e., including the wave operator along with the resolvent of the Laplace-Beltrami operator (and also the heat operator, time-dependent Schrödinger operator, etc.)–leads to many new questions as well as important connections to other fields. Amongst the most important of these is the connection with the study of solutions of the wave equation associated to a Lorentzian metric, in particular on spaces which do not naturally split as $\mathbb{R} \times M$. The most natural and important examples of such Lorentzian spaces are the vacuum solutions of the Einstein equations, sometimes called cosmological spacetimes. There is extensive ongoing work aimed at understanding the stability under the nonlinear Einstein evolution of even the most simple of these spacetimes. For example, the proof of the stability of Minkowski space, by Christodoulou and Klainerman [3], over twenty years ago, is still being digested by the community, and simplifications and extensions of that work are still of immediate interest. The current main focus here is to prove the stability of the Kerr family of spacetimes, which are rotating black holes. The current state of knowledge now rests on a detailed understanding of the linear wave evolution on these spaces, but many of the nonlinear aspects of the problem remain out of reach. Geometric scattering has a lot to say about all of this. In particular, something still poorly understood is how one should define resonances for these operators when the time variable does not split off as a factor. This is quite important because the location of resonances affects the rates of linear wave decay, which in turn is important to understand precisely as input to the nonlinear theory.

Let us discuss only one further aspect of geometric scattering theory, which is the connection between scattering theory on asymptotically hyperbolic manifolds and conformal geometry. That there should be some connection between asymptotically hyperbolic and conformal geometries was presciently foreseen by Fefferman and Graham in the early 1980's [4, 12], which now falls under the rubric of Fefferman's ambient metric program. This correspondence was discovered independently by the string theorists and is known in that community as the holographic principle, also called the AdS/CFT or Maldacena correspondence. The mathematical aspects of this were established in the seminal paper of Graham and Zworski [7], which explained, amongst other things, how the higher order conformally covariant operators (the so-called GJMS operators) of conformal geometry can be realized as residues of poles of the scattering operator for the Laplace-Beltrami operator on an associated asymptotically hyperbolic Einstein space. Other major discoveries here include the study of renormalized volumes, as defined by Graham and Witten [6] and Juhl's theory of generalized intertwining operators [10].

We have necessarily omitted many important aspects, questions and tools of the subject, but the description above gives some indication of the vitality of the subject and its deep connections with many other parts of mathematics.

Description of the meeting

The BIRS meeting itself was intended as a gathering of researchers from disparate parts of the field, to help disseminate advances in one part of the subject to specialists in other parts, and also to help introduce the many younger researchers in the field to the broader areas of investigation and the many senior researchers. Particular effort was focussed on inviting young researchers, spotlighting their work, and giving them an opportunity to interact with senior researchers in their fields. In all of this, the meeting was a great success, as we describe below.

A meeting with very similar themes was held at BIRS in the Spring of 2003; this was the second meeting in the history of BIRS, and we hope that BIRS will continue to be the venue for future meetings which follow the continuing developments and successes of this field.

Focus of the meeting

Set into the backdrop of this general field of geometric scattering, and based on the very enthusiastic response by researchers, in particular the junior ones, the organizers decided to focus on just a few of these themes, with emphasis on the contributions of younger participants complemented by talks from senior researchers chosen for their expository abilities who provided overview of some of the most important new directions.

We describe now the sets of topics discussed in the lectures of this meeting, divided into slightly arbitrary groups:

- Classical geometric scattering: Guillarmou, Borthwick, Christiansen, Datchev, Nonnenmacher, Aldana, Marazzi;

- Connections with conformal geometry and AdS/CFT: Graham, Juhl, Gover, Hirachi;
- Connections with mathematical relativity: Tohaneanu, Alexakis, Wunsch, Baskin, Wang, Vasy, Häfner;
- Other: Zelditch (Quantum ergodic restriction theorems), Albin (Signature theorems on stratified spaces).

Presentation Highlights

Rather than discuss all the talks in detail, let us focus on a representative sample of these presentations.

- Andreas Juhl lectured on his surprising new discoveries about the the universal recursive structure of Branson's Q-curvature, which shows that the Q-curvature in a given dimension and order can be written in terms Q-curvatures and GJMS operators of lower degrees and orders. The Q-curvature has emerged as a basic curvature invariant in conformal geometry, but its geometric meaning is still mostly mysterious. Juhl's results are likely to play a major role in the continuing efforts to understand its geometric content and uses.
- Colin Guillarmou presented his joint work with Rafe Mazzeo [8] which extends the theory of the meromorphic continuation of the resolvent of the Laplacian to arbitrary geometrically finite hyperbolic manifolds. This completes an old program in the subject, historically one of the first in geometric scattering theory, by finally incorporating intermediate rank cusps with irrational holonomy.
- Spyros Alexakis presented his recent work with A. D. Ionescu and Sergiu Klainerman which gives a solution to the old conjecture that any solution of the vacuum Einstein equation which is equal to the Kerr solution outside the event horizon is in fact globally equal to the Kerr solution. Their work requires an assumption (smallness of the Mars tensor) which they hope eventually to remove. Nonetheless, the basic analysis here contains an important new unique continuation theorem.
- Stéphane Nonnenmacher lectured on his work with Johannes Sjöstrand and Maciej Zworski in which they show that the study of the resolvent, and hence of scattering operator and resonances, can be reduced to the study of a family of 'open quantum maps', which are finite-dimensional operators constructed by quantizing the Poincaré map associated with the geodesic flow near the set of trapped trajectories.

Scientific Progress Resulting from the Meeting

The following items are distilled from an email survey of participants following the conference.

- Pierre Albin, Hans Christianson, and Colin Guillarmou were able to make progress on their ongoing project concerning the existence of quasimodes for the Schrödinger operator near a hyperbolic geodesic.
- Dean Baskin was able to use ideas from conversations with Colin Guillarmou and from Guillarmou's talk to obtain some new results about resonances for the wave operator on the AdS-Schwarzschild spacetime.
- Rod Gover and Jean-Philippe Nicolas initiated a collaboration to apply ideas from conformal geometry to understand decay of curvature and other fields in relativity.
- Hans Christianson continued his joint work with Steven Zelditch on quantum unique ergodic restriction theorems; he was also able to work with Pierre Albin, Colin Guillarmou and Jeremy Marzuola on the construction of soliton-like solutions to the nonlinear Schrödinger equation on compact manifolds. Finally, he made progress with Jared Wunsch on proving local smoothing for manifolds with degenerate trapping, and also with Kiril Datchev and Colin Guillarmou on the random walk operator on manifolds with cusp ends.

- Stéphane Nonnenmacher initiated work on a number of open problems with Tanya Christiansen (on "generic" fractal Weyl laws), with Frééric Naud (on spectral gap results of Bourgain-Gamburd-Sarnak and their possible application to resonance-free regions in congruence quotients of $\mathbb{H}^2$), and with Andras Vasy on high-energy resolvent estimates and their application to similar problems
- Jean-Phillipe Nicolas and Dietrich Häfner were able to use time during the meeting to finish a joint paper; they also began a new research project with Rod Gover.
- David Borthwick, Tanya Christiansen, Peter Hislop, and Peter Perry made progress on a joint work concerning generic properties of the distribution of resonances for manifolds hyperbolic at infinity
- Clara Aldana and Pierre Albin continued their joint work on isoresonant surfaces. This is a generalization of older work of Borthwick and Perry.
- Robin Graham engaged in extended conversations with Yoshihiko Matsumoto, a current graduate student of Kengo Hirachi, and provided significant assistance on his current thesis work.

Responses from participants

One of the most positive outcomes of the meeting was the interaction between senior and junior researchers. The conference was structured to highlight the work of younger researchers and provide opportunities for new collaborations. Here are some representative comments of younger researchers about the conference.

> "The conference was very useful to me because it gave me the opportunity to give a talk about my work on determinants of Laplacian and Ricci flow ... to a very suitable audience. ... On the other hand, I got to talk to people on my area who I had not met before."
>
> "In addition to a number of stimulating talks, it was a great opportunity to continue or begin new research."
>
> "My participation in this workshop allowed me to have some fresh insight in to a field to which I am a relative newcomer. I saw connections between one of my current research projects and the work of several speakers... The workshop gave me the opportunity to meet new people and establish more significant relationships with people I had met previously."

Outcome of the Meeting

While it is hard to quantify specific outcomes of any given meeting, there are some indicators including papers written as a direct outgrowth of conversations at the conference, or at the very least, the formation of new collaborations which will eventually lead to publications. (We are aware of several papers resulting from such interactions which have not yet been completed, which is reasonable given the relatively brief time between the conference and when this report is being written.) We have already indicated several new and ongoing collaborations which were certainly expedited by this conference. Less tangible outcomes include the possibility of cross-disciplinary interaction, which was in any case one of the stated goals of the meeting. For example, we feel that the heavy emphasis we placed to spotlight the techniques of geometric scattering to problems in mathematical relativity not only helped illuminate the great progress that has been made at this interface between fields in the past few years, but has stimulated many of the young researchers to work on problems in these directions.

Publications and preprints

Dmitry Jakobson and Frédéric Naud were able to prove a "spectral gap" estimate for resonances of convex co-compact subgroups of arithmetic groups [9]. More specifically they prove a lower bound on the distance between the first non-trivial scattering resonance and remaining resonances. The spectral gap for resonances is analogous to the spectral gap between the lowest and next eigenvalue of the Laplacian, but the problem is much subtler since the resonances are determined by a non-self-adjoint eigenvalue problem. Jakobson and Naud exploit known Selberg trace formula techniques

Hans Christianson, Colin Guillarmou, and Laurent Michel completed a paper [2] about the spectral gap for the operator associated to random walks on finite-volume, non-compact surfaces with hyperbolic cusps. The study of this type of operator is relatively new in microlocal theory, and was brought to the attention of Gilles Lebeau by the probabilist Persi Diaconis a few years ago. They had given a thorough analysis of it in Euclidean space, but through that work it was realized that there are some important corresponding analytic questions that should be studied for other classes of manifolds. This paper is an important first step in that direction.

David Borthwick, Tanya Christiansen, Peter Hislop and Peter Perry [1] prove that the counting function for resonances on manifolds of constant negative curvature "near infinity" generically saturates known upper bounds for resonances. Deterministic lower bounds on counting for resonances are typically very difficult to obtain (and reasonable conjectures for the lower bounds are known to be false in many cases of interest). The approach of proving "generic" lower bounds provides a powerful tool for the study of resonances which has now been extended to an important geometric setting. This approach may lead to similar generic lower bounds on the counting function of resonances in strips in terms of the fractal dimension of trapped sets of geodesics.

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Chapter 11

Volume Inequalities (10w5114)

Mar 28 - Apr 02, 2010

Organizer(s): Karoly Bezdek (University of Calgary), Robert Connelly (Cornell University), Alexander Litvak (University of Alberta), Frank Morgan (Williams College)

Volume is one of the most fundamental concepts of mathematics and in particular, of geometry. Also, it plays a central role in discrete geometry, geometric measure theory as well as in asymptotic geometric analysis. Our major goal was to discuss the possibility of further progress on a number of important research problems of the above mentioned three fields by bringing together a good number of leading experts. There have been 25 lectures on attractive recent results that on the one hand, have given a focused overview of the state of the art of the matters within the given research area on the other hand, have proposed new techniques as well as conjectured new results.

In the following we give a brief overview of a selection of lectures. Out of the 25 lectures delivered at our conference 6, 9 and 10 reported on (significant) progress on a number of (fundamental) problems of geometric measure theory, asymptotic geometric analysis and discrete geometry. Here we just highlight some of the major results discussed in the lectures and refer the interested reader for more details to the complete list of lectures and abstracts on the workshop webpage. Also, we wish to mention that almost all lectures reported on some recent results that generated informal discussions among the conference participants representing all three major research areas at focus.

Geometric Measure Theory: Simon Coxs lecture *"The minimal perimeter for N confined deformable bubbles of equal are"* reported on candidates to the least perimeter partition of various polygonal shapes into N planar connected equal-area regions for N $<$43. Also, candidates to the least perimeter partition of the surface of the sphere into N connected equal-area regions have been listed. For small N these can be related to simple polyhedra and for N $>$13 they consist of 12 pentagons and N ? 12 hexagons. Max Engelsteins lecture *"The Least-Perimeter Partition of the Sphere into Four Equal Areas"* proved that the least-perimeter partition of the sphere into four equal areas is the regular tetrahedral partition. *Frank Morgans* lecture *"The Isoperimetric Problem in Spaces with Density"* discussed recent results on the isoperimetric problem in Euclidean space with density whenever the log of the density is convex. The lecture of *John M. Sullivan* under title *"Rope length and related packing problems"* investigated the rope length problem that considers curves of thickness at least one, and asks to minimize the tube volume (or equivalently length) within a given knot type.

Asymptotic Geometric Analysis: *Vitali Milman* delivered a survey lecture on the role of polarity and stability in high-dimensional convex geometry. *Emanuel Milman* proved a generalization of Caffarellis Theorem and showed its relation to the Gaussian correlation conjecture and similar correlation inequalities for non-Gaussian measures. *Peter Pivovarov* discussed super-Gaussian bounds for the volume of caps of convex isotropic bodies and their relations to the mean-widths. *Elisabeth Werner* introduced a new affine invariant of a convex body, which can be found as the relative entropy of the cone measure of the body, and showed new affine isoperimetric inequalities. *Vlad Yaskin* presented solutions of two open problems on unique determination of convex polytopes. *Artem Zvavitch* proved that if a convex body K is close to the unit ball and the intersection body of K is equal to K, then K is the unit ball. He also discussed a harmonic analysis version of this question.

Discrete Geometry: *Karoly Bezdeks* lecture entitled *"Illuminating Ball-Polyhedra"* has given an extension of the well-known theorem of Schramm on illuminating convex bodies of constant width and proved the Boltyanski-Hadwiger conjecture for fat ball-polyhedra. Here ball-polyhedra are intersections of finitely many congruent balls in Euclidean space. Moreover, the ball-polyhedron is called a fat one, if it contains the centers of its generating balls. The probabilistic method of the proof is centered around estimating the volume of convex bodies of constant width in spherical d-space. *Gabor Fejes Toths* lecture *Partial covering of a convex domain with translates of a centrally symmetric convex disc* generalized some old theorems of L. Fejes Toth and C. A. Rogers as follows. Let D be a convex domain in the plain and let S be a family of n translates of a centrally symmetric convex disc C. An upper bound was proved for the area of the part of D covered by the discs of S. The bound is best possible in the sense that it is asymptotically tight when n and the area of D approach infinity so that the density of the discs relative to D is fixed. *Igors Gorbovickiss* lecture *"Kneser-Poulsen conjecture for low density configurations"* was centered around the Kneser-Poulsen conjecture according to which if a finite set of balls in Euclidean d-space is rearranged so that the distance between each pair of centers does not decrease, then the volume of the union does not decrease. It was proved that if before the rearrangement each ball is intersected with no more than d + 2 other balls, then the conjecture holds. The central problem of *Oleg R. Musins* lecture *"The Tammes problem for N=13"* asked for the arrangement and the maximum radius of 13 equal size non-overlapping spheres touching the unit sphere. The lecture reported on a computer-assisted solution based on the enumeration of the so-called irreducible graphs. *Rolf Schneiders* lecture *"A Volume inequality and coverings of the sphere"* proved that among spherically convex bodies of given inradius in spherical d-space the lune has the largest possible volume. Based on this a Tarski-type result was proved including the statement that if the d-dimensional unit sphere is covered by finitely many spherically convex bodies, then the sum of the inradii of these bodies is at least π.

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Chapter 12

Coordinated Mathematical Modeling of Internal Waves (10w5083)

Apr 04 - Apr 09, 2010

Organizer(s): Thomas Peacock (Massachusetts Institute of Technology), Neil Balmforth (University of British Columbia), Gordon Ogilvie (University of Cambridge), Bruce Sutherland (University of Alberta)

This report presents a review of the material covered at the workshop on ”Coordinated Mathematical Modeling of Internal Waves”. The scope of the workshop was very broad, covering internal wave dynamics that arises in geophysical and astrophysical contexts. Five plenary lectures were given on the topics of oceanic, atmospheric and astrophysical internal waves. The presenters of these five lectures herein provide an overview of the state-of-play of research in each of these fields, and furthermore summarize the major outstanding issues and questions that were raised at the workshop.

Astrophysical Internal Waves I (by J. Goodman)

If internal waves are defined as periodic fluid motions restored by buoyancy and coriolis forces, then the internal waves observed in astronomical bodies are mainly global modes of oscillation rather than traveling waves such as those observed in the Earth's atmosphere and oceans. This is largely a selection effect, since at astronomical distances only waves that modulate the net light output from the nearer face of a star can be directly detected. Small-scale traveling waves are probably excited by instabilities, turbulence, and sometimes astronomical tides, and such waves may be important for mixing and momentum transport. But the absence of *in situ* measurements makes them difficult to constrain. This review concentrates on directly observed or potentially observable modes/waves; the subject of tidally excited internal waves—dear to my own heart—has been taken up by G. Ogilvie and others at this meeting.

A *g-mode* is the usual astronomical term for a global oscillation supported mainly by buoyancy due to stable stratification of entropy or composition. The radiatively diffusive core of the Sun, which encompasses 70% of its radius and more than 97% of its mass, is stratified, and g-modes surely exist there, but none have yet been securely detected [7]. Their eigenfunctions are evanescent in the outer 30% of the Sun, which is convective and therefore unstratified. The predicted velocity amplitude at the photosphere (visible surface) is $\lesssim 1\,\mathrm{mm\,s^{-1}}$ if the g-modes are excited by the convective turbulence, as the p-modes are. The latter are basically sound waves; $\sim 10^6$ p-modes are seen with typical amplitudes $\sim 10\ \mathrm{cm\,s^{-1}}$ and periods 3-6 min, and these have been used extensively to probe the Sun's internal structure [15].

A possible example of the indirect influence of astrophysical internal waves is the suggestion that g-mode coupling explains why the core rotates synchronously with the convection zone, as is inferred from p-mode rotational splittings, even though the Sun has gradually lost angular momentum to the solar wind over its lifetime [60]. As is often the case with indirect effects of internal waves in astrophysics, however, there are competing candidates for the coupling mechanism.

Many stars pulsate at amplitudes much larger than would be expected from turbulent forcing. Some of the frequencies are compatible with g-modes. These include subclasses of main-sequence B stars (i.e., surface temperatures 10^4-$10^{4.5}\,\mathrm{K}$) [20]. The excitation mechanisms are thermal: modulation of the radiative or convective heat flux (luminosity) of the star produces mechanical work in a manner somewhat analogous to—-but thermodynamically much less efficient than—a Carnot engine [17]. That this does not occur in all stars is due to requirements on the thermal timescale at those depths where modulation is possible, which translate to requirements on the surface temperature. It is worth noting that whereas the real parts of the mode frequencies are straightforwardly calculable by linear theory,[1] calculation of growth rates, stochastic forcing, and nonlinear saturation are challenging and more vulnerable to uncertainties in the input physics: e.g. radiative opacities, turbulent viscosities, etc.

By far the best observed and perhaps best understood g-mode pulsators are not main-sequence stars but white dwarfs. These are "dead" stars supported against their own gravity by electron degeneracy rather than thermal pressure and composed mainly of thermonuclear ash (helium through magnesium) rather than hydrogen. The residual heat supports, in addition to the observable luminosity of these objects, a slight thermal stratification of the outermost layers; additional stratification occurs deeper at the interfaces among helium, carbon, oxygen (etc.) zones due to the slight differences in nuclear mass per (pressure-ionized) electron rather than the molecular weight *per se*. In particular, the DAVs (a.k.a. ZZ Ceti stars) are white-dwarf pulsators with surface temperatures in the range $11,000 - 12,000\,\mathrm{K}$. Due to the compactness of white dwarfs ($R \sim 10^3$-$10^4\,\mathrm{km}$, $\bar{\rho} \gtrsim 10^6\,\mathrm{g\,cm^{-3}}$), the g-mode periods are 10^2-10^3 seconds—as compared to hours to days for main-sequence pulsators—enabling useful time series to be obtained relatively quickly. Precise measurements of mode frequencies diagnose the internal structure of the white dwarfs. The intrinsic linewidths are so small and the mode lifetimes so long in some cases that the gradual change in frequencies due to cooling—on timescales of order $10^9\,\mathrm{yr}$—is directly detected ([63] and references therein).

Excitation of DAV g-modes is understood to occur by a thermal instability in which the surface convection zone is crucial to modulating the heat flux, even though it contains only $\sim 10^{-14}$ of the stellar mass [13, 30]. As with any linear instability, it is necessary to address nonlinear saturation. This is less well understood than excitation (and much less well than the linear eigenfrequencies), but for the smaller-amplitude pulsators with many active modes, there are quantitative reasons to believe that saturation occurs by three-mode couplings, and in particular by parametric instabilities [65].[2]

This review includes a brief discussion of *r-modes* in neutron stars. The maximum observed rate of rotation of neutron stars, $\approx 700\,\mathrm{Hz}$, is less than the "break-up" rate where centrifugal force balances gravity (thought to be $\approx 1\,\mathrm{kHz}$); it is speculated this is due to loss of angular momentum by gravitational radiation [11], which requires the star to be slightly nonaxisymmetric. This may occur by linear instability of r-modes, which can be spontaneously excited by emission of gravitational waves at high rotation rates if the viscosity of the neutron star is sufficiently small [6]. This is another example of a somewhat speculative indirect effect of internal waves. There is, however, hope that the gravitational waves may be directly detected in the not too distant future [62].

Unlike g-modes, r-modes are restored by Coriolis rather than buoyancy forces. They are a special case of the more general class of rotationally supported internal waves, namely inertial oscillations. r-modes are distinguished by their long wavelengths and simple dispersion relation; in fact they are approximately polynomial in Cartesian coordinates. Quadrupolar modes varying longitudinally $\propto \exp(2i\phi)$ have angular frequency $\approx 4\Omega/3$ in an inertial frame, where Ω is the rotational frequency of the star, but $\approx -2\Omega/3$ in the rotating frame. This makes them modes of negative energy and angular momentum, so that they can be excited by emission of positive-energy gravitational waves; since the emitted power is proportional to the square of the wave amplitude (and to the sixth power of frequency), this produces linear instability. Here too saturation may occur via a network of nonlinear three-mode couplings [14, 54]. However, it appears that a steady balance between parametric growth and viscous dissipation of the daughter modes is not possible,

[1] This is true at least for nonrotating, spherical stars; the basic equations are summarized in the accompanying presentation. Even linear theory can be conceptually challenging with rotation, however, as witnessed by the talks given at this meeting by B. Dinstrans, G. Ogilvie, J. Papaloizou, M. Rieutord, & Y. Wu.

[2] There may be close parallels here to three-mode couplings of oceanic internal waves, discussed at this conference by J. MacKinnon and N. Balmforth, among others.

so that growth and saturation of the primary mode—and its potentially observable gravitational waves—may undergo limit cycles.

Astrophysical Internal Waves II (by G.I. Ogilvie)

Internal waves play an important role in astrophysics, in the context of tidal interactions between stars and planets. In comparison with terrestrial studies, the astrophysical approach takes a broad and often simplistic view, because we must deal with a vast range of systems and parameters, and have very few observational data, usually of a highly indirect nature.

Tidal interactions can have a significant effect on the orbital and spin evolution of binary stars over astronomical timescales if the orbital period is less than ten days or so [68]. They have also affected the Earth–Moon system and the satellites of other planets in the solar system [49]. Interest has been rekindled in this subject through the ongoing discovery of many extrasolar planets that orbit very close to their host stars [69].

Typically, tidal interactions lead to a synchronization and alignment of the spin of the bodies with their orbital motion, together with a circularization of the orbit. These dissipative processes are accompanied by heating, which can have dramatic consequences, as in the case of Jupiter's closest moon, Io. In systems of extreme mass ratio, such as planets orbiting stars, the large body usually cannot achieve synchronization, and the tidal exchange of angular momentum leads instead to orbital migration, which is inward if the large body spins more slowly than the orbit. This process limits the lifetime of planets found in close orbits around stars.

A general mathematical formalism can be constructed for problems of tidal forcing, in which the tidal potential experienced by a body is expanded in solid spherical harmonics and in a Fourier series in time. For orbits of significant eccentricity, a broad spectrum of forcing frequencies is present [64]. At least in linear theory, our aim is to calculate the potential Love number, which is a dimensionless measure of the response of the body to periodic forcing; it depends on the degree and order of the spherical harmonic that is applied, and also on the tidal frequency. The Love number measures the external gravitational potential perturbation generated by the deformed body, which is the only means by which energy and angular momentum can be exchanged with the companion. It is a complex response function, and its imaginary part $\mathrm{Im}(k)$, which determines the part of the response that is out of phase with the forcing, governs the energy and angular momentum exchanges.

One possible viewpoint is that an astrophysical body supports a spectrum of discrete global oscillation modes, which might form a complete set of orthogonal functions under certain conditions. These modes would typically be computed for an ideal fluid, and their damping rates due to non-adiabatic effects or viscosity would be estimated by perturbative methods. Each mode can then be expected to respond to periodic forcing in the same way as a damped harmonic oscillator, and the overall response function of the body would contain a succession of Lorentzian peaks corresponding to the various modes with the appropriate natural frequencies and damping constants, and weighted according to their spatial overlap with the tidal potential.

There are at least two important ways in which this viewpoint is questionable. First, the relevant low-frequency oscillation modes in convective regions of stars and giant planets are thought to be inertial waves, which do not generally form discrete oscillation modes in an ideal fluid unless they propagate within simple containers such as a full sphere. If the inertial waves are confined to a spherical shell, for example because of the presence of a dense planetary core or stellar radiative zone, then after multiple reflections they exhibit a complicated behavior that depends strongly on the tidal frequency [47, 52]. Singularities associated with the critical latitude and with wave attractors have been found to be important, and connections can be made with problems studied in the Earth's ocean and in laboratory experiments. The tidal response is much more complicated than a succession of Lorentzian peaks, but on the other hand $\mathrm{Im}(k)$ may achieve a viscosity-independent asymptotic regime in restricted intervals. Recent work by several participants at the workshop has revealed the importance of inertial waves for tidal dissipation in astrophysical bodies as well as their remarkable complexity [10, 32, 36, 48, 53, 66]. Broadly speaking, this work implies that global modes are relevant when the inertial waves propagate in a full sphere, while singularities dominate the response when the core exceeds a certain size.

Second, when internal waves are involved, global oscillation modes may not be established because the waves can break. This is a problem especially for internal gravity waves that are excited in stellar radiative zones. Since the tidal frequency is usually much smaller than the Brunt–Väisälä frequency, the gravity waves can have a very short radial wavelength and propagate slowly. They are especially susceptible to breaking as they approach the surface of a star (for stars more massive than the Sun) or the center (for solar-type stars). Wave breaking can prevent the resonant excitation of global modes and leads instead to efficient tidal dissipation over a broad range of frequencies [29, 31]. This is an example of a situation in which the nonlinear behaviour is much simpler, in broad terms, than the linear behaviour. It is also an area in which terrestrial studies can provide valuable information for astrophysicists.

Atmospheric Internal Waves (by D.C. Fritts)

Internal Gravity Waves (IGWs) play enormous roles in the dynamics, structure, and variability of Earth's atmosphere extending from the surface well into the thermosphere ($\sim$500 km and above). Their importance derives from their many sources, their efficient transport of energy and momentum to higher altitudes, and increases in their amplitudes and effects accompanying rapid density decreases with altitude (see [22], for a recent review). The dominant sources for smaller-scale IGWs include topography, convection, and wind shears. Wavelengths arising from these sources range from $\sim$10 to 100's of km in the horizontal and $\sim$1 to 100 km or more in the vertical, with the larger scales more prevalent at higher altitudes. Unbalanced jet stream flows, solar energy inputs in the auroral zones, and body forces accompanying IGW dissipation processes at higher altitudes yield larger-scale IGWs which have influences at lower or higher altitudes depending on their phase speeds.

The IGWs having the largest influences on atmospheric circulation and structure, and the weather and climate processes driving our forecasting needs, are the subset accounting for the dominant transport of energy and momentum from source regions to higher altitudes. These are the IGWs having the largest amplitudes, vertical group velocities, and energy and momentum fluxes at each altitude. IGWs excited at larger amplitudes and smaller scales account for the dominant fluxes and play the major roles in the troposphere and stratosphere. Because atmospheric density decreases by $\sim 10^6$ and $\sim 10^{11}$ from Earth's surface to $\sim$100 and $\sim$300 km (for mean solar conditions), respectively, the dominant IGWs in the mesosphere and thermosphere have larger scales and amplitudes than at lower altitudes by $\sim$1 to 2 decades.

IGW amplitudes increase strongly with increasing altitude because conservative IGW motions maintain a constant pseudo-momentum flux, $F = < u'_h w' (1 - f^2/\omega^2) >$ as they propagate, where $\rho_0(z) \sim e^{-z/H}$ is mean density, $H \sim 7$ km at lower altitudes, u'_h and w' are the IGW horizontal and vertical perturbation velocities in the plane of propagation, f and ω are the inertial and IGW intrinsic frequencies, and primes and angle brackets denote perturbations and a suitable spatial or temporal average, respectively. This implies IGW amplitudes that vary with density or altitude as $(u'_h,\, w',\, \rho'/\rho_0) \sim \rho_0^{-1/2}(z) \sim e^{z/2H}$. However, increasing amplitudes cause IGWs to be increasingly susceptible to various non-conservative instability processes which constrain IGW amplitudes, induce various interaction and instability dynamics, and drive IGW energy and momentum deposition. Larger-scale effects of these dynamics include: 1) systematic changes in the mean circulation and thermal structure throughout the atmosphere, 2) generation of secondary IGWs at higher altitudes, 3) modulation of, and by, tidal and planetary wave motions and mapping of these structures to much higher altitudes, and 4) apparently strong influences of these neutral dynamics on plasma dynamics and instabilities throughout the ionosphere. Smaller-scale effects include: 5) turbulence and mixing throughout the atmosphere with intensities and influences that increase with altitude into the thermosphere, and 6) an approximately "universal" IGW spectrum in wavenumber and frequency remote from IGW sources.

Stability theory provides valuable guidance on the occurrence, character, and time scales of the instability dynamics influencing IGWs (e.g., [1, 43, 57]), while numerical modeling provides insights into the instability and turbulence dynamics and mixing in idealized environments (e.g., [23, 24]). Despite many advances in theoretical, modeling, and observational studies, however, current parameterizations of these dynamics, and their influences on the large-scale circulation and structure of the atmosphere, are recognized to have major deficiencies due to an incomplete understanding of these dynamics at present (e.g., [40, 56]).

Solar tides are also important components of the atmospheric motion field at higher altitudes. They can be viewed as large-scale IGWs forced by solar thermal absorption and modified by Earth's curvature and rotation. Thermal absorption in the troposphere excites deep tropical convection exhibiting maxima over

Africa, the Amazon basin, and the western Pacific (except during El Niño) that induces both migrating (sun synchronous) and non-migrating modes (having eastward and westward phase speeds different than the sun) at harmonics of a solar day. Solar UV absorption by ozone in the stratosphere yields additional tidal forcing at larger vertical scales. The result of these thermal sources and interactions among the various tidal modes and planetary waves is a rich superposition of tidal harmonics exhibiting complex but systematic phase structures and winds of 50 to 100 ms^{-1} or larger extending from $\sim$80 km well into the thermosphere. Like IGWs at smaller spatial scales, the tides contribute to energy and momentum transport over considerable depths. Major tidal roles include the modulation of IGW propagation and transport to higher altitudes extending well into the thermosphere and tidal influences on plasma dynamics and instabilities in the ionosphere.

Despite significant progress to date in many areas, there remain major unknowns spanning the spectrum of linear, quasi-linear, and nonlinear dynamics of IGWs in Earth's atmosphere. While linear theory provides a reasonable, though qualitative, description of the dominant IGW sources and propagation in variable environments, it often fails to describe the details. This is surely due, in part, to the lack of complete characterization of the spatial and temporal scales of the IGW sources and the environments in which they arise and through which they propagate. Observations cannot describe the airflow over terrain at high resolution and thus are unable to describe the effects of boundary layer dynamics, separation, or temporal modulation. Similarly, convection is poorly defined in space and time (in observations and models) relative to the scales of the most intense updrafts (and strongest IGW sources). Hence even an accurate statistical description of IGW responses to convection is beyond our present capabilities. Other IGW sources, such as jet streams, wind shears, or body forces, are even less well characterized.

Fine structure in the wind and/or temperature fields through which IGWs propagate almost certainly influences their propagation and tendency for instability throughout the atmosphere. Yet we have limited abilities to characterize these influences at present, despite indications that such superpositions of spatial scales may dramatically influence the tendency toward, and character of, instabilities influencing IGW amplitudes and transport. Likewise, quasi-linear influences (e.g., IGW-induced mean flows) are well documented at larger scales throughout the atmosphere, but we know little about transient or localized body forcing or their influences on IGW propagation, interaction, and instability dynamics.

By far the largest current unknowns concerning IGWs, however, are the nonlinear dynamics and spectral transfers accompanying wave-wave interactions and IGW instability and turbulence generation. While valuable insights have come from theory, laboratory studies, and atmospheric observations, the parameter space for these dynamics is enormous, and studies to date have only provided a few enticing glimpses of the likely diversity. These dynamics and their effects depend in detail on both the dominant properties of these flows (i.e., IGW and environmental parameters) as well as the fine-structure flow that may or may not be observable, but which may have significant influences on the flow evolution. Key questions include: 1) when are linear or quasi-linear dynamics sufficient to describe IGW effects, 2) when are nonlinear effects essential to account for observed IGW character, 3) which dynamics determine the IGW spectrum with altitude (and under what conditions), and 4) what dynamics are critical to parameterize these IGW effects in our numerical weather prediction, climate, and general circulation models?

Oceanic Internal Waves I (by J.A. MacKinnon)

Internal gravity waves are ubiquitous in the stratified ocean, and play an important role in both local dynamics and ecology and the Earth's climate as a whole. Oceanic internal waves are Boussinesq and often have low enough amplitudes that a linear dispersion relation accurately describes their polarization and propagation characteristics (see, e.g. [28]). Vertical wavelengths range from the full ocean depth (km) to tens of meters. Wave frequencies are bounded at the low end by the local (latitude-varying) inertial frequency and at the high end by the local buoyancy frequency. Oceanic internal waves tend to be spectrally red in both frequency and wavenumber, with variance dominated by low-vertical-mode, low-frequency waves [25].

Though there are many motivations to study internal waves in the ocean (heaving of density surfaces affects everything from sound propagation to light limitation for phytoplankton), most research is inspired by the large role internal waves in diapycnal mixing. Away from surface and bottom boundary layers the magnitude and geography of diapycnal mixing in the ocean interior is largely set by the dynamics of breaking internal gravity waves. Over the last two decades it has become clear that wave breaking, and the resultant turbulent mixing, are strong inhomogeneous in both space and time. The patterns are driven by details of internal wave generation, propagation, interaction, and dissipation. In turn, the patchiness of diapycnal mixing has significant consequences for both regional and global flow patterns. Current generation climate models include little if any of these patterns or the internal wave dynamics that produce them [33, 38, 55]. Climate models that do not appropriately represent the turbulent fluxes of heat, momentum, and CO_2 across critical interfaces will not accurately represent the ocean's role in present or future climate.

Open questions remain for every stage of the internal wave life cycle. Energy is input into the internal wave field primarily by the tides and wind [67]. Internal tides are generated where the barotropic tide rubs over rough topography. Near the generation site, internal tides often take beam-like form, with the detailed structure dependent on tidal strength and shape of the topography [8, 16, 26]. Some of the resultant baroclinic energy dissipates locally, producing a global map of mixing hotspots that mirrors internal tide generation sites [59]. However, most of the energy radiates away in the form of low (vertical) mode waves [58]. Where this low-mode energy dissipates is still very much up in the air - contenders include scattering over deep topography [39], breaking on the continental slope [46], nonlinear interactions with the ambient internal wave field, including the special case of parametric subharmonic instability [5, 34, 45, 44], or interactions with mesoscale features [50, 51].

Near-inertial internal waves start with surface wind forcing of near-inertial motions in the mixed layer [3]. Beta-plane and eddy-interactions change the horizontal wavenumber so this variance can move equatorward and into the pycnocline, turning purely inertial motions into near-inertial waves that can propagate [18, 19]. Subsequent interactions within the internal wave field and with topography likely determine their role in turbulence production but these pieces of the puzzle are not well-understood. Local dissipation of higher-mode near-inertial waves plays a large role in turbulent fluxes of heat, dissolved gases, and nutrients in the stratified transition layer just beneath the mixed layer. As with internal tides, higher-mode waves are likely to be generated and dissipated locally, while low-mode waves escape to propagate thousands of km across ocean basins [4].

Oceanic Internal Waves II (By G.N. Ivey)

In the coastal ocean environment, the combination of finite depth and often complex coastal bathymetry means the role of boundaries becomes all important in the internal wave dynamics. The interaction of internal waves with the boundaries often promotes turbulent mixing, of central importance not only to local coastal ocean dynamics but also to basin-scale dynamics. The coastal region is also of particular importance to industry such as the offshore oil and gas industry, fisheries and the ecological functioning of the region.

Internal waves at density interfaces can grow from an initial small amplitude η_0 to form large amplitude highly non-linear internal wave trains. The final state of these evolving internal waves is dependent upon the two parameters η_0/H and h/H, where h is the upper layer depth and H the total depth [35]. In extreme cases, the induced interfacial shear can be so strong that mixing occurs, but the occurrence of mixing is very dependent upon both the strength of the shear as well as how long the shear is locally sustained [9]. Rather than in the interior, internal waves at density interfaces are most easily broken down when shoaling over sloping bottoms where, depending on relative magnitudes of the bottom slope and wave slope, from zero up to a maximum of 25% of wave energy can be converted to increased PE [2, 12].

In continuously stratified environments, a feature of both observational and numerical modeling work, particularly in the coastal ocean, is the crossing of obliquely propagating internal wave beams. Resonant interactions and turbulent can occur at these intersection regions and, while this has been demonstrated in the laboratory [61], it has not been observed in the field but could well be important in coastal regions such as Monterey Bay or the South China Sea with complex and energetic internal wave fields. Internal wave breakdown is clearly more dramatic and active near boundaries and especially due to wave reflection at critical slopes where energy conversions can again be up to 25% efficient [37]. While the process is well known, the sensitivity of the process to topographic shape and near boundary ambient flows is less understood.

In general more is known about internal wave reflection than generation. The major generation mechanisms are from turbulence in the surface mixing layer and particularly tidally forced flow over bottom topography which can generate both modal and beam-like responses [21]. Field measurements suggest highly dynamic mean flow fields and intense turbulent mixing in boundary regions and it remains unclear how this impacts the effectiveness of wave generation, particularly in the beam case [27, 42]

Some implications for field scale numerical models are clearly the need for three-dimensional effects, but there remains challenges over when (or where in domain) non-hydrostatic models are needed, and how to deal with the resulting computational constraints for field scale applications. What spatial resolution is needed, especially near boundaries, to describe the topographic shape, horizontal excursion length and (especially) in vertical? It is not clear how these factors influence internal wave beam width as it leaves the bottom. Intimately linked to this is the need for simple but dynamic parameterization of turbulence [41] in the vicinity of topography where waves may overturn and break.

Concluding Q & A

In a concluding session, the following questions were posed and answered by the participants. This is a brief synopsis of this session.

What is the spectrum of internal waves produced by turbulence or penetrative convection?

There appears to be some organization/weak coupling with a preferred excitation frequency $\omega \sim 0.6N - 0.8N$ (Sutherland). Some evidence for support of this in ocean data (MacKinnon). Basically a complicated broad spectrum in stars (Rogers). BV frequency varies significantly with location in stars (Goodman). Interaction sites between waves set the spectrum; after that it is just propagation (Sutherland).

Is geometric focusing relevant in a domain with a large aspect ratio?

Focusing was first studied in a thin shell case around the equator. Important when waves only get trapped in an equatorial region (Rieutord).

”Universal” wave spectrum - what causes it?

In atmosphere it is instability processes (Fritts). Saturation phenomena due to wave-wave interactions in the ocean. Reproduced by numerical models. GM spectrum established since 1970’s and proven if energy enters in $M2$ and $K1$. Not necessarily triad interactions (StLaurent). Lots of tests/foundation came from near Woods Hole. There have been ocean observations elsewhere that disagree (Alford). Ocean expressed in terms of modes. Atmosphere has very different processes (Sutherland). Maybe some small-scale processes are the same in the ocean and atmosphere (MacKinnon). Don’t need breaking to achieve saturation (StLaurent). Energy dissipation timescales are different in the ocean (50 days) and atmosphere (10 days). Scales in the ocean different to atmosphere. Ocean is limited to 10km vertical scales whereas atmosphere can go upto 100km (general comments).

Why isn’t momentum deposition important in the ocean?

Not necessarily true. In Antarctic Circumpolar Current it may be that momentum deposition by lee waves is important. Also in equatorial undercurrent (MacKinnon). Momentum deposition in the ocean appears not to have been measured (Sommeria,StLaurent).

Why perform lab experiments?

Basically there are still processes that are challenging for numerics. Can see unexpected things in the lab. Numerical models are for finite periods of time; if you are interested in long time behavior then need experimental validation (general comments).

Is there an atmospheric tide?

Yes. Created by heating and cooling. Also gravitational tides. This is very important in the ionosphere (Fritts).

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[69] see *http://exoplanet.eu*

Chapter 13

Generalized complex and holomorphic Poisson geometry (10w5072)

Apr 11 - Apr 16, 2010

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Overview of the Field

Generalized complex geometry is a relatively new subject in differential geometry, originating in 2001 with the work of Hitchin on geometries defined by differential forms of mixed degree. It has the particularly interesting feature that it interpolates between two very classical areas in geometry: complex algebraic geometry on the one hand, and symplectic geometry on the other hand. As such, it has bearing on some of the most intriguing geometrical problems of the last few decades, namely the suggestion by physicists that a duality of quantum field theories leads to a ”mirror symmetry” between complex and symplectic geometry.

Examples of generalized complex manifolds include complex and symplectic manifolds; these are at opposite extremes of the spectrum of possibilities. Because of this fact, there are many connections between the subject and existing work on complex and symplectic geometry. More intriguing is the fact that complex and symplectic methods often apply, with subtle modifications, to the study of the intermediate cases. Unlike symplectic or complex geometry, the local behaviour of a generalized complex manifold is not uniform. Indeed, its local structure is characterized by a Poisson bracket, whose rank at any given point characterizes the local geometry. For this reason, the study of Poisson structures is central to the understanding of generalized complex manifolds which are neither complex nor symplectic. Recently (Cavalcanti and Gualtieri 2007-8), the first examples were found of generalized complex 4-manifolds which admit neither complex nor symplectic structures; methods of Poisson geometry were central to the effort. This opens up the question of what obstructions there are to the existence of generalized complex structures.

While the local structure of generalized complex manifolds may be non-uniform, it is often describable as a deformation of a complex structure, where the deformation parameter is itself a holomorphic Poisson structure. This places strong constraints on the behaviour of the geometry, and allows the use of our knowledge of holomorphic Poisson manifolds coming from the study of integrable systems, mechanics, and algebraic geometry. Using this approach, we have gained a greater understanding of generalized complex manifolds, especially in dimension 4, in parallel with the recent completion of the classification of holomorphic Poisson surfaces (Bartocci-Macrì 2004).

Another surprising connection with holomorphic Poisson geometry arises from the study of a distinguished class of sub-objects of a generalized complex manifold, called D-branes because they correspond to Dirichlet boundary conditions on open strings with ends on a membrane in string theory (Kapustin-Li 2005). One finds that D-branes in a usual symplectic manifold correspond not only to Lagrangian submanifolds but also to new objects in symplectic geometry called co-isotropic A-branes (Kapustin-Orlov 2001). The presence of such branes may induce on the symplectic manifold the structure of a holomorphic symplectic structure. This was used to great effect in the recent work of Kapustin-Witten (2006) and Gukov-Witten (2008) on the geometric Langlands program, in which a D-brane on the Hitchin moduli space of Higgs bundles leads to the appearance of D-modules, a key step in establishing the Langlands correspondence.

Just as complex and symplectic geometry may be made compatible with a Riemannian metric, a generalized complex structure may be equipped with a compatible Riemannian metric to form a generalized Kähler structure. It can be shown (Gualtieri 2004) that generalized Kähler geometry is equivalent to the most general $N = (2, 2)$ supersymmetric sigma model target geometry, as described in 1984 by Gates-Hull-Roček. In fact, a generalized Kähler structure comprises not one but *two* integrable complex structures, each Hermitian with respect to the Riemannian metric. For this reason, the subject has great relevance to bi-Hermitian geometry, a subject which has been studied from the point of view of twistor theory for several decades (Apostolov-Gauduchon-Grantcharov 1988). In a generalized Kähler manifold, the difference between the two complex structures is, remarkably, measured by a holomorphic Poisson structure (Hitchin 2005). We see again the emergence of a Poisson structure in describing how far the generalized structure is from the usual one.

The construction of examples of generalized Kähler manifolds has proven surprisingly challenging. Without the standard tools of algebraic geometry for constructing usual Kähler manifolds, one must discover new methods of construction. Much effort has recently been expended in this aim. In (Hitchin 2005), examples are produced under homogeneity assumptions. In (Bursztyn-Cavalcanti-Gualtieri 2005) and (Lin-Tolman 2005), examples are produced via the development of a reduction procedure analogous to the Marsden-Weinstein symplectic reduction. In (Goto 2005), a large class of examples are produced by deformation of usual Kähler structures, and in (Hitchin 2006), new examples are produced via Hamiltonian deformation. There is much work under way on new methods of construction as well as better conceptual frameworks for understanding the presence of generalized Kähler geometry.

In the same way that Kähler geometry is generalized, other geometries of special Holonomy, such as Calabi-Yau and G2 manifolds, have extensions to generalized geometry. In fact, Generalized Calabi-Yau geometry was one of Hitchin's original motivations in the subject (Hitchin 2001), and such a structure was used shortly thereafter in (Huybrechts 2003) to establish an isomorphism between the moduli space of Generalized Calabi-Yau metrics on the K3 surface and its moduli space of $N = (2, 2)$ super-conformal field theories in the sense of (Aspinwall-Morrison 1997). For generalized G2 structures on 7-manifolds, (Witt 2004) shows that the presence of generalized G2 structure provides a solution to the supersymmetry equations on spinors in type IIA/B supergravity, and studies the resulting geometrical structure using Riemannian connections with skew torsion.

The major challenges in the emerging field of generalized geometry include the following three items. First, to achieve a greater understanding of the intrinsic structures involved, such as generalized complex or Kähler manifolds, and their relation to standard structures in Kähler or Poisson geometry. Second, to construct new examples of generalized complex and Kähler structures, hopefully with very general methods. Third, the development of an algebraic theory capturing a hypothesized categorical structure for generalized complex manifolds analogous to the Fukaya category of symplectic manifolds or the category of coherent sheaves on a complex manifold.

Objectives of the workshop

Before this BIRS workshop, a meeting gathering the growing number of researchers investigating the various forms of generalized geometry, such as generalized complex and Kähler geometry, had never been held. There was a general consensus among many of the researchers mentioned above that a meeting focused on the subject would be of great benefit to progress in the field.

The primary objective of the workshop was to gather together, in the secluded and stimulating environment of BIRS, the mathematicians who work on generalized complex geometry and closely related fields such as Poisson geometry, non-Kähler complex geometry, and integrable systems, so that they may combine their tools and approaches to further our understanding of these subjects. In particular, we worked to further the following goals.

- The myriad examples of holomorphic Poisson manifolds and dynamical systems studied in integrable systems should be better-known to the fields of Poisson geometry and generalized complex geometry and will hopefully provide new areas of investigation.
- Within Poisson geometry, much effort has been expended in recent years (Crainic-Fernandes 2001) to construct and study the symplectic groupoid, which is a kind of "resolution" of a Poisson manifold to a symplectic manifold with groupoid structure. Recently (Crainic 2004, Stiénon-Xu 2006) the notion of symplectic groupoid has been extended to generalized complex manifolds in an effort to resolve their complicated local structure. This project is still ongoing, as our understanding of the intrinsic structure of the groupoid is not complete. However it promises to shed enormous light on the problem of developing a generalized complex category in analogy to the symplectic and Poisson categories in the sense of Weinstein.
- The algebro-geometric approach to Poisson structures provides a wide set of tools for constructing objects such as Poisson modules on Poisson manifolds; by learning about and furthering these methods, we shall better understand the construction of D-branes on generalized complex manifolds.
- The known exotic examples of generalized complex 4-manifolds were constructed by surgery methods analogous to those used in complex algebraic geometry as well as Poisson geometry. A better understanding of these tools may lead to new constructions of generalized complex manifolds in dimension 4 and 6, especially.
- The well-developed theory of reduction in Poisson and symplectic geometry, including the theory of group-valued moment maps (Alekseev-Malkin-Meinrenken 1997, Alekseev-Bursztyn-Meinrenken 2007) has only begun to be extended and applied in a consistent fashion to generalized geometrical structures such as Dirac structures and generalized complex structures, and more effort in this direction will be helpful to clarify the study of geometrical structures admitting symmetries.

The workshop was intended as a 5-day workshop involving the main researchers in the fields above, both faculty and postdoctoral, together with the graduate students which have taken up the subject in their doctoral work.

Overview of the meeting

Here are the abstracts of the talks, in alphabetical order by speaker surname:

Speaker: **Marco Aldi** (UC Berkeley)
Title: "Twisted T-duality and Quantization"

Abstract: The goal of this talk is to describe some mathematical aspects of the so called "doubled formalism". Our main application is a detailed study, in the language of vertex algebras, of the (twisted) T-duality relating the Heisenberg nilmanifold and the H-twisted 3-torus. This is joint work with Reimundo Heluani.

Speaker: **Sergey Arkhipov** (University of Toronto)
Title: "Conducting bundles of gerbes with connective structure and categorical symmetries"

Abstract: following Severa and Bressler-Chervov, we recall the definition of the Courant algebroid playing the role of the Atiyah algebroid for a gerbe with connective structure and known under the name of the conducting bundle of the gerbe. We consider the category of gerbe-twisted coherent sheaves with connection and relate the conducting bundle with the homotopy Lie algebra of the categorical group of autoequivalences of this category. The material of the talk is a joint project with Xinwen Zhu.

Speaker: **Tom Baird** (Memorial University)
Title: "A Poisson structure on the moduli space of flat connections over a non-orientable surface"

Abstract: Let G be a simple Lie group and S a two dimensional manifold, and let $M(S, G)$ denote the moduli space of flat G-connections over S. When S is orientable, $M(S, G)$ is a (singular) Poisson manifold arising as the phase space of Chern-Simons theory and so has deep connections with low dimensional topology and mathematical physics.

In this lecture, we explain how to construct a Poisson structure on $M(S, G)$ when S is non-orientable. The construction will make use of the quasi-Hamiltonian reduction of Alekseev-Malkin-Meinrenken's, in the Dirac geometry framework developed by Bursztyn-Crainic-Weinstein-Zhu.

Speaker: **Claudio Bartocci** (Università degli Studi di Genova)
Title: "Geometric interpretation of the bi-hamiltonian structure of the Calogero-Moser system"

Abstract: We shall show that the bi-Hamiltonian structure of the rational n-particle (attractive) Calogero-Moser system can be obtained by means of a double projection from a very simple Poisson pair on the cotangent bundle of gl(n,R). The relation with the Lax formalism will be also discussed. Joint work with G. Falqui, I. Mencattini, G. Ortenzi and M. Pedroni.

Speaker: **Ragnar-Olaf Buchweitz** (University of Toronto)
Title: "The super poisson structure on a Gerstenhaber algebra"

Abstract: A Gerstenhaber algebra is a graded algebra G that carries both a graded commutative product and, on the shifted copy G[1], a super Lie algebra structure such that the bracket g,- from G to G becomes a graded derivation for every element of g. In this way, bracketing with elements from G induces a map from G into the graded derivations or vectorfields of G.

In analogy, as Drinfeld pointed out, one may view G as the algebra of functions on a Poisson super-space, and the question is: What else can we say about these spaces? So far, very little! However, the geometry should be rich, as there are often additional features, such as a Hodge decomposition on a "virtual" tangent cone.

We hope that insight from ordinary Poisson geometry might be transferable to this super context.

We will discuss in some detail two examples: Hochschild cohomology, concretely, say, for flat morphisms between smooth spaces and their fibres, on the one hand, and the cobar construction over a Lie algebra that underlies the the theory of Classical (CYBE) and Quantum Yang-Baxter Equations (QYBE) on the other. In general, these two classical examples, due originally to Gerstenhaber, are related and give rise to universal deformation formulas.

Speaker: **Arlo Caine** (University of Notre Dame)
Title: "Poisson Structures on Toric Varieties"

*Abstract:*Let $X(\Sigma)$ be a smooth projective toric variety for a complex torus $T_{\mathbb{C}}$. Through a GIT construction, $X(\Sigma)$ can be given a number of Poisson structures which are invariant under the action of the complex group $T_{\mathbb{C}}$. Examples include holomorphic Poisson structures on $X(\Sigma)$ as well as smooth real Poisson structures. Of particular interest will be the Poisson structure Π_Σ associated to the standard Poisson structure π on $\mathbb{C}^d$. The symplectic leaves of Π_Σ are the $T_{\mathbb{C}} - orbits$ in $X(\Sigma)$. Hence, Π_Σ is non-degenerate on an open dense set but is not symplectic. It will be shown that each leaf admits a Hamiltonian action by a sub-torus of the compact torus $T \subset T_{\mathbb{C}}$, but that the global action of $T_{\mathbb{C}}$ on $(X(\Sigma), \Pi_\Sigma)$ is Poisson but not Hamiltonian. I will discuss some work on understanding the Poisson cohomology of this structure, including a lower bound for the dimension of $H^1(X(\Sigma), \Pi_\Sigma)$, and conclude with a discussion of the curious geometry of modular vector field of Π_Σ with the Delzant Liouville form.

Speaker: **Alberto Cattaneo** (Universität Zürich)
Title: "Reduction via Graded Geometry"

Abstract: Various geometric (e.g. Poisson, Courant, generalized complex) structures may be rephrased in terms of graded symplectic manifolds endowed with functions satisfying certain equations. From the latter point of view the most general reduction is just that of graded presymplectic submanifolds compatible with the given functions. By translating this back to the language of ordinary differential geometry, we recover all the known reduction procedures plus new ones. For example, in the Poisson world we get various generalizations of the Marsden-Ratiu reduction. This is based on joint work with Bursztyn, Mehta, and Zambon.

Speaker: **Georges Dloussky** (Université de Provence)
Title: "Normal singularities and holomorphic Poisson structures associated to a family of non-Kähler compact complex surfaces"

Abstract: Complex surfaces S containing global spherical shells (GSS) with Betti numbers $b_1(S) = 1$ and $n = b_2(S) > 0$ contain n rational curves. When the intersection matrix of the rational curves $M(S)$ is negative definite a Grauert theorem insures that the maximal divisor can be contracted to one or two normal isolated singularities. We show that the genus of the singularities are one or two, may be Gorenstein. This local property is equivalent to the existence of a holomorphic Poisson structure on S. The topological invariant $k(S) = \sqrt{detM(S)} + 1$ plays an important role in the study of surfaces with GSS, non-invertible contracting germs of mappings and some birationnal mappings of $P^2(C)$. We explain how to compute the integer $k(S)$ using a family of polynomials.

Speaker: **Ryushi Goto** (Osaka University)
Title: "Unobstructed K-deformations of generalized complex structures and bihermitian structures"

*Abstract:*We survey our results on deformations of generalized complex and Kähler structures. At first, we introduce K-deformations of generalized complex structures on a compact Kähler manifold with effective anti-canonical line bundle. It turns out that K-deformations are always unobstructed. This is a generalization of unobstructedness theorem of deformations of Calabi-Yaus by Bogomolov-Tian-Todorov to two directions: from ordinary complex structures to generalized complex structures, and from trivial canonical line bundle to effective anti-canonical line bundle.

Next we explain the stability theorem of generalized Kähler structures with one pure spinor, which shows that generalized Kähler structures are stable under small deformations of generalized complex structures. This is regarded as a generalization of the stability theorem of ordinary Kähler structures by Kodaira-Spencer. Then a non-zero holomorphic Poisson structure gives rise to deformations of generalized Kähler manifolds starting with ordinary Kähler manifolds.

As an application, we construct bihermitian structures on compact Kähler manifolds with holomorphic Poisson structures by using K-deformations and the stability theorem together. In particular, we show that a compact Kähler surface S admits a non-trivial bihermitian structure if and only if S has a non-zero holomorphic Poisson structure. Examples of bihermitian structures on del Pezzo surfaces, degenerate del Pezzo surfaces, Hirzebruch surfaces and some ruled surfaces are discussed.

[1] Unobstructed K-deformations of Generalized Complex Structures and Bihermitian Structures, arXiv:1002.0391.

[2] Poisson structures and generalized Kähler structures, arXiv:0712.2685, J. Math. Soc. Japan, Vol. 61, No. 1 (2009) pp.107-132.

[3] Deformations of generalized complex and generalized Kähler structures, arXiv:0705.2495.

[4] On deformations of generalized Calabi-Yau, hyperKähler, G_2 and Spin(7) structures I, arXiv:math/0512211.

Speaker: **Marco Gualtieri** (University of Toronto)
Title: "Gerbes and Poisson structures in generalized complex and Kähler geometry"

Abstract: I will review and explain the mechanism by which Poisson geometry enters in generalized complex geometry and generalized Kähler geometry, as a sort of introduction to the topic of the conference. I will then use this to deduce some algebraic relationships between the two possibly non-isomorphic complex structures occurring in a generalized Kähler structure.

Speaker: **Nigel Hitchin** (University of Oxford)
Title: "Generalized holomorphic bundles and the B-field action"

Abstract: Gualtieri introduced the notion of a generalized holomorphic vector bundle over a generalized complex manifold. If a closed 2-form preserves the generalized complex structure then it transforms as a B-field one generalized holomorphic vector bundle to another and acts on the moduli space. We look at some examples of this and also describe twisted structures which involves a cocycle of B-field actions, spectral covers and holomorphic gerbes.

Speaker: **Conan Leung** (Institute of Mathematical Sciences and Chinese University of Hong Kong)
Title: "Geometric Structures on Riemannian manifolds"

Abstract: In this talk, I will describe various geometric structures from a unified approach using normed division algebras. By doubling the geometry, this method also give a nice description of all Riemannian symmetric spaces as Grassmannians.

Speaker: **Eckhard Meinrenken** (University of Toronto)
Title: "Twisted Spin^c structures on conjugacy classes"

Abstract: Let G be a compact, connected Lie group. An essential ingredient in the Borel-Weil construction of irreducible G-representations is the fact that the co-adjoint orbits $\mathcal{O} \subset \mathfrak{g}^*$ carry distinguished Kähler structures. More generally, Hamiltonian G-spaces in symplectic geometry carry distinguished Spin^c structures, and the associated Dirac operators are used in their quantization.

By contrast, conjugacy classes $\mathcal{C} \subset G$ need not admit complex structures in general, or even Spin^c structures. I will explain in this talk that the conjugacy classes, and more generally all quasi-Hamiltonian G-spaces, carry canonical *twisted* Spin^c structures, with twisting by a distinguished background 'gerbe' over G. The twisted Spin^c structures appear in a quantization procedure for quasi-Hamiltonian spaces.

This talk is based on joint work with Anton Alekseev.

Speaker: **Justin Sawon** (University of North Carolina)
Title: "Fourier-Mukai transforms and deformations in generalized complex geometry"

Abstract: In this talk I will describe Toda's results on deformations of the category Coh(X) of coherent sheaves on a complex manifold X. They come from deformations of X as a complex manifold, non-commutative deformations, and gerby deformations (which can all be interpreted as deformations of X as a generalized complex manifold). Toda also described how to deform Fourier-Mukai equivalences, and I will present some examples coming from mirror SYZ fibrations.

Speaker: **Andrei Teleman** (Université de Provence)
Title: "Using moduli spaces of holomorphic bundles to prove existence of curves on class VII surfaces"

Abstract: The classification of complex surfaces is not finished yet. The most important gap in the Kodaira-Enriques classification table concerns the Kodaira class VII, e.g. the class of surfaces X having $\mathrm{kod(X)} = -\infty$, $b_1(X) = 1$. These surfaces are interesting from a differential topological point of view, because they are non-simply connected 4-manifolds with definite intersection form. Class VII surfaces with $b_2 = 0$ are completely classified, but the methods used for this subclass do not extend to the general case. In the case $b_2 > 0$

important progress has been obtained by Kato, Nakamura, Dloussky and later by Dloussky-Oeljeklaus-Toma, but the complete classification has been considered since many years to be a hopeless goal. The difficulty is to show that any minimal class VII surface with $b_2 > 0$ admits sufficiently many curves. I will explain my program (based on ideas from Donaldson theory) to prove existence of curves on minimal class VII surfaces with $b_2 > 0$ and the first effective results obtained using this program: the classification up to biholomorphism for $b_2 = 1$ and up to deformation equivalence for $b_2 = 2$. Finally I will discuss the challenges to overcome (but also the expectations) for extending these methods to the case $b_2 > 2$.

Speaker: **Susan Tolman** (University of Illinois at Urbana-Champaign)
Title: "Symplectic circle actions with minimal fixed points"

Abstract: The purpose of this talk is to show that there are very few "extremely simple" symplectic manifolds with sympliectic actions. For example, consider a Hamiltonian circle action on a compact symplectic manifold (M, ω). It is easy to check that the sum of $\dim(F) + 2$ over all fixed components is greater than or equal to $\dim(M) + 2$. We show that, in certain cases, equality implies that the manifold "looks like" one of a handful of standard examples. This can be viewed as a symplectic analog of the Petrie conjecture. We will also discuss related results for non-Hamiltonian actions. Based on joint work with Hui Li and Alvaro Pelayo.

Speaker: **Frederik Witt** (Universität München)
Title: "Calibrations, D-branes and B-fields"

Abstract: In their quest for minimal submanifolds, Harvey and Lawson introduced the notion of a calibrated submanifold. In this talk, I shall present a natural extension of this concept to the generalised geometry framework and explain how this relates to D-branes in type II string theory.

Speaker: **Maxim Zabzine** (Uppsala Universitet)
Title: "Why strings love generalized geometry"

Abstract: I will review the relation between sigma models, Poisson vertex algebras and vertex algebras. The generalized geometry plays a central role in this relation. I will discuss the recent results on the connection between the sheaves of susy vertex algebras and the different aspects of generalized geometry.

Presentation Highlights/Scientific Progress Made

Examples of recent breakthroughs:

1. Prof. Hitchin described new work in progress concerning generalized holomorphic bundles over generalized complex manifolds. These are generalizations of usual holomorphic bundles and they may be approached with the same questions that have been applied to holomorphic bundles. For example, do they have moduli spaces? How can we construct examples? He focused on a particularly intriguing case of viewing a complex manifold as a generalized complex manifold. In this case, the notion of a generalized holomorphic bundle coincides with the usual notion of a holomorphic bundle, except that it is equipped with a co-Higgs field. Hitchin explained how the co-Higgs field leads to a spectral description of the bundle, as in the case of Higgs bundles. Even more interesting was the observation that the complex manifold may support a nontrivial holomorphic gerbe, in which case the generalized holomorphic bundles are related to twisted coherent sheaves. This provides a novel differential-geometric interpretation of these objects.

2. Prof. Goto described his recent project of studying deformation theory of generalized complex and Kähler manifolds, which has led to many successes in the search for examples of bi-Hermitian manifolds. A particularly striking result which he emphasized in his talk was that his theory has something

new to say even about deformations of usual complex manifolds. That is, if we consider complex deformations of a Kähler manifold which fix an anti-canonical divisor, then the deformation theory is *unobstructed*. In other words, the celebrated Tian-Todorov lemma which describes deformations of Calabi-Yau manifolds actually applies to any Kahler manifold once we fix an anti-canonical divisor. Goto's more general theorem is a statement about unobstructedness of certain deformations of generalized Kähler manifolds, and it guarantees the existence of many bi-Hermitian structures with non-isomorphic constituent complex structures.

3. The classification of complex surfaces is not yet complete. Prof. Dloussky and Prof. Teleman gave an overview of the state of the art in the classification of surfaces, focusing on the topic of global spherical shells, which come up in the study of class VII surfaces, which are those that remain to be completely classified. Interestingly, there is a relationship between these surfaces and the presence of nontrivial holomorphic gerbes, making an intriguing connection to Hitchin's recent work. In the case of the Hopf surface, for example, which has a global spherical shell, the study of nontrivial holomorphic gerbes is essential in understanding the generalized geometry of the space. We also saw how gauge theory in the guise of Donaldson theory can be used to study the still-open question of classifying these manifolds.

4. Dr. Aldi's talk introduced a mysterious and quite intriguing generalization of the vast topic of vertex operator algebras. His generalization (joint with Heluani) is motivated from the study of T-duality, an operation which forms part of the formalism of generalized geometry. By T-dualizing a torus, he obtains an exotic version of the usual algebra of operators in the conformal field theory associated to the torus, which contains terms in its operator product expansion which are disallowed in the usual theory of vertex operator algebras. These di-logarithmic terms represent a new direction in the subject, motivated from dualities in quantum field theory.

Outcome of the Meeting

We had 41 participants. It was important to us that the participants not only be main researchers in the area, both faculty and postdoctoral, but also graduate students who have taken up the subject in their doctoral work. We were very successful in that respect, with the participation of 8 graduate students from the Universities of British Columbia, Toronto, McGill, California at Berkeley, and Stony Brook. The topics of the conference were directly relevant to the thesis topics of several of those graduate students present, and they were highly motivated by the opportunity to talk with experts in the field. There were also 5 postdoctoral researchers, from the Universities of Toronto, Waterloo, California at Berkeley, and Notre Dame.

We also had the participation of physicists. The origins of Poisson and generalized complex geometry can be traced back to physics, and many of the questions studied in the field are motivated by physics. In fact, two of the talks were given by physicists, Prof. Zabzine and Dr. Aldi. There were many interactions between the mathematicians and the physicists, and at least one collaboration emerged from them, between Prof. Zabzine and Dr. Cabrera.

The workshop, as well as the extended time at BIRS due to the intervening volcano, stimulated a number of collaborations. Those we are aware of are as follows: One began between Profs. Dancer and Tolman after her talk about the symplectic Petrie conjecture. The collaboration between Profs. Karigiannis and Leung was also nourished by the conference. A new collaboration between Profs. Apostolov and Gauduchon concerning generalized Kähler metrics was also begun. Furthermore, collaborations began between Profs. Gualtieri and Bursztyn as well as Profs. Gualtieri and Moraru.

The participants were very enthusiastic about the scientific content of the workshop, as well as the facilities and breathtaking natural setting of BIRS. Moreover, the warm hospitality and professionalism of the staff were very much appreciated, and we would in particular like to thank the Scientific Director and Scientific Coordinator of BIRS for being so helpful and accommodating to European participants stranded in Banff due to the eruptions of Eyjafjallajökull.

Participants

Aldi, Marco (UC Berkeley)
Apostolov, Vestislav (Université du Québec à Montréal)
Arkhipov, Sergey (University of Toronto)
Bailey, Michael (University of Toronto)
Baird, Tom (University of Oxford)
Bartocci, Claudio (University of Genoa)
Brav, Chris (University of Toronto)
Buchweitz, Ragnar-Olaf (University of Toronto Scarborough)
Bursztyn, Henrique (IMPA - Instituto Nacional de Matematica Pura e Aplicada Rio de Janeiro)
Cabrera, Alejandro (IMPA)
Caine, Arlo (Notre Dame University)
Canez, Santiago (University of California, Berkeley)
Cattaneo, Alberto (Zurich University)
Cavalcanti, Gil (Utrecht University)
Dancer, Andrew (University of Oxford)
Dixon, Kael (University of British Columbia)
Dloussky, Georges (Université de Provence)
Gauduchon, Paul (Recherche Centre National de la Recherche Scientifique (CNRS))
Gindi, Steve (Stony Brook University)
Goto, Ryushi (Osaka University)
Gualtieri, Marco (University of Toronto)
Hitchin, Nigel (Oxford University)
Hu, Shengda (University of Waterloo)
Hurtubise, Jacques (McGill University)
Karigiannis, Spiro (University of Waterloo)
Leung, Naichung Conan (Chinese University of Hong Kong)
Li, Travis Songhao (University of Toronto)
Li-Bland, David (University of Toronto)
Mare, Augustin-Liviu (University of Regina)
Meinrenken, Eckhard (University of Toronto)
Moraru, Ruxandra (University of Waterloo)
Poon, Yat-Sun (University of California Riverside)
Pym, Brent (University of Toronto)
Sawon, Justin (Colorado State University)
Sniatycki, Jedrzej (University of Calgary)
Teleman, Andrei (Universite de Provence)
Tolman, Susan (University of Illinois at Urbana-Champaign)
Wade, Aissa (Penn State University)
Witt, Frederik (LMU München)
Wong, Michael Lennox (McGill University)
Zabzine, Maxim (Uppsala University)

Chapter 14

Optimal transportation and applications (10w5025)

Apr 18 - Apr 23, 2010

Organizer(s): Alessio Figalli (The University of Texas at Austin) Yuxin Ge (Universite Paris Est Creteil) Young-Heon Kim (University of British Columbia) Robert McCann (University of Toronto) Neil Trudinger (Australian National University)

Summary

Our meeting took place during a week of many flight cancellations, due to the eruption of a volcano in Iceland. This caused a number of European participants to arrive late and prevented several more — 10 total, including one organizer — from attending at all. Nevertheless, by rearranging the planned activities, a lively and stimulating program was achieved involving the 32 odd participants who managed to attend. In particular, several summaries of striking progress were presented, directions for further research identified, introductions were made, collaborations advanced, and some new ones established.

Background

Optimal mass transportation can be traced back to Gaspard Monge's famous paper of 1781: 'Mémoire sur la théorie des déblais et des remblais'. The problem there is to minimize the cost of transporting a given distribution of mass from one location to another. Since then, it has become a classical subject in probability theory, economics and optimization. Following the seminal discoveries of Brenier in his 1987 paper 'Décomposition polaire et réarrangement monotone des champs de vecteurs' [6], optimal transportation has received much renewed attention in the last 20 years. It has become an increasingly common and powerful tool, at the interface between partial differential equations, fluid mechanics, geometry, probability theory, and functional analysis. At the same time, it has lead to significant developments in applied mathematics, including for instance in economics, biology, meteorology, design, and image processing.

Regularity of optimal transportation, fully nonlinear partial differential equations, and Riemannian geometry

The smoothness of optimal transport maps is an important issue in transportation theory since it gives information about qualitative behavior of the map, as well as simplifying computations and algorithms in numerical and theoretical implementations. Thanks to the results of Brenier [6, 7] and McCann [31], it is well known that the potential function of the map satisfies a Monge-Ampère type equation, an important fully nonlinear second order elliptic PDE arising in differential geometry. In the case of the quadratic cost function in Euclidean space, pioneering papers in this field are due to Delanoë [3], Caffarelli [8, 9, 7, 11], and Urbas [86]. More recently, Ma, Trudinger and Wang [69, 84] (see also [83]) discovered a mysterious analytical condition, now called the Ma-Trudinger-Wang condition (or simply MTW condition) to prove regularity estimates for general cost functions. Costs functions which satisfy such a condition are called regular. At this point, Loeper [6] gave a geometric description of this regularity condition, and he proved that the distance squared on the sphere is a uniformly regular cost, giving the first non-trivial example on curved manifolds. The Ma-Trudinger-Wang tensor is reinterpreted by Kim-McCann [52] in an intrinsic way, and they show that it can be identified as the sectional curvature tensor on the product manifold equipped with a pseudo-Riemannian metric with signature (n, n). Also, recent results of Loeper-Villani [61] and Figalli-Rifford [40] show that the regularity condition on the square distance of a Riemannian manifold implies geometric results, like the convexity of the cut-loci. Developments discussed at the workshop highlighted many fruitful interactions between analysis and geometry around optimal transportation.

Geometry of the space of probability measures, and it applications to geometric inequalities and nonlinear diffusion

Links from optimal transport to geometric analysis, including to the theory of Ricci curvature and Ricci flow, take their origin in the work of Otto and Villani [74], and have received even more attention after the recent works of Lott and Villani [61], Sturm [80, 81], McCann and Topping [68]. The possibility to define useful analogs of such concepts in a metric measure space setting has been a tantalizing goal, only partly realized so far. Still this progress, together with the original contribution due to Otto [73] on the formal Riemannian structure of the Wasserstein space and its application on PDE, is having a strong impact on the research community.

Indeed, on the one hand one exploits that geometric/functional inequalities are related to hidden convexity of appropriate entropy functionals, and thus governs the rate of convergence of the corresponding gradient flows. This framework yields a lot of interesting results, including extensions of (log-)Sobolev inequalities with completely new proofs of the original ones, as well as quantitative study of asymptotic structure of nonlinear diffusion processes, including the porous-medium equations and fast diffusion equations. There are a lot of literature in this direction: see, e.g., the references in [1, 10, 11].

On the other hand, optimal transportation has also provided a new and simpler way to establish sharp geometric inequalities like the isoperimetric theorem, optimal Sobolev inequalities and optimal Gagliardo-Nirenberg inequalities: see e.g., [74, 10, 11, 2, 3]. More recently, Figalli, Maggi and Pratelli [39] were able to exploit Gromov's proof of the anisotropic isoperimetric inequality via optimal transport to prove a sharp quantitative version of the Wulff inequality. This result shows that optimal transportation's proofs of functional inequalities, apart from being generally very short and elegant, are also very stable and can be used to get improved versions of the original inequality, see also for instance [38].

Application to economics, meteorology, design problems, image processing,

There are numerous applications of optimal transport, among which we concentrate on economics, meteorology, and design problems.

Economics

Mass transportation duality is useful in formulating the problem of existence, uniqueness and purity for equilibrium in hedonic models. Recent works of Ekeland [29, 30], Chiappori, McCann and Nesheim [16] have shown that optimal transportation techniques are powerful tools for the analysis of matching problems and hedonic equilibria. Work of Rochet and Choné [78] and Carlier [15] also exposed applications to the principal agent problem – a central paradigm in microeconomic theory, which models the optimal decision problem facing a monopolist whose must act based on statistical information about her clients. Although existence has generally been established in such models, characterization of the solutions, including uniqueness, smoothness, and comparative statics remain pressing open questions. Transportation theory has a wide range of further potential applications in econometrics, urban economics, adverse selection problems and nonlinear pricing. These were highlighted in a talk of Robert McCann concerning recent work with Figalli and Kim.

Geophysical dynamics

Geophysical dynamics seeks to understand the evolution of the atmosphere and oceans, which is fundamental to weather and climate prediction. It has been shown by Cullen and his collaborators that mass transportation theory can be applied to fluid dynamical problems, for instance those governing the large-scale behaviour of the atmosphere and oceans (see e.g., [21]). Here discontinuous solutions find important applications as models for atmospheric fronts, where the point is to analyze the geometry and dynamics of the discontinuity. The theory can also be given a geometrical interpretation, which has led to important ex- tensions in its applicability, and can be used to investigate the qualitative impact of geographical formations, such as mountain ranges. A related open problem to which mass transportation is relevant is the incorporation moisture and thermodynamics into the dry dynamics, to model, e.g., rainstorms. Since Cullen was one of the researchers who participation was prevented by the volcanic eruption in Iceland, his collaborator Mikhail Feldman gave beautiful survey of mathematical developments surrounding the semigeostrophic theory.

Engineering design

Mass transportation theory has a number of promising applications in engineering design – ranging from the construction of reflector antennas or shapes which minimize wind resistance, to problems in computer vision. Oliker [72] and X-J Wang [90] have pioneered the use of transportation theory in reflector design, while Plakhov has been exploring novel applications in aerodynamics, see e.g., [76, 77]. Image registration offers medical applications, in which the goal is establish a common geometric reference frame between two or more diagnostic images captured at different times. Based on the mass transportation theory, Tannenbaum and his group developed powerful algorithms for computing elastic registration and warping maps: see e.g., [4, 49, 28].

Open Problems and Progresses

When studying regularity of optimal maps, one of the major open problems is to find extensive classes of cost functions and domains where the MTW condition holds. In relation to geometry, the Riemannian distance squared cost on a manifold may be the most natural case to consider. In this direction, so far the list of manifolds where MTW is satisfied, includes tori, C^4-perturbations of the round sphere, and Riemannian products and submersions of the round sphere: see e.g., [6, 54, 61, 40, 13]. An important open problem is to relate a local geometric Riemannian curvature condition to MTW condition which is global in nature – but the relevant data are concentrated along geodesic paths. For example, can an estimate on the derivative of the sectional curvature imply MTW condition? Some partial results in this direction have been provided by [13, 42, 26]. Another angle is to understand what geometric restrictions the MTW condition gives. So far progress has been made regarding convexity of tangent cut loci in [61, 40, 41, 42, 43, 44].

Establishing regularity of optimal maps for a cost satisfying MTW condition is a separate issue. Continuity of optimal maps with bounded transported mass distributions are now known on the manifolds satisfying the strong MTW condition due to the results in [6, 54, 63, 61, 40, 44], while the higher regularity of optimal maps for more regular mass distributions is still open for perturbation cases (though, there are some partial results [12, 61, 13]). There has been also progress in related problem, called reflector antenna in the works [90, 48, 91, 69, 13, 6, 50]: especially, in [50] it is identified the range of regions where regularity holds for general data. For a degenerate MTW condition, where the analysis is more subtle due to lack of strong local estimates, a global higher regularity is known [84] on domains in $\mathbf{R}^n$. For continuity with rough data, there has been a substantial progress in [34, 36] assuming a slightly stronger but still degenerate version of MTW condition, so-called nonnegative cross-curvature. The higher regularity in [34, 36] uses recently found interior a priori estimates of [65] (see also [64]). The work [36] on multiple products of spheres is the first time higher regularity is obtained on non-flat manifold satisfying only degenerate MTW condition. For general degenerate MTW case, continuity with rough data and interior regularity remain open.

A wide open problem of regularity theory is to understand the nature of discontinuity/singularity set of optimal maps when the MTW condition is not satisfied, e.g., the distance squared cost on negatively curved Riemannian manifolds. As Villani asked in his book [11], does such set have nice geometry or does it show fractal nature? Partial results in this direction have been recently proved in [31, 33], but a complete answer to this problem is still missing.

As (quite surplisingly) shown by the recent work in [35], a variant of the MTW condition naturally arises in the principal agent problem in multi-dimensional setting. More precisely, the authors identify a structural condition on the value $b(x, y)$ of product type y to agent type x – and on the principal's costs $c(y)$ – which is necessary and sufficient for reducing the profit maximization problem faced by the principal to a convex program. This is a key step toward making the principal's problem theoretically and computationally tractable; in particular, it allows us to derive uniqueness and stability of the principal's optimum strategy – and similarly of the strategy maximizing the expected welfare of the agents when the principal's profitability is constrained. This fact shows how the MTW condition plays a key role as a structural condition in principal agent problem, and it is likely that this fact could be useful in the future also in other problems coming from economics.

New applications for optimal transport are also appearing in statistical mechanics. The recent work described by Sei [79] concerned applications to directional statistics, and showed that a convex combination of optimal transport plans on a sphere gives a way to construct a family of probability distributions. Moreover, the the work in [36] allows Sei's result to be generalized to multiple products of spheres. Let us also observe that, since the state of a spin system is classically modeled as a point in the phase space obtained by taking many products of spheres, one may expect that optimal transportation will prove useful to estimate rates of decay for correlations in other models from statistical mechanics, with the goal of establishing phase transitions. The hope is that, in contrast with current methods that take advantage of the specific structure of models, convexity methods will be robust under small changes to the model.

Other important open problems arise in the contest of the theory of Lott-Villani [61] and Sturm [80, 81] of metric-measure spaces with Ricci curvature bounded from below. Indeed, still the theory presents many open problem, as the recent work of Bacher and Sturm shows (see also the discussion on the talk of Sturm below): indeed, the authors introduce a new curvature-dimension condition which is more flexible than the original one introduced by Sturm, and allows to obtain much more general result (at least at the moment) with the drawback of producing slightly worse constants in some inequalities. So, it becomes natural now to try to understand which is the right condition to consider on metric spaces (note that the two conditions coincide on Riemannian manifolds). Another important question concerns the study of gradient flows in these class of metric spaces. As shown by Gigli [45], the heat flow on a metric space with Ricci curvature bounded from below exists and is unique. However, questions concerning stability and long-time asymptotics are widely open.

Presentation Highlights

Theoretical aspects of optimal transportation

Regularity of optimal transportation, nonlinear PDE, and related geometry.

A number of speakers discussed topics concerning the Ma, Trudinger and Wang conditions for regularity of optimal transportations and fully nonlinear elliptic Hessian equations.

Jiakun Liu presented his joint work [65] with Xu-Jia Wang and Neil Trudinger on the continuity of second derivatives of solutions to the Monge-Ampère type equations arising in optimal transportation. His result includes Hölder and more general continuity estimates for second derivatives, when the inhomogeneous term in the equation is Hölder and Dini continuous, together with corresponding regularity results for the potentials in optimal transportation.

Ludovic Rifford discussed joint work [44] with Alessio Figalli and Cédric Villani on the regularity of optimal transport maps associated with quadratic costs on Riemannian manifolds. He gave necessary and sufficient conditions related to the so-called Ma-Trudinger-Wang and extended Ma-Trudinger-Wang conditions, with examples and counterexamples.

Micah Warren presented a joint work [55] with Young-Heon Kim and Robert McCann. He introduced a new pseudo-Riemannian metric on the products space of source and target domains of optimal transportation. This metric involves both the mass densities and the cost; it is a conformal perturbation of the metric previously defined by Kim and McCann [52], which gives a geometrization of the condition of Ma, Trudinger and Wang as a curvature condition of the metric. It leads to a new geometrical extremization property of optimal maps. Namely, in the conformally perturbed metric, the graph of the optimal map between two given smooth densities becomes a calibrated maximal Lagrangian rectifiable n-current, thus special Lagrangian in the sense of Hitchin; it has zero mean curvature as an embedded submanifold. This gives an unexpected link between optimal transportation and the more classical problem of finding mass minimizing currents in geometric measure theory. The calibrations which detect these special Lagrangians are pseudo-Riemannian analogues of the special Lagrangian calibrations for Calabi-Yau manifolds.

Simon Brendle talked about his joint work [5] with Micah Warren concerning existence results for minimal Lagrangian graphs. Given two uniformly convex domains in $\mathbf{R}^n$, he showed existence of a diffeomorphism between them, whose graph is a minimal Lagrangian submanifold. This question comes down to a boundary value problem for a fully nonlinear PDE, and is in the similar spirit as the second boundary value problems of Monge-Ampère type equations arising in optimal transportation, and is also related in broader sense to the talk of Micah Warren. Brendle also discussed a similar question for domains in the hyperbolic plane.

Paul Lee discussed transportation costs arising from natural mechanical actions. He reported a joint work with R. McCann [57], where they found a class of costs based on Lagrangian actions, which satisfy the Ma, Trudinger and Wang conditions for regularity of optimal transportation.

Geometry of the space of probability measures

Nicola Gigli discussed heat flow in metric measure spaces [45]. Under the assumption of Ricci curvature bounded from below, he obtained well-posedness of the definition of of the heat flow as the gradient flow of the Entropy with respect to the quadratic Wasserstein distance. In particular, uniqueness is proved.

Karl-Theodor Sturm presented some partial results (joint work with K. Bacher) to open questions concerning the curvature-dimension condition $CD(K;N)$ for metric measure spaces. They introduced a new version $CD^*(K;N)$ (called reduced curvature-dimension condition) of $CD(K;N)$. Like the original condition, on Riemannian manifolds this new condition it is equivalent (roughly speaking) to the conditions "Ricci bounded from below by K" and "dimension bounded from above by N". However, it provides worse constants in functional inequalities than the ones that can be deduced from $CD(K,N)$. On the other hand, it has properties which make it more suitable for many applications. Indeed, it satisfies a local-to-global property: that is, if it holds locally then it is also true globally (a fact not known for $CD(K,N)$). Moreover, it satisfies a tensorization property, which allows to deduce $CD(K;N)$ for metric cones and suspensions, under suitable assumptions on the basis. As an application of these results, they can prove finiteness of the fundamental group of any metric measure space $(M;d;m)$ which satisfies $CD(K;N)$ locally with positive K and finite N.

Asuka Takatsu reported a joint work with Shin-ichi Ohta [71] on an extension of the notion of displacement convexity to a more general entropy functional, called the Tsallis entropy. This convexity induces new examples of measure concentration.

Gershon Wolansky presented his investigation [92] of a link between optimal transformations obtained by different Lagrangian actions on Riemannian manifolds. In particular, he explained how the 1-Wasserstein metric arises as a limit of the p-Wasserstein distance W_p between two small perturbations of a suitably chosen reference measure μ: for any non-negative measures λ^+, λ^- of equal mass

$$W_1(\lambda^-,\lambda^+) = \lim_{\epsilon\to 0} \epsilon^{-1} \inf_{\mu} W_p(\mu+\epsilon\lambda^-, \mu+\epsilon\lambda^+),$$

where the infimum is over the set of probability measures μ on the ambient space M. He used a version of this limit theorem as the foundation for a series of developments concerning optimal network theory.

Extensions of the notion of optimal transportation

A couple of speakers discussed how to extend the notion of optimal transportation.

First, Brendan Pass talked about his result [75] on multi-marginal optimal transportation where the goal is to minimize matching of multiple (more than two) mass distributions. To study the local structure of the optimal plan in this multi-marginal setting, he used a family of semi-Riemannian metrics derived from the mixed, second order partials derivatives of the cost function, which is a reminiscence of the metric of [52], to provide upper bounds on the dimension of the support of the optimal measure.

Qinglan Xia discussed the ramified optimal transportation which he has been developing in a series of papers since 2003: see e.g., [93, 95] . Here, he allows more flexible geometry for each path of the transportation plan. Namely, each such path is allowed to branch out, while each branching point contributes some weight in the transportation cost. This theory has many nice applications. In particular, he successfully modeled the formation of a tree leaf for various tree types [94]. In his talk, he connected his theory to another variational problem: p-harmonic maps on graphs.

Application of optimal transportation:

There were talks concerning various applications of optimal transportation.

Chris Budd showed how optimal transport ideas can be used to generate a mesh suitable for discretize time-dependent partial differential equations. The point is that the mesh should also evolve to capture the change of the underlying structure so that the computations are efficient, accurate and reliable. The meshes are constructed by optimally transporting a reference mesh according to a metric dictated by the solution of the underlying PDE. He showed how this procedure is applied to a series of problems, including the formation of tropical storms in meteorological systems.

Mikhail Feldman discussed a model in geophysical dynamics (e.g. meteorology) called semi-geostrophic system. He presented his recent work with A. Tudorascu showing rigorously energy conservation property for weak Lagrangian solutions to this system. Though formally well-known, finding solutions which respect conservation of energy is both important and delicate.

Wilfrid Gangbo reported a joint work with Alessio Figalli and Turkay Yolcu [32], where they extend De Giorgi's interpolation method to a class of parabolic equations which are not gradient flows but possess an entropy functional and an underlying Lagrangian. The new fact in the study is that not only the Lagrangian may depend on spatial variables, but it does not induce a metric. Assuming the initial condition to be a density function, not necessarily smooth, but solely of bounded first moments and finite "entropy", they could use a variational scheme to discretize the equation in time and construct approximate solutions (this scheme is analogous to the minimizing movement scheme introduced by De Giorgi to construct gradient flows in metric spaces). Then, De Giorgi's interpolation method turns out to be a powerful tool for proving convergence of the algorithm. Finally, they show uniqueness and stability in L^1 of their solutions.

Robert McCann described recent work with A. Figalli and Y.-H. Kim [35] on the principal agent problem in multi-dimensional setting. He showed that some Ma-Truginder-Wang type conditions give a general structural conditions on the value $b(X, Y)$ of product X to buyer Y, and on monopolists cost $c(X)$ of producing X, which reduce the relevant minimizing problem to a convex program in a Banach space– leading to uniqueness and stability results for its solution, confirming robustness of certain economic phenomena observed in previous researches. This results extends the special cases when either in 1 dimension or $b(X, Y)$ is linear, to a much general class of situations.

Quentin Merigot [70] explained topological inference problem, which addresses the question of recovering the topology (eg. homotopy type) of a compact subset K of $\mathbf{R}^d$ using approximation by a discrete set. In his work, he defined a notion of distance function to a probability measure on $\mathbf{R}^d$ whose sub-level sets can be used to associate a geometry and topology to the measure. This function has a Lipschitz-dependence on the measure with respect to the quadratic Wasserstein distance, and can be used to obtain topological reconstruction results in the presence of noise.

Garry Newsam reviewed two practical issues in transport problems: The first is the issue of appropriate function space settings for objects such as images and whether the penalty functions used to distinguish specific transportations / registrations from the class of all possible maps are consistent with these settings. The second is the opportunity to match theory to data opened up by new massive data records on real transportation flows, such as those on maritime cargo traffic provided by signals from the Automatic Identification System (AIS) transmitters now carried by all ships.

Tomanari Sei explained two topics on statistics which relate to the optimal transportation theory [79].

One is directional statistics, where convex combination of optimal transport plans on a manifold gives a way to construct a family of probability distributions on the manifold. The mathematical method behind is closely related to the talk of McCann [35]. Another topic is on information geometry, where he discussed the dual structure of a cost function, called divergence in statistics.

Results in other related areas

Maria Gualdani reported on a mean field model arising in price formation. Her result on this free boundary problem uses tools from non-interacting stochastic particle systems and multiscale analysis.

Amir Moradifam discussed the regularity issue of biharmonic equation of the form $\Delta^2 u = \frac{\lambda}{(1-u)^2}$, which is originated from the theory of Micro-Electro-Mechanical Systems (MEMS). He demonstrated that the regularity depends on the dimension, with a proof is based on certain improved Hardy-Rellich inequalities.

Shawn Xianfu Wang addressed an issue in convex analysis, describing how the proximal average method can be used to find the least norm minimizers of a convex function and its Fenchel conjugate.

Ramon Zaraté presented results from his thesis, on how to apply variational method to finding the unknown nonlinearity of given partial differential equations, ranging from equations of Euler-Lagrange type to parabolic equations.

Outcome of the Meeting

It was unfortunate that airport closures due to volcanic eruptions in Iceland prevented several European participants — many of them distinguished scientists — from attending. These included: Stefano Bianchini, Guillaume Carlier, Mike Cullen, Luigi de Pascale, Yuxin Ge, Peter Topping, Alexander Plakhov, Max von Renesse, and Cédric Villani.

However, those who were in attendance rose to the occasion and filled the breach admirably. Indeed, the workshop succeeded in addressing many of the most important research directions in optimal transportation theory in spite of these absences, through talks that included those of Gigli, Feldman, Liu, McCann, Rifford, Sturm and Warren. Other such as Brendle and Gualdani gave lucid and stimulating lectures on complementary topics. There was a high level of participation by young people, including graduate students, recent postdoctoral fellows, minorities and women, who benefitted from a relaxed schedule allowing additional time for interactions with researchers both senior and junior.

This workshop brought together researchers from a range of different fields with common interests in subjects related to the mathematics of optimal transportation, both theoretical and practical aspects. It showcased recent progress and set the stage for future developments, while stimulating new collaborations, new questions, and new lines of research. By making these connections, we believe that the meeting has accelerated the rate of progress within mathematics and in the transfer and application of mathematical techniques between mathematics and adjacent areas of science, including economics and statistics. Its lasting impact will be reflected in research directions which grow from the interactions which were catalyzed here.

Participants

Brendle, Simon (Stanford University)
Chen, Shibing (University of Toronto)
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Figalli, Alessio (The University of Texas at Austin)
Gallouet, Thomas ('Ecole Normale Sup'erieure de Lyon)
Gangbo, Wilfrid (Georgia Institute of Technology)
Gigli, Nicola (University of Nice)
Gualdani, Maria (University of Texas at Austin)
Indrei, Emanuel (University of Texas at Austin)
Kim, Young-Heon (University of British Columbia)
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Liu, Jiakun (Australian National University)

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Sturm, Karl-Theodor (University of Bonn)
Takatsu, Asuka (Tohoku University)
Trudinger, Neil (Australian National University)
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Chapter 15

Character Varieties in the Geometry and Topology of Low-dimensional Manifolds (10w5094)

Apr 25 - Apr 30, 2010

Organizer(s): Alan Reid (University of Texas at Austin), Steve Boyer (Universite du Quebec a Montreal), Dick Canary (University of Michigan), William Goldman (University of Maryland)

Overview and Introduction

The workshop (the first of its kind) brought together researchers who use character variety methods and related techniques to study the geometry and topology of low-dimensional manifolds.

We briefly recall some background. Suppose that H is a finitely generated group and G a real or complex algebraic Lie group. The set of representations of H in G, denoted $R_G(H)$, can be given the structure of a real or complex algebraic set called the *G-representation variety of H*. In addition, the algebro-geometric quotient of $R_G(H)$ by G determines an algebraic set $X_G(H)$ called the *G-character variety of H*.

The main areas that were focused on were:

- Teichmüller theory and connections to the $SL(2, \mathbf{C})$- character variety of a surface group;
- surface group representations with more general Lie groups G as targets;
- applications of the $SL(2, \mathbf{C})$-character variety to the study of bounded 3-manifolds;
- connections between $SU(2)$ character varieties, gauge theory, and 3-manifold topology;
- the role of the character varieties in deformations of geometric structures.

Rather than having a specific set of open problems to focus on, one of the motivating goals of the workshop was to foster a better understanding of the different aspects of the character variety as well exposing both junior and senior people to the panorama of mathematics that exists in the study of character varieties in connection with the topics mentioned above.

Recent Developments

Let G be $SL(2, \mathbf{R})$ or $SL(2, \mathbf{C})$ and let H be the fundamental group of a compact, orientable, hyperbolizable 3-manifold M with incompressible boundary containing a closed orientable surface Σ of genus at least 2. When $M = \Sigma \times I$, H is a surface group and $X_G(H)$ has been of central importance in the study of the geometry of M and Σ over many decades. Discrete embeddings of H in G correspond to hyperbolic structures and display remarkable flexibility. These ideas, which form a part of Teichmuller theory, were subsequently vital to Thurston's work on geometrization of 3-manifolds. The last few years have seen spectacular developments in our understanding of the topology of the general M, such as the solutions of the Tameness Conjecture (by Agol, and independently Calegari-Gabai) and of the Ending Lamination Conjecture (by Brock-Canary-Minsky). This work leads to a classification of hyperbolic manifolds homotopy equivalent to M which, in turn, gives a better understanding of part of the $SL(2, \mathbf{C})$-character varieties of these groups H. Other recent developments regarding the $SL(2, \mathbf{C})$-character variety can be found in the proofs of the orbifold theorem by Boileau-Leeb-Porti and Cooper-Hodgson-Kerckhoff. We were fortunate in that Brock, Canary, Hodgson, Kerckhoff Minsky and Porti all attended the workshop (Boileau unfortunately had to cancel at the last minute because of disruption to air travel caused by a volcanic eruption).

For groups G more complicated than $SL(2, \mathbf{C})$, the G-character variety of Σ also has special properties, such as components corresponding to the Hitchin-Labourie-Fock-Goncharov "higher Teichmuller spaces". These representations correspond to more general geometric structures, such as real projective structures. There has been a lot of recent work in this area, and one of the leaders in the field (A. Wienhard) attended the meeting.

Next let $G = SL(2, \mathbf{C})$ and suppose H is the fundamental group of a non-compact, orientable, finite volume hyperbolic 3-manifold. Embedded, incompressible, non-boundary-parallel surfaces in compact 3-manifolds are one of the most important structural tools in 3-manifold topology. However, producing such surfaces remains an elusive problem. The seminal work of Culler and Shalen on the $SL(2, \mathbf{C})$-character variety of such groups yields a general method of producing them, and in particular, ones with non-empty boundary. Their work remains one of the few general methods for constructing such surfaces. This subsequently led to the notion of the A-polynomial, a powerful invariant of a knot.

Culler and Shalen as well as several other of the main people who were at the forefront of these developments attended.

Presentation Highlights

The organizers selected five participants to each give 2 lectures. These reflected the main themes of the workshop and had both an introductory part as well as a discussion of more recent developments. These were:

Hans Boden: *Connections between $SU(2)$ character varieties, gauge theory, and 3-manifold topology.*

Ken Bromberg: *Teichmuller theory and the character variety.*

Daryl Cooper: *The role of the character variety in deformations of geometric structures.*

Peter Shalen: *The character variety and the topology of 3-dimensional manifolds.*

Anna Wienhard: *Surface group representations in Lie groups.*

As well as these lectures, there were lectures by both junior and senior people that illustrated recent developments in the various fields. The senior people giving talks were:

Tsachik Gelander (*On the dynamics of $Aut(F_n)$ on character varieties*), Ursula Hamenstadt (*Bounded cohomology: Its construction and use*), Yair Minsky (*Primitive stability and the action of $Out(F_n)$ on character varieties*) and Joan Porti (*Regenerating hyperbolic cone 3-manifolds from dimension 2*).

Junior people giving talks were:

Shinpei Baba (2π-*graftings on complex projective structures*), Melissa Macasieb (*On character varieties of 2-bridge knot groups*), Aaron Magid (*Local connectivity of deformation spaces of Kleinian groups*), Stephan Tillmann (*Representations of closed 3-manifold groups*)

Some particular highlights of the lectures were Wienhard's lectures that described recent work on giving a geometric interpretation to representations in the Hitchin component for $SL(4, \mathbf{R})$ that generalizes work of Goldman in the case of $SL(3, \mathbf{R})$.

Other highlights include the lectures of Gelander and Minsky that discussed the dynamics of the action of $Aut(F_n)$ and $Out(F_n)$ on $X(F_n)$. In particular, Minsky described his work on the existence of an open subset of $X(F_n)$ that properly contains the so-called Schottky characters which is $Out(F_n)$ invariant, and on which $Out(F_n)$ acts properly discontinuously.

Scientific Progress Made

The meeting proved to be a fertile ground for people from a variety of backgrounds who study the character variety. Many of the attendee's are now involved in some way, as part of a proposed Research Network in Topology, Geometry, and Dynamics of Character Varieties submitted to NSF.

Participants

Baba, Shinpei (Bonn University)
Biringer, Ian (Yale University)
Boden, Hans (McMaster University)
Boyer, Steve (Universite du Quebec a Montreal)
Brock, Jeffrey (Brown University)
Bromberg, Kenneth (University of Utah)
Canary, Dick (University of Michigan)
Cavendish, Will (Princeton University)
Charette, Virginie (Universite de Sherbrooke)
Chesebro, Eric (University of Montana)
Cooper, Daryl (University of California Santa Barbara)
Culler, Marc (University of Illinois, Chicago)
DeBlois, Jason (University of Illionis at Chicago)
Do, Norman (McGill University)
Dumas, David (University of Illinois at Chicago)
Gelander, Tsachik (Hebrew University)
Goldman, William (University of Maryland)
Hamenstaedt, Ursula (UniversitŁt Bonn)
Kent, Richard (Brown University)
Kerckhoff, Steve (Stanford University)
Landes, Emily (University of Texas)
Lawton, Sean (University of Texas-Pan American)
Lecuire, Cyril (Univ. Paul Sabatier)
Lee, Michelle (University of Michigan)
Leininger, Chris (University of Illinois Urbana Champaign)
Long, Darren (University of California, Santa Barbara)
Macasieb, Melissa (University of Maryland)
Magid, Aaron (University of Maryland)
Mattman, Thomas (California State University, Chico)
McShane, Greg (Universite de Grenoble)
Minsky, Yair (Yale University)
Petersen, Kate (Florida State University)
Porti, Joan (Universitat Autonoma de Barcelona)
Reid, Alan (University of Texas at Austin)

Segerman, Henry (University of Texas)
Shalen, Peter (University of Illinois at Chicago)
Sikora, Adam (State University of New York (SUNY) - Buffalo)
Souto, Juan (University of Michigan)
Tan, Ser-Peow (National University of Singapore)
Tillmann, Stephan (University of Queensland)
Walsh, Genevieve (Tufts University)
Wienhard, Anna (Princeton University)

Chapter 16

Creative Writing in Mathematics and Science (10w5057)

May 02 - May 07, 2010

Organizer(s): Marjorie Senechal (Smith College), Florin Diacu (University of Victoria)

May 2, 2012

Introduction

The 4th BIRS workshop of *Creative Writing in Mathematics and Science* brought together 19 mathematicians, scientists, and journalists who actively write about mathematics[1] for a general public. Some of the participants had attended at one or several of the previous workshops, but most of them were new to an event of this kind. They were (in alphabetical order):

- Madhur Anand, an ecology professor at the Univeristy of Guelph,
- Steve Batterson, a mathematics professor and historian of science at Emory University,
- John Bohannon, a freelance science journalist affiliated with Harvard University,
- Wendy Brandts, a biology researcher at the University of Ottawa,
- Sarah Isabel Burgess, a Ph.D. candidate in physics at the University of Toronto,
- Robin Chapman, a psychology professor (emerita) at the University of Wisconsin,
- Barry Cipra, a freelance mathematics writer based in Minneapolis,
- Chandler Davis, a mathematics professor (emeritus) at the University of Toronto,
- Robert Dawson, a mathematics professor at St. Mary's University,
- Florin Diacu, a mathematics professor at the University of Victoria,
- Adam Dickinson, an English professor at Brock University,
- Philip Holmes, a mathematics and engineering professor at Princeton University,
- Gizem Karaali, a mathematics professor at Pomona College,
- Joseph Mazur, a mathematics professor (emeritus) at Marlboro College,
- Siobhan Roberts, a freelance science journalist affiliated with the Institute for Advanced Study in Princeton,
- Mari-Lou Rowley, an English professor at the University of Saskatchewan,
- Marjorie Senechal, a mathematics professor (emerita) at Smith College,

[1] Throughout this report, we use the term "mathematics" inclusively, to encompass the sciences that make heavy use of it.

- Vladimir Tasic, a mathematics professor at the University of New Brunswick,
- Dragana Varagic, an actor and art director of April Productions in Toronto.

Objectives

The main goals of the workshop were to continue to expand and encourage the small community of writers actively seeking to engage the larger public in mathematics in a broadly creative way, and to increase the cooperation between BIRS and the Banff Center's Writing and Publishing program, to the benefit of both. Since this is the longest direct collaboration BIRS has established with the Banff Centre for the Arts, we aimed to further strengthen the ties.

The sound achievements of previous BIRS/Banff workshops include, in addition to publications of individual participants, the well-attended public reading in Max Bell Hall in June 2006, and playwright Ellen Maddow's math-laced music comedy "Delicious Rivers," written in collaboration with Marjorie Senechal and performed at La Mama Cafe in New York and at Smith College in 2006. The writing of twenty past workshop participants is showcased in *The Shape of Content*, an anthology of creative writing in mathematics edited by the three co-organizers of the third workshop (Marjorie Senechal, Jan Zwicky, and Chandler Davis) and published by A.K. Peters Ltd. in November, 2008. The current workshop aimed to match or exceed the success of these past achievements.

Workshop Presentations

Each participant in this workshop made a presentation to be critiqued by all the others. The atmosphere was collegial. Each participant received constructive feedback about his/her work and learned from the other critiques as well. These brainstorming sessions matched the spirit of any mathematics workshop held at BIRS.

Madhur Anand, a published poet, presented 10 poems from her first book-length poetry manuscript-in-progress. These poems contain scientific ideas and concepts to varying degrees and in differing manifestations. Ecological objects and systems are used for imagery and to describe narratives that transcend traditional scientific boundaries, in which humans are objective observers of nature to socio-ecological systems, while human stories can find metaphor in ecological histories and be informed by them. In several poems the poet becomes entwined in the narrative through personal experience. The method of inquiry taken in these poems is not unlike those of simulation experiments she conducts in her research in ecological modelling. Some ecological modelling has recently come to be appreciated as a form of experiment. This is particularly true of simulation in which each individual evolves in some computer-generated world according to a set of rules and assumptions as well as parameters that can be manipulated beyond values observed in real data. The poet finds that simulation modelling can lead to realities not originally imagined by the modeler, just as a poem can lead to realities not originally imagined by the poet.

Steve Batterson, known best for his biography of Steven Smale, presented a chapter from a book he is working on about the changes in American mathematics from 1890 to 1913. At the beginning of this period, pure mathematical research barely existed on campuses in the United States; to obtain graduate level training in the subject, American students typically went to Germany. Over the last decade of the nineteenth century, several of these young scholars obtained positions in United States universities. Despite heavy teaching loads, they managed to transplant the European mathematical ethos to their own country, turning out high level research and creating solid graduate programs. By 1913 mathematical research in the United States was self-sustaining and worthy of international respect. Batterson's book focuses on these intellectual pioneers and the cultural and institutional barriers they overcame.

John Bohannon, who is a frequent contributor to *Science*, presented several short movies he has worked on with the actor and film director Isabela Rosellini. Mostly interested in writing scripts, he sought the workshop's advice on several mathematical and science ideas he is considering.

Wendy Brandts's fiction involves science in two ways. She uses characters who are mathematicians and scientists, and also uses ideas and metaphors from math and science to convey the thoughts and emotions of her characters. The work she presented at the workshop tries to change the general public perception, which sees mathematicians and scientists as nerdy, crazy, or sociopathic. She aims to present us as we really are: people with feelings, but who try to make a difference through their research and teaching. Her manuscript also tries to deepen the understanding of the arrow of time, with the help of a character who has researched that area.

Sarah Isabel Burges presented three poems. The first two are extended sequences based on recollections from her childhood. They focus on her first experiences of "scientific wonder," the fascination with the natural world that led her to become a scientist, and which keeps her in science. The third poem explores her experiences of the relationship and tensions between religion and science, and offers a view of scientific practice as an expression of reverence for the natural world.

Robin Chapman has published several highly acclaimed books of poetry. She presented several poems from a manuscript-in-progress, *The Eelgrass Meadow*. These poems deal with the philosophy of knowing, the science of seeing, and the evolution of the planet and its species.

Barry Cipra presented a short story written—literally—on a Möbius strip (see Figure 16.1). The idea was to experiment with integrating the mathematical properties of the Möbius strip into the structure of a story. The Möbius strip's endlessly looping nature and the twist that turns the surface's two sides into one suggested, to him, a story about an ongoing love/hate relationship, with no beginning, no middle, and no end, that switches points of view back and forth between the two narrators. This form is also an experiment in the kinesthetic experience of reading: "scrolling" a Mobius strip is a novel tactile sensation that surely influences the reader's reaction to what's written on it.

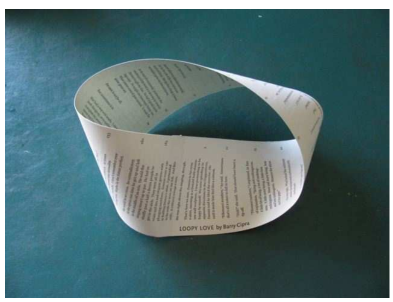

Figure 16.1: A story without beginning or ending, written on a Möbius strip

Chandler Davis, better known for his science-fiction writing, presented experiments in mathematics and music. The musical score in Figure 16.2, for instance, is based on a mathematical rule. Davis explained in his written piece how this and several other musical pieces work, and played the tunes for us on a piano in the lounge.

Robert Dawson presented a short story initially entitled "The Exam" (the much stronger name "Final Exam" was suggested in the workshop, and he adopted it.) A professor, bitter about the attitudes and behaviour of some of his first year calculus students, sets a more-or-less-impossible final examination (with a twist that is not revealed until the end of the story). The choice of calculus as the subject is not coincidental: outsiders see calculus as obscure and difficult; those familiar with it know its high potential for tricky questions.

Florin Diacu presented a chapter on his book-in-progress on the theory of voting, *Random Democracy*. How fair is our voting system? Are we electing the leaders the majority wants? *Random Democracy* presents examples from everyday life, ranging from sports to politics, and shows how election procedures influence the course of history. An exploration of voting systems used worldwide, *Random Democracy* concludes

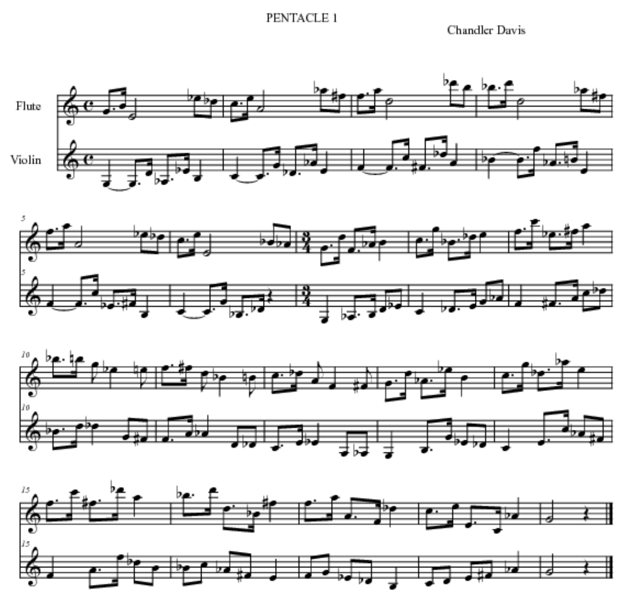

Figure 16.2: The musical score of a pentacle piece composed with the help of some mathematical rules

that all electoral models distort the voters' message. Fortunately some methods are better than others. The author makes the case for proportional representation methods (in particular the single transferable vote), which—though far from perfect—reflect peoples wishes better than other models.

The project Adam Dickinson was working on for BIRS is part of a book-length poetry manuscript about plastic and plasticity entitled *The Polymers*. Polymers are biologically ubiquitous; and plastic, as a cultural and industrial commodity, is similarly omnipresent. This marks a curious contradictory tension: plastic is at once banal and futuristic, colloquial and scientific, a polluting substance that is also intimately associated with our lives—including our thoughts, given that the brain's polymer structure makes possible conceptual "plasticity." The origins of plastic, as an industrial material, have extended and continue to extend out of attempts to mimic or substitute for materials in the natural world. Dickinson juxtaposes distant and differing contexts of behaviour and meaning in order to underscore the chains (and repeated units) of unexpected associations that inform contemporary cultural practices and assumptions. His poems employ the discourses and techniques of polymer science as an alternate way of reading the "giant molecules" of cultural formations (memes, styles, ideologies) that might be said to characterize the global plastic of human behaviour.

Phil Holmes read and discussed two new poems ("Minding one's business" and "Gaps") that use mathematical and scientific findings and language to probe the brain and how it creates the mind, i.e., our notion of ourselves. In the latter an exact mathematical construction of a Cantor set serves as a metaphor for gaps, or absences, of memories that constitutes our sense of self. He also presented a translation of a Hungarian poem for children that plays on a single rhyme repeated with minor variations throughout, to illustrate difficulties in preserving both meaning and form in translation of poetry. More generally, he is interested in parallels and differences between the relations between form and content in science and literature.

Gizem Karaali presented an alternative genesis tale, a brief parable of how the universe got started and how its creator, the nameless goddess who is the main protagonist of the piece, got into mathematics. The story line follows her development into a mathematician, from her point of view, as she meets new challenges and learns to resolve them in satisfactory ways. She creates humans on a whim but then is irrevocably changed by her interactions with them. In particular it is her interactions with the human mathematicians that transform her most. The story follows the nameless goddess in her brief encounters with various mathematicians as they tackle issues of mathematical concern, and see her eventually become more and more enthralled with mathematics itself.

Joseph Mazur's manuscript was an exercise in mixing genres. He usually writes nonfiction. In this piece, however, he crosses the boundaries, blending narrative mathematics with fiction. Poincaré returns to Paris after a 99-year absence, marveling at the changed way of life, and explaining, to his fellow denizens of the Academie the recent solution of his conjecture. In this story Mazur explores good and bad aspects of change and progress in human thought and seeks bridges between distant generations.

Siobhan Roberts read an excerpt from the first chapter of her forthcoming biography of the Princeton University mathematician John Horton Conway. The working title is *Making a Game of Life*, and the book will be published by Walker & Company/Bloomsbury USA circa 2012. In the introductory chapter she seeks to draw the reader into the story and establish the style and pace of her narrative. The chapter revolves around Conway's Free Will Theorem, a motley combination of geometry, physics and philosophy. This theorem serves as a leitmotif throughout the biography.

Mari-Lou Rowley's work as a poet has been inspired by science and the researchers she has interviewed in her science writing career. As the most abstract of all sciences, she finds mathematics the ultimate challenge to write about, both journalistically and creatively. Her current manuscript, *NumenRology*, is based on mathematics and mathematicians; at the workshop, she sought advice from experts. The result, as she claims, "was a true interdisciplinary confluence—the poetry of science and the science of poetry."

Marjorie Senechal presented a 7-page account from the scientific biography she is writing about Dorothy Wrinch (1894–1976), a controversial mathematician/philosopher/protein-chemist/crystallographer. A student of Bertrand Russell, Wrinch was the first woman to receive a D.Sc. from Oxford. (Fittingly, Senechal's book will be published by Oxford University Press.) Wrinch's geometrical model for protein structure (the first ever) catalyzed research in the 1930s on both sides of the Atlantic. But "mathematical biology" had yet to be coined, and she herself was pushed out of the field. The controversy is still discussed by chemists today with much heat but little light. (True, she was her own worst enemy, but so were they all.) To shed real light on this story, Senechal walks in Wrinch's footsteps as well as her own. The 40 papers in applied mathematics and scientific method Wrinch wrote before turning to proteins show where she was coming from. Senechal's presentation dealt with Wrinch's fascination with repeating patterns, and the thread of the story was structured as a repeating pattern.

Vladimir Tasic presented an excerpt from a book he is writing about the French philosopher Alain Badiou. Many consider Badiou to be the greatest living philosopher in France; others think he spouts nonsense. All agree, however, that mathematics plays a central role in his work. He relies on nontrivial results of mathematical logic and category theory; his understanding of sophisticated mathematics and his emphasis on what he calls "mathematical truth-procedures" make him a rarity in contemporary philosophy. At the same time, his system places equal importance on art, especially poetry, and he is rebuilding the common ground that has been damaged by the so-called science wars. Thus, writing a book about him is a multidisciplinary project, which poses the usual problem of boundaries between disciplines.

As a theatre practitioner who plays with mathematical and scientific principles as metaphors in her drama work and teaching, Dragana Varagic presented a play in progress about Mileva Einstein, Albert Eistein's first wife and the mother of his two sons. The play includes ideas from Solomon Marcus's book "Poetica Matematica," originally published in Romanian, the translation of Albrecht Folsing's "Albert Einstein," some material on neurolinguistics, and an ecological model for simple interactions between populations. Varagic keeps a Greek tragedy structure for her piece, but breaks Aristotelian time-space principles, and plays freely with the theatrical notions of time and space.

Breaking Barriers

One highlight of the workshop was a public reading and panel discussion, on the evening of May 5, 2010 at the TransCanada PipeLines Pavilion, called *Breaking Barriers: Writers, Scientists, and Mathematicians in Conversation*. The auditorium was packed, and an internal TV system was needed to accommodate the overflow.

The event, a collaboration between our workshop and the Literary Arts Programme (LAP) at the Banff Centre, consisted of two parts: (1) readings by Don McKay (LAP), Siobhan Roberts, and Adam Dickinson and (2) a panel discussion among Joseph Mazur, Don Mckay (LAP), Philip Holmes, Stephanie Bolster (LAP), and Elena Johnson (LAP). Steven Ross Smith, the director of the Literary Arts Programme, posed general questions and moderated the discussion:

- where do science and literature meet and what are we trying to break?
- are the barriers real?
- do the different languages of mathematics and literature create barriers or provide opportunity?
- is the resultant collaboration or cross-disciplinary thinking creating something else?

At the end, the panel took questions from the floor.

To our pleasant surprise, no one on the panel or in the audience believed there are any barriers at all. Instead, the questions and answers explored the wide and deep relations between C.P. Snow's supposed "two cultures" and encouraged participants in our workshop and the Banff Literary Arts program to keep up their good work.

The success of this event prompted the group of writers-in-residence at the Banff Centre to invite all BIRS participants to an impromptu reading in their lounge on the next evening. About 20 people from both groups read 5-minute excerpts from their published pieces or work-in-progress. Lively group discussions followed the readings.

Conclusions

When the first BIRS creative writing workshop was held, in 2003, writing (plays, poems, fiction, nonfiction) about mathematics was rare. Today, just seven years and four workshops later, mathematics is becoming a popular theme in literature and on the stage. By encouraging mathematicians in their creative writing, and professional writers to adopt mathematical themes, BIRS is playing a catalytic role to influence this growth. The location of BIRS at the Banff Centre also allows a rich exchange of ideas between professional writers-in-residence and BIRS participants in the creative writing workshops.

The 4th BIRS workshop of *Creative Writing in Mathematics and Science* not only succeeded to achieve its goals, but also exceeded the expectations. We believe there is enough material sprouting from this event to plan a new anthology of mathematical writing. One publisher has contacted us already.

We would like to use this opportunity to thank BIRS for the excellent working conditions provided before and during the meeting, for its continuous support, of which we hope to further benefit in the future towards making mathematics understood and appreciated by the general public.

Marjorie Senechal and Florin Diacu

Participants

Anand, Madhur (University of Guelph)
Batterson, Steve (Emory University)
Bohannon, John (Harvard University)
Brandts, Wendy (University of Ottawa)
Burgess, Sarah Isabel (University of Toronto)
Chapman, Robin (University of Wisconsin)
Cipra, Barry (Freelance)
Davis, Chandler (University of Toronto)
Dawson, Robert (St. Mary's University)
Diacu, Florin (University of Victoria)
Dickinson, Adam (Brock University)
Holmes, Philip (Princeton University)
Karaali, Gizem (Pomona College)
Mazur, Joseph (Marlboro College)
Roberts, Siobhan (Institute for Advanced Study)
Rowley, Mari-Lou (University of Saskatchewan)
Senechal, Marjorie (Smith College)
Tasic, Vladimir (University of New Brunswick)
Varagic, Dragana (Freelance, Art. Dir. April Productions)

Chapter 17

Functional Data Analysis: Future Directions (10w5027)

May 02 - May 07, 2010

Organizer(s): Jason Nielsen (Carleton University), Jim Ramsay (McGill University), Jiguo Cao (Simon Fraser University), Fang Yao (University of Toronto)

Overview of the Field

Functional data analysis concerns data providing information about curves, surfaces or anything else varying over a continuum. The continuum is often time, but may also be spatial location, wavelength, probability and etc.

The data may be so accurate that error can be ignored, may be subject to substantial measurement error, or even have a complex indirect relationship to the curve that they define. For example, measurements of the heights of children over a wide range of ages have an error level so small as to be ignorable for many purposes, but daily records of precipitation at a weather station are so variable as to require careful and sophisticated analyses in order to extract something like a mean precipitation curve.

However these curves are estimated, it is the assumption that they are intrinsically smooth that often defines a functional data analysis. In particular, functional data analyses often make use of the information in the slopes and curvatures of curves, as reflected in their derivatives. Plots of first and second derivatives, or plots of second derivative values as functions of first derivative values, may reveal important aspects of the processes generating the data. As a consequence, curve estimation methods designed to yield good derivative estimates can play a critical role in functional data analysis. Regularization is routinely employed to ensure smoothness in a derivative of a specified order, and also to quantify fidelity to a differential equation that may explain a substantial amount of the shape of the curve or surface.

Models for functional data and methods for their analysis may resemble those for conventional multivariate data, including linear and nonlinear regression models, principal components analysis, cluster analysis and most others. But the possibility of using derivative information greatly extends the power of these methods, and also leads to functional models defined by differential equations or dynamic systems, or other types of functional equations.

It has been clear from the beginning that curves and surfaces as data exhibit both phase and amplitude variation, where phase variation refers to the location on the continuous substrate of salient features in the curves. The first clear example of this was the temporal variation in the age of puberty in human growth curves, but subsequently phase variation became evident in many if not most samples of functional data. This has posed severe problems for the use of common descriptive statistics adapted to functional data, such as cross-sectional means, variances and correlations, as well as tools like principal components and regression analysis; all of which are designed to describe only amplitude variation. This bi–stochastic nature of functional data has since been recognized in many other branches of statistics, such as image analysis, shape analysis and tree-structured models.

The term “functional data analysis” was first used by [6], the first monograph was [3], and this was followed by [4] and [5]. [2] has subsequently appeared, and a number of other books are known to be in preparation.

As the workshop title indicates, the focus was less on surveying current and past research, and more on taking stock of where we’ve come, and then looking forward to anticipate the problems that we hope will inspire research in the coming years. We tried to divide the invitees to the workshop roughly evenly between the more senior members in the field who have already done much to define what FDA is today, and the young researchers with the potential to take this field to new places.

BIRS has moved this year to funding half workshops as well as the usual full workshop involving about 40 participants. We, as a half workshop, shared the facilities with another group over the Monday to Friday period of May 3 to 7. Our partner workshop was on Creative Writing in Mathematics and Science, and it would have been hard to choose a companion topic of more importance to the development of statistics. A number of us attended the Thursday evening session of the other workshop, and there was discussion of a more systematic interaction in the future.

Subtracting Wednesday afternoon, which by sacred tradition is given over to exploring the Rocky Mountains, this gave us nine morning/afternoon sessions of roughly three hours each, allowing for break time. We divided each of these in two, making 18 sessions of 1.5 hours each. This format gave us the opportunity to devote much more of the workshop to free unstructured exchanges than is typically the case, as well as making it possible for each of us to present our own work and exchange thoughts on the future of FDA. The amount and quality of the exchange was considered in our final evaluation to be perhaps the most important outcome of the week.

Recent Developments and Open Problems

We structured the week into themes:

- Random functions and inference and prediction
- Software, computational, numerical analysis and publication issues
- Estimating covariance structure, principal components analysis and functional variance components
- Statistical dynamics, both deterministic and stochastic
- Extension to spatial, spatial/temporal and other multidimensional domains
- Joint variation in amplitude and phase, the use of tensor methods
- Functional linear models, and input/output systems in general
- Native and observed coordinate and frame systems
- Applications

We also called attention to the forthcoming SAMSI Program on the Analysis of Object Oriented Data that aims to link functional data analysis, dynamic systems, shape analysis, image analysis and the analysis of tree-structured and other strongly non-Euclidean data. See http://www.samsi.info/programs/2010aoodprogram.shtml for more information.

Presentation Highlights

One of us (Ramsay) offered the following reflections.

When Bernard Silverman and I met in 1992 to write our first book, we knew a number of things. Our perspective on this emerging area would quickly be seen as too narrow. But a useful treatment of a restricted range of topics seemed much preferable to a scattered and disorganized account of everything that might come to mind. Keeping the math simple seemed paramount in order to maximize access to FDA methodology by researchers with data to analyze. Although we did take a functional analytic approach in our own discussions, we knew the danger of even using the term "functional" in the title of the book, and we have heard so many times since that something deserving that qualifier must surely be too deep for ordinary people. As a consequence, we sacrificed depth in both mathematical and statistical terms to accessibility. The subsequent literature has done a fine job of providing much that we might have included and could not have provided due to our own limitations. Some advance was made in the 2005 edition, but much remains to be done.

But the workshop stretched the meaning of FDA far beyond what either of us could have envisaged, and Steve Marron's opening talk on object oriented data analysis was a tour de force of scene-setting in this sense. We learned from both Steve and Hans-Georg Müller that both the domains of functional data models and their range in some function space can have a manifold structure induced by a finite dimensional coordinate or chart system, which may or may not be local, that spans the actual variation in either of these spaces. This point was emphasized further by a number of applications as well as by the excellent discussion of the implications of "phase variation" and of the nature of a functional "feature".

The use of a dynamic system, either as a regularizer of a high-dimensional model, or as a model in its own right, also induces a manifold structure into the function space where the data are modeled. Both the null space of the associated differential operator and the variation in that null space induced by varying the parameters of the system seem important new aspects that we need to consider further. In addition to Hans-Georg's talk, that of Laura Sangalli also addressed directly the issue of how to estimate a manifold in model space. How do we estimate a space curve when there is no domain available except arc length, which of course only is defined by the estimate itself? And this in the presence of noisy data? The talk by Jianhua Huang on estimating the variation in boundaries of particles also seemed to fit into this manifold-structured data and model context.

Not nearly enough discussion was possible of extending the domain of functional data and models beyond one dimension to data distributed over space, space/time, and other multidimensional continua; but this seems surely a big topic for the time that we had available. We need another workshop on this alone, and a number of us are poised to extend FDA into spatial data analysis in the next couple of years.

But even in one-dimensional domains, we had a good deal of useful discussion of alternative measures of time that would be more appropriate to the data. Surjit Ray's presentation of the landsat data especially highlighted this issue. Debashis Paul's talk posed the question of how to work with intervals whose initial or final values are not known. It was recognized, too, that functional data often come as single or a small set of long series of observations having layers of structure, rather than as largish samples of "independent" functional observations, and that methods assuming replications, such as principal components analysis, need revisiting within this context. Simon Bonner's talk further developed this issue.

Bernard and I certainly did not appreciate how central the issue of the "right" coordinate system would become in FDA. Our first inkling of this was the appreciation of the need to estimate "system" time as opposed to clock time as a substrate for growth and weather data. Nevertheless, we too often used off-the-rack coordinate systems, such as orthogonal Cartesian coordinates for the handwriting and juggling data or latitude and longitude for spatial data, even when the data themselves clearly suggested better coordinate axes. Steve's "M-reps" as a boundary-defining method were especially striking. Diffusion-tensor imaging is also a recent approach to defining "intrinsic" coordinates for complex functional data. Triangulation methods using obvious feature-defined locations or cluster centers seems really natural in higher-dimensional settings.

It was inevitable that such a fascinating collection of data objects would inspire many comments on better ways to do functional data analysis. I can't do much better than listing a few of my favorites in point form.

- Neglecting auto-correlation over time or spatial covariation is a dangerous business, and that we did so little about this in both our books and in our software packages is embarrassing. This seems easy to correct, and we have to get at it.
- Methods like principal components analysis are essentially exploratory, and known components of variation such as mean effects, influences of obvious covariates like latitude and so forth, ought to be removed before using PCA and CCA on the residual structure. Otherwise we risk, or even will surely, mask interesting variation by using PCA to do the job that projections and regression methods were meant to do.
- We have to be careful with terminology. "Mean", "variance" and so forth are tightly tied to Hilbert space structures, and will mislead our collaborators when our models and analyses go beyond these frameworks. Marc Genton's talk on displaying curve variation by functional box plots and Ivan Mizera's use of quantile regression seem just what we need in this regard. Finding better terminology might involve collaboration with the creative writing team that shared the BIRS facility with us.
- The issue of adding noise to models comes up every time I talk about dynamic systems. You all know now that this confuses me. I thought models were supposed to simplify the information in data, rather than simulating their complexity. Perhaps everyone should just give up on me.
- Outliers are a fact of life, and Liangliang Wang offered some radiosonde data that sure drove this point home, along with Ivan's emphasis on L1 based methodology. We need to improve our capacity to deal with this in the FDA toolbox.

I dove into the business of setting up an object-oriented FDA software package, first in Matlab and later in S-PLUS and R, with an enthusiasm that only can come with having no idea what one is getting into. Bernard warned me, but I refused to listen. Now I know, but at least I can say that people like Spencer Graves have come to my rescue in my worst moments, as well as those who wrote innumerable emails suggests corrections to errors and needed extensions.

Jason Nielsen's talk provided an exceptional overview of the positives and negatives of R and Matlab as software environments. He helped us all to understand why R is so slow, and how much faster it would run if it could be compiled. I can only say that we should all do a bit of fund-raising to give him the time he needs to finish his R compiler.

I've already mentioned tensor analysis as an essential tool as we get into manifolds and other aspects of differential geometry. How can we help our statistical colleagues to acquire this expertise with minimal effort? This is a question that has an analogue with respect to dynamic systems modeling. I've also mentioned the need to expand the FDA software to permit the modeling of auto- and spatial correlation, a simple task, it would seem.

Spatial and space-time FDA will require a rather more serious effort, but experience shows that there is no way around this task; if software is not readily available, they won't use it. In this respect, we seem stuck with the R environment for a long time to come. Basis function tools were commented on directly or indirectly many times. The use of what are called "empirical orthogonal functions" or "EOF's" in the physical science literature, but principal components by the rest of us, is now standard practice; and in my view a little too standard since it risks throwing away interesting variation. But it's here to stay and I'm extending the packages to allow for bases to be defined by eigenfunctions specifically and any functional data object in general. Also needed is the capacity to combine bases ($+$, $-$, and $*$ operators essentially) to allow for multilevel variation and other things. Jiguo and I [1] offer some tips in our paper on functional linear mixed modeling in the issue of JASA that has just appeared, and this will be in the next package releases. Not mentioned at the workshop but too important to omit here is the fact that Giles Hooker and a couple friends have released an R package CollocInfer for dynamic systems estimation along with a long manual.

Chunming Zhang was almost alone in considering the issue of inference for functional data, but in the balance this seems less surprising now than it did a couple of weeks ago. Inference is based on probability, and dare to question whether what is taught these days in courses on the subject will ever be of much help in this high-dimensional context. Perhaps probability theory is just low dimensional by its nature. How good it would be to be proven wrong about this!

Scientific Progress Made

Although the workshop could only bring together a small set of the rapidly expanding community of researchers and practitioners involved in functional data analysis, it did gather those who were exceptionally effective communicators and facilitators of discussion. Especially appreciated was the facilitation of involvement by new researchers in the discussion and the affirmation of their already significant achievements. The community development contribution of the workshop was therefore exceptional.

Outcome of the Meeting

The workshop will have a substantial impact on the SAMSI year-long project Analysis of Object Oriented Data. Many of the participants will also be involved in the opening SAMSI workshop in Sept. 12-15, 2010, and later on as organizers and researchers in residence.

The potential role of differential geometry in further developments in this field seemed obvious, and to suggest some hard work helping our colleagues to master tools such as tensor analysis. It was hoped that future workshops will bring together applied and pure mathematicians as well as statisticians in order to reflect in more depth on this theme.

The BIRS facility cannot be beat for its ambiance, which ensures delightful, leisurely and thoughtful discussion on a wide range of topics by participants coming to an area from many scientific domains. We particularly appreciated the warm hospitality and constant attention to supporting our work by Brenda Williams and her colleagues that were on site. The dining facilities at BIRS seemed like a week-long banquet, and the proximity of Banff town and Park, with their many opportunities for relaxation and exercise, contributed abundantly to the success of the workshop.

Participants

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Ray, Surajit (Boston University)
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Chapter 18

Inverse Transport Theory and Tomography (10w5063)

May 16 - May 21, 2010

Organizer(s): Plamen Stefanov (Purdue University), Guillaume Bal (Columbia University), Gunther Uhlmann (University of Washington)

Activity Report

This workshop brought together experts in inverse problems with interest in the broadly defined field of transport theory. The workshop balanced research in theoretical and computational inverse transport and in experimental atmospheric science and biomedical imaging with four speakers (and a few more in the audience) coming from the Engineering and Applied Science communities and the rest of the speakers coming from the applied analysis and applied mathematics communities. Some of the main objectives of this workshop was to provide a cohesive summary of the very active research activities performed over the past five years in the field of inverse problems and to identify potential areas of research where collaborations between mathematicians and engineers and both necessary and fruitful.

Integral geometry

Inverse transport theory may be separated broadly into two categories. The first category involves propagation in the absence of scattering and is closely related to the broad field of integral geometry. An important problem consists of inverting attenuated ray transforms as their appear in, e.g., medical and geophysical imaging. Mikko Salo presented recently obtained uniqueness results with Gunther Uhlmann for the attenuated geodesic ray transform of functions and 1-forms on simple 2D Riemannian manifolds with an arbitrary known absorption coefficient. The approach is constructive, as well.

Alexandre Bukhgeim considered the problem of the reconstruction of both the source term and the absorption coefficient in Euclidean geometry using the tools of A-analytic functions that he and collaborators had introduced in the past. This remains an open problem.

Nick Hoell (graduate student) showed explicit reconstruction formulas for the attenuated integral of functions along the integrals of specific vector fields in the analytic category, whereby generalizing earlier results obtained for the hyperbolic geometry.

Sean Holman analyzed the problem of polarization tomography on a Riemannian manifold and generalized to this setting results of generic reconstructions that were obtained by, e.g., Stefanov and Uhlmann, in the setting of the reconstruction of functions from their geodesic ray transform.

Discretization aspects

The above formulas apply in the presence of a continuum of data. The practical problem of reconstructions with sparse and limited data was considered by Matti Lassas. His presentation analyzes the interplay between noise and discretization effects and which numerical algorithms should be used to perform inversions in X-ray tomography and more generally in all linear inverse problems of the form $m = Af + e$ with e random noise.

In the presence of extremely noisy data as they appear in, e.g., detection of low emission radioactive sources, detailed statistical models need to be introduced. Peter Kuchment reported on recent results in the reconstruction of sources whose intensity can be as weak as one part in a thousand of the noise level.

Inverse transport theory

Many important recent results were reported in inverse transport theory when scattering is taken into account. From the theoretical viewpoint, Alexandru Tamasan presented joint results with McDowall and Stefanov about full characterizations of non-uniqueness (gauge equivalence) results in transport theory when the absorption coefficient depends on the velocity variable, with important applications for reconstructions in anisotropic media. A notable result is that the reconstruction of anisotropic absorption coefficients can be made stable on the support of the scattering coefficient and not elsewhere.

Alexandre Jollivet reviewed recent stability analyses of inverse transport reconstructions in the different regimes that appear in applications. Which coefficients may be reconstructed from available data and with which stability properties strongly depends on the available measurements, for instance whether time-dependent measurements or angularly resolved measurements are accessible.

Vadim Markel presented explicit reconstructions formulas when only single scattering is taken into account. Neglecting multiple scattering allows one to obtain stable and explicit reconstructions of the scattering and absorption coefficients in geometries of practical interest.

Numerical aspects of inverse transport

Several presentations reported on recent results in the numerical simulations of forward and inverse transport problems. Although many numerical methods have been proposed to solve transport equations, the solution of inverse transport problems requires specific treatment. A novel forward transport solver based on a few multigrid method with optical molecular imaging applications was presented by Hongkai Zhao.

Nonlinear kinetic models also find important applications of inverse transport theory. The reconstruction of doping profiles in semi-conductors may be accurately described by a Boltzmann-Poisson system of equations. Heuristic arguments then show that the reconstruction of the doping profile is a severely ill-posed problem. Numerical algorithms presented by Kui Ren show that limited of practically useful information can nonetheless be reconstructed from available measurements of current-voltage curves. Moreover, these studies show that less accurate forward descriptions than the Boltzmann-Poisson system such as drift-diffusion models fail to adequately reconstruct this information.

Stability of inverse transport problems as they appear in Jollivéts talk comes from the fact that singularities in the object we wish to reconstruct propagate to the available data. In transport, such singularities are singularities in the angular and spatial variables. It is notoriously difficulty to capture such singularities numerically. Based on a spectrally accurate algorithm to rotate domains of interest, Francois Monard (graduate students) presented a new discretization of the transport equation that allows one to accurately capture all relevant transport singularities and obtain stable numerical reconstructions of the optical parameters in cases of limited amounts of scattering.

Deterministic numerical transport solutions are expensive and have difficulties handling complex geometries. Many solvers have thus been developed to use the probabilistic representation of transport solutions and devise Monte-Carlo statistical algorithms. The main difficulty with such algorithms is their sometimes large variance, which results in expensive numerical simulations to combat statistical noise. Ian Langmore presented recent results of variance reduction techniques based on deterministic adjoint calculations and showed how variance could be significantly reduced in numerical simulations of transport equations as they arise, e.g., in remote sensing.

Large scattering limits and diffusion models

In many applications of forward and inverse transport, the transport mean free path (the main distance between successive interactions of the particles with the underlying medium) is so small that more macroscopic models such as the diffusion equation are more appropriate. Several presentations were devoted to the theoretical and numerical analysis of inverse diffusion problems. A major drawback of inverse diffusion problems of course is their severe ill-posedness. In order to stabilize the reconstructions, either more data need to be acquired or prior information needs to be included. Pedro González presented recent results where diffuse optical tomography (an inverse diffusion problem) can be somewhat stabilized by the acquisition of spectral data, since the absorption and scattering coefficients behave differently as a function of the color (wavelength) of the probing light. His talk gave numerical evidence that spectral information allows us to better distinguish between healthy and non-healthy tissues.

Arnold Kim introduced prior information by assuming a simple two-layer half space geometry of the problem and by reconstructing point-like absorbers from boundary measurements of back-scattered light. Such formulations are useful to devise at which stage cancer development can be detected in epithelial tissues.

Tanja Tarvainen presented the Bayesian method as a versatile statistical mean to introduce prior information into the reconstructions. The framework was then used to incorporate pre-computed errors between the accurate transport model of photon propagation in optical tomography and its diffusion approximation. The methodology allows one to obtain reconstructions with the accuracy of the transport solution at the cost of the much less expensive diffusion model.

Gen Nakamura considered the framework of time-dependent measurements to mitigate the ill-posedness of diffuse optical tomography and in applications of heat diffusion. He presented theoretical and numerical evidence of improvements of reconstructions in this setting.

Theoretical results in connected areas

We have seen that the transport of particles was often modeled using kinetic equations or their diffusive limits. Similar equations are used to model many fields of applied science and share similar difficulties as far as inverse problems are concerned.

One such problem is the inverse spectral problem for weighted Laplacians on Riemannian manifolds with singularities in one of its dimensions leading to n-1 dimensional Riemannian orbifolds. Using the Gromov-Hausdorff metric that is adapted to the reconstruction of geometric objects (defined independent of re-parameterization), Yaroslav Kurylev presented results of stability of the reconstruction of the geometry of such Riemannian manifolds from boundary spectral information.

We have already mentioned that inverse diffusion problems were severely ill-posed. It turns out that singular diffusion tensors may sometimes not be visible from outside measurements, with applications in the cloaking of objects. Since invisibility requires that one constructs un-physical singular conductivities, there has been a lot of recent activity to try and understand how accurate cloaking might be for less singular conductivities as they can be engineered in practice. Hongyu Liu presented recent results on approximate cloaking when wave propagation is no longer necessary a low-frequency approximation of diffusion type but takes the more general form of acoustic and electromagnetic systems of equations.

Such systems of equations are more difficult to analyze mathematically if only because the standard complex geometric solutions of the form $e^{\rho\cdot x}$ with ρ a complex vector are much more involved for systems of equations as they are for scalar equations. Ting Zhou presented results on the use of such complicated complex geometric optics solutions to reconstruct obstacles in a system of Maxwell equations by using the so-called enclosure method.

Applications of inverse transport in biomedical imaging and atmospheric science

Transport of particles finds many applications in medical and geophysical imaging. An important application in medical imaging is optical tomography. Several theoretical and numerical results presented during this workshop have been mentioned already. Andreas Hielscher reported on recent applications of optical tomography in small animal and human imaging. Optical tomography is an important modality as the optical properties of healthy and non-healthy tissues are quite different. Specifically, tumors absorb near infra red light much more so than healthy tissues and may be characterized by detailed reconstructions of oxy- and deoxy-hemoglobin concentrations. The presentation reviewed potential strengths and limitations of the practical implementation of optical tomography and gave examples of applications encountered in clinical and pre-clinical imaging such as monitoring of tumor growth and regression, effects of anti-angiogenic drugs in pediatric cancer treatment, breast cancer screening, and detection of arthritis.

Transport theory is also important in remote sensing as it is applied, e.g., to reconstruct cloud and aerosol properties in the Earth atmosphere. Quantifying their optical properties remains a hard problem in the global climate models used, e.g., to understand global warming. At present, very crude models for the cloud geometry are used in practical implementation. Anthony Davis surveyed in this presentation the recent steps that have been taken toward fully three dimensional atmospheric tomography and covered the analogies that can be made between inverse transport in atmospheric imaging and in medical imaging. A fully integrated three dimensional inverse transport setting in atmospheric tomography is still very much in the making. Once the technical challenge and observational resources are understood, the Earth's particulate atmosphere may inspire new applications for advanced methods in inverse transport theory as well as in physics-based tomography.

PAT and TAT

As was mentioned several times above, optical tomography and more generally inverse transport theory in highly scattering environments is a severely ill-posed problem. This prevents the method to be used as a stand alone imaging technique for human beings when millimeter or sub-millimeter resolution is required. Yet, the good discrimination properties of optical waves provides an important diagnostic for the presence of, e.g., malign tumors. Ultrasound tomography somehow suffers from opposite defects. Healthy and non-healthy tissues display very similar sound speeds at least in early stage tumors. In spite of sub-millimeter resolution capabilities, ultrasounds are therefore difficult to use in this context. Several recent imaging modalities have been proposed recently that aim to combine the good discrimination properties of light with the high resolution capabilities of acoustic waves. One such modality is photo-acoustic tomography (PAT). A similar modality combining microwave radiation (to obtain good discrimination properties) with acoustic waves (to obtain good resolution) is called thermo-acoustic tomography (TAT).

Several experts on PAT, TAT, and ultrasound tomography presented their recent research at the workshop. Lihong Wang is a pioneer in the experimental aspects of PAT and TAT. His group has developed photo-acoustic imaging technologies for in vivo early-cancer detection and functional imaging by physically combining non-ionizing electromagnetic and ultrasonic waves. The hybrid imaging modality provides relatively deep penetration at high ultrasonic resolution and yield speckle-free images with high electromagnetic contrast. With this technique, optical contrast can be used to quantify the concentration of total hemoglobin, the oxygen saturation of hemoglobin, and the concentration of melanin. Melanoma and other tumors have been imaged in vivo in small animals.

Sarah Patch was a pioneer in the development of reconstruction algorithms in TAT. Her talk presented the device used at the university of Wisconsin-Milwaukee to perform TAT experiments and underlined the many difficulties associated with generating non-resonant electromagnetic signal excitations.

Reconstructions in photo-acoustics and thermo-acoustics can be separated into two steps. The first step consists of reconstructing the amount of absorbed radiation by the tissues from measurements of ultrasounds at the boundary of the domain. The latter quantity is, however, a functional of the optical parameters of the tissues, which depends on unknown solutions to a partial differential equation. The second step consists then of reconstructing the optical parameters from the now known absorbed radiation. This second step is called quantitative photo-acoustics. Roger Zemp addressed this issue and presented results of simultaneous reconstructions of both the absorption and the scattering coefficients from knowledge of absorbed radiation corresponding to several illuminations of the sample. Quantitative photo-acoustic is known in some cases to correspond to a well-posed problem (more precisely very mildly ill-posed) unlike optical tomography. This was confirmed by spatially accurate and robust numerical reconstructions.

Most photo-acoustic and thermo-acoustic reconstructions ignore acoustic wave absorption. However, high frequencies are significantly attenuated causing difficulties to achieve sub-millimeter resolution at a depth of several centimeters in human tissues. Otmar Scherzer presented recent results on the modeling of absorption and its impact on thermo-acoustic reconstructions. Absorption modeling is rendered extremely complicated by the fact that different frequencies are attenuated differently. Causality must be preserved, which generates well-recognized difficulties. The talk detailed a specific attenuation law used in other contexts and analyzed its effects on reconstructions in thermo-acoustics.

Although radiation transport is an important step in photo-acoustics, a central step is the reconstruction of amount of absorbed radiation from measured ultrasounds. Mathematically, this takes the form of an inverse wave problem where the initial condition is sought from boundary measurements. This problem belongs to the broad family of inverse source problems which can be tacked by time reversion since the wave propagation solution operator is a unitary operator. Alison Malcolm analyzed the time reversal methodology to address the underground sequestering of CO2 and determine whether changes in the underlying medium (such as cracks) is important or not and possibly reconstruct such changes. More specifically, the shape and frequency of correlations of the coda of multiply scattered waves were exploited to obtain localization of such potential changes.

Where is the field going?

The workshop was successful in bringing together mathematicians, applied scientists and engineers who specialize in the analysis and applications of forward and inverse transport theory. Although many inverse problems remain to be addressed in this broad field, significant, practically relevant, theoretical results have been obtained in recent years. This workshop allowed the participants to obtain an up-to-date cross section of the field. The workshop also presented several applications of inverse transport as they are studied in the applied sciences and engineering disciplines. This generated discussions between the communities represented at the workshop, which was an important organizational objective.

The workshop also helped identify some areas in which mathematical analysis may very well be useful for practitioners. Let us give one such example in the field of photo- and thermo-acoustics. Although the wave inversion problem is well understood for propagation in smoothly varying media with sufficient information at the domain's boundary, significant difficulties arise when the refractive effects of, e.g., the skull are taken into account. Understanding this problem is one of the major roadblocks to brain imaging using thermo-acoustic tomography.

The problem of simultaneously recovery of the absorption and the source in the attenuated X-ray transform remains a challenging open theoretical problem.

Participants

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Chapter 19

Self-Assembly of Block Copolymers: Theoretical Models and Mathematical Challenges (10w5105)

May 23 - May 28, 2010

Organizer(s): Rustum Choksi (Simon Fraser University), Yasumasa Nishiura (Hokkaido University), An-Chang Shi (McMaster University)

Overview of the Field

Block copolymers are macromolecules composed of two or more chemically distinct polymer chains linked together by covalent bonds. The thermodynamical incompatiblility between the different sub-chains drives the system to phase separate. However the covalent bonds between the different sub-chains prevent phase separation at a macroscopic length scale. As a result of these two competing trends, block copolymers undergo phase separation at a nanometer length scale, leading to an amazingly rich array of nanostructures. These structures present tremendous potentials for technological application because they allow for the synthesis of materials with tailored mechanical, electrical and chemical properties (see [1, 8, 11]).

The main challenge of block copolymer self-assembly is to describe and predict the possible nanostructures for a given set of molecular parameters such as the polymer architecture and monomer-monomer interactions. Searching different nanostructures and constructing phase diagrams for block copolymers have been very active research areas in soft matter physics involving physicists, chemists and materials scientists. Due to the virtually endless possibilities of block copolymer architectures, the phase space of the possible nanostructures is formidably large. Therefore theory and simulation are indispensable in the study of block copolymer self-assembly. In particular, theoretical results provide crucial understanding of the formation mechanism of these nanostructures, as well as useful guidance to the synthesis of block copolymers for particular complex nanostructures.

Most of the theoretical studies of block copolymers are based on a framework termed the self-consistent field theory (SCFT) [8]. The SCFT of polymers is a field theoretical representation of the statistical mechanics of polymers. It transforms the formidable task of integrating contributions to the partition function from many-chain interactions to the computation of the contribution of one polymer in a self-consistent field. Efforts from the physics and materials science communities have shown that SCFT is a powerful framework which is capable of describing and predicting the nanostructures of block copolymers ([8, 14, 21]). Specifically, the mean-field equations of SCFT are a set of highly nonlinearly and nonlocally coupled equations, whose solutions can be periodic functions corresponding to ordered three-dimensional structures. The challenge is to finding these solutions without *a priori* knowledge about the phases, which is equivalent to finding solutions of a nonlinear and nonlocal optimization problem. Although great progresses on the SCFT of block copolymers have been made in the last decades, many challenges still remain ([8, 14, 10]). From the perspective of applied mathematics, two of these challenges are the understanding of the mathematical structure of the SCFT equations and the development of efficient computation techniques for complex ordered nanostructures.

To date, most mathematical work has centered on a simple theoretical model of block copolymers, the Ohta-Kawasaki model. Using an expansion in terms of monomer densities, the SCFT of block copolymers can be approximated by a Landau-type free energy functional, as shown by Leibler [6] in 1980. A variation of this expansion was proposed by Ohta and Kawasaki [18], leading to a simple theoretical model for diblock copolymers. As first noted in [17], the Ohta-Kawasaki model gives rise to a nonlocal perturbation of the ubiquitous Cahn-Hilliard problem which has been the generator of an immense body of work in applied math and nonlinear partial differential equations ([7]). However simple, the Ohta-Kawasaki functional has a tremendously rich mathematical structure, and is in fact the natural higher-dimensional analogue of a functional written down by S. Müller [15] as a toy problem to capture multiple scales. It can also simply be viewed as a paradigm for pattern formation induced by short and long-range interactions. The study of its rich energy landscape is central to our understanding of nonconvex and nonlocal variational problems, and it has lead to new mathematics. Examples include a deep and intricate spectral analysis [19]; a novel application of modular functions [5]; a rare two-dimensional result characterizing certain aspects of the ground state [16]; fascinating geometric questions on the relationship to stable constant mean curvature surfaces [20]; the creation of nonlocal extensions to standard second variation inequalities involving the mean curvature [6]; the analysis of rich multiscale variational problems [9]. Furthermore, it has fostered a very general result on the inherent periodicity of minimizers in the presence of long-range interactions [1].

Objectives of the Workshop

Given this rich mathematical progress, it is timely to draw the attention of applied mathematicians to the full self-consistent field theory and other recent developments in the statistical physics of inhomogeneous polymers.

The main objective of this workshop is to bring together for the first time two groups of researchers:

1) applied mathematicians with training in the calculus of variations and nonlinear PDE, scientific computing, applied probability, and with core interests in problems stemming from the material sciences, particularly polymeric materials;

2) physicists and engineers at the forefront of equilibrium models for inhomogeneous polymers, particularly self-assembly of block copolymers, whose work has a substantial mathematical component.

Given the tremendous activities and interests in block copolymer structures, it is important and timely to bring together these two communities, who have, as yet, had only limited interactions. So far, most mathematical work on block copolymer phases has centred on the simplified Ohta-Kawasaki model. These activities have lead to some rich mathematics and will no doubt continue to drive mathematical work in the future. It is therefore natural to extend the activities of applied mathematicians to other underlying equilibrium theories of inhomogeneous polymers. From a scientific point of view, the field theoretical models such as the SCFT have had a massive impact in many areas of physics and engineering. However these models have largely been untouched by applied mathematicians. Given the complex nonlinear and nonlocal structure of the SCFT equations, it is very likely that the SCFT model could lead to some interesting new mathematics. Furthermore, the substantial computational components in the theoretical studies of block copolymers makes the area ripe for a more mathematical perspective – be it in terms of rigor or in terms of computational sophistication. For the latter, recent collaborations [8, 4] of applied mathematicians with the Fredrickson group at UC Santa Barbara have revealed that such interactions can be fruitful. On the other hand, the materials sciences have proven to be an important source of problems in the modern calculus of variations and PDE, often provide a guiding force behind the exploration of certain classes of nonlinear PDEs and infinite dimensional, non-convex variational problems [12]. In this respect, exposing mathematicians to widely-used variational theories in contemporary polymer physics could only prove beneficial.

Presentation Highlights

The speakers at this workshop represent a wide array of progresses in the study of self-assembly of block copolymers. Topics include numerical implementation of SCFT and Ohta-Kawasaki density functional theory, methodology to obtain solutions of ordered phases for complex block copolymers, self-assembly of block copolymers under confinement, dynamics of structural formation, as well as the effect of electrostatics. Among these diverse problems addressed by the speakers, a few important topics emerged from them.

The first challenge to the applied mathematics and physics community is the development of efficient methods for the discovery of new ordered phases. Within the content of SCFT, this task corresponds to finding solutions for a nonlinear and nonlocal optimization problem. The theme of exploring complex ordered phases of block copolymers are contained in a number of talks, noticeably the presentations by Feng Qiu, Friederike Schmid, Marcus Muller, Weihua Li, Maso Doi, Zhao-Yan Sun and Carlos Garcia Cevera. A recent progress in this area is the development of a generic reciprocal-space method, as given by Feng Qiu. In this method, the SCFT theory is formulated in the Fourier space, leading to a set of nonlinear algebraic equations. Feng Qiu demonstrated that this method can be used to obtain a large number of preciously unknown ordered structures for ABC linear and start triblock copolymers. Another interesting progress in this area is the development of more realistic and fast simulation methods for block copolymers (Marcus Muller, Qiang Wang). Despite all these progresses, obtaining novel ordered phases from SCFT is still a challenging task. The general theme emerged from the discussions at the workshop is that a combination of real-space and reciprocal space methods presents a possible route for the search of ordered phases within the content of SCFT.

The second challenge to the applied mathematics and physics community is the understanding of block copolymers under confinement. In the talks by Baohui Li, Toshihoro Kawakatsu, and to some extent Xiaogfeng Ren, it has been clearly shown that confinement can lead to an amazingly rich array of ordered structures, which are not available in the bulk systems. In fact, block copolymers under confined have become an intensively researched area in the past few years in polymer physics community. From a theoretical point of view, confinement leads to extra controlling parameters for the self-assembly of block copolymers, corresponding to a nonlinear, nonlocal optimization problem within a finite domain of complex boundary conditions. So far, most of the novel structures were discovered from simulations. It is desirable to develop mathematical techniques for the systematic search of ordered phases for the confined system.

The third challenge to the applied mathematics and physics community is the study of phase transition dynamics. A couple of talks have been devoted to this topic (Takao Ohta and Andrei Zvelindovsky). Phase ordering dynamics is an extremely important topic but our understanding of the dynamics is still quite limited. The two talks presented in the workshop present an effort to study the phase transition dynamics using an extension of the SCFT. This approach does give us some important information about the kinetic pathways of the order to order phase transitions. The phase transition pathways can also be examined by studying the landscape of the SCFT free energy functional (An-Chang Shi et al). Despite all these progresses, dynamics of order-to-order phase transitions in soft matter is still a major challenge to the scientific community.

A forth challenge lies in an understanding of the SCFT in the strong segregation limit. To this end, there were two talks (Matsen and Muratov) with similar goals but completely different approaches and perspectives.

Besides the above highlights, another important topic in soft matter is the effect of charges on the equilibrium and dynamic properties of the materials, as represented by Zhen-Gang Wang, Michael Schick and Chun Liu. The challenge in the charged system is that the Coulombic interaction between charged species is long-range. New ideas and methods are needed for the study of these systems. Charged soft matter is a rapidly developing research area. It is hoped that this topics can be discussed in future BIRS workshop.

Finally we would like to emphasize there is an importance existence of the applied mathematicians to the research in this area, as demonstrated by the large number of talks from this group of researchers (e.g. Garcia-Cevera, Glasner, Muratov, Oshita, Ren, Williams). One interesting observation is that theory of Ohta-Kawasaki is remarkably successful given its simplicity. We expect that the Ohta-Kawasaki framework will continue to provide a platform for the mathematicians to study the self-assembly of ordered phases. Furthermore, we hope that the SCFT framework, given its nonlinear and nonlocal nature, will provide a ground for the development of some interesting new mathematics.

Conclusions of the Workshop and Future Directions

The workshop was successful on many grounds. Firstly, it built new contacts between applied mathematicians with physicists and engineers which hopefully will result in future collaborations. It also exposed certain fundamental questions and problems for future study:

- Many issues surrounding the Self-Consistent Mean Field Theory (SCFT) remain unclear:
  (i) a rigorous framework and or some justifications/validations for the approximations used
  (ii) computational challenges in the strong segregation regime,
  (iii) the exact nature and predictions of the theory in the strong segregation limit,
  (iv) extensions to dynamics.
  To this end, it is hopefully that mathematicians can have an impact.

- Confinement issues are of great contemporary interest (both from the point of view of theory and synthesis). Restricting the size of the sample to length scales on the level of the chain length gives rise to an enormous number of complex structures. There is definitely a need for a geometric classification, and at the very least, the formation of a catalogue for experimentally and computationally observed structures.

- The (perhaps overly) simplified Ohta-Kawasaki theory is remarkable successful from a qualitative point of view. A full analysis of its predictions in 3D near the order-disorder transition could prove useful.

- Block copolymer thin films are also of significant interest, and computational tools for solving PDEs on surfaces will prove useful.

In view of these open problems and the recently developed connections, a second BIRS workshop could prove very fruitful.

Talks and Abstracts

Speaker: Masao Doi
Title: Computational Implementation of Ohta-Kawasaki Density Functional for Block Polymers having General Architecture
Abstract: The Ohta-Kawasaki theory gives a simple expression for the free energy of the melt of block copolymers as a functional of the density distribution of each blocks. Here I will discuss how to generalize

this theory for the block copolymers of general architecture, and how to implement it in computational code. This talk is based on the work: ”Density functional theory for block copolymer melts and blends”, Takashi Uneyama and Masao Doi, Macromolecules, 38, 196-205 (2005).

Speaker: Tetsuo Deguchi, Department of Physics, Ochanomizu University
Title: Random Knotting and applications to Polymer Physics
Abstract: Recently, topological effects of ring polymers have attracted much attention in various fields of science such as physics, biology and chemistry. DNA knots, knots in proteins, and synthetic ring polymers have been extensively studied not only theoretically but also experimentally. Interestingly, their mesoscopic or macroscopic properties may depend on their topology. The topology of a ring polymer is given by its knot type, and it does not change under thermal fluctuations. Here the conformations of real ring polymers in solution are modeled by those of random polygons or self-avoiding polygons under some topological constraint.

In this talk, we discuss application of knot invariants to the statistical mechanics of physical systems of ring polymers in solution. We first formulate simulation scheme making use of knot invariants, and then systematically evaluate physical quantities of the system of ring polymers in solution [1,2,3]. In order to analyze the simulation data, we introduce so called scaling arguments, and derive approximate formulas for describing the parameter-dependence of some physical quantity. As such a parameter, we often consider the number of segments, N (in the unit of the Kuhn length).

In particular, we discuss the probability of random knotting and the average size (mean square radius of gyration) of random polygons with a fixed knot type as functions of N. We show swelling of ring polymers due to topological constraints in the theta solution. We also introduce an effective formula for the distribution function of the distance between two given segments of a polygon.

Through some examples we show that simulation using knot invariants should be useful in application to real ring polymers. In fact, the results of the present talk can be checked in experiments of polymers near future. We thus connect the mathematics of knots with polymer physics.

[1] T. Deguchi and K. Tsurusaki, Random knots and links and applications to polymer physics, in “Lectures at Knots ’96, edited by S. Suzuki, (World Scientific, Singapore, 1997) pp. 95-122. [2] M. K. Shimamura and T. Deguchi, Finite-size and asymptotic behaviors of the gyration radius of knotted cylindrical self-avoiding polygons, Phys. Rev. E 65, 051802 (2002). (9 pages) [3] M. K. Shimamura and T. Deguchi, On the mean gyration radius and the radial distribution function of ring polymers with excluded-volume under a topological constraint, in “Physical and Numerical Models in Knot Theory, edited by J.A. Calvo, K.C. Millett and E.J. Rawdon, (World Scientific, Singapore, 2005) pp. 399 – 419.

Speaker: Karl Glasner, Department of Mathematics, University of Arizona
Title: The Subcritical Regime of Copolymer Mixtures
Abstract: Most of the attention given to theoretical descriptions of BCPs is concerned with supercritical pattern formation, in particular periodic or nearly periodic equilibria. In contrast, nontrivial localized equilibria can also exist over a range of parameters below the point of phase separation. In the abstract theory of pattern formation (described e.g. by the Swift-Hohenberg equation) this phenomenon has been studied at length. For A-B copolymer mixtures, these describe localized micelles or bilayer structures. This talk will discuss recent advances in understanding the complex bifurcation diagram for localized equilibria, and their implications for density functional models of BCPs. Aspects of dynamics will also be considered, including instabilities and self-replication phenomenon.

Speaker: Carlos Garcia Cevera, Department of Mathematics, UC Santa Barbara
Title: Numerical advances in Self-Consistent Field Theory simulations, and applications to block copolymer lithography.

Abstract: I will discuss some recent developments in the numerical simulation of self-consistent field theory (SCFT) for block copolymers. I will focus on the following applications:
(i) SCFT simulations of block copolymers laterally confined in a square well: Here we explore the conditions for which self-assembly in laterally confined thin block copolymer films results in tetragonal square arrays of standing up cylinders. More specifically, we study the equilibrium phase behavior of thin films composed of a blend of AB block copolymer and A homopolymer laterally confined in square wells. By using suitable homopolymer additives and appropriately sized wells, we observed square lattices of upright B cylinders that are not stable in pure AB block copolymer systems. Considering the potential application of such films in block copolymer lithography, we also conducted numerical SCFT simulations of the role of line edge roughness at the periphery of the square well on feature defect populations. Our results indicate that the tetragonal ordering observed under square confinement is robust to a wide range of boundary perturbations.
(ii) SCFT simulations of block copolymers on the surface of a sphere: In this model, we assume that the composition of the thin block copolymer film is independent of the radial direction. Using this approach we were able to study the phase separation process, and specifically the formation of defects in the lamellar and cylindrical phases, and its dependence on the radius of the sphere. If time permits, I will discuss recent work on polymer brushes.
(iii) Numerical Solution of the complex Langevin (CL) equations in polymer field theory: I will discussed some improved time integration schemes for solving the nonlinear, nonlocal stochastic CL equations. These methods can decrease the computation time required by orders of magnitude. Further, I will show how the spatial and temporal multiscale nature of the system can be addressed by the use of Fourier acceleration.

Speaker: Toshihiro Kawakatsu, Department of Physics, Tohoku University
Title: Self-consistent field theory for polymers under confinement
Abstract: In the problem of polymer confinement in a narrow container, reduction in the entropy of the chain conformation plays an important role. As a result of this conformation entropy effect, confined block copolymers show various complex mesophases such as hexagonally perforated lamellar phase (in a thin layer) or helical domain phase (in a thin cylinder), which are not be stable in 3-dimensional bulk phase. We simulate the dynamics of phase transitions of such confined systems by using dynamical self-consistent field theory with which one can take the conformation entropy into account. We also discuss effect of soft confinement by flexible container as another interesting topic on polymer confinement.

Speaker: Baohui Li, School of Physics, Nankai University
Title: Block Copolymers Under Various Spatial Confinements
Abstract: Block copolymers have attracted increasing interest both scientifically and in view of a growing number of technological applications because they are capable of forming different ordered phases at nanoscopic length scales. Nano-confinement of block copolymers can be used to produce novel morphologies with potentially novel applications. The influence of confinement on the microphase separation and morphology of block copolymers is also of fundamental interest in polymer science. In a spatially confined environment, structural frustration, confinement-induced entropy loss and surface-polymer interactions can strongly influence the molecular organization. We have systemically investigated the self-assembly of diblock copolymers in various geometric confinements using a simulated annealing simulations. A rich variety of novel morphologies is obtained, depending on the copolymer component and the confinement geometry. The morphological transitions can be understood based on the degree of structural frustration parametrized by the ratio of the confining size to the characteristic length of the bulk phase. The studies demonstrate that confined self-assembly of block copolymers provides a robust method to produce nanoscopic structures which are not accessible in the unconfined state.

Speaker: Weihua Li, Department of Macromolecular Science, Fudan University
Title: Applications of real-space SCFT on the study of self-assembly of block copolymers
Abstract: The self-consistent field theory (SCFT) has been proven to be one of the most successful theories

in the study of self-assembling behaviors of block copolymers. The application of the real-space approach of SCFT has been broadened by the development of the high-efficient pseudo-spectral method. It can be readily used to study the self-assembly of block copolymers under geometrical confinement and the self-assembly of complex block copolymers. Though it cannot have free energy accuracy as high as that of reciprocal method, it can calculate reliable phase diagrams. A few examples of its applications, including AB diblock copolymers in nanopores, linear multiblock copolymers, and ABC star triblock copolymers, are discussed here. A lot of interesting structures are observed in these block copolymer systems, and some of them have been seen by experiments.

Speaker: Chun Liu, Department of Mathematics, Penn State
Title: Energetic Variational Approaches in the Modeling of Ionic Solutions and Ion Channels
Abstract: Ion channels are key components in a wide variety of biological processes. The selectivity of ion channels is the key to many biological processes. Selectivities in both calcium and sodium channels can be described by the reduced models, taking into consideration of dielectric coefficient and ion particle sizes, as well as their very different primary structure and properties. These self-organized systems will be modeled and analyzed with energetic variational approaches (EnVarA) that were motivated by classical works of Rayleigh and Onsager. The resulting/derived multiphysics multiscale systems automatically satisfy the Second Laws of Thermodynamics and the basic physics that are involved in the system, such as the microscopic diffusion, the electrostatics and the macroscopic conservation of momentum, as well as the physical boundary conditions. In this talk, I will discuss the some of the related biological, physics, chemistry and mathematical issues arising in this area.

Speaker: Mark Matsen, Department of Mathematics, University of Reading
Title: The strong-segregation limit of SCFT
Abstract: Helfand's SCFT for block copolymer melts has two analytical limits: the weak-segregation regime described by Leibler's RPA theory and the strong-segregation regime treated by Semenov's SST calculation. The validity of the weak-segregation theory is easily established, but all previous attempts have failed to demonstrate the convergence of the SCFT to the analytical strong-segregation theory. This raises a question of whether or not something is missing from the current formulation of SST. We re-address the convergence by pushing the numerical SCFT calculations to ultra-high degrees of segregation and by examining finite-segregation corrections to SST.

Speaker: Marcus Muller, Institut fr Theoretische Physik Georg-August-UniversitŁt
Title: Structure formation in block copolymers and polymer blends
Abstract: Using soft, coarse-grained models we study the kinetics of structure formation in dense, multi-component polymer liquids. In the first part, I will discuss the consequences of soft potentials that naturally arise from a coarse-graining procedure and allow for an overlap of the coarse-grained interaction centers (segments). This feature allows to increase the segment density and to model experimental values of the invariant degree of polymerization resulting in a realistic strength of fluctuations. The softness, however, does not prevent the bonds to cross each other during the course of their motion. The role of non-crossability on the kinetics of self-assembly is briefly illustrated and a slip-link model a la Likhtman is employed to mimic entanglement effects in an effective way.

In the second part, I will discuss how to couple a particle model of a dense, binary polymer melt to a Ginzburg-Landau description. Coupling the order-parameter field, m, of the Ginzburg-Landau description to the particle model by restraining the composition fluctuations of the particle model, we can calculate the chemical potential field, mu, that corresponds to the order-parameter field, m. This information allows to reconstruct the underlying free-energy functional of the Ginzburg-Landau description. We use a simple trial form of the free-energy functional containing a small number of parameters – i.e., the Flory-Huggins parameter and the coefficient in front of the square gradient term – and determine these free parameters from a short simulation of the coupled system. Then, we use the so-parameterized Ginzburg-Landau description to propagate the order-parameter field in time and couple the particle-based model to the new order-parameter field configuration. The strong coupling makes the particle-based model quickly adapt to the new m, and the simulation cycle commences again. The advantages of this computational technique are two-fold: (i) it provides an approximation for the free-energy functional for the Ginzburg-Landau description of the particle model and (ii) the coupling speeds up the simulation of the particle-based system. The latter effect is related to the scale separation between the strong bonded forces, that dictate the time step in the particle model, and the weak non-bonded forces, that drive the structure formation.

Speaker: Cyrill Muratov, Department of Mathematical Sciences, NJIT
Title: Droplet phases in compositionally asymmetric diblock copolymer melts in two dimensions
Abstract: In this talk, I will discuss the energetics of diblock copolymer melts under strong segregation and high compositional asymmetry, which favor periodic lattices of compact droplets of the minority phase as energy minimizers. I will begin by identifying the contribution of the lattice geometry to the energy which is responsible for the lattice selection and show that in two dimensions a hexagonal lattice is optimal among simple lattices. I will then present an analysis of the same problem in the two-dimensional Ohta-Kawasaki model near the onset of multi-droplet patterns. As a first step, I will show that under suitable scaling the energy of minimizers becomes asymptotically equal to that of a sharp interface energy with screened Coulomb interaction. I will then show that the minimizers of the corresponding sharp interface energy consist of nearly identical circular droplets of small size separated by large distances. I will finally show that in a suitable limit these droplets become uniformly distributed throughout the domain.

Speaker: Takao Ohta, Department of Physics, Kyoto University
Title: Dynamics of gyroid structure in microphase separation
Abstract: We study dynamics of microphase separation in diblock copolymer melts focusing on the double gyroid structure based on the Cahn-Hilliard type equation for local concentration. The theoretical results by means of the mode expansion method are given for formation of gyroid, structural transitions between gyroid and other states [1], and the viscoelastic response [2]. The real space numerical results for a coexistence state of gyroid and lamellar structures are also shown [3]. Some of the related results obtained by the self-consistent mean field theory [4] are discussed. Furthermore, we describe formation of interconnected structures in Turing pattern in three dimensions, which is mathematically related to the microphase separation problem [5]. Extension of the theory introducing the variables other than concentration is also briefly mentioned.

[1] K. Yamada, M. Nonomura and T. Ohta, Kinetics of morphological transitions in microphase-separated diblock copolymers, Macromolecules 37, 5762 (2004). [2] R. Tamate, K. Yamada, J. Vinals, and T. Ohta, ”Structural rheology of microphase separated diblock copolymers”, J. Phys. Soc. Jpn., 77 034802 (2008). [3] K. Yamada and T. Ohta, ”Interface between lamellar and gyroid structures in diblock copolymer melts”, J. Phys. Soc. Jpn., 76, 084801 (2007). [4] C. A. Tyler and D. C. Morse, ”Linear elasticity of cubic phases in block copolymer melts by self-consistemt field theory”, Macromolecules, 36, 3764 (2003). [5] H. Shoji, K. Yamada, D. Ueyama and T. Ohta, ”Turing patterns in three dimensions” Phys. Rev. E 75, 046212 (2007).

Speaker: Yoshihito OSHITA, Okayama University
Title: A rigorous derivation of mean-field models for diblock copolymer melts
Abstract: We study the free boundary problem describing the micro phase separation of diblock copolymer melts in the regime that one component has small volume fraction such that micro phase separation results in an ensemble of small balls of one component. Mean-field models for the evolution of a large ensemble of such spheres have been formally derived in Glasner and Choksi (Physica D, 238:12411255, 2009), Helmers et al. (Netw Heterog Media, 3(3):615632, 2008). It turns out that on a time scale of the order of the average volume of the spheres, the evolution is dominated by coarsening and subsequent stabilization of the radii of the spheres, whereas migration becomes only relevant on a larger time scale. Starting from the free boundary

problem restricted to balls we rigorously derive the mean-field equations in the early time regime. Our analysis is based on passing to the homogenization limit in the variational framework of a gradient flow.

Speaker: Feng Qui, Department of Macromolecular Science, Fudan University
Title: Discovering Ordered Phases of Multi-block Copolymers: A Generic Fourier-Space Approach
Abstract: We propose a generic approach to solve the self-consistent field theory (SCFT) equations for the discovery of complex ordered structures of block copolymers. In our method, all spatially varying functions are expanded in terms of Fourier series which are essentially determined by computational box parameters. Then SCFT equations can be cast in terms of expansion coefficients. The solutions of the SCFT equations can then be obtained using any of the available numerical techniques. The essence of this approach is to use the full-power of the spectral method, in which the symmetry of the ordered phases is not presumed. Furthermore, our Fourier-space method has the advantage of identifying new complex structures, especially continuous structures, more easily and definitively.

With this method, we successfully reproduce phases observed in diblock copolymers. We have confirmed that the generic Fourier-space method leads to equilibrated lamella, cylinder, gyroid, O70, and sphere phases at the compositions and values consistent with the Matsen-Schick phase diagrams. Our emphasis has been focused on phase behaviors of ABC linear and star-shaped triblock copolymers, in which both centro- and noncentro-symmetric phases can be formed. The phase diagram of a model frustrated ABC triblock copolymer is constructed. A number of new phases are predicted for the linear triblock copolymers. Then the method is further applied to a more realistic model of SEBM triblock copolymer, in which the fascinating KP phase is predicted to occur at the parameters that mostly match the experiment conditions.

For ABC star triblock copolymers, the most important architectural feature is that their three blocks are joined at one junction point. In an ordered phase the junction points are constrained in one-dimensional lines, resulting novel microphase-separated morphologies such as tiling patterns. A variety of tiling patterns in ABC star triblocks have been predicted using the Fourier-space method and relevant phase diagrams have been constructed. The predicted phase transition sequences from the SCFT calculations are in qualitative agreement with experimental and Monte Carlo simulation results.

We believe that the generic Fourier-space approach is a powerful method to predict novel ordered phases for complex block copolymers. These ordered structures can be used as input for the more accurate and efficient real-space or reciprocal-space methods.

Speaker: Xiaofeng Ren, Department of Mathematics, George Washington University
Title: Ansatze of the curvature-potential equation from morphology and morphogenesis problems
Abstract: Pattern formation problems arise in many physical and biological systems as orderly outcomes of self-organization principles. Examples include animal coats, skin pigmentation, and morphological phases in block copolymers. Recent advances in singular perturbation theory and asymptotic analysis have made it possible to study these problems rigorously. In this talk I will discuss a central theme in the construction of various patterns as solutions to some well known PDE and geometric problems: how a single piece of structure built on the entire space can be used as an ansatz to produce a near periodic pattern on a bounded domain. We start with the simple disc and show how the spot pattern in morphogenesis and the cylindrical phase in diblock copolymers can be mathematically explained. More complex are the ring structure and the oval structure which can also be used to construct solutions on bounded domains. Finally we discuss the newly discovered smoke-ring structure and the toroidal tube structure in space. The results presented in this lecture come from joint works with Kang, Kolokolnikov, and Wei.

Speaker: Michael Schick, Department of Physics, University of Washington
Title: Ionic Effects on the Electric Field needed to Orient Dielectric Lamellae
Abstract: We consider the effect of mobile ions on the applied potential needed to reorient a lamellar system of two different materials placed between two planar electrodes. The reorientation occurs from a configura-

tion parallel to the electrodes favored by surface interactions to an orientation perpendicular to the electrodes favored by the electric field. The system consists of alternating A and B layers with different dielectric constants. The mobile ions are assumed to be insoluble in the B layers and hence confined to the A layers. We find that the ions reduce the needed voltage most strongly when they are constrained such that each A lamella is electrically neutral. In this case, a macroscopic separation of charge and its concomitant lowering of free energy, is attained only in the perpendicular orientation. When the ions are free to move between different A layers, such that charge neutrality is only required globally, their effect is smaller and depends upon the preferred surface interaction of the two materials. Under some conditions, the addition of ions can actually stabilize the parallel configuration. Our predictions are relevant to recent experiments conducted on lamellar phases of diblock copolymer films with ionic selective impurities.

Speaker: Friederike Schmid, Institut fuer Physik. Universitaet Mainz
Introductory Minicourse: Self-Consistent Field Theories of Inhomogeneous (Co)polymer blends
Abstract: The course gives an introduction into basic concepts of the theory of polymer/copolymer blends, with a particular emphasis on the so-called 'self-consistent field theory' (SCF theory). It is aimed at an audience who is not familiar with this theory. Everybody else should sleep in or have coffee instead. The topics to be covered include

General introduction in polymer models Flory Huggins theory and chi-parameter Detailed introduction into the SCF theory Limiting behavior at 'strong' and 'weak' segregation, in particular, connection to Ginzburg-Landau theories like the Ohta-Kawasaki functional Fluctuation effects Time-dependent density-functional theory and time-dependent Ginzburg-Landau theory Applications

Speaker: Friederike Schmid, Institut fuer Physik. Universitaet Mainz
Title: Copolymer self-assembly at nonequilibrium and in networks
Abstract: The talk will have two parts. The first part deals with the kinetics of nanostructure formation in amphiphilic copolymer solutions. Copolymers in solution spontaneously aggregate into a variety of nanostructures, e.g., micelles or vesicles, which can be tuned by tuning system parameters such as the chain lengths, the block lengths, the composition etc, This can be used to prepare nanoscaled materials with well-defined properties. Using a dynamic density functional approach, we studied the dynamical processes leading to spontaneous vesicle formation in copolymer solutions. Depending on the system parameters, vesicle formation is found to proceed via different pathways. The final structure depends on the pathway. Under certain conditions, toroidal and even cagelike micelles (i.e., perforated vesicles) can be obtained.

In the second part, a method to construct a self-consistent field theory for crosslinked systems is proposed. The original SCF theory is devised for polymer fluids; however, many polymeric materials have a network structure, which means that they respond elastically to stress and that deformations are restored. A generalized SCF theory for networks shall be devised and first application examples shall be presented.

Speaker: Zhao-Yan Sun, Changchun Institute of Applied Chemistry
Title: Effects of Architecture and Composition on the Microphase Separation of Block Copolymers
Abstract: It is well-known that block copolymer systems have fascinating ability to self-assemble into a variety of smart soft materials and well-controlled micro-phase structures on nanometer scale. With the development of synthetic methods, multi-component block copolymer systems with complex chain architectures such as pi-shaped and H-shaped block copolymer can be synthesized easily in experiments. These block copolymers may have some important applications in the fields such as macromolecular self-assembly, controlled drug delivery, and the preparation of advanced materials. Therefore, it is very important to explore the self-assembly of block copolymers with complex chain architecture. In this work, the combinatorial screening method based on the self-consistent field theory (SCFT) proposed by Drolet and Fredrickson is employed to investigate the self-assembly of pi-shaped and H-shaped block copolymers. Our results may provide some theoretical guidance for exploring the self-assembly of multi-component block copolymer sys-

tems with complex chain architectures.

Speaker: Zhen-Gang Wang, Division of Chemistry and Chemical Engineering, California Institute of Technology
Title: Self Energy of Small Ions
Abstract: We address the issue of the self energy of the mobile ions in electrolyte solutions within a general Gaussian renormalized fluctuation theory using a field-theoretic approach. We introduce the Born radii of the ions in the form of a charge distribution allowing for different Born radii between the cations and anions. The model thus automatically yields a theory free of divergences and accounts for the solvation of the ions at the level of continuous dielectric media. In an inhomogeneous dielectric medium, the self energy is in general position dependent and differences in the self energy between cations and anions can give rise to local charge separation in a macroscopically neutral system. Treating the Born radius a as a smallness parameter, we show that the self energy can be split into an O(a-1) nonuniversal contribution and an O(a-0) universal contribution that depends only on the ion concentration, valency, and the spatially varying dielectric constant. For a weakly inhomogeneous dielectric medium, the nonuniversal part of the self energy is shown to have the form of the Born energy with the local dielectric constant. This self energy can be incorporated into the Poisson-Boltzmann equation, in conjunction with other mean-field approaches, such as self-consistent field theory for polymers, as a simple means of including this local fluctuation effect at a mean-field level. We illustrate the application of this born-energy augmented Poisson-Boltzmann approach to the problem of interface tension between two salt containing solutions, highlighting the effects of the interfacial widths and salt concentration.

Speaker: Qiang (David) Wang, Department of Chemical and Biological Engineering, Colorado State University
Title: Some Applications of SCFT and Its Quantitative Test by Fast Lattice Monte Carlo Simulation
Abstract: I will first present some of our recent work using real-space self-consistent field (SCF) calculations with high accuracy to study (1) diblock copolymers (DBC) under nano-confinement, (2) stimuli-responsive surfaces from DBC brushes, and (3) polyelectrolyte adsorption and layer-by-layer assembly. I will then talk about comparisons between lattice SCF theory and fast lattice Monte Carlo (FLMC) simulations that are based on exactly the same Hamiltonian, thus with no parameter-fitting between the two. Such comparisons provide the most stringent test of the SCF theory, and unambiguously and quantitatively reveal the system fluctuations/correlations neglected in the theory.

Speaker: JF Williams, Department of Mathematics, Simon Fraser University
Title: Asymptotic analysis and computation for minimizers of a modified Cahn-Hilliard energy in 3D.
Abstract: In this talk I will present an asymptotic analysis of the energy-driven pattern formation induced by competing short and long range effects in a model for self-assembly of diblock copolymers. This work shows that structures predicted by the self-consistent mean field theory may be constructed via asymptotic analysis of the associated PDE. Additionally, local minimizers, such as the perforated lamella, may also be understood. All asymptotic constructions are verified by simulation of an evolutionary PDE via modified gradient descent starting from random initial conditions.

Speaker: Vanessa Weith, Theoretische Physik I, Universitaet Bayreuth
Title: Dynamics of Janus particles in a phase-separating binary mixture
Abstract: Adding particles to a binary mixture induces an interesting dynamic coupling between the wetting of the particles and the phase separation of the mixture. Recently a new class of colloidal particles, so-called Janus particles, have been synthesized in large quantities [1]. Janus particles, named after the Roman god Janus, represent colloids with a different chemical composition of the surface of the two halves of a particle. Accordingly each half of a particle may be wetted preferentially by one component of the mixture. We present the results of numerical simulations of the dynamics of Janus particles immersed in a phase-separating binary

mixture based on a meanfield approach. When the two constituents of a binary mixture wet the two sides of a Janus particle differently, the particle induces a spatial variation of the concentration in their neighborhood. Accordingly, Janus particles in phase separating mixtures are trapped to interfaces, which leads to a complex dynamics. Due to the strong localization of an interface, the diffusion of Janus particles is much more pronounced compared with isotropic particles. As a result of this fast diffusion the Janus particles placed initially at large distances may effectively approach each other and they can remain coupled in the case of an appropriate orientation. [1] A. Walther and A. H. E. Mueller, Soft Matter 4, 663-668 (2008).

Speaker: Andrei V. Zvelindovsky, University of Central Lancashire
Title: Kinetics of block copolymer phase transitions under electric field
Abstract: Mesophases of block copolymers with blocks of different dielectric constants might undergo transformations under an applied electric field. These include orientational phase transitions of a particular phase or order-order transitions between phases of different symmetries. We modified dynamic SCFT in order to account for a non-isotropic diffusion due to the dielectric mismatch of blocks. We review our works, in which we study lamellar, cylindrical, spherical and gyroid phases under electric field. The results are compared with available experimental data and findings based on Ginzburg-Landau type theories.

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Chapter 20

Diophantine Approximation and Analytic Number Theory: A Tribute to Cam Stewart (10w5032)

May 30 - Jun 04, 2010

Organizer(s): Gary Walsh (University of Ottawa and CSE), Michael Bennett (University of British Columbia), Andrew Granville (Universite de Montreal), Jeff Thunder (Northern Illinois University)

Introduction

This conference dealt with two areas of Number Theory, "the queen of mathematics." Diophantine approximation can be broadly described as the solvability in rational integers to various inequalities. The name comes from the later Greek mathematician Diophantus, who studied the solutions to certain equations. Though clearly a very old branch of mathematics, it remains a vibrant area of study to this day. The last century saw many deep and powerful results: the theorems of Thue, Siegel and later Roth, Baker's linear forms in logarithms, and Schmidt's subspace theorem, to name but a few. Much recent work has melded the arithmetic nature of the subject with advances in algebraic geometry (e.g., the work of Faltings and Vojta), where one is interested in the properties of rational points on algebraic varieties defined over a number field. Recent successes in this area have lead to the solutions to many old and notoriously difficult problems.

Many mathematicians when asked about analytic number theory immediately think of the famous Riemann hypothesis and perhaps the Goldbach conjecture. In fact, the area is much more rich than that. Early last century Ramanujan together with Hardy, Littlewood and others developed analytic methods to answer questions about Diophantine equations. A famous example here would be Waring's problem, where one is concerned with writing an integer as a sum of equal powers of integers. This particular area has seen a recent resurgence of activity, spurred on by the work of Vaughn and Wooley. Another more recent line of work has brought probabilistic methods into the mix. The celebrated results of Green and Tao here bear testament to the efficacy of these ideas; they proved that the sequence of prime numbers contains arbitrarily long arithmetic progressions. Along more classical lines, Goldston and Yildirim have within the last five years made stunning progress on the study of gaps between prime numbers.

These two areas of number theory are far from being isolated "islands" in mathematics. Besides the obvious connections to algebra, geometry, complex variables, etc., these areas touch upon subjects as disparate as logic (via model theory), coding theory and cryptography. A glance at Math Reviews immediately confirms that Number Theory continues to be one of the most active subjects in all of mathematics, one that benefits from and employs tools from many areas, and where new applications continue to arise.

Finally, we note that this meeting was a tribute to the work of Cameron Stewart in celebration of his sixtieth birthday. Cam, as he is known to his friends and colleagues, has a lengthy record in these two areas of number theory and has made a great many outstanding contributions to the subject.

Overview of the Fields

It was observed early on that in order to find integer solutions to many Diophantine equations, one is naturally lead to approximating certain real numbers by rational numbers. For example, the old question of finding numbers that are both square and "triangular" results in a Pell equation, and as is well-known, the solutions to such equations come from good approximations to quadratic irrational numbers. These good approximations can be found, for example, using continued fractions. Unfortunately, finding such "good approximations" for algebraic numbers of higher degree still remains problematic to this day.

Let α be a real number. At its most basic, Diophantine approximation deals with finding rational numbers p/q (here p and q are relatively prime integers) with

$$\left|\alpha - \frac{p}{q}\right| < \frac{c(\alpha)}{q^\delta}, \qquad (*)$$

where $c(\alpha)$ is some positive number and $\delta \geq 2$. Liouville showed that for an algebraic number α of degree $d \geq 2$, there is a $c(\alpha)$ such that (*) has no solutions for $\delta \geq d$. On the other hand, Dirichlet showed that for any real number α, there are infinitely many solutions to (*) with $c(\alpha) = 1$ and $\delta = 2$.

Early last century Thue made a great breakthrough: he showed that for any algebraic α of degree $d \geq 3$, there are only finitely many solutions to (*) with $\delta > (d/2) + 1$. Unfortunately, while the methods of Thue allow one to get upper bounds on the *number* of such solutions, one has absolutely no information on the *size* (i.e., how large the denominator q may be) of such solutions. The method is called *ineffective*, as it doesn't allow one to find all such solutions (since the upper bounds one can derive for their number is most certainly larger than the "truth"). Nevertheless, a great deal of mathematics over the years has been devoted to extending and improving on Thue's original ideas. Two highlights are Roth's famous result [5] where he replaced Thue's bound above with the more simple $\delta > 2$, (Roth was awarded the Fields medal for his work) and Schmidt's famous subspace theorem (see [6], for example) which pushed things to higher dimensions (he won the Cole prize for his work).

Another great stride forward was made by A. Baker (see [1]). Briefly, he was able to prove effective upper bounds on the size of solutions to (*). This method, called linear forms in logarithms, is a major tool in solving Diophantine equations (Baker was awarded the Fields medal for his work). It does not make the Thue methods obsolete, however, since it yields rather large upper bounds on the size of the possible solutions. For example, Tijdeman used linear forms in logarithms to essentially "solve" Catalan's conjecture in 1976. But improvements to the method and quantum leaps in computing power were still unable to exhaust all possible solutions before the problem was completely resolved via algebraic number theoretic methods by Mihailescu in 2002.

The use of analytical tools and methods to solve questions about integers has a long history. One can start with Euler's product formula which relates the Riemann zeta function with the primes. The proof of the prime number theorem late in the nineteenth century was a great achievment and a testament to the power of complex analysis. More recently, Bombieri's development of the large sieve in the 1960s (see [3]) has led to many deep and interesting results. (Bombieri was awarded the Fields medal for his work.) As a testimony to the continued vibrancy of research in this area, one might note the number of first-rate mathematicians currently working in areas related to the field, including Sarnak, Granville, Friedlander, Green, Iwaniec, Soundararajan, Tao, Bourgain and Connes.

Recent Developments

Though Thue's original method of proof was "ineffective" as described above, it was clear that one could derive upper bounds for the *number* of exceptional solutions. This has carried through to Roth's theorem and the subspace theorem; versions of these results where one has such upper bounds are called quantitative. There has been much effort to make stronger quantitative versions of both Roth's theorem and the subspace theorem. Also, there have been quantitative versions involving other absolute values and even a "absolute" version [4] over the field of all algebraic numbers. In a similar manner, there are more recent versions of linear forms in logarithms which give better bounds [2], as well as linear forms in p-adic, elliptic and even hyperelliptic logarithms.

While the above efforts to improve on machinery is clearly fundamental, the majority of work in the area has been applying these tools to solving actual Diophantine equations and inequalities. One major topic here deals with S-unit equations, the simplest of which is just

$$a + b = 1$$

where a and b are S-units in a given number field (or perhaps a function field). Every number field (finite algebraic extension of the rational numbers) has a countable colletion of places which correspond to topologically inequivalent absolute values on the field. These places are in one-to-one correspondence with the embeddings of the field into the complex numbers (these are the "infinite" places") and the non-zero prime ideals in the ring of integers of the field. Given a finite set S of such places containing all of the infinite places, an S-integer is an element a of the field which has absolute value $|a|_v = 1$ for all places v not in S. It turns out that many Diophantine questions are equivalent to solving a particular S-unit equation or family of such.

In analytic number theory, work continues on using the machinery already on hand to answer deep questions about the primes and other sets of interest, as well as on applications of new techniques coming from additive combinatorics and the theory of automorphic forms. Progress is also being made on the methods themselves, where one often looks to optimize the techniques to suit the particular question at hand. An example here would be Vaughan and Wooley's improvements on the circle method to answer then-open questions regarding Waring's problem. In addition, work continues on the Riemann zeta function. The Riemann hypothesis is obviously the "holy grail" here, but more modest goals are still very important. Recent work of Soundararajan has increased our knowledge of the moments of the zeta function, for example.

Presentation Highlights

Yann Bugeaud of Strasbourg spoke on the irrationality exponent of a certain type of number. Given a real number α, the irrationality exponent of α is the infimum of the set of δ for which the inequality (*) above has infinitely many solutions in rational numbers p/q. Thus, by Roth's theorem the irrationality exponent of any algebraic number is simply 2. Computing the irrationality exponent of non-algebraic numbers is typically an extremely difficult task. Often we must be content trying simply to prove upper bounds for the irrationality exponent. This is the case, for example, with the number π (presently the best upper bound for its irrationality exponent is approximately 8, while it is generally thought that the actual irrationality exponent here is 2).

Bugeaud discussed α of the following form. Start with the Thue-Morse sequence $\{t_n\}_{n\geq 0}$ defined recursively by $t_0 = 0$, $t_{2n} = t_n$ and $t_{2n+1} = 1 - t_n$. Choose an integer $b \geq 2$. Bugeaud proved that the irrationality exponent of the number $\alpha = \sum_{n\geq 0} t_n b^{-n}$ is 2.

Jan-Hendrik Evertse of Leiden discussed orders of number fields which are generated (as modules over the integers) by a single element. Such orders are called “monogenic.” When the order in question is the maximal order, i.e., the ring of integers of the field, one says there is a power basis if it is monogenic. This is usually not the case, but it is extremely useful when it is. If one has a monogenic order O of the form $Z[\alpha]$, then clearly $O = Z[\beta]$ for any β of the form $\beta = \pm\alpha + a$ for some $a \in Z$. We say such β are equivalent to α. Given a monogenic order O, one is interested in the number of inequivalent α which generate O. Evertse proved that for orders in number fields of degree at least 3, only finitely many can be monogenic with at least three inequivalent generators. Also, for non-CM fields, there are infinitely many monogenic orders with exactly two non-equivalent generators. The method of proof here relies on previous results dealing with S-unit equations in two variables.

Noriko Hirata-Kohno of Tokyo discussed Iwasawa p-adic logarithms and showed how one could use these in the p-adic linear forms in logarithms machinery. The goal here is to improve/extend the machinery to give better estimates and/or be more widely applicable.

Helmut Maier of Ulm spoke on exponential sums over prime numbers. He presented a conjecture for such sums over “short” intervals which is reasonably natural, and showed how this conjecture implies the twin prime conjecture. Further, he showed that an analogous conjecture is true when the set of prime numbers is replaced by a set of integers without small prime factors.

Two speakers, Andras Sárközy and Rob Tijdeman, spoke directly about the work of Cam Stewart. Both are frequent coauthors with Cam; Sárközy has written more than 15 papers with him.

Andras gave a history of his work with Cam on sums $a+b$ and shifted products $ab+1$. Given sufficiently large sets A and B, one is interested in the arithmetic properties of sums of the form $a+b$ where $a \in A$ and $b \in B$ and also of the form $ab+1$. Such questions go back all the way to Diophantus. By “arithmetic properties” here we mean questions about the prime factors, square factors, etc. Together with Cam, and occasionally other authors, Andras has proven many results in this area.

Rob’s talk concentrated on Cam’s work involving linear forms in logarithms. Cam’s first paper appeared in the journal Acta Arithmetica in 1975. It dealt with the largest prime factor of sums of the form $a^n - b^n$. If we denote the largest such prime factor by P, then Cam proved that

$$\frac{P(a^n - b^n)}{n} \to \infty$$

as n tends to ∞ through some well-defined set of density 1. Stewart and Tijdeman together worked on the abc-conjecture. Suppose $a,\ b$ and c are positive integers with $a + b = c$. Denote their conductor by N; N is the product of all primes dividing abc. The abc-conjecture states that, for all $\epsilon > 0$, one has $N^{1+\epsilon} \gg_\epsilon c$, where the implicit constant in the Vinogradov notation here depends only on ϵ. In an important paper from 1985, Stewart and Tijdeman proved that $\log c \ll N^{15}$ and also that

$$c > N \exp\left((4-\delta)\frac{\sqrt{\log N}}{\log\log N}\right)$$

for infinitely many cases, where $\delta > 0$ is arbitrary. In particular, the ϵ in the abc-conjecture is necessary. Rob further spoke on Cam’s work involving S-unit equations and Thue-Mahler equations.

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Chapter 21

Whittaker Functions, Crystal Bases, and Quantum Groups (10w5096)

Jun 06 - Jun 11, 2010

Organizer(s): Paul Gunnells (University of Massachusetts Amherst), Ben Brubaker (Massachusetts Institute of Technology), Dan Bump (Stanford), Gautam Chinta (City College of New York)

Objectives of the workshop

The goals of the workshop were to explore several new connections between Whittaker functions and combinatorial representation theory that have recently emerged, and to encourage collaboration between researchers in number theory, combinatorial representation theory, physics, and special functions. We hoped that the balance between the lectures and free time as well as the intimate setting of the Banff Research Station would stimulate many informal discussions and collaborations. We were delighted to see that these objectives were fulfilled.

We would like to thank the BIRS staff for their hospitality and efficiency.

Topics of the workshop

The Casselman-Shalika formula and its generalizations

Given a Lie group or p-adic group, and "Langlands parameters"— a conjugacy class in its Langlands dual group (a complex analytic Lie group)—one may define a spherical Whittaker function. When the group is $\mathrm{GL}(2,\mathbb{R}\diagdown)$ these functions are the confluent hypergeometric functions introduced by Whittaker and Watson [**?**], hence the name.

The Casselman-Shalika formula describes the values of a spherical p-adic Whittaker function in a surprising and beautiful way [**?**]. The values are simply the characters of the finite-dimensional irreducible representations of the dual group evaluated at the Langlands parameter conjugacy class. This formula has many applications in automorphic forms and number theory, being basic to both the Rankin-Selberg method and the Langlands-Shahidi method of constructing L-functions. It has also recently attracted the attention of physicists, as in the work of Gerasimov, Lebedev and Oblezin in connection with Givental's work on mirror symmetry [**?**, **?**].

Whittaker functions on metaplectic covers have also been a subject of study since the fundamental work of Kazhdan and Patterson [**?**], but the problem of extending the Casselman-Shalika formula to metaplectic groups was not considered much until recently due to lack of uniqueness of Whittaker models. These obstacles have been overcome by emphasizing newly discovered connections with representation theory, particularly with crystal graphs and quantum groups.

There are now two distinct types of generalizations of the Casselman-Shalika formula to metaplectic covers. To explain these, we note that by the Weyl character formula, the characters that are the special values of the original Casselman-Shalika formula are expressed as alternating sums of characters over the Weyl group. One generalization (primarily due to Chinta and Gunnells [**?**]) is again a sum over the Weyl group where these characters are replaced by products of Gauss sums. In the other generalization (primarily due to Brubaker, Bump, and Friedberg), the sum is similar to the realization of the character as a sum over basis vectors of a certain highest weight vector, though the monomials attached to each weight are multiplied by a function defined on the associated crystal graph. A complete understanding of these two approaches and their connection to Whittaker coefficients and to each other has only been established in type A. Partial results exist for other types, but it appears that a deeper understanding of the relationships between automorphic forms and combinatorics, particularly crystal bases, may be needed to move further.

When the metaplectic cover is trivial, these new formulas for Whittaker functions should recover the character predicted by the Casselman-Shalika formula. Remarkably, several such identities existed as purely combinatorial results in the literature. In this context, they are deformations of the Weyl character formula and the Weyl denominator formula found by Tokuyama (type A), Hamel and King (type C), Okada (type B) and others.

Crystal Bases

Crystal graphs and crystal bases were introduced by Kashiwara as combinatorial structures on representations of quantum groups. In the context of Whittaker functions, the relevant quantum group required is the quantized enveloping algebra of the Langlands dual group. Crystal bases provide a better context for an enormous amount of existing literature on tableaux, which are fundamental objects of study in combinatorics.

For examples of representations of Whittaker functions as sums over crystal bases, see Brubaker, Bump and Friedberg [**?**, **?**], Beineke, Brubaker and Frechette [**?**, **?**], and Chinta and Gunnells [**?**].

The construction of p-adic Whittaker coefficients via crystal graphs should have connections to Berenstein and Kazhdan's theory of geometric crystals [**?**, **?**]. This work gives new constructions of Kashiwara crystals, including those for modules over the Langlands dual group $\hat{G}$, using so-called positive unipotent bicrystals on the open Bruhat cell Bw_0B, where w_0 denotes the longest element of the Weyl group of G. Their method uses tropical geometry to make the transfer between the two types of crystals. Given that the p-adic integral defining the Whittaker coefficient is supported on the big Bruhat cell, and that the ingredients used to construct it have such strong resemblance to the ingredients and properties of objects in the theory of geometric crystals, we expect further investigation of these connections will lead to a better understanding of the ways in which finite dimensional representations appear in automorphic forms.

Kac-Moody developments

Since crystal bases and quantum groups can be defined in the general context of Kac-Moody Lie algebras, it becomes natural to ask whether the theory described above has generalizations to affine and other infinite root systems. This is being investigated, and there is some reason to hope for an affirmative answer. Two promising developments along these lines are the work of Garland on Eisenstein series on loop groups [**?**, **?**, **?**, **?**] and of Braverman and Kazhdan on spherical Hecke algebras on affine Kac-Moody groups over local non-archimedean fields.

However another potential approach can be imagined. The theory of metaplectic Whittaker functions can be developed independently of its origin in the representation theory of p-adic groups as the study of a class of multiple Dirichlet series with functional equations. In this approach, one uses the combinatorics of crystal graphs to define the coefficients of the Dirchlet series. A prototype was work of Bucur and Diaconu [**?**] (in the function field case) in which the group of functional equations was the affine Weyl group $D_4^{(1)}$. This Dirichlet series was selected due to an arithmetic application to fourth moments of L-functions, but for this proposal the relevance of their work is that it gives hope that one might be able to avoid technical complications by not basing the foundations on the representation theory mentioned above.

Another prototype of this question would be to express a deformation of the Jacobi triple product as a sum over an infinite crystal for the quantum group $A_1^{(1)}$ (in Kac's notation). Preliminary investigations suggest that this will be possible.

Real groups and further deformations

Stade developed important integral representations of Whittaker functions for $\mathrm{GL}(n, \mathbb{R}\setminus)$ that allow one to express certain integrals as products of Gamma functions. These have applications in the Rankin-Selberg method. Oda, Hirano, and Ishii have developed formulas for archimedean Whittaker functions that might have connections with the p-adic theory, since for $\mathrm{Sp}(6)$ their formula is a sum over Gelfand-Tsetlin patterns, which are in bijection with elements of crystal bases for $\mathrm{GL}(3)$. Stade's work, as well as this work of Oda, Hirano, and Ishii, are points where there are strong analogies between the real and p-adic theories.

Furthermore, the physicists Gerasimov, Lebedev and Oblezin's obtained a deformation of the Casselman-Shalika formula [**?**, **?**] in connection with Givental's work on mirror symmetry, which has been recently generalized beyond type A by Cherednik [**?**]. Strikingly, their theory simultaneously connects both the real and p-adic Whittaker functions: their deformations have two parameters q and t, and taking $q \to 1$ gives the classical Whittaker function, while $q \to 0$ gives the p-adic Whittaker function. This may be related to the fact that the Macdonald polynomials interpolate between archimedean and p-adic spherical functions [**?**], which is a point of contact with the theory of double affine Hecke operators, that was discussed by two speakers at the conference.

Statistical Mechanical Interpretations

It has been realized that Whittaker functions may be realized as partition functions of statistical-mechanical systems. These are exactly-solved lattice models, amenable to the methods of Baxter [**?**]. There is a potential point of contact here with the work of Gerasimov, Lebedev and Oblezin [**?**], for their emphasis on the Baxter Q-operator in the connection with their investigations of Whittaker functions, both real and archimedean. It is connected with both the crystal base description, since crystals may be used to parametrize the states of the physical system, and with the method of Chinta and Gunnells [**?**], since the functional equations that are the basis of their work express the commutativity of transfer matrices, which may be studied using the Yang-Baxter equation. Finally, it is well-known in physics that two-dimensional statistical mechanical models are equivalent to one-dimensional quantum mechanical models such as spin chains, and so there is a large amount of potentially relevant mathematical physics. See Brubaker, Bump, Chinta, Friedberg and Gunnells [**?**], Brubaker, Bump and Friedberg [**?**], Brubaker, Bump, Chinta and Gunnells [**?**], Hamel and King [**?**], and Ivanov [**?**].

Contents of the talks

The talks at the workshop reported on many new results related to the above list of topics. There were also some expository talks from experts, on both the automorphic and representation theory sides, designed to help build bridges between the different topics. Finally, there was an evening problem session that both summarized open questions mentioned in the talks and also generated new ideas. In the following we summarize the contents of each talk. Junior speakers are indicated by a bullet (•).

Arkady Berenstein (University of Oregon) spoke on *From geometric crystals to crystal bases*. The goal of his talk was to construct crystal bases (for irreducible modules over semisimple Lie algebras) by means of geometric crystals. Geometric and unipotent crystals were introduced a few years ago in a joint work with David Kazhdan as a useful geometric analogue of Kashiwara crystals [**?**, **?**]. More recent observations (based on his recent joint paper with David Kazhdan) show that geometric crystals, in addition to providing families of piecewise-linear parametrizations of crystal bases, also reveal such hidden combinatorial structures as 'crystal multiplication' and 'central charge' on tensor products of crystal bases.

Thomas Bliem (•) (San Francisco State University) spoke on *Expected degree of weights in Demazure modules of* $\widehat{\mathfrak{sl}}_2$. He reported on a recent result [**?**], joint wiht S. Kousidis, about the characters of Demazure modules for the affine Lie algebra $\widehat{\mathfrak{sl}}_2$. Namely, they calculate the derivative of these characters at $h = 0$. One can immediately reduce this to only considering the "basic specialization" of the character, i.e., the generating function of the dimensions of the eigenspaces for a scaling element d. In this language, they compute the derivative of this function at $q = 1$. For the proof, they still use another language and say that we compute the expected value of the degree distribution. En passant they obtain a new proof of Sanderson's dimension formula for these Demazure modules.

Ben Brubaker (MIT) spoke on *Modeling* p*-adic Whittaker functions I*. This talk, which was expository, introduced the themes of the workshop through a discussion of p-adic Whittaker functions for unramified principal series. He mentioned known methods for giving explicit descriptions of these Whittaker functions, including new expressions as generating functions on crystal bases and other combinatorially defined data associated to bases for highest weight representations.

Daniel Bump (Stanford University) presented *Modeling* p*-adic Whittaker functions II*, which was a continuation of Brubaker's talk. This talk looked deeper into representations of p-adic Whittaker functions. For spherical Whittaker functions on an algebraic group, these are the same as the characters of the irreducible characters of the L-group, but the speaker was also interested in metaplectic covers of the algebraic group, in which case these are similar to but different from such characters. The speaker discussed representations coming from the six-vertex model in statistical physics and explained their relationship to the crystal base description.

Both parts of this talk were videotaped.

Adrian Diaconu (University of Minnesota) gave the talk *Trace formulas and multiple Dirichlet series*. He discussed the multiple Dirichlet series attached to the problem of computing higher moments of quadratic L-functions [**?**]. Such series are analogues of Weyl group multiple Dirichlet series, but correspond to general Kac–Moody lie algebras. The speaker explained why results connecting character sums to automorphic forms indicate new complications in constructing the correct multiple Dirichlet series.

Solomon Friedberg (Boston College) spoke on *Global objects attached to* p*-adic Whittaker functions*. He described some of the connections between p-adic Whittaker functions and global objects, and their implications for number theory.

Angèle Hamel (Wilfried Laurier University) presented the talk *Bijective Proofs of Schur Function and Symplectic Schur Function Identities*. She gave modified jeu de taquin proofs of two symmetric function identities. The first relates shifted $GL(n)$-standard tableaux to the product of a Schur function and $\prod_{i<j}(x_i + y_j)$. This result generalizes the work of Robbins and Rumsey, Tokuyama, Okada, and others. The second identity is a symplectic character identity relating the sum of a product of symplectic Schur functions to the product $\prod_{i=1}^{m}\prod_{j=1}^{n}(x_i + x_i^{-1} + y_j + y_j^{-1})$. This result has its origin in work of Hasegawa, King, and Jimbo and Miwa. It has previously been proved by Terada and Bump and Gamburd. This is joint work of Hamel with Ron King [**?**].

Joel Kamnitzer (University of Toronto) spoke on *Mirkovic-Vilonen cycles and MV basis*. Mirkovic-Vilonen cycles are a family of subvarieties of the affine Grassmannian, which under the geometric Satake correspondence give a basis for representations of reductive groups. The speaker began with older work giving a description of MV cycles using MV polytopes [**?**]. Then he explained more recent results, joint with Pierre Baumann, on properties of the resulting MV basis.

Alex Kontorovich (•) (Brown University) presented *Sieving in groups*. He discussed recent progress on the Affine Sieve, which aims to find primes or almost-primes in sets of integers generated by group actions. Applications include the Apollonian circle packing and prime entries in matrix groups. Portions of his talk were joint with Hee Oh, Jean Bourgain, and Peter Sarnak [**?**].

Kyu-Hwan Lee (•) (UConn) spoke on *Representation theory of p-adic groups and canonical bases*. In his talk, he interpreted the Gindikin-Karpelevich formula and the Casselman-Shalika formula as sums over Lusztig's canonical bases, generalizing the results of Bump-Nakasuji and Tokuyama to arbitrary split reductive groups. He also showed how to rewrite formulas for spherical vectors and zonal spherical functions in terms of canonical bases [**?**].

Peter McNamara (•) (MIT) gave the talk *Crystals and Metaplectic Whittaker Functions*. He studied Whittaker functions on nonlinear coverings of simple algebraic groups over a non-archimedean local field, and produced a recipe for expressing such a Whittaker function as a weighted sum over a crystal graph. In type A, he showed that these expressions agree with known formulae for the prime power supported coefficients of multiple Dirichlet series [**?**].

Ivan Mirkovic (UMass-Amherst) spoke on *Lusztig's Conjecture for Lie algebras in positive characteristic*, which is joint work with Bezrukavnikov and Rumynin. Their method is to reformulate a certain representation-theoretic problem in positive characteristic in terms of D-modules on flag varieties, coherent sheaves on the cotangent bundle of the flag variety and perverse sheaves on affine flag variety. His talk concluded with the remark that the same techniques should apply to quantum groups at roots of unity, but some parts of this investigation have not been worked out [**?**].

Maki Nakasuji (•) (Stanford University) talked on *Casselman's basis of Iwahori vectors and the Bruhat order*, which was joint work with Daniel Bump. Casselman defined a basis of the vectors in a spherical representation of a reductive p-adic group which is defined as being dual to the intertwining operators. They studied the explicit expression of this basis and obtained a conjecture, which is a generalization of the formula of Gindikin and Karpelevich. In this talk, she presented this conjecture and gave partial results using Hecke algebra with some examples and related combinatorial conjectures [**?**].

Sergey Oblezin (ITEP) *Whittaker functions and topological field theories* This talk was a survey of his recent results (in collaboration with A.Gerasimov and D.Lebedev) on $GL(N,\mathbb{R}\diagdown)$-Whittaker function and their q-deformations [**?**, **?**] In the first part of the talk he constructed an element $Q(g)$ of spherical Hecke algebra $H(G,K)$ with $G = GL(N,\mathbb{R}\diagdown)$ and $K = SO(N)$, acting in the space of K-invariant functions on G. Then the Whittaker function is an eigenfunction of $Q(g)$, with the eigenvalue given by a product of Gamma-functions. Actually, the eigenvalue of the Whittaker function can be identified with the Archimedean L-function $L(s,\mathbb{C}^N)$.

Next he explained how the Archimedean L-function can be interpreted as correlation functions in (a pair of mirror dual) topological sigma-models on two-dimensional disk. In particular, the Archimedean L-function was identified with an equivariant symplectic volume of the space of maps of a disk into a complex space $\mathbb{C}^N$ with certain boundary conditions.

In the second part of the talk he defined a q-deformed $GL(N,\mathbb{R}\diagdown)$-Whittaker function and introduced a pair of its integral representations. He showed that the q-deformed Whittaker function coincides with a character of a Demazure module of affine Lie algebra $\hat{gl}(N)$. This result can be interpreted as an (Archimedean) q-version of the Casselman-Shalika formula for p-adic Whittaker function. Then he explained an interpretation of q-deformed Whittaker functions in terms of the spaces of maps of projective line into (partial) flag varieties.

The talk concluded by outlining directions of further research and generalizations to other Lie algebras. This was the second lecture that was videotaped.

Omer Offen (•) (Technion) spoke on *Spherical Whittaker functions on metaplectic GL(r)*. He proved a formula for a basis of spherical Whittaker functions with a fixed Hecke eigenvalue of the n-fold metaplectic cover of $GL(r)$. The formula expresses the Whittaker function as a sum over the Weyl group. He then showed that the p-part of the Weyl group multiple Dirichlet series of type A constructed by Chinta-Gunnells is expressed in terms of such a spherical Whittaker function. The computation adapts the method of Casselman and Shalika to the case that multiplicity is finite but not one. In the case of $n = 1$ the speaker recovers the Shintani, Casselman-Shalika formula. This was joint work with G. Chinta [**?**].

Soichi Okada (Nagoya University) gave the talk *Symmetric functions and spinor representations*. Symmetric functions are useful to the representation theory of classical groups. In this talk, the speaker introduced a family of symmetric functions with coefficients in the ring of integers adjoining a new element e with the property $e^2 = 1$, and investigated their properties. These symmetric functions can be used to describe the structure of the representation ring involving spinor representations of the Pin groups [**?**].

Manish Patnaik (•) (Harvard University) presented *Hecke algebras for p-adic loop groups*. He explained how to make sense of convolution algebras of double cosets in p-adic loop groups. In the spherical case, there is a Satake isomorhism which identifies this algebra explicitly. Moreover, he described an explicit form of this isomorphism (due in the classical case to Langlands and Macdonald) and its connection to the affine Gindikin-Karpelevic formula. He also explained an "Iwahoric" version of this construction. This is joint work with Gaitsgory and Kazhdan [**?**].

Samuel Patterson (Göttingen) spoke on *Some challenges from number theory*. One of the major applications of the ideas discussed at this conference was to the distribution of the values of Gauss sums, that is, to the circle of ideas around the Kummer Conjecture. This application is by way of the theory of metaplectic groups and forms. Although much has already been achieved, and the necessary tools exist, the speaker pointed out that there is still unfinished business. In particular one has to move from the local theory to the framework of Dedekind rings. In the talk he described the approach of Chinta and Gunnells [**?**] and attempted to clarify what still needs to be done.

Arun Ram (University of Melbourne) spoke on *Combinatorics and spherical functions*. This talk gave a dictionary between the affine Hecke language and the Whittaker function language. He defined the affine Hecke algebra, stated the affine Hecke algebra version of the Gindikin-Karpilevic formula, and discussed the Casselman-Shalika formula [**?**] from the point of view of Lusztig's 1981 paper on q-weight multiplicities [**?**] and from the point of view of Macdonald polynomials [**?**]. At the end of the talk he explained why Whittaker functions and their relatives have natural expressions with terms indexed by paths in the path model (crystal).

Siddhartha Sahi (Rutgers University) presented *An introduction to Double affine Hecke algebras*. Double affine Hecke algebras were introduced by Cherednik who used them to prove the Macdonald cojectures on root systems. In this talk Sahi provided an introduction to double affine Hecke algebras following his joint work with Bogdan Ion [**?**].

Gordan Savin (University of Utah) gave the talk *Two Bernstein components for the metaplectic group*. The Weil representation decomposes as a sum of two irreducible representations, odd and even Weil representations. Let $M(e)$ and $M(o)$ be the components, in the sense of Bernstein, of the category of smooth representations of the metaplectic group $Mp(2n)$ containing the even and the odd Weil representation, respectively. Let V^+ and V^- be two orthogonal p-adic spaces of dimension $2n + 1$, with the trivial and non-trivial Hasse invariant, respectively. Let $B(+)$ and $B(-)$ be the Bernstein components of SO(V^+) and SO(V^-) containing the trivial representation. He described canonical equivalences of $M(e)$ and $B(+)$ and of $M(o)$ and $B(-)$. This was joint work with Wee Teck Gan.

Anne Schilling (UC Davis) spoke on *Combinatorics of Kirillov-Reshetikhin crystals*. She reviewed recent work with several coauthors (Masato Okado, Ghislain Fourier, Brant Jones) on combinatorial models for Kirillov-Reshetikhin crystals [**?**, **?**, **?**]. These are affine finite-dimensional crystals that play an important role in mathematical physics and representation theory. The affine structure makes it possible to define an energy statistics that can be used to define partition functions. At the end of her talk, she explained how the Kirillov-Reshetikhin crystals can be used to find expression for fusion/quantum cohomology coefficients.

Feedback and response from the conference

The workshop was well-attended by researchers at all points in their careers, and from countries all around the world, including Canada, USA, Israel, Russia, Japan, Germany, and Australia. After the completion of the workshop, the organizers received many positive comments from both senior and junior participants. One junior participant wrote "*It was great to learn about new connections between Whittaker functions (which I feel like I know pretty well) and exotic objects from representation theory.*" A senior participant wrote "*The range of perspectives about the subject of the conference—automorphic, representation theoretic, combinatorial, quantum, analytic—made this an especially exciting and valuable meeting. The organizers are to be congratulated for their excellent work.*" Another senior participant wrote "*This workshop really opened my eyes to a lot of beautiful stuff. I feel like my research has been jump-started.*" One senior participant wrote "*Two research projects have grown directly out of ideas I gleaned from some of the talks, and/or from discussions I had in Banff with other attendees. I appreciate that opportunity.*"

Based on these comments, we believe that the conference was successful. We also believe that by bringing together people from different fields with different strengths and interests, we have faciliated new collaborations. Because of the success of the workshop, we hope to apply to Banff in the future for another week, perhaps with the intent of running in 2012 or 2013, so that participants can give updates and progress reports, and so that new junior people can be introduced to this material.

Participants

Beineke, Jennifer (Western New England College)
Berenstein, Arkady (University of Oregon)
Bliem, Thomas (San Francisco State University)
Brubaker, Ben (Massachusetts Institute of Technology)
Bucur, Alina (UC San Diego)
Bump, Dan (Stanford)
Chinta, Gautam (City College of New York)
Diaconu, Adrian (Minnesota)
Frechette, Sharon (College of the Holy Cross)
Friedberg, Solomon (Boston College)
Gannon, Terry (University of Alberta)
Garland, Howard (Yale University)
Goldfeld, Dorian (Columbia University)
Goodman, Roe (Rutgers University)
Gunnells, Paul (University of Massachusetts Amherst)
Hamel, Angele (Wilfrid Laurier University)
Hoffstein, Jeffrey (Brown)
Ivanov, Dmitriy (Stanford University)
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Chapter 22

Inclusive fitness in evolutionary modeling (10w5017)

Jun 13 - Jun 18, 2010

Organizer(s): Peter Taylor (Queen's University), Geoff Wild (University of Western Ontario), Stuart West (University of Oxford)

Introduction

The notion of Darwinian fitness allows us to understand how natural selection influences the evolution of organismal traits. For example, we might explain a plant's morphology, or a bird's behaviour in terms of the fitness advantages (reproductive or survival benefits) such morphology or behaviour confers.

The notion of **inclusive fitness** is used specifically to understand how selection will act on those traits that influence the fitness of several genetically-related individuals simultaneously. Inclusive fitness recognizes that an individual may have a "genetic share" in the fitness of its neighbours, and so it is a more general (more "inclusive") measure of evolutionary success.

The development of inclusive fitness is usually credited to the biologist W. D. Hamilton, who used the idea to explain the selective advantage of altruistic traits [12]. Before Hamilton's seminal work was published, the advantage of altruistic traits was difficult to explain using fitness alone. The fact that an individual would be willing to decrease its fitness by some amount (traditionally denoted, c) to increase the fitness of a neighbour by some other amount (traditionally denoted, b) seemed counterintuitive to many evolutionary biologists. Hamilton, showed, that the selective advantage of these "problematic" traits is clear provided the recipient of the altruistic act is genetically related to the actor, and provided one adopts an inclusive fitness perspective. In this case, the fitness of the actor is $1 - c$, and the fitness of the recipient is $1 + b$; if the actor and the recipient are related to one another by a factor r, then the actor's inclusive fitness is simply, $1 - c + (1 + b)r$. Relative to the situation in which the actor does nothing (i.e. the situation in which both actor and recipient fitness is 1), the inclusive-fitness change is

$$-c + br. \tag{22.1}$$

A selective advantage is obtained whenever this change is positive, or, in biological terms, whenever b is large enough and the actor and recipient are sufficiently close genetic relatives.

This report details the activities and outcomes of our 5-day half-workshop devoted to inclusive fitness and evolutionary biology—the first such meeting of its kind. Ours was a real "workshop" in that, rather than focus on talks, we spent most of our time in discussion clarifying and amplifying a number of issues around the nature and scope of inclusive fitness theory. The next section gives an overview of the current state of inclusive-fitness theory; it also outlines how the current state of the theory shaped our goals. Although our workshop did not focus on talks, there were a number of short ones that served to connect our ongoing discussion with the major themes and ideas of the speaker. Sections 3 and 4 provide highlights from the various talks given and, in some cases, the discussion that followed. Section 5 details the outcome of the workshop and the new research directions it has spawned.

Overview of the Field and Recent Developments

Since Hamilton's work on altruism [12] was published, the inclusive-fitness approach to evolutionary modelling has been generalized and modified to deal with a wide range of biological scenarios. Inclusive fitness can now be used to study class-structured populations (in other words, populations composed of different kinds or "classes" of individual, e.g. males/females, young/old) [29], or populations that experience stochastic demographic fluctuations [26]. The inclusive-fitness approach can also effectively complement the application of other modelling tools (e.g. optimal control theory [4]), making mathematical results more palatable to even the most math-averse evolutionary biologist.

The success of Hamilton's central idea has also been buoyed by the development of an alternative modelling approach known as the **direct-fitness** method [31]. In fact we decided to revert to Maynard Smith's original terminology and designate this the **neighbour-modulated fitness** approach. This approach can be thought of as a "sister" to the inclusive-fitness approach. While inclusive fitness places an actor at the centre of the analysis, neighbour-modulated fitness focuses attention on the recipient (Fig. 22.1). Although inclusive fitness and neighbour-modulated fitness are, in most cases equivalent [32], neighbour-modulated fitness corresponds more closely to the approaches used in other mathematical treatments of evolution (e.g. game theory, and population genetics). In fact, links between inclusive-fitness and other mathematical treatments are sometimes more easily established using neighbour-modulated fitness [28, 24]. Whatever their relative advantages or disadvantages may be, inclusive fitness and neighbour-modulated fitness have emerged as a the primary tools for modelling what evolutionary biologists call **kin selection**.

The recent literature has seen a number of papers that either focus on the limitations of kin-selection theory [33, 7], or marvel at the breadth of its scope [35]. Although conflicting opinions have long been a part of kin-selection's history, their continued prominence is, at least in part, due to simple misunderstanding (misunderstanding that exists even among the theory's practitioners). One overall goal ("Goal I") of the workshop, then, was to **clear up misconceptions** by investigating our own assumptions and by **investigating theoretical connections** between inclusive fitness and other approaches to modelling evolution.

Theoretical developments aside, kin-selection theory has played a major role in developing our understanding of many natural systems [15]. We were interested, therefore, in determining what **future contributions** kin selection theory might make to biology as a whole ("Goal II").

Highlights, Goal I – Misconceptions and Theoretical Connections

Confusion between kin selection and inclusive fitness

In some treatments the terms "kin selection" and "inclusive fitness" seem to be used interchangeably. In other cases authors make a strict distinction between these terms. As we have suggested above, they are not really parallel terms but refer to different levels of organization. Our discussions identified the confusion between the notions of kin selection and inclusive fitness as a major problem in the current literature.

We took kin selection to be a process—the process whereby the frequency of particular copies of a gene (alleles) is affected when the behaviour of a bearer of that allele affects the fitness of relatives (kin) who will carry that allele with some positive probability. Kin selection is very often at work in social behaviour, as an organisms neighbours tend often to be kin.

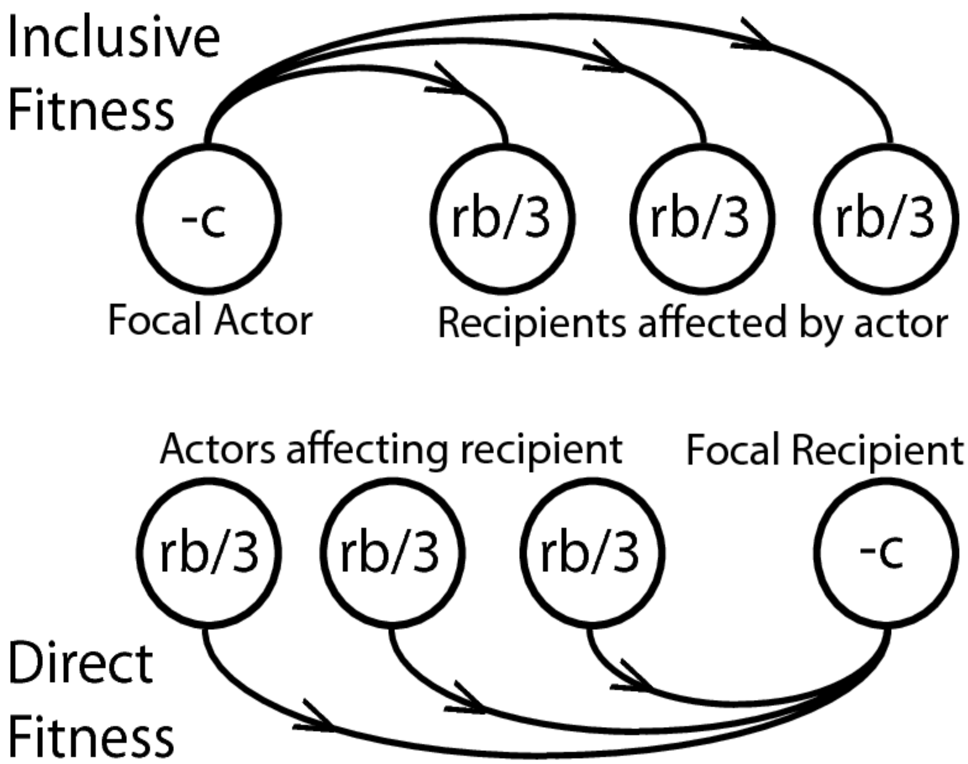

Figure 22.1: The inclusive-fitness approach (top) makes kin-selection based arguments by fixing attention on one actor, supposing that actor exhibits deviant behaviour and summing all the fitness consequences that deviant behaviour has for recipients related to the actor. As an example, suppose the actor's deviant behaviour causes it to decrease is own fitness by an amount c, but confers a benefit of $b/3$ to each of three recipients that are related to the actor by a factor of r. In this case the direction of allele frequency change is correctly predicted by $-c + 3 \times rb/3 = -c + rb$. In contrast, the neighbour-modulated fitness approach (bottom) makes a kin selection based argument by fixing attention on one recipient and supposing that its deviant genotype alters its behaviour and alters the behaviour of nearby actors at rate r. The same example above is now described as follows: the altered genotype of the recipient means that its fitness is reduced by c and that each of three actors are r times as deviant as the recipient, with each "unit of deviation" benefitting the recipient by an amount $b/3$. The allele-frequency change is again correctly predicted by $-c + rb$, but this result has been achieved by a different method of counting.

Inclusive fitness on the other hand is a method of keeping track of the frequency of an allele under the effects of selection. It is an accounting scheme cleverly designed to keep track of changing numbers of an allele over a generation of selection under precisely those circumstances in which kin selection operates, situations in which behaviour affects the fitness of kin. This accounting method has significant power both computationally and conceptually. Computationally, the focus of inclusive fitness at the individual rather than the genetic level, on whole organisms rather than on alleles, simplifies the calculations and in some cases can perform them when a more elemental population genetics approach would be intractable. Conceptually, the expressions provided by an inclusive fitness analysis can readily be interpreted in terms of fitness effects and relatedness between interactants and thereby it can tell us a story which enriches our understanding of the process and the different selective forces at work.

What (Who) are kin?

This is perhaps one of the most obscure questions in the field. From the beginning [12] "kin" were conceived either as relatives that bore standard labels (e.g. offspring, cousins, great uncles, etc.), or as neighbours in structured populations who, because of limited dispersal, were likely to share genes with the focal individual. In the former case, an individual's precise genetic relationship is known; in the latter case relatedness is entirely probabilistic in nature.

Although a considerable body of work has focused on the effect of kin selection on interactions in structured populations (interactions among "probabilistic relatives"), some researchers still to use the term "kin" in the narrow, "standard label" context only. For example, there has been much work on tag-based interactions, where tags (sometimes called "greenbeards") can be used to estimate the level of probabilistic relationship between interactants [9]. Here, individuals with similar tags are not considered "kin" per se, and so it is difficult for the average evolutionary biologist to determine whether kin selection is indeed at work.

Where do we draw the line between interactions that are kin-based and those that are not? In David Queller's presentation he raised the age-old distinction between "kin" and "kith" and suggested that this might be a useful distinction for our purposes. David put forward the idea that tag-based assortment be considered to be influenced by something he called **kith selection**. Discussion raised some doubt that a firm or useful line between kin and kith could be drawn.

Additivity and frequency dependence

Hamilton [12] did not require that the different fitness effects (i.e the costs and benefits) of an interaction be additive, but he did point out that relatedness could only be easily calculated – either through a pedigree or a recursive analysis – under an assumption of additivity of gene action both within and between individuals. When interactions have synergistic effects assumptions of additivity fail. While calculations can still be made in certain simple population structures, generalized relatedness measures (ones that depend on higher-order moments of the distribution of alleles) have to be used; these tend to be frequency dependent and difficult to calculate.

Andy Gardner and David Queller each presented a different perspective on dealing with synergy with the inclusive-fitness approach. Both perspectives were based on the well-known Price equation [22]. The Price equation expresses the change that occurs in the expected individual phenotype (a random variable, P) over the course of a single generation in terms of an individual's fitness (a random variable, W) and genetic make-up (a random variable, G). In the simplest of cases, the Price equation says,

$$\Delta \mathrm{E}(P) = \frac{\mathrm{Cov}(W, G)}{\mathrm{E}(W)}. \tag{22.2}$$

Gardner pointed out that, even with synergistic effects, the covariance in equation (22.2) can be decomposed using additional information about the phenotypes of its neighbour, say P', so that

$$\mathrm{E}(W)\Delta \mathrm{E}(P) = \beta\,\mathrm{Cov}(G, P) + \beta' \mathrm{Cov}(G, P'), \tag{22.3}$$

where β denotes the average effect of an individual's phenotype on its own fitness, and where β' denotes the average effect of a neighbour's phenotype on an individual's fitness. Note that β and β' are least-squares regression coefficients and may, in principle, depend on the frequency distribution of a particular allele ($\mathbf{p}$). The coefficients β and β' also analogues to the cost and benefit terms in equation (22.1), respectively. With this in mind, we might re-write equation (22.3) as

$$\mathrm{E}(W)\Delta\mathrm{E}(P) = \mathrm{Cov}(G, P)\left(-c(\mathbf{p}) + b(\mathbf{p})r\right). \tag{22.4}$$

By definition, $\mathrm{E}(W)$ is positive; we can assume (wlog) that $\mathrm{Cov}(G, P)$ is also positive. And so (22.4) tells us that the sign of the average change in phenotype is correctly predicted by a frequency-dependent version of line (22.1):

$$-c(\mathbf{p}) + b(\mathbf{p})r,$$

where $r = \mathrm{Cov}(G, P')/\mathrm{Cov}(G, P)$. In short, Gardner showed that the structure of Hamilton's expression (22.1) can be preserved in the face of synergistic interactions.

Using a different covariance decomposition, Queller showed

$$\Delta\mathrm{E}(P) \propto -c + br + d\tilde{r}, \tag{22.5}$$

where b and c are *exactly* the same as they were in equation (22.1), and $\tilde{r}$ is a coefficient of synergy. Equation (22.5) shows that synergistic effects can also be studied by adding frequency-dependent terms to Hamilton's classical frequency-independent expression (22.1).

While in certain cases the choice between (22.4) and (22.5) comes down to modeller's preference, in other cases the choice may have important practical consequences. In particular it was suggested that Queller's formulation (22.5) might be more amenable to experimental testing, or at least more convenient for purposes of experimental design. This suggestion is particularly interesting, but was not explored in depth during the workshop.

Relationship with evolutionary game dynamics

Interestingly, our half-workshop was twinned with another focused on Evolutionary Game Dynamics. There has been much confused debate over the past few years on the relationship between this active area of investigation and inclusive fitness, and we scheduled a number of common sessions in order to take advantage of this conjunction. Our view is that the opportunity to share ideas with those involved in evolutionary game dynamics was a valuable one, as was the chance to simply get to know one another better. It appears that new collaborations are already emerging from this time together.

On a more technical note, we should stress that both approaches – inclusive fitness and evolutionary game theory – address evolutionary change in behaviour, and although they are often equivalent [1, 5, 30] the approaches typically emphasize different model assumptions.

Wild presented some recent results [34] that take a kin-selection view of the branching-processes models sometimes used in evolutionary game dynamics [6]. Wild showed that, when the action of selection is weak, rare deviant strategies tend approximately to a quasi-stationary distribution in the population, and that relatedness coefficients used in kin-selection theory are simply expectations based on such distributions. He also suggested that expressions like those in (22.1) could be used in the same way the basic reproduction number is used in mathematical epidemiology—as a heuristic (but formally justifiable) substitute for less biologically transparent tools for testing the stability of dynamic systems.

Evolutionary game dynamics, of late, has paid much attention to evolution in lattice-structured populations, employing the moment-closure methods from statistical physics to make analytical progress [18, 19]. Lion presented results that use the moment closure methods, but he was able to interpret the results explicitly in terms of inclusive fitness. Although the main point of Lion's talk was to show how different assumptions about the way in which costs are incurred and benefits are accrued influence model predictions, the ease with which the kin-selection version of his analysis proceeded highlighted the fact that inclusive fitness can be used to streamline game-theoretic arguments.

Relationship with population genetics

Population genetics is the "gold standard" method against which other methods of modelling evolution are measured. Unfortunately when confronted with population structure, the calculations population-genetic methods require are often intractable. In such cases, inclusive fitness can provide a feasible way forward, but one must be willing to accept its technical assumptions.

Much the work carried out by Rousset and his colleagues over the past 10 years [23, 24, 25, 26] has focused on establishing a strong connection between results that are of interest to population geneticists (i.e. results related to the **fixation probability**, a type of probability of absorption), and results typically obtained through kin-selection means. Rousset detailed some of his work for us, and though it has been quite successful, challenges related to model populations with a particular structure ("isolation-by-distance" models) remain.

In his talk, Whitlock reviewed ideas of mutation rate, hard and soft selection, frequency-dependent selection, non-additivity, all familiar to us, but in quite a different context. He also pointed out that statistical methods for estimating the extent of population subdivision (and, by extension, relatedness [25]) in nature are readily available. The availability of these measures suggests that opportunities to test kin-selection theory in the "real world" abound.

Confusion among proponents of group selection/multilevel selection

There have been claims made in the literature that selection favours adaptations that cannot be understood in inclusive-fitness terms [13, 27, 37, 38]; only selection at the level of the group, it is argued, is able to provide the necessary adaptive context. As demonstrated elsewhere though [35], claims like these tend to misunderstand the the scope of kin-selection theory and its technical limitations. There was no disagreement within our workshop on the connections between kin selection theory and the theory that explicitly considers the action of selection at multiple levels of biological organization, and we did not discuss the issue very much (we mention it in this report only because the issue was raised in our workshop proposal). Furthermore, (as discussed below) Alan Grafen's presentation illustrated that inclusive fitness is not just an accounting method, but also an answer to the problem of what organisms should appear designed to maximise.

A role for group theory

In one of our final talks, Taylor outlined some remarkable work that uses ideas from group theory to solve kin selection problems in an elegant manner. Briefly, Taylor used the symmetry found in certain graph theoretic descriptions of social interactions to impose an algebraic group structure on his model population that made potentially difficult calculations rather easy. Given the success enjoyed by "evolutionary graph theory" [16], the workshop participants wondered if we will now see "evolutionary group theory."

Highlights, Goal II – Future Applications of Kin Selection

Inclusive fitness as a maximand

The inclusive fitness of an actor can, in some cases, serve as an objective function whose value will increase under the action of selection. In these cases, an actor's behaviour can be understood as an adaptation "designed" for the purpose of maximizing this objective function. This result can sometimes be misunderstood; it does not say inclusive fitness must always be maximized. As Grafen's presentation pointed out, the result outlines the conditions under which inclusive fitness should to be maximized in nature.

The inclusive-fitness-as-a-maximand result provides formal, mathematical justification for the explanations routinely used by field biologists [10]. As our discussions indicated, inclusive fitness maximization is taken for granted across much of biology; it is the basis for a great deal of field work and for grants awarded for field work [14]; it is also arguably the reason why higher organisms appear to have a sense of purpose that guides their behaviour. Understanding the extent to which biologists are justified in using inclusive-fitness theory in the field, then, is of utmost importance and more work needs to be done. In particular, Grafen's result needs to be extended to address cases in which the rates at which inclusive fitness costs and benefits accrue change with changing allele frequency.

Our discussion also revealed that there is currently no maximization result based on neighbour-modulated fitness (NMF). Given the preference some theoreticians have for this approach, we asked whether an NMF-based maximization result could be developed (and we conjectured that this might well be the case). Some members of our workshop will investigate this issue further.

Kin selection in realistic ecological scenarios

With kin-selection theory one is often able to find simplifications that make even complicated models tractable. In his talk, Alizon showed how he used this advantage of kin-selection theory to investigate how competition among the various pathogen strains that infect a host ultimately influence evolution.

In contrast, to Alizon's work, van Baalen reported that he had experienced tremendous difficulty when attempting to use inclusive fitness to model the evolution of certain colonial species of insect. This difficulty led van Baalen to suggest that inclusive-fitness methodology (or even direct-fitness methodology), may not be the appropriate tool for dealing with some of the more ecologically complex systems (participants did, however, offer suggestions to address van Baalen's concerns). Subsequent discussion revealed that several workshop participants were eager to establish a more general inclusive-fitness methodology—one which could handle even difficult sets of ecological assumptions.

Kin selection, autism and psychiatric disorders

In many instances, two neighbours have different "genetic interests" in their neighbourhoods. As a result their inclusive fitness interests are said to be **in conflict** and selection favours different conditional behaviours in each of the conflicting parties [8, 20, 21, 36]. When the "neighbours" in question are actually homologous genes, a phenomenon called **genomic imprinting** can result [11].

Úbeda's presentation addressed the conflict between (and genomic imprinting of) genes expressed in the mammalian brain—a genes thought to be involved in autism and psychiatric disorders like schizophrenia [2]. Specifically, Úbeda showed how kin-selection theory can inform clinical studies of these disorders. By combining inclusive fitness and life-history theory, he showed that sex-specific patterns of dispersal and sex-specific variation in mating success have the potential to influence patterns of genomic imprinting in genes disorder-related genes. His work demonstrated how human ecology might actually set the stage for the evolution of those patterns of imprinting now linked to autism and psychoses. The idea that kin-selection theory might act as a bridge connecting human ecology and psychiatry/medical genetics is an intriguing one that the members of the group will pursue.

A kin-selection perspective for sexual-selection theory

Alonzo's presentation focused on the possibility of new applications for kin-selection theory. In particular, she emphasised that whilst interactions between mates involves much potential for cooperation and conflict, the methods and insights of kin selection and inclusive fitness theory have rarely been applied to the field of sexual selection. A number of topics were raised where interactions between these areas could be useful, and several of of the participants are actively investigating these questions. Wild and West are examining how structured populations and relatedness between individuals could influence the strength of selection for conflict between mates. West, Wild and Gardner are using a combination of theoretical and empirical approaches to examine how promiscuity can reduce relatedness within families and hence reduce selection for cooperation, across a range of organisms from wasps to birds [3].

Outcome of the Meeting

Overall, the meeting served to focus our future research endeavours. Our attempts to eliminate sources of confusion within this key group of people identified points of disagreement that, in turn, put a spotlight on new questions to tackle. In particular,

- we will explore the utility of Queller's notion of "kith selection";
- we will determine whether there are indeed practical advantages to keeping frequency-dependent fitness changes separate from frequency independent ones, as was done in equation (22.5);
- we will investigate the extent to which algebraic group theory can be used to improve kin-selection methodology;
- we will investigate how reasonable it is to consider neighbour-modulated fitness (NMF) to be a maximand like inclusive fitness.

Points on which we could agree were equally valuable. Agreement established a common ground that will form the foundation for future meetings, at BIRS or elsewhere. Many participants found they had common interests, despite their (arguably) disparate backgrounds. Indeed, it appears that this meeting will help smaller groups of workshop participants achieve progress on issues related to the application of kin-selection theory to

- the evolution of complex ecological interactions;
- the interplay between human ecology and psychiatry/medical genetics;
- the evolution of cooperative and antagonistic interactions between the sexes.

In closing, we wish to thank BIRS for helping us bring together researchers from around the world to discuss inclusive-fitness theory. We certainly look forward to the future progress this meeting will have enabled.

Participants

Alizon, Samuel (ETH Zentrum, Zrich)
Alonzo, Suzanne (Yale University)
Day, Troy (Queens University)
El Mouden, Claire (Department of Zoology)
Foster, Kevin (Harvard University)
Gardner, Andy (University of Oxford)
Grafen, Alan (Oxford University)
Greenwood-Lee, James (University of Calgary)
Lehmann, Laurent (Stanford University)
Lion, Sébastien (Royal Holloway, University of London)
Pen, Ido (University of Groningen)
Queller, David (Rice University)
Ronce, Ophelie (University of Montpellier 2 CNRS)
Rousset, Francois (Montpelier University)
Taylor, Peter (Queen's University)
Ubeda, Francisco (University of Tennessee)
Van Baalen, Minus (CNRS UMR 7625 Ecologie et Evolution)
West, Stuart (University of Oxford)

Whitlock, Mike (University of British Columbia)
Wild, Geoff (University of Western Ontario)

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Chapter 23

Evolutionary Games (10w5020)

Jun 13 - Jun 18, 2010

Organizer(s): Karl Sigmund (University of Vienna), Ross Cressman (Wilfrid Laurier University), Christine Taylor (Harvard University)

Overview of the Field

Since the workshop held at BIRS in 2006 on the same topic, evolutionary game theory has continued to expand in the directions identified there as well as in several new directions. There seems to be a tendency to reach out from the founding concept of an evolutionarily stable strategy, towards related concepts such as continuously stable strategies and stochastically stable strategies, towards the analysis of polymorphic equilibria and complex population structures, towards a dynamic underpinning of the evolutionary process based on different transmission mechanisms, towards the investigation of how individual information and ongoing interactions impact population behavior, towards a reinterpretation of existing models of population dynamics using a game-theoretic perspective. These directions lead to a large variety of stochastic processes and deterministic dynamics whose interrelation is far from being fully understood.

The 2010 workshop aimed to bring together people with different modeling approaches and to allow them to appraise the state of the art in the neighboring fields. This seems all the more useful as evolutionary games have been approached within several different disciplines with very different traditions and also different channels of communication (journals, conferences etc). We mention here classical, economy-based game theory versus biology-driven evolutionary models; probabilistic reasoning based on finite population models versus ordinary differential equations assuming infinite, well mixed populations; equilibrium concepts versus complex attractors; long-term versus short-term evolution; frequency-dependent population genetics versus learning models based on imitation, or endogenous aspiration levels, etc.

To give some specific examples, extensive-form games have for decades been analyzed entirely by static classical game theory techniques based on rationality assumptions, but have recently been exhaustively studied from a dynamic perspective in a monograph [8] on evolutionary games and applied to existing models such as signaling games[19]. Classical stochastic processes used in genetics, as for instance the Moran process, have provided the basis for an entirely new analysis of evolutionary dynamics in games in finite populations[15, 23], using concepts such as substitution and fixation. There are surprising relations between different types of deterministic game dynamics, as for instance between the orbits of the best-reply dynamics and the time-averages of solutions of the replicator equation[18]. Non-linear payoff functions are increasingly well understood, for instance through adaptive dynamics[20]; population games have been investigated in depth[28]; games with continuous strategy spaces become increasingly important, and often lead to other predictions than in the discrete case[17]; games on graphs [22, 25] and dynamic graphs [14, 26] are of obvious importance for the evolution of cooperation. The phase-transitions in spatial games attract more and more investigators wielding the tool-box of statistical mechanics and power laws[31], etc.

The main focus of the workshop was on mathematical methodology. However, since most of the new methods have been devised by applying them to very concrete examples from biology or experimental games, it was important to also have several lectures concentrating on new applications. These include the study of animal movement between spatially separated patches through the habitat selection game[1] . Such new directions enhance our understanding of evolutionary methods that predict individual behavior modeled by game interactions.

In addition, experimental work on the evolution of cooperation in Public Goods and Prisoner's Dilemma games pioneered by Fehr, Gächter, Milinski, et al. [12, 13] are gaining new impetus in the last couple of years. New results from groups led by Nowak and Cressman point to interesting cross-cultural similarities and differences.

Presentation Highlights

During the workshop week, there were two concurrent programs: one on Evolutionary Games and the other on Inclusive Fitness in Evolutionary Modeling. Many of the topics discussed in both workshops are of mutual interest to all participants, hence there were many interactions between the two workshop during open discussion sessions in the Max Bell Lecture Hall as well as informally in the lounge and dining hall.

In the first half of the morning, both workshops gathered together for lectures from the Inclusive Fitness group. David Queller (Rice University) spoke on non-additivity, joint effects, frequency dependence and green beard effect; Andy Gardner (University of Oxford) on the genetic theory of kin selection; Mike Whitlock (University of British Columbia) on applications of evolutionary model in discrete and spacial population to evolution of recessive alleles and social evolution; Sébastien Lion (University of London) on inclusive fitness theory applied to complex and realistic ecological dynamics; Samuel Alizon (ETH) on kin selection methods in evolutionary epidemiology; and finally Suzanne Alonzo (Yale University) on how interactions within and between sexes affect the evolution and ecology of reproductive traits, paternity and male tactics, sexual conflict and selection using phenotypic and genetic modeling approaches with ocellated wrasse as the focal species.

The rest of the day was filled with Evolutionary Games talks, with occasional visits from the Inclusive Fitness group as well from the Focused Research Group on Discrete Probability. All of our twenty participants gave talks covering a wide spectrum of themes:

- A few of our speakers presented work of interest to both workshops in attendance.
  - Jeff Fletcher (Portland State University) affirmed his belief that inclusive fitness is an accounting method, not a fundamental mechanism. He argued that various theories of the evolution of altruism rely on the same underlying requirement for sufficient assortment between the genotype in question and help from others.
  - Feng Fu (Harvard University) presented a minimal model of in-group favoritism in homogeneous populations. The population is divided in groups according to each individual's randomly assigned tag. Each individual has the same level of in/out group helping tendency. Individuals' tags and behavioral strategies are both heritable traits that are subject to mutation and selection. Feng derived an analytical condition for cooperation to evolve under weak selection using coalescent theory. The critical benefit-to-cost ratio reaches minimum when individuals only help in-group members and refrain from helping out-group members.

  - Sabin Lessard (Montréal University) discussed the effects of relatedness and population subdivision on long-term evolution based on interactions in finite group-structured populations[21].
  - Recent work of Hisashi Ohtsuki (Tokyo Institute of Technology) on evolutionary games in island model is of particular interest to the inclusive fitness group. Hisashi investigated the evolutionary dynamics of games played in a subdivided population which follows the Wright's island model. He found that limited dispersal produces positive association among neighbors' strategies, hence coefficients of relatedness appear in the main equation. His results can be interpreted in terms of inclusive fitness, and several previous results follow this setup.

- Theoretical studies of evolutionary games continues to flourish.

  - Tibor Antal (Harvard University) presented his recent work with Fu, Nowak, Ohtsuki, Tarnita, Taylor, Traulsen, Wage and Wakeley using perturbation theory to study games in phenotype space under weak selection[2, 3]. The main focus is on determining the strategy that is most abundant in the long run. The technique developed can be applied to games with multiple strategies and games in structured populations.
  - Joseph Apaloo (St. Francis Xavier University) gave an overview on the mathematical theory for describing the eventual outcome of evolutionary games involving single species as well as multi-species evolutionary models[4].

- The effect of reputation, reward, and punishment on the evolution of cooperation and altruism remains a fascinating topic. Prisoner's Dilemma and Public Goods games have become the mathematical metaphors for game theoretical investigations of cooperative behavior in respectively pairs and groups of interacting individuals. Cooperation is a conundrum because cooperators make a sacrifice to benefit others at some cost to themselves. Exploiters or defectors reap the benefits and forgo costs. Despite the fact that groups of cooperators outperform groups of defectors, Darwinian selection or utilitarian principles based on rational choice should favor defectors.

  - Indirect reciprocity is one of the main mechanisms to explain the evolution of cooperation. Ulrich Berger (Vienna University of Economics Business Administration) introduced a new notion of "tolerant scoring", a first-order assessment rule with built-in tolerance against single defections, to understand the evolution of cooperation in Prisoner's Dilemma Game[6]. The upshot of the analysis in this framework is that all individuals are discriminators and most cooperate.
  - There have been much interest and progress in experimental study [11, 12, 13, 27] on the evolutionary of cooperation. Ross Cressman (Wilfrid Laurier University) reported results from two experiments [34] that test the effects of punishment and/or reward schemes on the cooperative behavior of players in repeated Prisoner's Dilemma (PD) and Public Goods (PGG) games. Subjects for both game experiments were university students in Beijing. For the PD experiment, costly punishment does not increase the average level of cooperation compared to the control experiment where this option is not available. This result contrasts with several similar experiments conducted in western societies. On the other hand, in the PGG control experiment (i.e. the standard repeated PGG without reward or punishment), the average contribution levels to the public good match closely those found in the same control conducted in Boston. The PGG experiment shows that combined reward and punishment schemes are most effective in increasing contributions, followed by punishment on its own and that reward on its own has no significant effect on contributions. These results differ from those in Boston that exhibited little difference in contribution levels when players reward, punish, or reward and punish each other between rounds. The experiments are discussed in relation to cultural differences in attitudes to a player's reputation and to institutional incentive schemes to increase the cooperative behavior of its members.

  - Christoph Hauert (University of British Columbia) outlined his recent work with Peter Forsyth, an undergraduate student, on incentives for cooperation which may defeat the social dilemma of cooperation. Negative incentives based on the punishment of shirkers are efficient in stabilizing cooperation once established but fail to initiate cooperation. In the complementary case of positive incentives created by rewarding those that did contribute to the public good, cooperation can be initiated in interaction groups of arbitrary size but, in contrast to punishment, can not be stabilized. In fact, the dynamics of reward is complex and dominated by unpredictable oscillations.
  - József Garay (Eötvös University) considered the four behavioral traits: envy (reducing the fitness of more successful individuals at one's own cost), charity (increasing the fitness of less successful individuals at one's own cost), spitefulness (decreasing others' fitness unconditionally at one's own cost), and selfishness (neither decreasing nor increasing others' fitness). He found that when damage is additive, envy dominates selfishness if the cost of envy is low, envy and selfishness can replace spitefulness when cost of damage is high, moreover, envy is selected in a mixed population of all four strategies. When damage is multiplicative, coexistence of selfish and envious strategists is possible. Envy is a conditional spiteful strategy, so in envious groups there is less damage than in spiteful groups, hence envy decreases the total cost of the spiteful competition. In a simple kin-selection scenario the envious-spiteful strategists (envious within its kin and spiteful outside its kin) outperform selfish and spiteful ones as well.
  - Karl Sigmund (University of Vienna) provided yet another perspective on the effect of punishment in the evolution of cooperation. Karl and his colleagues analyzed the effect and dynamics of peer versus pool punishment in public goods games. It is well known that sanctions promote collaboration in public goods games, but since they are themselves a public good, second-order free riders, who do not punish defectors, can exploit this and subvert cooperation. The punishment of second-order defectors is called second-order punishment. Most experiments use peer punishment, which is ill suited for second-order punishment[9, 30]. But another form of punishment, called pool punishment, is better suited to the task. In an open competition of peer with pool punishment, the latter prevails if and only if second order punishment is included. Pool punishment trades efficiency for stability. It is an implementation of the self-financed contract enforcement mechanisms which are frequently found in real-life institutions implementing the 'governance of the commons'.

- Michael Doebeli discussed his recent work with Ispolatov on the origin and maintenance of phenotypic diversity in a population or species[10]. They extend the classical Gaussian model for frequency-dependent competition from one to many phenotypic dimensions. Their analysis indicates that for a number of phenotypes, each of which is under stabilizing selection and frequency-dependent selection, where frequency-dependence is sufficiently weak to induce maintenance of diversity along any of the phenotypic components in isolation, then any interaction between phenotypes strongly increases the tendancy for diversification.

- Vlastimil Krivan (Academy of Sciences of the Czech Republic) analyzed models of optimal foraging theory with respect to evolutionarily stability of optimal strategies[1]. An improvement is made on the original prey and patch models introduced by Charnov which assume frequency independent fitness functions that are proportional to energy intake rate by a single consumer. In the dynamic setting with frequency dependent fitness functions and corresponding evolutionarily stable strategies, partial preferences for food types arise.

- At our 2006 workshop, Hauert, Lieberman, and Ohtsuki showed a simple rule ($r > k$) for the evolution of cooperation on graphs and social networks[25], namely the benefit to cost ratio must exceed the average degree of a node. Since then, Pacheco and Santos showed that social diversity promotes the emergence of cooperation in Public Goods Games, particularly with fixed contribution[29].

- Building upon these work on games on graphs, Cong Li (Chinese Academy of Science) together with Cressman and Tao explored three main questions: How does network structure affect the evolution of cooperation? Do different network structures work similarly? Which is the best network structure for the promotion of cooperation? Many biological, technological and social networks lie somewhere between two extremes which are regular and random networks. Watts and Strogatz [33] found these systems can be highly clustered, like regular lattices, yet have small characteristic path lengths, like random graphs, and they called these networks the 'small-world' networks. Barabási and Albert [5] also noticed that a common property of many large networks is that the vertex connectivities follow a scale-free power distribution, i.e., $P(k) \sim k^{-\gamma}$, where $P(k)$ is the probability that a vertex in the network interacts with other vertices. Cong and his colleagues found that for 'small-world' networks, network structure makes no difference in promoting cooperation under weak selection, regular graphs does best in PG games, promotion of cooperation is however sensitive to network structure under strong selection, and fixed contribution works to promote cooperation in 'small-world' and random graph for PD games but not for PG games under weak selection. For scale-free networks, the simple rule $r > k$ fails for some PD and PG games, and furthermore, scale-free network promotes cooperation more efficiently than regular, small-world, and random network.
- Jacek Miękisz (Warsaw University) discussed the Prisoner's Dilemma game on the Barabási-Albert scale-free network with costs of maintaining links. He showed that a population of players undergoes a sharp transition from the cooperation phase to a mixed cooperation/defection phase as the cost passes through its critical value. In the random matching model, players are randomly matched with a finite number of opponents - equal to the number of neighbors in the corresponding spatial model. Jacek showed that for the snow drift game, spatial structure promotes cooperation much better than the random matching of players.
- György Szabó (Research Institute for Technical Physics and Materials Science) talked about his work on social dilemmas in spatial systems with collective strategy updates[32]. Social dilemmas are studied with players following unconditional cooperative or defective strategies. The players are located on a square lattice and each player's income is collected from 2×2 games (including Prisoner's Dilemma, Stag Hunt and Hawk-Dove games) with the four nearest neighbors. The evolution of strategy distribution is governed by random sequential strategy updates. During an elementary process several players choose new strategies at random in a way favoring the income increase of a group they belong to. The strategy update is stochastic and the magnitude of noise is characterized by a "temperature" parameter using the Fermi-Dirac function that provides smooth transition from 0 to 1 in the strategy adoption probability. Systematic investigations are performed to determine the average frequency of cooperators in the stationary state when varying the payoffs, the size of group, and also the number of players who can modify their strategy simultaneously for a fixed noise level. The present dynamical rules support the maintenance of cooperation in two ways. On the one hand, cooperators and defectors can form chessboard like structure providing optimum income for the whole society if the sum of sucker's payoff and temptation to choose defection is sufficiently high. On the other hand, the enforcement of group interest supports cooperation within the region of Prisoner's Dilemma even if only one or two players can choose new strategy within an elementary step.

• Evolutionary game dynamics continue to spark interesting work, both in existing and new directions.

- Marius Ochea (Tilburg University) , an economist, studied repeated Prisoner's Dilemma game under logit dynamics[24], focusing on five strategies: AllC (unconditional cooperators), AllD (unconditional defectors), TFT (reactive players), GTFT (Generous Tit-for-Tat), and Pavlov (Win-StayLoseShift). He discovered that the Rock-Paper-Scissors (RPS) phenomenon is abundant in the 3×3 ecologies involving Pavlov and GTFT players, and in the 4×4 ecology without GTFT, RPS cycles coexists with a chaotic attractor. AllC is detrimental to the TFT, GTFT, and Pavlov players in the 4×4 ecologies leading to AllD monomorphism, and Pavlov players succeeds in the 4×4 ecologies without AllC and goes to extinction in the 5×5 setting with AllC.

- Another economist, Bill Sandholm (University of Wisconsin), discussed his recent work on sampling best response dynamics and deterministic equilibrium selection. Bill and his colleagues consider a model of evolution in games in which revising agents observe the strategies of k randomly sampled opponents and then choose a best response to the distribution of strategies in the sample. They prove that under the resulting deterministic evolutionary dynamics, which they call k-sampling best response dynamics, any iterated $(1/k)$- dominant equilibrium is almost globally asymptotically stable. They show as well that this sufficient condition for stability is also necessary in super-modular games. Since the selection occurs by way of a deterministic dynamic, the selected equilibrium is reached quickly; in particular, the long waiting times associated with equilibrium selection in stochastic stability models are absent.

  Bill also demonstrated the latest version of his shareware program **Dynamo**, a suite of easy-to-use Mathematica notebooks for generating phase diagrams, vector fields, and other graphics related to evolutionary game dynamics. The software is a great tool which provides intuitive and geometric perspective for researchers. The software is publicly available at

  `http://www.ssc.wisc.edu/˜whs/dynamo/index.html`

  Bill's forthcoming book, Population Games and Evolutionary Dynamics, offers a systematic, rigorous, and unified presentation of evolutionary game theory, covering the core developments of the theory from its inception in biology in the 1970s through recent advances. It will be a valuable resource for students and researchers in the field.

- Evolutionary game dynamics of two players with two strategies has been studied in great detail. These games have been used to model many biologically relevant scenarios, ranging from social dilemmas in mammals to microbial diversity. Some of these games may, in fact, take place among an artbitary number of individuals and not just between two. Two participants presented interesting work on the dynamics of multiplayer games.

  - It is often difficult to determine the exact payoffs in a game, furthermore, payoff values are frequently variable rather than constant. In finite random games, where there are n players, each having finitely many strategies with payoffs that are independent and identical continuous distributions, cooperation is preferable when a Nash equilibrium is not Pareto-optimal. Christine Taylor (Harvard University) gave a brief overview on the Pareto-inefficiency of Nash equilibrium solutions in finite random games[7], and then explored the relationship between cooperation and self-interest in certain classes of two-player multi-strategy games and multi-player two-strategy symmetric games. She found that cooperation is more advantageous in two-player multi-strategy random games as the number of strategies increases, and as the correlation between the two player's payoffs increases. For symmetric multiplayer two-strategy random games, cooperation becomes more beneficial as the number of players increases.
  - Arne Traulsen (Max-Planck-Institute for Evolutionary Biology) studied game dynamics of symmetric two-strategy multiplayer games[16]. In this setting, one can calculate fixation probabilities and compare them to each other or to neutral selection in the spirit of the $1/3$-rule. For games with multiple players and more than two strategies, some statements derived for pairwise interactions no longer hold. For example, in two player games with any number of strategies there can

be at most one isolated internal equilibrium. For d players with n strategies, there can be at most $(d-1)^{n-1}$ isolated internal equilibria. Multiplayer games show a great dynamical complexity that cannot be captured based on pairwise interactions. The results hold for any game and can easily be applied to specific cases, such as public goods games or multiplayer stag hunts.

Many of the presentation slides are posted online at

`http://temple.birs.ca/~10w5020/`

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Outcome of the Meeting

We are most grateful to BIRS for the opportunity to bring together a group of researchers from scientifically as well as geographically diverse areas to the majestic setting of Banff National Park again, 4 years after our 2006 workshop. All participants have enjoyed learning the latest work of their colleagues, not to mention the incredible views, great selection of food in the dining hall, excellent lodging, and inviting atmosphere of the common lounge. As the presentation summaries illustrate, our colleagues have made considerable advances in various branches of evolutionary games since our previous meeting, along the paths highlighted in our 2006 workshop and in new directions. We are particularly appreciative of the hospitality and administrative support from Brenda Williams and her staff. The organizers are unanimous that the efficient BIRS staff has made the BIRS workshops the easiest conference to organize.

The reduced group size for this workshop has not dampened the enthusiasm of participants. Many fruitful exchanges took place during the presentations, as well as in the lounge, dining hall, not only within Evolutionary Games workshop, but also with members of the Inclusive Fitness workshop. BIRS workshops, as always, have left participants feeling refreshed and inspired to forge new collaborations. We are already looking forward to meeting again to discover our progresses at the next Banff workshop.

The rainy weather for most of the week kept participants working together longer than otherwise. A large number of our workshop participants, who stayed on to attend the 14th International Symposium on Dynamic Games and Applications conveniently held in Banff immediately after our workshop, reported that they were rewarded with sunny skies and great hikes at the week's end.

Participants

Antal, Tibor (Harvard University)
Apaloo, Joe (St. Francis Xavier University)
Berger, Ulrich (WU Vienna)
Cressman, Ross (Wilfrid Laurier University)
Doebeli, Michael (University of British Columbia)
Fletcher, Jeff (Portland State University)
Fu, Feng (Peking University)
Garay, József (Eötvös Loránd University)
Hauert, Christoph (UBC)
Krivan, Vlastimil (Biological Research Center)
Lessard, Sabin (Université de Montréal)
Li, Cong (Chinese Academy of Sciences)
Miekisz, Jacek (Warsaw University)
Ochea, Marius (University of Tilburg)
Ohtsuki, Hisashi (Japan Science and Technology Agency, Tokyo Institute of Technology)

Sandholm, Bill (University of Wisconsin)
Sigmund, Karl (University of Vienna)
Szabo, Gyorgy (Research Institute for Technical Physics and Materials Science)
Taylor, Christine (Harvard University)
Traulsen, Arne (Max-Planck-Institute for Evolutionary Biology)

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Chapter 24

Geometric Analysis and General Relativity (10w5011)

Jun 20 - Jun 25, 2010

Organizer(s): Lars Andersson (Max-Planck-Institut fur Gravitationsphysik) Mihalis Dafermos (University of Cambridge) Greg Galloway (University of Miami) Daniel Pollack (University of Washington)

Overview of the Field

General Relativity is one of the fundamental theories of modern physics. Since its formulation by Einstein in 1915, it has been a cornerstone of our understanding of the universe. Mathematical research on the problems of general relativity brings together many important areas of research in partial differential equations, differential geometry, dynamical systems and analysis. The fundamental mathematical questions which arise in general relativity have stimulated the development of substantial new tools in analysis and geometry. Conversely, the introduction of modern tools from these fields have recently led to significant developments in general relativity, shedding new light on a number of deep and far reaching conjectures.

The area of interaction between the analysis of the Lorentzian Einstein equation, the field equation of general relativity, and other geometric partial differential equations is large. Important classes of hyperbolic equations such as the wave maps equation and the Yang-Mills equation are connected with the Einstein equation at a fundamental level, and harmonic analysis methods used in the study of those equations are being applied to the Einstein equation. Fluids as well as kinetic models such as the Vlasov equation appear as matter models.

The Einstein equation shares issues of convergence, collapse and stability with important geometric evolution equations such as the Ricci flow and the mean curvature flow. Asymptotic behavior at singularities as well as questions related to asymptotic geometrization are being intensely studied in the case of the Einstein equation as well as in the cases of the Ricci and the mean curvature flows. There is the potential for continued cross fertilization between these fields. Elliptic problems and techniques arise in studying the initial data sets in the context of the Cauchy problem.

The analysis of the Riemannian Einstein equation plays a fundamental role in modern Riemannian geometry and geometric analysis. Recent developments in General Relativity have brought many ideas and techniques which have been developed in the Riemannian context to bear on the Lorentzian Einstein equations. An example of this type of development is the realization that apparent horizons, which are relevant for our understanding of quasilocal aspects of black holds, have many properties in common with minimal surfaces. Many recent results in this area have been inspired in part by this connection. Other areas of geometry which have played a significant role in general relativity in recent years include the geometrization of three-manifolds; convergence and collapsing phenomena in Riemannian manifolds with bounds on their curvatures, the study of manifolds admitting metrics of positive scalar curvature, and curvature flows for hypersurfaces.

Recent Developments and Open Problems

One of the fundamental mathematical results in relativity is the establishment of the global nonlinear stability of Minkowski space due to Christadoulou and Klainerman. Important recent work by Lindblad and Rodnianski has provided an alternative treatment of this. One of the most outstanding problems in the field concerns the analogous question for black hole spacetimes, namely the nonlinear stability of the Kerr black holes. While this problem is unlikely to be resolved in the near future a number of recent results are relevant to it and will likely be part of the ultimate resolution. This includes the analysis of the interior of black holes for certain spherically symmetric non-vacuum spacetimes due to Dafermos; and the analysis of the decay for solutions of the wave equation and Price Law decay within black hole spacetimes due to Dafermos and Rodnianski. Stability results have also been recently established for $U(1)$-symmetric spacetimes by Choquet-Bruhat and for certain hyperbolic models by Andersson and Moncrief.

Intimately related to these questions are the Cosmic Censorship Conjectures due to Penrose, which relate to the presence of naked singularities and the fundamental issue of determinism for the physical model posed by the Einstein field equations. The recent verification of the Strong Cosmic Censorship for the Gowdy spacetimes by Ringström represents a significant positive result in this area.

Christodoulou has proved that a concentration of radiation can lead to the formation of closed trapped surfaces in vacuum, in particular assuming the standard weak cosmic censorship schenario this leads to formation of black holes arising solely from the focusing of sufficiently strong incoming gravitational waves. This result and the so-called short-pulse method it relies on can be expected to lead to important advances and there is already related work by Klainerman and Rodnianski as well as others. This work complements the earlier work of Schoen and Yau, and others on the formation of black holes due to concentration of matter. There remain important open problems in this direction.

Other important recent advances concerning the Cauchy problem for the Einstein equations have come from Klainerman-Rodnianski and Szeftel on well-posedness and extention criteria for the vacuum equations and from Planchon-Rodnianski on the question of uniqueness without a loss in regularity.

The quasi-local model for black holes alluded to above is developed in the context of the study of marginally outer trapped tubes. This notion was introduced by Hayward and subsequently developed by Ashtekar and Krishnan. Significant recent mathematical work in this area has been done by Andersson, Dafermos, Galloway, Mars, Metzger, Schoen and Simon. New PhDs such as Eichmair and Williams have recently emerged into the field having done work in this area.

Global inequalities have played a large role in general relativity, going back at least as far as the proof the positive mass theorem due to Schoen and Yau. An important generalization of this was recently obtained via the proofs of the Riemannian Penrose inequality due to Huisken-Ilmanen and Bray. The long standing attempt to generalize the notion of mass in relativity to one which is locally defined has seen new ideas introduced due to the work of Shi and Tam and the subsequent results of Liu-Yau and Wang-Yau. Recognizing the need for low regularity formulations of the fundamental quantities in relativity Huisken has recently developed formulations of these global inequalities in terms of isoparametric inequalities which hold in a very rough setting.

The analysis of initial data sets and the implications of this for their spacetime developments has been the subject of a great deal of recent attention. Many mathematical developments in this area stem from the introduction of gluing techniques from geometric analysis. Corvino's construction of vacuum spacetimes which are Schwarzschild outside of a compact set, and the extension of this method by Corvino-Schoen and Chruściel-Delay have had a significant impact. The combination of this with conformal gluing methods by Chruściel, Isenberg and Pollack have led to examples of vacuum spacetimes with no constant mean curvature slices. Building on work of Holst, Nagy and Tsogtgerel, Maxwell has very recently produced the first general existence result for the vacuum constraint equations with no restrictions on the mean curvature. Nonetheless the issue of understanding the basic questions of the existence and uniqueness for solutions of the Einstein constraint equations remains largely open in general for initial data sets with arbitrary mean curvature.

Presentation Highlights

The talks for the meeting were solicited in two ways. The organizers asked all of the participants to send us a title and abstract if they wanted to give a talk. In addition we asked specific participants, whose recent work was known to be of widespread interest, to give talks. All daytime talks were scheduled for 50 minutes, to allow sufficient time afterward for questions and discussion. Rather than fill every available slot with talks, we made an effort to preserve a good deal of time for informal discussion and collaboration. This was very successful and groups formed spontaneously in the lecture room and lounge as well as in outdoor excursions around BIRS.

One particularly successful aspect of the meeting were the four post-dinner talks which we arranged to be given by Gerhard Huisken, Richard Schoen, Igor Rodnianski and Shing-Tung Yau. These hour long talks by well established leaders in the field were meant to introduce the background and most recent developments in primary and active areas of study within Geometric Analysis and General Relativity. This led to four wonderful talks, which were very much appreciated by all participants.

A summary of each of the talks given at the meeting follows.

Mihalis Dafermos, Superradiance, trapping, and decay for waves on Kerr spacetimes in the general subextremal case $|a| < M$

Mihalis Dafermos spoke on his joint work with Igor Rodnianski on boundedness and decay estimates for the free scalar wave equation on the exterior Kerr spacetime. A proof of boundedness and decay for the scalar wave equation on the Kerr exterior spacetime is an important test case for the black hole stability problem, a special case of which is the problem of non-linear stability in vacuum for the Kerr black hole spacetime. The black hole stability problem is one of the central open mathematical problems motivated general relativity. Recent work of Dafermos and Rodnianski, Tataru and collaborators as well as Andersson and Blue has provided such estimates for the case of a slow rotating Kerr spacetime, i.e. $|a| \ll M$. This case is characterised by the fact that superradiance can be treated as a small parameter. In his talk, Dafermos reported on his recent joint work with Rodnianski proving decay in the general subextreme case $|a| < M$. Key to this approach is the construction of distinct multiplier estimates taylored to the superradiant and trapped frequency ranges, respectively. The approach exploits in particular the insight that for the entire subextremal range, superradiant frequencies are not trapped in the high frequency limit.

Gustav Holzegel, Asymptotic behavior of spacetimes approaching a Schwarzschild solution

In his talk, Gustav Holzegel considered the problem of proving, given a vacuum spacetime which approaches a Schwarzschild solution, decay to the future for the spacetime curvature. In particular, assuming decay of appropriate norms of the Ricci rotation coefficients and their derivatives, he proved boundedness and decay for the curvature components and their derivatives. Some important difficulties arise from the fact that not all curvature components decay. An important ingredient in this work is to generalize recent work of Dafermos and Rodnianski regarding decay for the wave equation to the setting of the Bianchi equations.

Alan Rendall, Higher dimensional cosmological models

Alan Rendall presented some joint results with Arne Goedeke on solutions of the vacuum Einstein equations in dimensions greater than four. The central question discussed is whether spatially homogeneous models which are forever expanding are geodesically complete in the future. This fact is known to hold in four dimensions, but the proof does not directly generalize to the higher dimensional case. Rendall introduced a sufficient condition for completeness and showed that it is satisfied in a class of models of dimension five by means of Kaluza-Klein reduction. The talk was concluded by a discussion of the prospects for obtaining a more global understanding of this problem.

Hans Ringström, Models of the universe with arbitrary compact spatial topology

The current standard model of the universe is spatially homogeneous, isotropic and spatially flat. Furthermore, the matter content is described by two perfect fluids (dust and radiation) and there is a positive cosmological constant. Such a model can be well approximated by a solution to the Einstein- Vlasov equations with a positive cosmological constant. Motivated by this observation, Hans Ringström has studied the properties of cosmological models with Vlasov matter and a positive cosmological constants. The results described in the talk included far-reaching statements on the stability of such models, as well as a proof that the assumption that the universe is close in our past to the standard Friedmann model does not restrict the spatial topology of the universe.

Shing-Tung Yau, Quasi-local mass in general relativity

Starting with a background for the notion energy and momentum in general relativity, Yau discussed his approach to the problem of defining a quasi-local mass in general relativity, which has been developed in collaboration with Mu-Tao Wang and Po-Ning Chen, based on earlier work of Shi and Tam, as well as Liu and Yau. An important background to the definition of quasi-local mass introduced by Yau is the Brown-York analysis of the boundary terms in in the gravitational Lagrangian. The above mentioned quasi-local mass definitions all rely on an imbedding of a 2-sphere in a reference space which gives a quasi-local mass notion via the Brown-York analysis after making a gauge choice. The novel idea in the approach of Wang and Yau is to make use of an optimal imbedding of the 2-sphere in Minkowski space. This essentially reduces the gauge freedom in the definition of the quasi-local mass to a choice of a vector in the reference Minkowski space, a notion related to a choice of observer. The talk of M-T Wang gave further details of this construction.

Mu-Tao Wang, Limit of quasilocal mass and isometric embeddings into Minkowski space

In his talk based on joint work with S.-T. Yau, Mu-Tao Wang discussed how the limit of quasilocal mass on a family of surfaces in spacetime can be evaluated in terms of the mean curvature vectors and showed that this gives a uniform description of ADM mass and Bond mass for asymptotically flat and asymptotically null spaces, respectively. He then explained how the related variational problem for quasilocal mass anchors a ground state as a hypersurface in Minkowski space.

Marcus Khuri, The Static Metric Extension Conjecture

There are several competing definitions of quasi-local mass in General Relativity. A very promising and natural candidate, proposed by R. Bartnik, seeks to localize the total or ADM mass. Fundamental to understanding Bartniks construction is the question of existence and uniqueness for a canonical geometric boundary value problem associated with the static vacuum Einstein equations. In his talk, Marcus Khuri discussed joint work with Michael Anderson, which confirms that existence holds (under a nondegeneracy condition) but also shows that uniqueness fails. He concluded by discussing the possible implications of this result.

Marc Mars, The Bray and Khuri approach to the general Penrose inequality in two particularly simple cases

Bray and Khuri have put forward an interesting new approach to address the Penrose inequality for arbitrary initial data sets. The two simplest possible situations where one can think of applying these results involve spherically symmetric initial data and static initial data. Restricting to the spherical case, Marc Mars was able to extend previous results by Bray and Khuri when the outermost horizon is strictly stable and non-minimal to the general case. For the static case, he showed that there are slices of the Kruskal spacetime with mass m for which the outermost generalized apparent horizon has area strictly larger than $16\pi m^2$ and presented a Penrose inequality for general static initial data sets satisfying the dominant energy condition, provided the mean curvature of the degenerate components satisfies an integral inequality.

Frans Pretorius, The instability of 5-dimensional black strings

5 dimensional black strings were shown to be unstable to long-wavelength perturbations by Gregory and Laflamme. Entropy considerations imply the prefered end-state of the unstable spacetime is a sequence of black holes with spherical topology. For this to happen, the black string event horizon would have to bifurcate, accompanied by a naked singularity. This would be an example of generic violation of cosmic censorship in 5 dimensional Einstein gravity. Frans Pretorius presented recent numerical results, joint with L. Lehner, which aim at illucidating the end-state of the Gregory-Laflamme instability.

Piotr Chruściel, 5-dimensional black holes

Piotr Chruściel started by discussing the current status of uniqueness results for 3+1 stationary electro-vac black hole spacetimes. He then gave a review of some higher dimensional black hole spacetimes and our knowledge of their global structures, including those of Myers-Perry (generalization of Kerr), Emparan-Reall and Pomeransky-Senkov (black ring) and Elvang-Figueras (Black Saturn). He then reported on recent work, joint with Cortier and Garcia-Parrado, and with Eckstein and Szybka on the global properties of higher dimensional black hole spacetimes. In particular, this work shows that the Pomeransky-Senkov and Black Saturn spacetimes are singularity-free in the exterior of the horizon, and gives an analytical extension which is a candidate for a maximal extension.

Gerhard Huisken, Foliations, flows and rigidity in asymptotically flat 3-manifolds

The talk of Gerhard Huisken was centered around the inverse mean curvature flow, the mean curvature flow and their role in proving geometric inequalities involving such notions as the isoperimetric ratio, quasi-local mass (eg. Geroch or Hawking mass) and the ADM mass defined at infinity. The just mentioned geometric flows define canonical foliations in 3-manifolds with interesting monotonicity properties which play a central role in the proofs of geometric inequalities. A prime example of such an application is the proof by Huisken and Illmanen of the Riemannian Penrose inequality.

David Maxwell, The Conformal Method and Concrete Examples

Recent advances by Holst, et. al and Maxwell concerning the conformal method and non-CMC initial data might have led an optimist to conjecture that the conformal method could be just as effective for constructing non-CMC data as it is in the CMC case. In his talk, David Maxwell discussed some concrete examples that indicate that this is not true. He showed that for certain reasonable conformal data violating a near-CMC condition there cannot be a unique solution: there are either no solutions or more than one. For some examples, he was able to establish that there exist multiple solutions. These concrete examples are independently interesting as they exhibit a number of new phenomena for the conformal method, including existence of certain solutions under a very weak near-CMC hypotheses, explicit dependence on the choice of conformal class representative, and extreme sensitivity of the solution theory with respect to a coupling constant in the Einstein constraints.

Hubert Bray, On Dark Matter, Spiral Galaxies, and the Axioms of General Relativity

Hubert Bray introduced geometric axioms for the metric and the connection of a spacetime where the gravitational influence of the connection may be interpreted as dark matter. In particular he showed how these axioms lead to the Einstein-Klein-Gordon equations with a cosmological constant, where the scalar field of the Klein-Gordon equation represents the deviation of the connection from the standard Levi-Civita connection on the tangent bundle and is interpreted as dark matter. This form of dark matter is compatible with the CDM cosmological model of the universe. In addition, unlike the WIMP model of dark matter, this dark matter is automatically cold (as is observed) in a homogeneous, isotropic universe. He concluded by showing how this scalar field dark matter, which naturally forms dark matter density waves due to its wave nature, may cause the observed barred spiral pattern density waves in many disk galaxies and triaxial shapes with plausible brightness profiles in many elliptical galaxies. If correct, this would provide a unified explanation for spirals and bars in spiral galaxies and for the brightness profiles of elliptical galaxies. The results of preliminary computer simulations were shown and compared with photos of actual galaxies.

Richard Schoen, Singularities in positive mass arguments

Richard Schoen discussed the obstructions to proving positive mass theorems in the presence of singularities. There have been a few instances when singularities have been shown to be allowable, but there is no comprehensive characterization of them.

Spyridon Alexakis, On the black hole uniqueness problem

The classical uniqueness theorem for stationary black hole spacetimes due to Carter and Robinson relies on the existence of a second, rotational, Killing field. A construction by Hawking yields such a Killing field under the assumption that the spacetime is analytic. However, until recently the existence of the Hawking Killing field for stationary black hole spacetimes containing a bifurcate Killing horizon has been open. In recent joint work with Ionescu and Klainerman, Alexakis has established the existence of a Hawking Killing field without assuming analyticity. The current version of the black hole uniqueness theorem requires a smallness assumption and is therefore valid only for spacetimes close, in a certain sense, to the Kerr spacetime. One of the main ideas in the proof is the use of an inequality of Carleman type to prove a uniqueness result for a wave equation on the exterior of the horizon, given data on the horizon.

Sergio Dain, Linear perturbations and mass conservation for axisymmetric Einstein equations

In axial symmetry, there exists a gauge for Einstein equations such that the total mass of the spacetime can be written as a conserved, positive definite, integral on the spacelike slices. This property can be expected to play an important role in the global evolution. In this gauge the equations reduce to a coupled hyperbolic-elliptic system which is formally singular at the axis. Due to this singular behavior, the local in time existence of this system can not be analyzed by standard methods. In his talk, based on joint work with Martin Reiris, Sergio Dain studied the linear perturbation of the flat solution in this gauge (with the purpose of analyzing the principal part of the equations, which represents the main source of the difficulties), and proved existence and uniqueness of solutions of this singular linear system. The solutions are obtained in terms of integral transformations in a remarkable simple form. This representation is suitable for proving useful estimates for the non-linear case. This result is expected open the door to the study of the full Einstein equations in this gauge.

Lydia Bieri, Null Asymptotics of Solutions of the Einstein-Maxwell Equations in General Relativity and Gravitational Radiation

A major goal of mathematical general relativity and astrophysics is to precisely describe and finally observe gravitational radiation, one of the predictions of general relativity. In order to do so, one has to study the null asymptotic limits of the spacetimes for typical sources, including binary neutron stars and binary black hole mergers. In these processes typically mass and momenta are radiated away in form of gravitational waves. Demetrios Christodoulou showed that every gravitational-wave burst has a nonlinear memory. In her talk, Lydia Bieri discussed the null asymptotics for spacetimes solving the Einstein-Maxwell equations, computed the radiated energy, and derive limits at null infinity. These limits were compared with the Einstein vacuum case. The methods used were introduced in the works of Christodoulou, Klainerman, Bieri and Zipser.

Pieter Blue, Hidden symmetries and decay for the wave equation outside a Kerr black hole

The Kerr solutions to Einstein's equations describe rotating black holes. For the wave equation in flat-space and outside the non-rotating, Schwarzschild black holes, one method for proving decay is the vector-field method, which uses the energy-momentum tensor and vector-fields. Outside the Schwarzschild black hole, a key intermediate step in proving decay involved proving a Morawetz estimate using a vector-field which pointed away from the photon sphere, where null geodesics orbit the black hole. Outside the Kerr black hole, the photon orbits have a more complicated structure. Pieter Blue, in a talk based on joint work with Lars Andersson, showed that by using the hidden symmetry of Kerr, it is possible to replace the Morawetz vector-field by a fifth-order operator which, in an appropriate sense, points away from the photon orbits. This allows one to prove the necessary Morawetz estimate, also called a local energy decay estimate, which is a key step in proving pointwise decay estimates.

Igor Rodnianski, On formation of trapped surfaces

Igor Rodnianski discussed joint work with Sergiu Klainerman which extends and refines the results of Demetrios Christodoulou on the formation of trapped surfaces due to the concentration of radiation. The result of Christodoulou shows that the existence of sufficiently strong pulses of radiation, entering from a finite interval of retarded time on past null infinity, results in the formation of a trapped surface. The proof requires the incoming pulse of radiation to be highly isotropic. One of the new features of the work of Klainerman and Rodnianski is that it handles the situation where the incoming radiation is anisotropic. In particular, conditions are given where an incoming pulse supported in only a part of the cross-sections of past null infinity can be shown to form a spacetime containing a trapped surface and more generally a "scarred surface". This work may be expected to be relevant to understanding break-down phenomena for solutions of the Einstein equations with low regularity.

Michael Eichmair, Some old and some new results on MOTS and Jang's equation

In this talk, Michael Eichmair presented a synthetic overview of the geometric theory of Jang's equation, pioneered by R. Schoen and S.-T. Yau in their proof of the spacetime positive energy theorem, and its recent application to the existence theory of marginally outer trapped surfaces in initial data sets by L. Andersson, J. Metzger, and himself. He discussed recent joint work with J. Metzger on the mixed blow up behavior of Jang's equation in certain exterior domains of initial data sets. These results are akin to the classical Jenkins-Serrin-Spruck theory for minimal and constant mean curvature graphs.

Participants

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Chapter 25

Noncommutative Lp spaces, Operator spaces and Applications (10w5005)

Jun 27 - Jul 02, 2010

Organizer(s): Quanhua Xu (Universite de Franche-Comte), Marius Junge (University of Illinois, Urbana-Champaign), Gilles Pisier (Texas A&M University)

Overview of the field. Noncommutative L_p-spaces are at the heart of this conference. These spaces have a long history going back to pioneering works by von Neumann, Dixmier and Segal. They are the analogues of the classical Lebesgue spaces of p-integrable functions, where now functions are replaced by operators. These spaces have been investigated for operator algebras with a trace, and then around 1980 generalizations to type III von Neumann algebras have appeared (Kosaki, Haagerup, Terp, Hilsum). These algebras have no trace and therefore the integration theory has to be entirely redone. These generalizations were motivated and made possible by the great progress in operator algebra theory, in particular the Tomita-Takesaki theory and Connes's spectacular results on the classification of type III factors.

Since the early nineties and the arrival of new theories like those of operator spaces and free probability, noncommutative integration is living another period of stimulating new developments. In particular, noncommutative Khintchine and martingale inequalities have opened new perspectives. It is well-known nowadays that the theory of noncommutative L_p-spaces is intimately related with many other fields such as:

- **Operator algebras.** By definition noncommutative L_1-spaces are the preduals of von Neumann algebras. The structure von Neumann algebras is naturally reflected in these spaces. More generally, noncommutative L_p-spaces allow to address many questions related to algebraic structures. For example, in Connes's noncommutative geometry, "Fredholm modules" are defined as elements of a noncommutative L_p-space adapted to the geometry. These different theories form an important field of research in functional analysis and have numerous interactions with other disciplines like algebras, K-theory, mathematical and theoretical physics.

- **Geometry of Banach spaces.** Noncommutative L_p-spaces are a generalization of classical L_p-spaces as well as Schatten classes. They have therefore provided - and continue to provide - many important examples and counterexamples for Banach space theory. Furthermore, their geometrical properties are sometimes crucial for certain problems in mathematical physics (see the works of Lieb and his collaborators).

- **Operator spaces.** This theory is placed at the intersection of the preceding two topics. It is of interest to researchers coming from other subjects such as operator algebras, quantum probability, or Banach spaces. Within this theory noncommutative L_p-spaces are experiencing a strong development. The research in this area is very active and there is a strong international competition. Let us mention the works of Blecher, Junge, Musat, Oikhberg, Ozawa, Randrianantoanina, Rosenthal and Ruan in the United States, Le Merdy, Lust-Piquard, Pisier, Raynaud, Ricard and Xu in France, and Bozejko, Defant, Haagerup, Lindsay and Parcet in the other European countries.

- **Quantum probability.** This field developed from the probabilistic interpretation of quantum mechanics. Its origins can be traced back to Bonn and von Neumann, but it is in the seventies and eighties that it grew into a separate theory through the works of Accardi, Bozejko, Hudson, Meyer, Parthasarathy, von Waldenfels, and many others. Noncommutative L_p-spaces arise naturally in the study of noncommutative martingale and ergodic theories. The work of Biane and Speicher has established a bridge to Voiculescu's free probability and underlines the interactions between this discipline, operator spaces/algebras, and random matrices.

- **Noncommutative harmonic analysis.** Matrix-valued harmonic analysis goes back to the classical works of Wiener-Masani and Helson-Lowdenslager on prediction theory. This led Arveson to introduce his theory of subdiagonal algebras (or noncommutative H_∞-spaces). This line of research continues to be very active, as show the recent works of Blecher-Labuschagne. On the other hand, the investigation of semigroups of completely positive maps on von Neumann algebras has recently shown to be an important tool in the work of Popa-Ozawa and Shlyakhtenko. Noncommutative L_p-spaces allow to formulate problems from classical harmonic analysis in the context of group von Neumann algebras.

- **Quantum information.** The interaction between operator algebras/spaces and quantum information theory is very recent and has brought some intriguing new ideas and concepts. One connection between them is the notion of channels, called completely positive maps in C*-algebras. Completely positive maps have been used in solving long-standing open problems, for example in Kirchbergs works on exact C*-algebras, and more recently in Popas works on rigidity of von Neumann algebras and groups. It is thus natural that quantum information has attracted attention and interest of researchers from operator algebras/spaces. From this point of view, the theory of operator algebras/spaces has many tools to offer. On the other hand, channels are the basic objects used in quantum information to model experiments.

The topics listed above correspond to separate mathematics communities and cultures, which nonetheless present many links and interactions. Noncommutative L_p-spaces have so far not been studied through these strong links to other topics.

Outline of the conference. A wide range of topics have been presented during this conference, including interactions of the theory of operator spaces and quantum probability with the following areas

- Quantum information theory
- Noncommutative harmonic analysis
- The theory of double integrals
- Quantum groups
- Operator algebras in connection with geometric group theory

At the planning stage of this conference it has been by no means clear that the interaction between quantum information theory and operator spaces/operator algebras could be as fruitful as it turns out to be during the conference. With C. King, D. Kribs, A. Winter, and P. Shor well-known researchers in quantum information could be attracted to participate in a conference whose title seem hardly be connected to quantum information theory. However, the Banff researchers center is one of the leading institutions supporting this exciting new area of interaction. Indeed, following up on problem due to A. Winter, and communicated to some fraction of the operator space community during the last workshop on interaction between operator spaces and quantum information, a major problem on tensor products of quantum channels could be solved (see Winter's problem below). The solution to Winter's problem is related to dilation properties of completely positive maps. Quite surprisingly these dilation properties also play an important role in certain aspects of noncommutative analysis. The new results in noncommutative analysis presented in this conference show that certain results from classical analysis are still meaningfull when replacing abelian discrete groups by their noncommutative counterparts. Further tools required in this recent research line are based on quantum probability. Thus, despite of the wide range of problems discussed in this conference, there is in fact a common ground and several connections between some of these topics. Last, but not least, the connection between Banach space and the Hastings' famous solution of the additivity problem also played an important role in this successful conference.

1) Noncommutative analysis and noncommutative probability. Despite its name harmonic analysis is not really the theory of harmonic functions. In fact, classical harmonic analysis is certainly concerned with Fourier analysis, abelian groups, and connection to number theory. In particular, fundamental results in the theory provide the analytic aspects of the Pontrajgin duality, such as Fourier transforms, multipliers, and properties of the heat semigroup in $\mathbb{Z}^n$ and $\mathbb{T}^n$. By now these properties are very well understood, and modern harmonic analysis moved on to different problems. However, by replacing the discrete groups by noncommutative discrete groups, one also has to replace their compact duals by the corresponding noncommutative space. This naturally leads to operator algebras and the corresponding L_p spaces associated with them. In this different setting very little is known. On this conference J. Parcet [13] presented a method, a suitable adaptation of the classical Calderón-Zygmund theory to the setting of finite dimensional cocyles on groups. Through discussions during the conference new mulitplier results for classical groups and Schur multipliers have been found. The talks by U. Haagerup [8] and E. Ricard [12] also concerned Schur-Herz multipliers on discrete groups. They computed the complete bounded norms of radial multipliers. These results have interesting applications to approximation properties of group von Neumann algebras and their noncommutative L_p spaces. See the paragraph below on Araki-Wood factors and also the recent work of M. de la Salle and V. Loforgue [7].

An important technical tool in the recent works on noncommutative harmonic analysis is the theory of generalized BMO spaces. In classical analysis this space of function with bounded mean oscillation replaces the space of bounded functions as an endpoint for interpolation. A similar role plays the corresponding the Hardy or the weak L_1 space. For BMO spaces this fundamental fact and further applications were presented by T. Mei, based on a series of recent works the first two of which were already published (see [18, 19]). Indeed, Mei invented an intrinsic definition of BMO spaces which seems new even in commutative setting. The interpolation result cannot be obtained from classical methods, but from probabilistic methods related to the dilation problem. In talks delivered by PhD students , S. Avsec gave an illustration of Mei's theory and its application to square functions for finite dimensional cocylces. M. Perrin outlined the theory of noncommutative H_p spaces for martingales with a continuous parameter set. Both talks are based on works in progress. This theory, together with the H_p theory developed by Le Merdy and a subset of the organizers, provides the backbone of the interpolation results.

2) The dilation problem. In operator algebras certain dilations or factorizations results are of fundamental importance. In this conference several talks were motivated by well-known results for positive maps on commutative spaces. The first instance of this result is the construction of a Markov process associated with a positive matrix. More generally Rota could construct a suitable probability measure on the space of pathes of a given set which encodes the transition probability of the underlying map. In the theory of semigroups a similar problem is known as the martingale problem. Here one requires in addition that the measure on the path space is supported on the space of continuous pathes.

A similar question arises for completely positive maps on operator algebras, in particular on matrix algebras. The addition“completely” here means that the map is positivity preserving even after adding an environment. M. Musat presented the surprising result (obtained with U. Haagerup; see [9]) that not all completely positive maps are factorizable. The notion of factorizability was invented by C. Anantharaman-Delaroche who showed that factorizable maps admit a Rota (or Markov) dilation. Due to the work of Haagerup and Musat the condition for a map to be factorizable is now very well understood and many examples are available. Moreover, the link to the notion of “dilation” previously studied by Kümmerer is clarified and the relation between Kümmerer’s examples and the new counterexamples is now clear.

Y. Dabrowski [6] (a PhD student) presented a result showing that for certain symmetric semigroups the dilation problem has a positive solution. Using slightly different methods a similar result has been obtained by one of the organizers and his coauthors (work in progress by M. Junge, E. Ricard and D. Shlyakhtenko).

It is probably fair to say that the Markov dilation problem for completely positive maps is now completely clarified, and this conference (and the previous conference on operator spaces at CIRM in Luminy) played an important role.

3) Winter’s problem. The starting point of Winter’s problem is Birkhoff’s classical theorem on the characterization of extreme points of the set of double stochastic matrices. Indeed, these extreme points are given by permutation matrices. In the context of quantum channels the analogue is a characterization of completely positive trace preserving maps. This characterization has been obtained by Choi, and there are recent results by Wolff on this subject. The nice aspect about the classical results is that permutation matrices are given by unitary maps. Winter’s problem itself is not about an individual channel, but about the n-fold tensor product. Winter asks whether eventually the cb distance to the convex hull of unitary channels goes to 0 (see [20]; see also the Report of the workshop on Operator structures in quantum information theory at BIRS, February 11-16, 2007). By the results of Haagerup and Musat the answer to this problem is negative. Indeed, those trace preserving completely positive maps which are not factorizable can never be in convex hull of unitaries and even not their tensor powers.

The history of this problem is a nice Banff success story because Winter’s problem become known to the operator space community on a prevrious meeting and then has been communicated to U. Haagerup by V. Paulsen, a participant of all the workshops in Banff connecting operator space theory and quantum information. Now, the solution had been presented again in a Banff workshop, and has since been picked up by the quantum information community.

4) Approximation problem for Araki-Wood factors. Araki-Wood factors have been introduced in the late sixties by physicists in the context of calculating thermodynamical limits of large systems. Since then they played a prominent role in operator algebras because they served as a model for Connes’ classification and the interesting invariants extracted from this work. More recently, D. Shlyakhtenko studied the free analogue of Araki-Wood factors and their properties. For example, in the context of S. Popa’s rigidity theory, it is important to know whether these factors have the approximation property, more precisely the completely contractive approximation property. Following the techniques for the free group this could be established under the additional assumption that the modular group of these factors is almost periodic. The case of continuous spectrum remained open. The solution to this problem by C. Houdayer and E. Ricard [12] had been presented by a talk of Ricard in this conference. The beautiful aspect of the solution is the clever use of Schur multipliers in a suitable larger algebra which then drop down to very useful maps on the factor.

5) Additivity conjecture and connections to Quantum Information. The additivity conjecture for the minimal entropy of quantum channels has recently been solved by M. Hastings [10]. This posed a longstanding problem in Quantum Information Theory. A number of talks were dedicated to this problem. New proofs and a better insight to why these counterexamples are positive were presented. Essentially there seem to be two avenues to simplify or extends Hastings’ approach which has its roots in the work of Haydon and Winter [20]. The first approach uses a basic but important observation which encodes a quantum channel, a completely positive trace preserving map, via a subspace of the tensor product of two Hilbert spaces. In this tensor product one may consider different norms induced by the Schatten norms. The way this approach is set up is that for $p = 2$ one finds the range of the partial isometry implementing the channel. However, the minimal entropy might be considered as a limit for p tending to 2 of the structure of these spaces with the inherited Schatten norm. Very small entropy is obtained if the norm for $p > 2$ is almost constant. But this corresponds to an almost isometric embedding of a Hilbert space in a Schatten p-class. Almost isometric embedding of Hilbert spaces in arbitrary Banach spaces have been studied in Banach space theory very intensively. This topic is particularly tied to the seminal work of Dvoretzky based on random techniques. S. Szarek has used and extended many of these techniques in particular in the connection with Gluskin spaces, estimates for eigenvalues of random matrices and many other topics. For fixed $p > 2$ one can find counterexamples (as observed by Haydon and Winter) simply by applying the known results for Dvoretzky's for Schatten p classes. However, Hastings's result even requires an improvement of standard Banach space result with better estimates of the error. In this case the desire to find a conceptual proof of Hastings's result lead to a deeper understanding of problems central to Banach space theory. S. Szarek clearly exposed in this conference his recent works [1, 2] with G. Aubrun and E. Werner on this subject.

B. Collins' talk presented another approach to these results relying on estimates from free probability, based on his joint works with I. Nechita [3, 4, 5]. These results provide new insights in the fine structure of random unitaries and random projections using deep combinatorial tools.

A different family of connections between operator space theory and quantum information theory concerns Bell inequalities and their generalizations. Bell inequalities are in the heart of the classical paper by A. Einstein, B. Podolsky, N. Rosen, and have ever since been used to indicate why quantum mechanics is not compatible with locality. In a talk by C. Palazuelos [15] new results on Bell inequalities and examples of violation were presented which provide asymptotically large violation in high dimension. In a talk by V.B. Scholz [14] the connection between Tsirelson's problem on calculating quantum probabilities with arbitrary commutating POVM's and tensor product structures was shown to follow from a positive solution of Connes' famous embedding problem. If in addition matrix valued coefficients are considered then Tsirelson's conjecture and Connes' embedding problem are indeed equivalent.

In addition to these talks there were additional informal talk on the connection of Entropy and Banach space or Operator space techniques in quantum information theory.

6) Additional Highlights It is a tradition in Operator Space Theory to include speakers from related topics, but not necessarily core subjects. This include beautiful talks of U. Haagerup and M. Bozejko on Schur multipliers and the connection to combinatorial objects.

The broad spectrum of talks was complemented by contributions on logmodular algebras (V. Paulsen), Lieb-Robinson bounds on operator inequalities based on deep results of Hastings (E. Carlen), operator space structure of certain multiplier spaces and Hausdorff-Young inequality in quantum groups (Z-J. Ruan and his student T. Cooney) and the recent solution by F. Sukochev and D. Potapov [16, 17] on bounds for double operator integrals.

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Chapter 26

Structure and representations of exceptional groups (10w5039)

Jul 04 - Jul 09, 2010

Organizer(s): Joseph Wolf (University of California - Berkeley), Wulf Rossmann (University of Ottawa), S. Twareque Ali (Concordia University), David Vogan (Massachusetts Institute of Technology)

Background

From Cartan and Killing's original classification of simple Lie groups in the 1890s, these groups have been understood to be of two rather different types: the infinite families of classical groups (related to classical linear algebra and geometry); and a finite number of exceptional groups, ranging from the 14-dimensional groups of type G_2 to the 248-dimensional groups of type E_8. Often it is possible to study all simple Lie groups at once, without reference to the classification; but for many fundamental problems, it is still necessary to treat each simple group separately.

For the classical groups, such case-by-case analysis often leads to arguments by induction on the dimension (as for instance in Gauss's method for solving systems of linear equations). This kind of structure and representation theory for classical groups brings tools from combinatorics (like the Robinson-Schensted algorithm), and leads to many beautiful and powerful results.

For the exceptional groups, such arguments are not available. The groups are not directly connected to classical combinatorics. A typical example of odd phenomena associated to the exceptional groups is the non-integrable almost complex structure on the six-dimensional sphere S^6, derived from the group G_2. What makes mathematics possible in this world is that there are only finitely many exceptional groups: some questions can be answered one group at a time, by hand or computer calculation.

The same peculiarity makes the possibility of connecting the exceptional groups to physics an extraordinarily appealing one. The geometry of special relativity is governed by the ten-dimensional Lorentz group of the quadratic form of signature $(3, 1)$. Mathematically this group is part of a family of Lorentz groups attached to signatures (p, q), for any non-negative integers p and q; there is no obvious mathematical reason to prefer the signature $(3, 1)$. A physical theory attached to an exceptional group - best of all, to the largest exceptional groups of type E_8 - would have no such mathematical cousins. There is only one E_8.

Recent Developments and Objectives

Two years ago Garrett Lisi proposed an extension of the Standard Model in physics, based on the structure of the 248-dimensional exceptional Lie algebra E_8. Lisi's paper raises a number of mathematically interesting questions about the structure of E_8, for instance this one: the work of Borel and de Siebenthal published in 1949, and Dynkin's work from around 1950, gave a great deal of information on the complex subgroups of complex simple Lie groups. For example, they independently showed that complex E_8 contains (up to conjugacy) just one subgroup locally isomorphic to $SL(5,\mathbb{C}) \times SL(5,\mathbb{C})$. For Lisi's work, one needs to know about *real* subgroups of *real* simple groups: which real forms of $SL(5,\mathbb{C}) \times SL(5,\mathbb{C})$ can appear in a particular real form of E_8? These are subtle questions, not yet completely understood. A mathematical study of these questions is interesting for its own sake, and may provide some constraints on the structure of the physical theories that can be built using E_8.

The goal of this workshop was to introduce mathematicians to these physical ideas, and to describe much of the recent mathematical work on the exceptional Lie groups.

Presentation Highlights

There were quite a few outstanding presentations, both formal and informal, concerning semisimple Lie groups (especially E_8) and their possible use in physical models. Among them, in alphabetical order of presenter's name, are

JEFF ADAMS (University of Maryland), "Elliptic elements of the Weyl group of E_8"

An element of a Weyl group W is *elliptic* if it has no fixed points in the reflection representation. An example is the Coxeter element, studied extensively by Kostant. Elliptic elements were classified by Carter in 1972, who discovered a relation with nilpotent conjugacy classes in the corresponding semisimple group G. Lusztig has recently studied this from a new point of view. Each elliptic conjugacy class in W is naturally a semisimple conjugacy class in G. Prof. Adams considered the elementary question: what is the map from elliptic conjugacy classes in W to W-orbits in T? He focused on the example of E_8 and presented a number of computer calculations. These examples suggested a particularly interesting class of elliptic elements, sharing some of the properties established by Kostant for the Coxeter element. He defined an elliptic conjugacy class in W to be *uniform* if each element acts freely on the set of roots, and if there is a representative of the class having length equal to the number of orbits on the roots. He showed that there are exactly 12 uniform conjugacy classes in the Weyl group of E_8.

DAN BARBASCH (Cornell University), "The spherical unitary dual for the quasisplit group of type E_6"

The presenter has in recent years described completely the spherical unitary representations of split groups over real and p-adic fields. A central feature of his work is a reduction to calculations in affine Hecke algebras, and ultimately to calculations related to finite-dimesnsional representations of Weyl groups. Attached to any diagram automorphism τ of finite order m for a simple Dynkin diagram, and to a cyclic Galois extension K of degree m of the base field k, there is a quasisplit group G over k. (In the case of exceptional groups, this means that there is a quasisplit group of type E_6 attached to each quadratic extension of k.) This talk offered a description of the spherical unitary dual of such a quasisplit group, in terms of the spherical unitary duals of smaller split groups (for E_6, split groups of type F_4).

BIRNE BINEGAR (Oklahoma State University), "W-graphs, nilpotent orbits, and primitive ideals"

Work of Howe and others in the 1970s attached to any irreducible representation of a semisimple Lie group some geometric invariants: for example, some nilpotent orbits in the dual of the Lie algebra. The presenter described his work using the `atlas` software to compute some of these invariants, using the Kazhdan-Lusztig notion of "W-graphs."

DAN CIUBOTARU (University of Utah), "The Dirac operator for graded affine Hecke algebras" (joint work with D. Barbasch and P. Trapa)

Prof. Ciubotaru defined an analogue of the Dirac operator for graded affine Hecke algebras of p-adic groups, and establish a version of Parthasarathys Dirac operator inequality. He then proved a version of Vogan's conjecture for Dirac cohomology. The formulation of the conjecture depends on a uniform parametrization of spin representations of Weyl groups. Prof. Ciubotaru applied these results to prove new results about unitary representations of graded affine Hecke algebras, and therefore of p-adic reductive groups.

MICHAEL EASTWOOD (Australian National University (Canberra)), "Representations from contact geometry"

Apart from $SL(2)$, each simple Lie group is the symmetry group of a contact manifold equipped with some extra geometric structure. This includes the exceptional groups. This fact can be used to give a geometric construction of the finite-dimensional representations of the simple groups, including the exceptional groups. Prof. Eastwood gave a useful introduction to contact geometry and indicated just how this gives a useful elegant construction of finite dimensional representations..

SKIP GARIBALDI (Emory University), "There is no (interesting) Theory of Everything inside E_8"

In joint work with Jacques Distler, Prof. Garibaldi proved that the real forms of E_8 (and the complex group E_8 regarded as a real group) cannot have subgroups with certain properties. Some widely accepted (this is meant to be a more neutral term than "well established") principles for mathematical models of physics suggest that a physical interpretation of this result is that the "Exceptionally Simple Theory of Everything" conflicts with widely accepted representation-theoretic properties of the Standard Model. He indicated that this interpretation is robust, in that the result also shows that a whole family of related "Theories of Everything" also conflict with these same properties of the Standard Model.

There was quite a bit of lively discussion here, as the mathematicians tried to pin down the precise meaning of various terms and conventions, and as Garrett Lisi questioned aspects of the presentation that were in contrast to his E_8 theory. Each of their viewpoints predicts some ("a handful of") unobserved particles and part of this discussion centered on how many unobserved particles were acceptable.

ALAN HUCKLEBERRY (Ruhr-Universität Bochum), "The role of Kobayashi hyperbolicity in the study of flag manifolds"

Open orbits D of simple real forms G_0 in flag manifolds $Z = G/Q$ of their complexifications G are considered. For any choice K_0 of a maximal compact subgroup of G_0, the minimal K_0-orbit in the flag domain D is a compact complex manfold referred to as the base cycle C_0 with respect to the choice of K_0. It can be regarded as a point in the Chow (or Barlet space) $\mathcal{C}_q(Z)$ of all cycles of the same dimension q. It is known that $\mathcal{C}_q(Z)$ is smooth at C_0 and therefore it makes sense to consider the irreducible compoment of $\mathcal{C}_q(Z)$ which contains C_0 and the open subset $\mathcal{C}_q(Z)$ of those cycles which are contained in D. The complex geometry of $\mathcal{C}_q(Z)$ was the theme of the talk. For example, using analytic properties of the intersection of the cycles with certain special Schubert varieties, the Kobayashi hyperbolicity of $\mathcal{C}_q(Z)$ is proved. This sheds light on the complex geometry of D, e.g., leading to a precise desciption of its group of holomorphic automorphisms. It should be emphasized that for fixed G_0 the cycle space $\mathcal{C}_q(Z)$ varies tremendously as D and Z vary, making it a rich source of interesting complex varieties with the potential of realizing nontrivial G_0-representations in a holomorphic context. A preprint (arXiv:1003:5974) is available.

TOSHIYUKI KOBAYASHI (Kyoto University), "Stable Spectrum on Locally Homogeneous Spaces"

Video: http://www.birs.ca/events/2010/5-day-workshops/10w5039/videos/watch/201007081615-Kobayashi.mp4

Questions of spectra and discontinuity are more delicate for homogeneous spaces G/H with H noncompact, than for those with compact H. Prof. T. Kobayashi discussed several aspects of this situation:
the existence question for $\Gamma \subset G$ with $\Gamma\backslash G/H$ compact
spectral analysis on compact quotient manifolds $\Gamma\backslash G/H$

deformation of Γ, e.g. to a subgroup $L \subset G$ for which $L \cap H$ is compact and Γ is uniform in L, and stable spectrum of $\Gamma \backslash G/H$

Here G is a noncompact simple Lie group, H is a closed reductive subgroup, and Γ is a discrete subgroup of G. Or G/H may be a pseudo–riemannian nilmanifold, e.g. Minkowski space. In any case, the first step is to find the condition for Γ to act freely and properly discontinuously on G/H, so that $\Gamma \backslash G/H$ is a pseudo–riemannian quotient manifold of G/H. Building on this, the presenter described the current state of these matters and contrasted the general pseudo–riemannian cases with the more classical riemannian cases.

BERTRAM KOSTANT (MIT) "Experimental evidence for the occurrence of E_8 in nature and the radii of the Gossett circles

Video: http://www.birs.ca/events/2010/5-day-workshops/10w5039/videos/watch/201007061330-Kostant.mp4

A recent experimental discovery involving spin structure of electrons in a cold one-dimensional magnet points to a validation of a (1989) Zamolodchikov model involving the exceptional Lie group E_8. The model predicts 8 particles and predicts the ratio of their masses. The conjectures have now been validated experimentally, at least for the first five masses. The Zamolodchikov model was extended in 1990 to a Kateev-Zamolodchikov model involving E_6 and E_7 as well. In a seemingly unrelated matter, the vertices of the 8-dimensional Gosset polytope identify with the 240 roots of E_8. Under the famous two-dimensional (Peter McMullen) projection of the polytope, the image of the vertices are arranged in 8 concentric circles, hereafter referred to as the Gosset circles. The McMullen projection generalizes to any complex simple Lie algebra (in particular not restricted to A-D-E types) whose rank is greater than 1. The Gosset circles generalize as well. Applying results in Prof. Kostant's AJM 1959 paper, he found some time ago a very easily defined operator A on a Cartan subalgebra, the ratios of whose eigenvalues are exactly the the ratios of squares of the radii r_i of the generalized Gosset circles. The two matters considered above relate to one another in that the ratio of the masses in the E_6, E_7, and E_8 Kateev-Zamolodchikov models are exactly equal to the ratios of the radii of the corresponding generalized Gosset circles.

GARRETT LISI, "Group-theoretic models in gravity, the standard model, and old-and-new ideas about unification"

This series of three informal lectures was the keynote of the conference. Meeting after dinner, each consisted of perhaps 30 minutes of exposition and 60 minutes of questions and answers. Most of the latter were clarifications to mathematicians, but some addressed the differences between Dr. Lisi's E_8 theory and the more conservative physical theory criteria described by Prof. Garibaldi, this in terms of properties that that one expects for a good physical model. The titles of the individual talks were "Unification"; "A physicist's topology—a group effort"; and "Massive speculation—trialities and tribulations".

TODOR MILEV (Jacobs Universität Bremen), "Computing regular subalgebras of simple Lie algebras"

Let $\mathfrak{g}$ be a finite dimensional simple Lie algebra and $\mathfrak{h}$ be a fixed Cartan subalgebra. Let $\mathfrak{l}$ be a subalgebra containing $\mathfrak{h}$ (non-zero nilradicals allowed) and let $\mathfrak{k} \supset \mathfrak{h}$ be the reductive part of $\mathfrak{l}$. A Fernando-Kac subalgebra of $\mathfrak{g}$, associated to an infinite dimensional $\mathfrak{g}$-module M, is defined as the set $\mathfrak{g}[M]$ of locally finitely acting elements of $\mathfrak{g}$. A subalgebra $\mathfrak{l}$ for which there exists an irreducible module M with $\mathfrak{g}[M] = \mathfrak{l}$ is called a Fernando-Kac subalgebra of $\mathfrak{g}$. A Fernando-Kac subalgebra is of finite type if there exists a module as above for which the Jordan-Hölder $\mathfrak{k}$-multiplicities of all simple $\mathfrak{k}$-modules are finite. A root system criterion describing all $\mathfrak{l} \supset \mathfrak{h}$ that are Fernando-Kac of finite type was conjectured by I. Penkov based on his joint work [PNZ] with V. Serganova and G. Zuckerman and a paper of S. Fernando. The presenter's Ph.D. thesis proves this criterion for all finite dimensional simple Lie algebras except E_8 (the case $\mathfrak{sl}(n)$ was already proved in [PSZ]). The proofs for exceptional Lie algebras F_4, E_6,and E_7 involved a computer computation. A regular subalgebra of a simple Lie algebra can be defined as a semisimple subalgebra spanned by root spaces of $\mathfrak{g}$. Regular subalgebras were classified in Dynkins fundamental paper "Semisimple Lie algebras of semisimple Lie algebras" (there are 75 proper isomorphism classes in E_8). Dynkin's classification automatically applies to root reductive subalgebras. In order to enumerate all possible nilradicals up to isomorphism one should first compute the $\mathfrak{k}$-module decomposition of $\mathfrak{g}$.

KARL-HERMANN NEEB (Universität Erlangen), "Semibounded representations of automorphism groups of Banach symmetric spaces"

The presenter discussed separable unitary representations of the automorphism group of a Hilbert hermitian symmetric space and its central extensions. He assumed that the representations are semibounded in the sense that, some element of the Lie algebra has a neighborhood on which the operators of the derived representation are uniformly bounded above. The methods to analyze such representations come from three sources: (1) Pickrells regularity results on separable representations of orthogonal and unitary groups, (2) some recent insights in the structure of invariant open convex cones in orthogonal and unitary Lie algebras, and (3) procedures to realize representations in Hilbert spaces of holomorphic sections of complex Hilbert bundles over the symmetric space.

BENT ØRSTED (Aarhus University), "Borel-de Siebenthal discrete series for exceptional groups"

For a semisimple Lie group admitting discrete series representations, it remains an interesting problem to find explicit realizations. In this lecture, based on joint work with Joseph Wolf, the presenter described the Borel-de Siebenthal discrete series, giving details about the geometry of the corresponding coadjoint orbits. In particular for some exceptional groups he described realizations allowing continuation in the discrete series parameter.

ROBERTO PERCACCI (International School for Advanced Studies, Trieste), "Elements of a GraviGUT"

A GraviGUT would be a theory where gravity is unified with the other interactions in a way that directly generalizes what is done in the grand unified theories of particle physics. The presenter described what one would need to do to construct such a theory, and the steps that have been successfully carried through so far. He concentrated on the case, developed in his work with Fabrizio Nesti, where the unifying group is $SO(3,11)$.

HADI SALMASIAN (University of Ottawa), "Unitary representations of supergroups and the method of orbits"

The main goal of this talk was to show that ideas of the orbit method can be applied to describe unitary representations of Lie supergroups. The presenter defined Lie supergroups and their unitary representations (in a global sense) and proved that for nilpotent Lie supergroups there exists a bijective correspondence between irreducible unitary representations and nonnegative coadjoint orbits. A simple branching rule for irreducible unitary representations to the even part followed.

GORDAN SAVIN (University of Utah), "Classifying discrete series representations of G_2 using minimal representations"

The presenter began with the classical inclusions

$$SL(3,\mathbb{C}) \hookrightarrow G_2(\mathbb{C}) \hookrightarrow Spin(7,\mathbb{C}).$$

Using Langlands functoriality conjectures, he deduced some (conjectural) relationships between discrete series representations for G_2 (over a p-adic field k) and representations of $PGL(3,k)$ and $PSp(6,k)$. Finally, he showed how to prove these conjectural relationships using theta-liftings related to minimal representations of E_6, E_7, and E_8.

DANIEL STERNHEIMER (Keio University and Université de Bourgogne) "Some instances of the unreasonable effectiveness (and limitations) of symmetries and deformations in fundamental physics"

The presenter gave a survey of some applications of group theory and deformation theory (including quantization) to mathematical physics. He discussed rotation and discrete groups in molecular physics ("dynamical" symmetry breaking in crystals, Racah-Flato-Kibler); chains of groups and symmetry breaking. He also discussed classification of Lie groups ("internal symmetries") in particle physics. Finally he addressed the topics of space-time symmetries and relations with internal symmetries. Then there was a discussion of deformation of symmetries, specifically deformation quantization, quantum groups and quantized spaces; of field theories and evolution equations from the point of view of nonlinear Lie group representations; of connections with some cosmology, including especially quantized anti-de Sitter groups and spaces; and of prospects for future developments between mathematics and physics.

Outcome of the Meeting

We enthusiastically thank BIRS for the opportunity to bring together a group of representation theorists with a group of physicists in circumstances that facilitated communication and understanding. The facilities and setting at BIRS are outstanding, as is the organization and infrastructure. In particular Brenda Williams and her staff made a big contribution to the success of the program.

For one reason or another, physics participation was less than we had hoped. This affected the balance of participants and the composition of the organizing committee. The BIRS staff was extremely helpful in dealing with that, and the organizers warmly thank them for their flexibility, which led to an exciting and fruitful conference.

The main progress was the increased understanding by mathematicians of the Standard Model and of the E_8 models in particle physics. There was some reciprocity here as the physics participants learned a good bit about the representation theory of semisimple Lie groups, E_8 in particular, and the ATLAS project in semisimple structure and representation theory.

A certain amount of mathematical software (especially ATLAS) was demonstrated and circulated. This will certainly have future impact.

With these two items of progress, the program more than satisfied its goals, and as nearly as we can tell all the participants were delighted with the way it worked out. But more than that, a number of participants took advantage of the presence of the others to advance individual or joint research projects; so the benefits of the meeting will continue to develop for some time.

David Vogan

Joseph Wolf

Participants

Achar, Pramod N. (Louisiana State University)
Adams, Jeffrey (University of Maryland)
Barbasch, Dan (Cornell University)
Binegar, Birne (Oklahoma State University)
Ciubotaru, Dan (University of Utah)
Cunningham, Clifton (University of Calgary)
Cushman, Richard (University of Calgary)
Dray, Tevian (Oregon State University)
Eastwood, Michael (Australian National University)
Garibaldi, Skip (Emory University)
Harris, Benjamin (MIT)
Howard, Tatiana Katarzyna (Univesity of Michigan)
Huang, Jing-Song (HKUST)
Huckleberry, Alan (Ruhr-Universitat Bochum)
Kobayashi, Toshiyuki (the University of Tokyo)
Kostant, Bertram (MIT)

Lisi, Garrett (Theoretical physicist)
Magaard, Kay (Birmingham)
Manogue, Corinne (Oregon State University)
Mare, Augustin-Liviu (University of Regina)
Milev, Todor (Jacobs University Bremen)
Neeb, Karl-Hermann (Darmstadt, Technichal University)
Orsted, Bent (University of Southern Denmark)
Percacci, Roberto (Perimeter Institute)
Rossmann, Wulf (University of Ottawa)
Salmasian, Hadi (University of Ottawa)
Savin, Gordan (Utah University)
Sternheimer, Daniel (Keio University)
Varadarajan, V. S. (UCLA)
Vogan, David (Massachusetts Institute of Technology)
Wilson, Rob (Queen Mary London)
Wolf, Joseph (University of California - Berkeley)
Yee, Wai Ling (University of Windsor)

Chapter 27

Statistical issues relevant to significance of discovery claims (10w5068)

Jul 11 - Jul 16, 2010

Organizer(s): Richard Lockhart (Simon Fraser University), James Linnemann (Michigan State University), Louis Lyons (University of Oxford)

Motivation for the meeting

In 2006 a workshop was held at BIRS titled "Statistical inference Problems in High Energy Physics and Astronomy". The outcome of the 2006 Workshop was so encouraging that we proposed another BIRS workshop for 2010. New facilities in Particle Physics and Astrophysics (e.g. the Large Hadron Collider and the GLAST telescope for gamma rays) are beginning to produce a large amount of data. There is a strong hope that these will result in exciting new discoveries. There are interesting statistical issues relating to discovery claims, and it is important to be able to give reliable, widely accepted statistical assessments of the evidence that the result is not due just to a statistical fluctuation.

A potentially disturbing example arises from an experimental Particle Physics collaboration who analyzed their data in 2003, and found that, at greater than a 5 sigma level, their data were inconsistent with the null hypothesis, and instead gave evidence for a new type of particle, the penta-quark. However a subsequent calculation of the Bayes factor comparing the null hypothesis with the alternative of a new particle was said to favour mildly the null hypothesis. This apparent sensitivity of an important conclusion to the statistical technique employed is worrying, and needs to be understood. The conflicting papers from the same authors analyzing the same data can be see at: `http://arxiv.org/abs/hep-ex/0307018` and `http://arxiv.org/abs/0709.3154`.

This workshop therefore brought together particle physicists, astronomers and statisticians to discuss:

1. Why Particle Physicists like 5 sigma as a discovery criterion; for Statisticians, requiring a 5 standard error deviation from the null, which corresponds to a significance level on the order of 1 in a million, is extraordinarily stringent.

2. Allowing for multiple tests; research groups carry out many tests on the same data.

3. Goodness of fit tests for comparing sparse multi-dimensional data with theory.

4. Comparison of different techniques for comparing 2 hypotheses, for example:

(a) p-values (including methods for combining p-values for different tests);

(b) The so-called CL_s (ratio of p-values for null hypothesis and alternative), an approach to setting upper confidence limits which is little known in the statistical community;

(c) Likelihood ratio tests, even when null and alternative hypotheses are composite;

(d) Difference in chi-squared of 2 separate fits to the same data;

(e) Model selection techniques such as AIC or BIC;

(f) Bayesian techniques such as posterior odds or Bayes factors (including the issue of choice of prior).

5. Adjusting for nuisance parameters in p-value and likelihood calculations.

6. Definitions of sensitivity of searches for new phenomena.

Presentation Highlights

The workshop format was very informal with the schedule being rejigged each evening in light of what happened that day. We wanted to focus on getting conversations and joint research projects going and we think we succeeded. In this section of the report we touch on main themes. Details of some presentations are provided in the next section.

The workshop opened with talks from a particle physicist (Louis Lyons) and an astronomer (Tom Laredo) setting the stage for the discussions and a response talk (Richard Lockhart) which tried to begin the process of translation from one technical language to another. We followed up by spending much of the first afternoon letting each participant say why he was there and what he hoped to get out of the meeting.

The second day began with talks from Jon Pumplin and Robert Thorne on parton distribution functions highlighting the following general problem. (Parton distribution functions describe the random partitioning of momentum among the quark and gluon constituents of a hadron such as a proton. When two hadrons collide it is really one of these constituents from each hadron which interact and these parton distribution functions then make it possible to describe the distribution of the momenta of the colliding constituents.) Several groups fit parton distribution function models to data arising from a variety of experiments. It is found that the fitted standard errors arising from standard chi-square approximations to log-likelihood ratio drops are unrealistic and that several experiments differ from the fitted values by more than is reasonable. It seems that differences of 50 need to be considered rather than differences of 1 or 2. This set of talks prompted much discussion and the talks had to be continued later in the meeting. See the commentary from Jon Pumplin, Robert Thorne and Steffen Lauritzen below.

Jim Linnemann talked about the on-off problem and Kyle Cranmer followed up with extensions therefrom. In particular he introduced the idea of “Asimov data sets”, new to statisticians and most physicist; for binned data an Asimov data set has bin counts equal to their expected value (even if that is not an integer). This sparked considerable discussion; see Kyle Cranmer’s remarks below. Also see Glen Cowan’s Wednesday talk on profile likelihood.

Elliott Bloom discussed the failure of Wilk’s theorem in an astrophysical example testing for source extension. Appropriate large sample approximations to the behaviour of likelihood ratio tests played an important role in the conference. See Eilam Gross and Ofer Vitells below. A talk by Glen Cowan on Wednesday touched on Wilk’s theorem

An important aspect of the workshop was the development of “Banff Challenge 2”. This challenge, running over fall 2010, is aimed at getting groups of statisticians and physicists to analyze data simulated data sets trying to detect signals either in analytically specified backgrounds or in situations where both the background and signals are described only by Monte Carlo data. An important component of the challenge, as with Banff Challenge 1, is the effect of systematic errors which are handled by either by specifying a prior of some sort or by auxiliary measurements.

The Challenge was discussed Wednesday morning in a series of presentations by workshop participants who had worked on a preliminary version of the problem. We returned to the discussion of the Challenge on Friday and a team led by Tom Junk and Wade Fisher has been working through the late summer to develop, distribute and publicize the challenge. Results are sought by early December in time for Phystat 2011 at CERN in January 2011.

One topic of intense discussion over the time period was the 'look elsewhere effect' or 'multiple testing' or 'multiple comparisons'. Louis introduced the issue on Monday. A number of other speakers touched on aspects of the question and Eilam Gross spoke on Wednesday about the issue and about 'trial factors' – the ratio of a P-values appropriate for a single hypothesis to that for testing several hypotheses. Thus a trial factor is a number which corresponds to the number of hypotheses examined in a simple Bonferroni correction.

In a search for a peak on a background, a canonical problem in discovery, tests can be run looking for a peak at each fixed point in the spectrum and then we can think of scanning over those points and picking the smallest P-value. This generates a look elsewhere effect; it could be corrected for if we had effective large sample theory for the overall likelihood ratio statistic. This is a problem, however, because Wilk's theorem does not apply in this context. This issue is at the heart of Eilam's presentation. See his remarks below.

Thursday had many talks covering a variety of topics before we turned to summary presentations. David van Dyke summarized from the point of view of a statistician, Roberto Trotta from the point of view of an astrophysicist and Luc Demortier from the point of view of a particle physicist.

Friday morning had a talk from Wolfgan Rolke about nearest neighbour methods for doing multivariate goodness-of-fit – an important interest in the area which the workshop was not able to focus on enough. Friday morning also considered the future of the Banff Challenge 2.

Individual Reports on Progress Resulting from the meeting.

In this section we have gathered commentary from individual participants hoping to highlight the diversity of benefits we each took from the workshop. What follows are direct quotes, slightly edited by the conference organizers; they are presented in alphabetical order.

Henrique Araujo & Alistair Currie: Statistical analyses of WIMP search results are coming under close scrutiny as direct search experiments begin to probe the 'hot regions' of favoured parameter space. The problem of assessing the presence of a signal on the tails of poorly characterized backgrounds is a recurrent one in rare event physics. No general solution exists; several ideas were discussed with Glen Cowan, Bob Cousins, Bodhi Sen, Wolfgang Rolke and others on topics such as blind analyses, Feldman-Cousins with uncertain backgrounds, profile likelihood analyses, Bayesian methods and other topics.

Banff Challenge 2 proved useful in preparing for the workshop, helping us to identify similarities and differences between direct dark matter searches and typical collider scenarios.

Our Imperial colleague Roberto Trotta persuaded us that a Bayesian analysis of dark matter experiments should address uncertainties on the technology together with those on the Astrophysics and we could end up collaborating on that. The Banff meeting was the perfect setting for these discussions and for our ideas to mature during the week.

Tests presented to quantify the similarity of multivariate datasets also suggest applications to dark matter searches, where data-to-data and MC-to-data comparisons figure in background estimation and signal modelling. Overall it was a most useful workshop in the most wonderful of settings!

Jim Berger: Bayesian hypothesis testing and model selection were reviewed and illustrated with a very recent example of Vaccine Trials, indicating the importance of looking at matters from a Bayesian as well as a frequentist perspective. The initial analyses — which were based solely on p-values — could have erroneously caused a major shift in scientific efforts towards a likely incorrect avenue of research.

The reasons for the differences between p-values and Bayesian assessments of evidence were then discussed, with special focus on the issue of systematics or bias in the model for analysis. There is an intriguing indication that Bayes factors may be more resistant to such bias than are p-values.

The major difficulty with the Bayesian approach to hypothesis testing and model selection is the choice of prior distributions — this was highlighted in the talk by Bob Cousins. The “solutions” to this problem that exist in the statistics literature were discussed, although it was acknowledged that only a robustness or sensitivity analysis can definitively settle the issue.

Finally, the Bayesian approach to the “look elsewhere effect” (“multiple testing” or, simply, the problem of “multiplicity” in the statistics literature) was also discussed. Of particular interest was that Bayesians and frequentists approach multiplicity from very different directions, and that it is crucial to understand — and utilize — the relevant strengths of each.

Elliott Bloom: I found the discovery statistics meeting to be an instructive and very interesting meeting. For a number of months I have been working with a group of staff, post docs and graduate students at KIPAC-SLAC trying to understand the asymptotic behavior of the Test Statistic resulting from our likelihood fitting routine by comparing MC simulations to the predictions of Chernoff’s theorem (I used to think that I was comparing to Wilks’ Theorem, but the discovery statistics workshop educated me on this point).

In my talk to the conference I showed that the asymptotic behavior expected from Chernoff’s theorem was badly violated in our MC simulations. Our results were received with interest by many people at the workshop and they made a number of valuable suggestions for further study by our group. This issue was also discussed in detail in the summary talk of David van Dyk, in which he also alluded to the result presented in my talk. Since returning we have tried a number of these suggestions and found that except for the absolute simplest case, fitting a peak with no background in a simple MC, Chernoff’s theorem is not satisfied by our MC simulations, and as we approach more realistic simulations of our actual Fermi data analysis this disagreement becomes more and more severe. We are still trying to pin down root cause for these disturbing trends. One suggestion made by Roberto Trotta, was to try a Bayesian approach, we have been using frequentist theory. We are seriously considering implementing his suggestion at this time.

Jim Chiang: I found the BIRS workshop to have been very useful in many respects. Among the talks, I found the ones by Tom Loredo, Jim Berger, Michael Woodroofe, Chad Shafer, and David van Dyk to be particularly useful. Tom’s discussions of the merits of the marginal likelihood vs the profile likelihood and the Neyman-Scott and related problems may be relevant for a bias we are finding in the analysis of Fermi data. David van Dyk’s slides on his team’s procedures for accounting for systematic uncertainties in the Chandra effective area described a framework in which similar sorts of calculations may be performed for Fermi data. He and his colleagues were kind enough to provide a draft of their paper in advance of publication, and we plan to implement some of their procedures. We are considering using the techniques Michael Woodroofe described for computing error probabilities via importance sampling for our own assessments of p-values. I’m happy to hear that Kyle and his student already have an implementation, and I have contacted Kyle about obtaining a copy of their code. As Kyle has already noted, he and I discussed RooStats at length, and I plan to implement some Fermi analysis using that framework and will provide feedback to Kyle and his colleagues that should help make that toolkit useful across disciplines. I had very useful discussions with Louis Lyons and Richard Lockhart on goodness-of-fit that helped clarify the relevant issues for me. My participation in this workshop inspired me to propose that the Fermi LAT team have a statistics board similar to those that exist for experiments such as CDF and ATLAS. A discussion that Elliott and I had with Joel Heinrich was extremely useful for defining the scope of the board functionality in this proposal, and the proposal was accepted by the LAT PI and analysis coordinators. Finally, I enjoyed the meals, hikes, BIRS lounge bull sessions, and after hours trips to the pub that helped make the whole event a very collegial experience.

Bob Cousins: This workshop was well worth my dedicated trip from CERN in Geneva, as it brought together a terrific mix of experts in a great environment. Thanks to excellent advance planning, the workshop attracted a nearly complete “Who’s Who” group of high energy physicists who have an impact on statistical techniques in our field. The equivalent among astronomers was well represented as well, and the always-insightful statisticians included those which have learned about our problems in previous workshops (such as Jim Berger, Steffen Lauritzen and Michael Woodroofe) as well as some new faces (at least to me) who were impressively adept at understanding our specific issues and helping us with them.

My own interest was particularly sparked in several discovery-oriented areas, notably the Jeffrey-Lindley paradox, the Look-Elsewhere Effect, and comparisons of different ways of dealing with nuisance parameters (e.g., marginalization and profiling). In all these cases, I came away from the workshop with important insights that will directly affect my work in high energy physics. In other areas, such as uncertainties in parton distribution functions, I believe that I and the others at the workshop materially helped those struggling with their problems, offering suggestions and establishing contacts that will be mutually beneficial in the future.

My talk was on the Jeffreys-Lindley paradox, about which I had only superficial knowledge before preparing for the workshop. In this example, a Bayesian model selection calculation and a Frequentist hypothesis test for the same problem have different scaling behavior with the sample size n, so that in the limit of large sample size they can reach opposite conclusions, each with overwhelming significance. The workshop provided motivation for me to read some 25 papers and books on this topic, and to try to relate it to the way we approach analogous cases in high energy physics. I will almost certainly try to find the time to write up what I have learned and to follow up on a conjecture or two that grew out of this work. The Banff Centre was a perfect location for such a workshop. In additions to animated conversations over the three meals, we had a number of late-evening discussions in the Corbett Hall lounge that calcified some issues each day. I look forward to returning some day to the Banff Centre.

Glen Cowan: The BIRS meeting on Statistical Methods for LHC Physics provided an outstanding opportunity to finalize and report on recent work carried out by myself and three other workshop participants (E. Gross, O. Vitells and K. Cranmer) on use of profile likelihood methods for discovery significance and for setting limits. A draft of our paper had been finished just prior to the meeting (e-print: arxiv:1007.1727), and this was the basis of the talk that I presented. We apply asymptotic distributions based on the approximations of Wald and Wilks to find p-values for either the background-only hypothesis or a hypothesized signal and also to find the expected (median) discovery or exclusion significance.

Feedback received during the meeting was positive, and a few important points emerged that we are now incorporating into the paper's final draft. For example, our paper now addresses a criticism concerning zero-length confidence intervals. We also benefited from discussion with the statisticians present on the relation of the so-called Asimov data set to the expected Fisher information.

Beyond the progress related to our paper, I found the entire programme of the meeting interesting and useful, especially the work on the "look-elsewhere effect".

Kyle Cranmer: The BIRS workshop was very useful and very enjoyable. A number of my projects and collaborations either got a boost or were formed at the workshop.

Through conversations with Richard Lockhart and Earl Lawrence, we were able to precisely show the relationship of the "Asimov" dataset and the Fisher information matrix, which was only a conjecture before coming to BIRS. This result is being included in the second version of our paper on the arxiv, which Eilam, Ofer, Glen, and I will submit for publication shortly. We have thanked Richard, Earl, and BIRS in the acknowledgements. The result is also relevant for speeding up the calculation of Jeffreys's prior, which may also impact the work on reference priors being done by Luc Demortier and Harrison Prosper.

During the workshop we discussed a number of ideas which I hope to see implemented in RooStats, which may have impact on the entire field. In particular, my graduate student, Sven Kreiss, has implemented the importance sampling techniques described by Michael Woodroofe, which can bring huge gains for the computationally expensive LHC Higgs combinations. That development should go into the next release of ROOT. Similarly, Luc, Harrison, and I were able to develop a plan for how their `refpriors` package can be interfaced and incorporated into RooStats. Steffen Lauritzen graciously sat with me to work through the graphical models corresponding to our HEP problems. Particularly interesting was the "max propagation" and "random propagation" algorithms, which may provide important speedups for our most common HEP problems. We hope to employ these new techniques in the context of the Banff challenge 2, which I hope will be as successful as the first Banff challenge.

I was happy to get back in touch with Bodhi Sen, who gave me some important insight into the relationship of the bootstrap and the algorithm we currently use to generalize of the Feldman-Cousins technique with nuisance parameters. Of course, I enjoyed lunch and dinner conversations with all of the participants, most memorably those with Jim Berger, Bob Cousins, Gary Feldman, and Tom Loredo.

Roberto Trotta and I were able to bring back to life a stalled project to estimate the coverage properties of current techniques that are used to infer regions of SUSY parameter space that compatible with a variety of experimental results. We hope to show some preliminary results at a conference in Stockholm in September.

Lastly, I had a long and pleasant conversation with Jim Chiang on our hike about the possibility of using RooStats in the analysis of data from the Fermi Gamma Ray Telescope. This development may have important consequences in our understanding of dark matter and a plausible combined analysis of LHC and Fermi data.

Luc Demortier: The most impressive aspect of the workshop was the high quality of all the talks. I learned something from each of them, but was particularly interested in some of the ideas presented by statisticians: a new importance sampling technique (M. Woodroofe), a goodness-of-fit test with Bayesian prior on alternatives (R. Lockhart), D. van Dyk's solution to the sensitivity problem in the calculation of upper limits, C. Schafer's decision-theoretic approach to parton densities and the Banff challenge, and Steffen Lauritzen's random effects model to determine the parton densities. Regarding the latter, the talks by J. Pumplin and R. Thorne were very useful and enlightening. It may be that one of the greatest successes of the workshop was the decision by these speakers to attempt a closure test on their procedure to determine the parton densities. On another front, there was a lot of discussion about the so-called Asimov data, but I remain somewhat skeptical of the validity of this method in more complicated settings than the usual illustrative examples. I enjoyed T. Loredo's talk on profile versus marginal likelihood. Finally, I should also mention several useful discussions I had with J. Berger about Bayes/frequentist points of contact.

With the help of a summer student I have done some work on the Banff challenge, and plan to write up our results for discussion with other interested parties. Many workshop participants showed interest in the look-elsewhere effect, and this has inspired me to try and write up a review of the extensive and still evolving statistics literature on the subject.

I gave one of the summary talks at the workshop, and the above is more or less a summary of that summary.

Eilam Gross: The Banff workshop was the most beneficial workshop I have been to in my life. Besides learning a great deal about statistics and meeting remarkable people, it is thanks to the Banff workshop that together with Ofer Vitells, we have managed to fully complete and understand our own research on the "Look Elsewhere Effect".

In his summary talk in the 2010 BANFF workshop Luc Demortier drew our attention to the work of Davies from 1977 which became the leading thread of our revised work. Michael Woodroofe whom we also met at BANFF, spent his valuable time to explain to us how to adopt the statistical language of Davies to the High Energy Physics jargon. He also spent valuable time in writing to us his impressions on the Look Elsewhere Effect. The revised version of our paper on the "look elsewhere effect" would have never been possible without the Banff workshop; for us this paper is a major scientific achievement.

On top of all this the magnificent atmosphere in Banff with the amazing hospitality set up the right ground for scientific developments. We have no words to express our thanks to the organizers and the team.

David Hand: The meeting was an eye-opener in revealing to me the breadth of statistical issues in which the particle physics and astronomy/cosmology communities had an interest. I knew of their interest in coping with massive data sets, but I had not realized that they also had a matching interest in the more philosophical subtleties of statistical inference. It served to reinforce my belief that those areas of physics are ones to which statisticians can make useful contributions. The recent surge of interest in these areas amongst statisticians (e.g. the establishment of the ISI group on astrostatistics) is very timely. I look forward to following up the various discussions I had outside the formal talks, and on the plans I made with various participants to collaborate on exploring some of their problems in detail.

Chris Hans: I found the Banff meeting to be very interesting. Most of the conferences I attend are organized by and for statisticians, and it was a pleasure to hear about statistical issues in astronomy and physics at this meeting directly from the source. While I can't say that I have developed any collaborations based on the meeting, I do feel that I gained a better understanding of which particular statistical areas are of interest – and importance – to researchers in these fields and will keep this in mind as I develop my research in these areas over the next few years. In terms of interactions at the meeting, I particularly enjoyed a few conversations I had with Tom Loredo about some of my work on Bayesian regularization priors and its connections to questions of model uncertainty. I also very much enjoyed meeting several statisticians who I had not yet met beyond earlier brief introductions (in particular Chad Schafer, Earl Lawrence, Nicolai Meinshausen and Bodhi Sen). In this sense, the meeting was successful in not only bringing together scientists across disciplines but also in bringing together statisticians across sub-disciplines who might not otherwise have an opportunity to interact and share ideas in such a small and productive setting.

Joel Heinrich: As a gathering of people from the HEP, Astrophysics, and Statistics worlds, the Banff meeting was helpful to me in several ways. I became informed on current trends in the HEP-statistics community, and the views of the statisticians regarding those trends. Learning about statistics practice in astrophysics provided a useful contrast to the practice in HEP which is familiar to me. Since the meeting, I have become involved in the design phase of Banff Challenge 2, which is intended to provide an additional forum for new methodology to be applied to the typical discovery problems in HEP.

Thomas Junk: This workshop was very productive. I met with other particle physicists, astrophysicists, and statisticians from July 11 to July 16. We discussed the issues related to how to make discoveries in particle physics and astrophysics; issues relating to the false discovery rate, such as Why do we like 5 sigma? What happened during historical non-discoveries like the Pentaquark and the 40-GeV top quark? Statisticians bring a unique point of view to the subject, and work is ongoing at CERN in the ATLAS and CMS statistics committees to work out their details of setting limits and discovery procedures. They were impressed with our care and rigor. I made three presentations, one on practical experimental details of interpreting search results, one on the challenge problems (homework for participants), filling in for Wade Fisher who could not attend, and one presentation on my solutions to the challenge problems. We will continue to work on these challenge problems to generalize them and make them more useful in the near future. I also learned about "power-limited Feldman-Cousins" and the simpler "power-limited CLs+b" techniques and will give them some thought. Techniques also for reducing our need to run computationally expensive exclusion and evidence/observation calculations were also brought up that I am interested in testing in the future. I learned that the look-elsewhere effect depends on the data sample size, an effect that in hindsight makes a lot of sense, but I was unaware of it before this meeting. I am also much happier and more comfortable with our treatment of the look-elsewhere effect, which has a degree of arbitrariness in defining "elsewhere"; There was more agreement on that subject than I was expecting, and now we can proceed with confidence.

Steffen Lauritzen: A very interesting meeting. I am in contact with Jon Pumplin and Robert Thorne [see the discussion from Robert Thorne below] to follow up on my remarks about parton distribution functions. I hope something comes out of that.

Jim Linnemann: I found the Banff workshop useful in a number of ways. First, I found many of the talks informative and stimulating. I was also able to use the occasion to communicate directly with colleagues on matters of interest. In particularly, I discussed with Robert Thorne (global parton distribution function fitting) and with Lorenzo Moneta some things I've learned in the last year on nonlinear fitting; I hope that Lorenzo can move some of this information into root where it will be accessible to a broad user community, and he seems interested in that path. I also found the discussion with colleagues on state ordering in the Look Elsewhere Effect to be clarifying, and expect this will be reflected in two physics papers in progress. Michael Woodroofe in particular has suggested some interesting ways to think about this problem, and I intend to follow up with him in this area. I have been involved in the setting of the initial Banff Challenge for this workshop, and also in the followup effort, which we expect will stimulate more effort and be reported on at the Phystat 2011 conference in Geneva. In addition, conversations with several statisticians (David Hand, Richard Lockhart, and Earl Lawrence) have identified common areas of interest which could lead to collaborations.

I also had interesting conversations with: Wolfgang Rolke on his proposed multidimensional goodness-of-fit (and pointed him to a paper by Friedman at an earlier phystat); Tom Loredo on 2-d angular difference measures in astrophysics; and with Gross et al's whose paper shed light on issues we'd seen in effective number of trials in an astrophysics experimentr.

Nicolai Meinshausen: The very stimulating meeting in Banff was interesting in many ways for me. The treatment of systematic errors in the particle physics simulation models is very much related to similar problems in climate models and I hope to be able to transfer some of the ideas between the fields in the future. It was also very fruitful to me meet some astronomers, notably Tom Loredo and people working on the Fermi experiment, and discuss the detection of periodic signals, a problem I have been working on and published about previously and which I intend to take up again, using partially the very useful input I got out of informal discussions at the meeting.

Lorenzo Moneta: This has been my first workshop at Banff and I have found it extremely useful for my work. It has been one of the most interesting and productive workshop I have participated. I have learned a lot about statistics at both theoretical and practical level from attending the lectures and participating in the discussions. For example, I have now a much clearer picture on what are the problemats in using the likelihood function to establish a discovery significance. This is very useful for my job to manage and develop software statistical tools for the data analysis of the LHC experiments.

I enjoyed very much the discussions with my colleagues from HEP, with the astro-particle physicists and the statisticians. The workshop provided a great opportunity to discuss together our statistical problems and to learn from each other. We have been discussing possible improvements for the RooStats package, like including the reference prior in the Bayesian analyses.

From listening to the lectures, I developed ideas for implementing new tools in the ROOT software package, such as automatic binning from histograms using Bayesian methods or new method for goodness of fit of multidimensional data. From discussing with Jim Linnemann, I will start investigating the possibility to improve the current minimization algorithm we are using in HEP (Minuit), to deal better with non linearity and with the problem of converging to a local minimum instead of the global minimum. This algorithm is the most common used algorithm in HEP for solving non linear fits, like those presented at the workshop for finding the parametrization of the parton structure function or for evaluating the discovery significance using the likelihood function. Furthermore, I enjoyed very much the pleasant atmosphere and the wonderful location. Thank you very much to the organizers and to BIRS.

Chad Schafer: The main point of my talk was to present an approach to constructing confidence regions/hypothesis tests which are optimal with respect to a clearly defined, yet user-specified, notion of performance. In particular, using standard decision theoretic ideas, one can construct decision procedures that possess frequentist coverage, but have maximal power against alternatives considered physically feasible. It is common that one seeks procedures with such properties, and standard approaches do exist (e.g, Wilks' Theorem) for well-behaved situations. For situations in which one has a complex model (likelihood function), care must be exercised. Although I did not describe it in any detail, there is a Monte Carlo procedure for approximating the aforementioned optimal procedure; it is designed to work in (indeed, it was motivated by) these cases where one has a complex likelihood function, or for some other reason cannot rely upon the asymptotic approximations of Wilks' Theorem. My hope is that this approach could be of value in addressing both the Second Banff Challenge, and the quantifying of the amount of uncertainty in the estimates of the Parton distribution function. I found the Workshop to be an ideal setting to explore the challenging inference problems in particle physics, and look forward to pursuing these further in direct collaboration with the physicists.

Jeffrey D. Scargle: I found the Banff workshop was very useful for me on both practical and theoretical levels. One of my main interests is in the use of modern statistical techniques to astrophysical data. As you know, the lines between astrophysics and particle physics are blurring – hence the field of astroparticle physics. There were many presentations extraordinarily well focused on the corresponding issues. I enjoyed very much working on the Banff Challenge Data; one always learns a lot by coming to grips with actual data – be they synthetic, experimental, or observational.

Bodhisattva Sen: The Banff workshop was very exciting. It was mostly an educational experience for me, as I am still trying to understand the major statistical issues in HEP. I discussed some related statistical concepts to some of the physicists in one-to-one conversations. I hope that some of these synergistic activities will lead to real collaborations in the future. I also plan to take a closer look at the Banff Challenge data, in the near future. The organization of the workshop was exemplary. I very much enjoyed the visit and most of the talks, although I think that a few of the talks could have highlighted the statistical aspects of the problem more clearly.

Paul Sommers: Thank you very much for inviting me to participate in the Banff workshop on "Statistical issues relevant to significance of discovery claims." This was a particularly valuable experience for me. As co-spokesperson for the Pierre Auger Collaboration, I am facing numerous problems that relate directly to statistical methods for assessing the significance of intriguing anisotropy correlations seen in our data, and also the problem of reporting sensible upper limits for point sources of neutral particles (neutrons and gamma rays). This was a great opportunity to learn from experts, and I was pleased to be able to present some results from the Auger Cosmic Ray Observatory.

The workshop was an opportunity to meet numerous distinguished persons whose work I know from the literature, and also to become acquainted with some outstanding scientists that I did not know about previously. It was an intellectually enriching experience in a delightful setting. Thanks again.

Robert Thorne: The Banff workshop was both useful and enjoyable, and from my viewpoint was unusual in the breadth of subject area expertise covered by the (relatively small number of) participants. However, this meant that my talk, which became talks, spent rather a longer time covering the basics than expected and did not really get to the precise details of how the procedures used by different groups differ in detail. However, it was gratifying that most (perhaps all) of the audience were happy to accept that this is a difficult problem, and also that the need to inflate the textbook determination for uncertainties of parton parameters was not found to be surprising.

It terms of determining more precise reasons for understanding why this inflation is necessary, the proposal to generate a set of data from the theory, but then to obtain the uncertainties by scattering according to the true experimental uncertainties in order to obtain a global set of data which is both consistent with itself and the theory will certainty be performed, and should be straightforward. Also generating a set from e.g. NNLO theory and attempting to fit with NLO, i.e. having self-consistent data set which does not match the theory perfectly is the obvious next step. Results will be interesting and I will keep people in touch.

I am also intrigued by various of the the proposals to solve the assumed problems of incompatibility of different data sets and/or of data and theory in a more statistically robust manner than used by the various groups at present. In particular that of Steffen Lauritzen to modify the χ^2 definition to account for different data sets preferring different values of the parameters using Random Effect models. The general principles behind this do indeed seem to match the problem and I hope to pursue this further, though it will require more new work than the simpler checks above.

Roberto Trotta: I found the meeting highly interesting and enjoyable. I valued in particular the opportunity to interact with Paul Summers, Tom Loredo, Bob Cousins, Jim Berger, Chad Shafer, with whom I had several interesting discussions regarding various aspects of my research. Kyle Cranmer and I took the opportunity of the workshop to restart a project we had been working on together, with the aim of publishing the results after the Summer. I also had the opportunity to give one of the summary talks of the meeting, in which I tried to describe synergies and differences between the problems and approaches discussed during the workshop and some of the currently ongoing research in cosmology.

Ofer Vitells: I found the BIRS workshop very useful and educational. Both the lectures and discussions provided many important insights into the statistical problem that were addressed. In particular we had useful discussion and feedback on our "Asimov" paper which is about to be submitted for publication soon (with Kyle, Eilam and Glen) as already mentioned by Kyle. In addition we got very helpful comments and references related to our work on the "look elsewhere effect". Michael Woodroofe and Luc Demortier pointed us to some related work that might help in placing some of our conjectures on a more solid ground. We are currently working on this in collaboration with Michael Woodroofe who has kindly agreed to help us with the mathematical formulation. I had also very interesting discussions with Henrique Araujo and Alastair Currie on their views on the statistical challenges of experiments that search for dark matter, and that will certainly contribute to our future work with the Xenon100 collaboration.

Michael Woodroofe: I got a better understanding of the physics and some new problems to pursue. I am following up with Eilam Gross and Jim Linnemann. With Eilam, I am working out the details of how Davies results apply to his problem. Jim's nested multiple hypotheses remind me a bit of a problem that arose in sequential analysis circa 1980. I think that a similar formulation might capture the effect that he wants. I spoke on how importance sampling was used in sequential analysis and how I think it can be used in the discovery problem.

Summary

This workshop started many useful collaborations and introduced many of us to new ideas. The follow up over the fall of the Banff Challenge 2 should be very productive. Finally, this workshop will set the stage for much useful discussion at PHYSTAT 2011 at CERN in January 2011.

Participants

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Gross, Eilam (Weizmann Institute)
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Lockhart, Richard (Simon Fraser University)
Loredo, Tom (Cornell University)

Lyons, Louis (University of Oxford)
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Murray, Bill (Rutherford Appleton Lab)
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Chapter 28

Statistical Genomics in Biomedical Research (10w5076)

Jul 18 - Jul 23, 2010

Organizer(s): Darlene Goldstein (Ecole Polytechnique Federale de Lausanne), Jennifer Bryan (University of British Columbia), Sandrine Dudoit (University of California, Berkeley), Jane Fridlyand (Genentech Inc.), Sunduz Keles (University of Wisconsin, Madison), Katherine Pollard (Gladstone Institutes, University of California, San Francisco)

Overview and Recent Developments in Statistical Genomics in Biomedical Research

Genetic research has been transformed by technological developments, and has by necessity become extremely quantitative, as massive quantities of varying complex data types can now be generated very rapidly. High-throughput data are being used in a variety of basic science investigations that have implications in the diagnosis and treatment of human disease: identification and characterization of genetic variants associated with a particular disease within and across populations; discovery of gene expression signatures associated with disease phenotypes; identification and testing of potential disease biomarkers. Methodological advances in the statistical treatment and interpretation of these data are needed in order to meet the pressing need for powerful, efficient and robust analyses.

Biomedical progress is increasingly dominated by high-throughput technologies, presenting new statistical and computational hurdles to overcome in order to make sound quantitative inferences. These technological advances provide unprecedented opportunity for understanding the genetic basis and molecular mechanisms of disease, as well as normal biological function. At the same time, they have given rise to multiple and complex data types, posing serious modeling and analytic challenges.

Fostered by the development of new techniques in molecular biology, translational research has become an important aspect of clinical research. The aim of translational research is to translate knowledge derived from laboratory work (basic research) into clinical applications. Translational research occurs at the interface between quantitative methodology and clinical treatment. The field is highly multidisciplinary and team-based, encompassing researchers with backgrounds in lab-based basic science, clinical investigation, statistical methodology and computational/algorithmic development. Moving these very high-dimensional data into clinical practice will require biologically-inspired expansion of the existing statistical framework for dealing with these complex structures.

This workshop will focus on key areas of basic and clinical biological research that generate very high dimensional, complex data structures and which require further development of statistical and computational methodology for their efficient use.

The targeted areas are briefly described below.

Population and Quantitative Genomics

Patterns of genetic variation in a population can reveal the dynamics of that species' history, disease susceptability, and response to changing environmental conditions. The focus is on genome features that vary among individuals within a species. While population genomics does not necessarily involve measuring a phenotype, studying the association between this genetic variation and variability in traits of interest across a population can shed light on the underlying biology, for example, helping to identify genetic risk factors associated with disease. Genetic variation consists of single nucleotide polymorphisms, large-scale polymorphism, copy number variation, and insertions, deletions, and rearragements in the genome. The major statistical challenges in population genomics are appropriately modeling and quantifying uncertainty about the historical events (recombination, mutation, migration, drift) that shape genetic variation. Coalescent theory and diffusion models provide a sound basis for these studies, but require extension and algorithmic improvements to handle the high-dimensional data sets from emerging technologies.

Quantitative traits of an individual (*e.g.* molecular biomarkers, drug concentrations, physical properties) are typically controlled by a collection of genetic loci, called quantitative trait loci (QTLs). Genomic technologies are enabling the measurement of many such traits and the simultaneous study of their association with millions of genetic markers. Quantitative genomics is facilitated by controlled breeding and/or knowledge of population history and structure. Furthermore, studies are now being conducted on huge panels of organisms in which distinct (combinations of) genes have been knocked out, or knocked down. This area of high-throughput phenotyping is another very powerful way to link genes to phenotypes and to identify the genetic interactions (*i.e.* epistasis) underlying multi-genic traits. Analysis of these complex data sets requires statistical methods for assessing power, modeling interactions, and accounting for multiple comparisons.

High-Throughput Sequencing Assays and Transcriptional Genomics

Advances in high-throughput sequencing capabilities have given rise to new, sequence-based versions of microarray-based assays. Common ones in current use include RNA-seq and ChIP-seq.

RNA-seq is a protocol for sequencing messenger RNA, and can be used as a tool to measure gene expression levels (e.g. for identifying differentially expressed genes) as well as for other aims requiring increased sensitivity compared to microarrays, notably to identify alternative splicing. This new technology requires a new generation of software for alignment to a reference genome. Software must be able to accommodate the reality that not all splice junctions are known, and the additional complications stemming from the large number of fragments with only very short overlaps. Some progress has already been made in this direction.

ChIP-seq is a sequencing-based alternative to (microarray-based) ChIP-chip that combines chromatin immunoprecipitation (ChIP) with DNA sequencing. This type of assay is used to study DNA-protein interactions. For example, gene expression is regulated by proteins known as transcription factors. Knowing how transcription factors and other proteins interact with DNA is crucial to understanding many types of biological functions.

ChIP-Seq has revolutionized experiments for genome-wide profiling of DNA-binding proteins, histone modifications, and nucleosome occupancy. As the cost of sequencing is decreasing, many researchers are switching from microarray-based technologies (ChIP-chip) to ChIP-Seq for genome-wide study of transcriptional regulation. Despite its increasing and well-deserved popularity, there is little work that investigates and accounts for sources of biases in the ChIP-Seq technology. These biases typically arise from both the standard pre-processing protocol and the underlying DNA sequence of the generated data.

Other difficulties arise in data analysis due to problems in peak identification/resolution (the precise DNA-protein binding location is not identified, only the ends of the ChIP fragments) and also due to regional biases such as sequencing and mapping biases. Model-based statistical approaches can be useful for resolving these difficulties.

Transcriptional genomics is concerned with approaches for understanding transcriptional regulation, based on data from both gene expression studies (by high-throughput sequencing and/or microarrays), chromatin immunoprecipitation assays, and promoter sequence data. One aim is to catalog and gain an understanding of single transcription factors; another is to identify transcriptional modules, sets of genes that are co-regulated in a set of experimental or in vivo conditions.

Basic and Clinical Research: Predictive Diagnostics and Designing Clinical Trials

Translational research aims to bridge the disconnect between new basic science discoveries and the ability to translate those discoveries into effective, affordable and safe medical treatments for patients. There is a need for cross-disciplinary work of basic science researchers, clinical scientists, computational scientists and statisticians to develop biologically meaningful yet quantitatively sound approaches to integrating genomic, experimental and computational evidence during research and clinical drug development. The statistical challenges include: evaluating accuracy and precision of the technology used to measure biomarkers; evaluating prediction accuracy and developing appropriate statistical measures (along with uncertainty estimates) for the performance of these potential biomarkers relative to any established benchmarks; and assessing the reproducibility of experimental outcomes and the resulting inferences, both within and across different populations.

For progress in diagnosis, prognosis and treatment of human disease, associations between disease with the avalanche of genomic information (SNP genotypes, haplotype blocks, candidate genes/alleles, proteins, and metabolites) must be reliably quantified and assessed. There is a strong need for biologically relevant, powerful computational methods and models to integrate multi-level genome-wide evidence and to interpret the resulting high-dimensional outcomes so that strategies for clinical implementation can be developed. The major fundamental statistical challenges occur at the data analytic stage, where diverse data elements from all sources need to be incorporated into comprehensive models for prediction, risk assessment, and/or efficiency.

Presentation Highlights and Scientific Progress

Here we give highlights from the talks presented at the meeting, along with the scientific progress that they represent as it pertains to the topics and problems described above.

Population and Quantitative Genomics

Jonathan Pritchard spoke about expression QTL mapping using RNA-Seq, a new, sequencing-based alternative to microarrays for measuring transcriptome activity. An important challenge of the post-genomic era is to make sense of how genome sequences control gene regulation. The talk discussed work using expression- and splicing-QTL (quantitative trait loci) in human lymphoblastoid cells as a model system for understanding how genetic variation can modify gene regulation. The focus was on the application of next-generation sequencing for measuring gene expression and splicing patterns and attempts to understand the mechanisms of action of eQTL SNPs.

Jeff Wall considered the problem of estimating human demographic parameters from sequence polymorphism data based on population genetic data. These data sets have the potential to inform about a species' demographic history, but most existing methods are not suitable for genomic-scale data. A composite-likelihood framework was presented for estimating demographic parameters such as split times and migration rates. The method was applied to the analysis of polymorphism data from different sub-Saharan African populations. His group has found evidence for population structure that likely predates the exodus of modern humans out of Africa. This finding has relevance with regard to current theories of human evolution.

Yoav Gilad has used next-generation sequencing to carry out comparative genomics in primates. Progress in evolutionary genomics is tightly coupled with the development of next-generation sequencing technologies, providing the ability to focus on a large number of outstanding questions that previously could not be addressed effectively. In the context of comparatives genomic studies in primates, new sequencing technologies have allowed collection of high resolution inter-individual and inter-species variation data from multiple dimensions of the regulatory landscape. These data are used to better understand the contribution of different regulatory mechanisms to overall inter-species differences in gene regulation, and allow identification of individual genes and entire pathways whose regulation evolves under natural selection in primates. These observations have the potential to help find functional genetic variation in humans. He provides an example where it was found that the set of genes previously associated with diseases that affect specific tissues is enriched for genes whose regulation evolves under stabilizing selection in the same tissues.

John Ngai presented insights gained by transcriptome profiling on regulation of olfactory stem cell renewal and differentiation. The process of tissue regeneration is complex, requiring coordination of stem cell proliferation and differentiation to maintain or repair the structure. The olfactory epithelium (OE) is a sensory neuroepithelium whose constituent cell types – including the olfactory sensory neurons – are continuously replaced during the lifetime of the animal. Following severe injury that results in the loss of mature cell types, the OE is rebuilt by the proliferation and differentiation of adult tissue stem cells. The regenerative capacity and limited number of cell types make the OE an excellent model for investigating stem cell regulation in vivo. He discussed previous studies that have identified the horizontal basal cell (HBC) as the multipotent neural stem cell of the OE. However, the molecules and pathways regulating this adult tissue stem cell are unknown. He used whole genome expression profiling of FACS-purified HBCs to characterize the mRNA and miRNA transcriptomes of HBCs under conditions of quiescence and proliferation/differentiation. These studies allowed identification of groups of genes associated with different phases of the HBC life cycle.

His group has found that p63, a member of the p53 tumor suppressor gene family, is highly enriched in quiescent HBCs. This finding is important because p63 is a key regulator of stem cell self-renewal and differentiation in all stratified epithelia investigated to date. Conditional inactivation of the p63 gene in HBCs results in the appearance of mature cells but loss of HBCs following regeneration. These results demonstrate a critical role of p63 in olfactory stem cell renewal and differentiation, and provide an entrée toward elucidating the downstream targets and interaction partners of this transcription factor. These studies provide the first molecular insights into the genetic network regulating stem cell dynamics in the OE and reveal an unexpected parallel between stem cell regulation in this sensory neuroepithelium and other epithelial tissues.

Transcriptional Genomics

Jason Lieb considered genome-wide measurement of transcription factor binding dynamics by competition ChIP. He presented a novel method applicable to a wide range of experimental next-generation sequencing datasets and signal patterns, including ChIP-seq, FAIRE-seq, and Histone Modification data. The method comprises a mixture regression-based framework that rigorously identifies, assesses and quantifies sets of factors that are relevant in explaining enriched and background signal in parallel. In addition, adjacent regions significantly enriched for signal are merged, allowing identification of both broad and short regions of activity. He provided a demonstration of how these factors play different roles across different data types, and showed how incorporating these factors into the modeling framework can lead to improved performance in the determination of biologically relevant loci. This method represents a significant shift away from earlier methods of peak calling/peak identification to a more flexible and unified modeling framework, applicable to many types of experimental situations.

Elodie Portales-Casamar discussed deciphering regulatory networks by transcription factor binding site analysis. She provided an introduction to regulation of gene expression, which can happen at multiple levels. These include chromatin modifications, initiation of transcription at gene promoters, alternative splicing and stability of RNA, protein modifications. The binding of transcription factors (TFs) to DNA sequences near or within genes is one of the primary mechanisms directing gene transcription. Understanding the interplay between TFs and their target genes is key to deciphering cellular regulatory networks that generate diverse types of cells and tissues within an organism.

She gave an overview of many of the common computational approaches to TF binding site analysis. Sets of known binding sequences are compared to construct TF binding models. Such necessary information is collected and disseminated through community-driven resources like PAZAR, a public database of transcription factor and regulatory sequence annotation, and the high-quality transcription factor binding profile database JASPAR. However, the compiled data still remains too sparse to cover the full spectrum of DNA-binding proteins. Genome-wide chromatin immunoprecipitation techniques (e.g. ChIP-Seq) are now providing larger data collections that allow for more accurate models and increase the quality of genome annotation. Such methods enable researchers to decipher entire regulatory networks in specific cellular contexts. The example included in the talk was for ChIP-Seq data analysis of the upregulation of detoxification systems by the Nrf2 transcription factor in cells exposed to stress.

Sunduz Keles presented her work on the development of MOSAiCS: Model-based One & Two Sample Analysis and Inference for ChIP-Seq data. This model addresses a range of problems, from multi-reads to background adjustment to peak calling. She discussed various statistical aspects of ChIP-Seq data analysis, including handling of multi-reads and developing background models that adjust for apparent sources of biases due to ChIP-Seq experimental protocol.

The particular focus was on data from a naked DNA sequencing experiment, which sequences non-cross-linked DNA after deproteinizing and shearing, to understand factors affecting background distribution of data generated in a ChIP-Seq experiment. She outlined a background model that accounts for the observed sources of biases such as mappability and GC content. She then presented MOSAiCS, a flexible mixture modeling approach for detecting peaks in ChIP-Seq data. This model incorporates the background component derived from n aked DNA experiments and introduces a flexible model for the actual signal component. This model fits actual ChIP-Seq data very well, and also has the important practical advantage that one-sample analysis of ChIP-Seq data with MOSAiCS performs as well as the two-sample ChIP-Seq data analysis that utilizes sequenced naked DNA as control. A further extension of this model was developed for two-sample ChIP-Seq data analysis with Input DNA control.

Ting Wang presented his work on mapping the human DNA methylome (regions of methylated DNA) with MeDIP-Seq and MRE-Seq technologies. These represent two complementary approaches to detect methylated and unmethylated genomic DNA. The first, methyl DNA immunoprecipitation and sequencing (MeDIP-Seq), uses antibody-based immunoprecipitation of 5-methylcytosine and sequencing to map the methylated fraction of the genome. In the second method, unmethylated CpG sites are identified by sequencing size-selected fragments from parallel DNA digestions with the methyl-sensitive restriction enzymes (MRE-Seq). Using these technologies, he as able to generate data providing a genome-wide, high-resolution methylome map of human brain tissue, and a second map of human ES cell H1. These maps on average interrogate close to 90% of all CpGs (25 million of 28 million total) and 98% of CpG islands in the human genome, at the modest expense of relatively small amount specimen and a few lanes of Illumina flowcell.

The role of DNA methylation in gene bodies was investigated with these methylome maps. From high-resolution coverage of CpG islands, the majority of methylated CpG islands were revealed to be in intragenic and intergenic regions, while less than 3% of CpG islands in 5′ promoters were methylated. The CpG islands in all three locations overlapped with RNA markers of transcription initiation, and unmethylated CpG islands also overlapped significantly with trimethylation of H3K4, a histone mark enriched at active promoters. The general and CpG-island-specific patterns of methylation are conserved in mouse tissues. These and other results support a major role for intragenic methylation in regulating cell context-specific alternative promoters in gene bodies.

High-Throughput Sequencing

James Bullard presented an overview of a new proprietary third generation sequencing technology from Pacific Biosciences, the PacBio RS, scheduled for full commercial release this year. The focus of this talk was on describing the types of data available to analysts, the open source software being produced by the company, and the repositories where example data can be obtained.

Margaret Taub talked about detection of single-nucleotide variants with high throughput sequencing, including current practices and pitfalls. The talke included results on one targeted re-sequencing dataset as well as some of the publicly available data from the 1000 genomes project. She explored the impacts of technical and sequence-specific properties on accurate variant detection.

Kaspar Hansen provided an overview of results from an investigation of empirical features of RNA-Seq data, including methods for examining base-level effects and measuring goodness-of-fit of read count models. He also presented some graphics that explore detection as a function of annotation and additional exploratory analyses of RNA-Seq data.

Wolfgang Huber presented methodology and software for differential expression analysis of sequence count data. High-throughput nucleotide sequencing provides quantitative readouts in assays for RNA expression (RNA-Seq), protein-DNA binding (ChIP-Seq) or cell counting (barcode sequencing). Statistical inference of differential signal in such data requires estimation of their variability throughout the dynamic range, which is typically much larger than the dynamic range of microarrays. When the number of replicates is small, error modeling can be used to achieve greater statistical power. He proposed an error model that uses the negative binomial distribution, with variance and mean linked by local regression, to model the null distribution of the count data. The method controls Type I error and is shown to provide good detection power for detection of differentially expressed genes. A free open-source R software package, DESeq, is available from the Bioconductor project.

High-Throughput Biological Assays

Laurent Jacob discussed obtaining higher statistical power for identification of differentially expressed pathways using known gene networks. The problem of identifying sets of genes which are differentially expressed between two clinical groups is cast as a multivariate two-sample test. Under the assumption that the shift of expression is coherent with a known network structure, he has shown that integrating this structure in the test statistic leads to more powerful tests. He also discussed systematic testing of all sub-networks of a large network for de novo pathway identification. The behaviour of this new approach was illustrated on both synthetic data and on a breast cancer hormone therapy resistance expression dataset.

Jean-Philippe Vert talked about including prior knowledge in shrinkage classifiers for genomic data. Estimating predictive models from high-dimensional and structured genomic data, such as gene expression of comparative genomic hybridization (CGH) data, measured on a small number of samples is one of the most challenging statistical problems raised by current needs in post-genomics. Popular tools in the fields of statistics and machine learning to address this issue are shrinkage estimators, which minimize an empirical risk regularized by a penalty term, and which include for example support vector machines or the LASSO. He discussed new penalty functions for shrinkage estimators, including generalizations of the LASSO which lead to particular sparsity patterns, and which can be seen as a way to include problem-specific prior information in the estimator. Several examples illustrating the approach were included, such as the classification of gene expression data using gene networks as prior knowledge, and the classification and detection of frequent breakpoints in CGH profiles.

Pierre Neuvial presented work on targeted maximum likelihood estimation of the relationship between copy number and gene expression in cancer studies, a specific type of data integration problem. Identification of genes whose DNA copy number is "associated" with their expression level in a cancer study can help pinpoint candidates implied in the disease and improve understanding of its molecular bases. DNA methylation is an important player to account for in this setting, as it can down-regulate gene expression. He developed a method based on Targeted Maximum Likelihood to quantify the relationship between copy number and expression, accounting for DNA methylation. He explained the method and its statistical properties. Some preliminary results were shown from a simulation study as well as from a real data set from the Cancer Genome Atlas project (TCGA).

Robert Scharpf discussed his work on a multilevel model to address batch effects in copy number estimation for high-throughput SNP arrays. Submicroscopic changes in chromosomal DNA copy number dosage are common and have been implicated in many heritable diseases and cancers. Recent high-throughput technologies have a resolution that permits the detection of segmental changes in DNA copy number that span thousands of basepairs across the genome. Genome-wide association studies may simultaneously screen for copy number-phenotype and SNP-phenotype associations as part of the analytic strategy. However, genome-wide array analyses are particularly susceptible to batch effects as the logistics of preparing DNA and processing thousands of arrays often involves multiple laboratories and technicians, or changes over calendar time to the reagents and laboratory equipment. Failure to adjust for batch effects can lead to incorrect inference and requires inefficient post-hoc quality control procedures that exclude regions that are associated with batch. His work extends previous model-based approaches for copy number estimation by explicitly modeling batch effects and using shrinkage to improve locus-specific estimates of copy number uncertainty. Key features of this approach include the use of diallelic genotype calls from experimental data to estimate batch- and locus-specific parameters of background and signal without the requirement of training data.

Jared Roach presented methodology and analysis of pedigree genome sequencing data for a small family with a rare disease. Full-genome sequences of a pedigree with p individuals can be represented as a series of genotype vectors. Consider a single chromosome with n positions. A genotype, $g_{i,p}$, is an observation of two alleles at a position i for individual p. For example, $g_{23145140,3}$ may be $\{A, C\}$. A genotype vector, $V_i = \{g_{i,1}, g_{i,2}, g_{i,3}, \ldots, g_{i,p}\}$, is an ordered list of genotypes for all individuals in the pedigree. The series of genotype vectors for a chromosome is thus $\{V_1, V_2, V_3, \ldots, V_n\}$. Binary inheritance vectors represent the not-directly-observed flow of alleles through the pedigree, and are parallel in structure to genotype vectors. These series of vectors can be regarded as emissions from Hidden Markov Models (HMMs) and illuminate underlying genetic features. He analyzed the whole-genome sequences of a family of four. HMMs enabled the precise identification of recombination sites and 70% of the sequencing errors. These analyses permit matching inheritance states and inheritance modes, and thus disease-gene identification.

Lei Sun presented work on a practical solution to the "winner's curse" in genome-wide scans. In genome-wide scans, the most significant variants detected in the original discovery study tend to have inflated effect size estimates due to the "winner's curse" phenomenon. The winner's curse has recently gained much attention in Genome-Wide Association Studies (GWAS), because it has been recognized as one of the major contributing factors to the failure of attempted replication studies. For example, five *Nature Genetics* publications in the first three months of 2009 acknowledged the effect of winner's curse in their discovery samples. However, none made statistical adjustments to the naive estimates.

Previous work (Sun and Bull, 2005) developed in the context of genome-wide linkage analyses has been extended to provide Bias-Reduced estimates via Bootstrap Re-sampling (BR-squared) for GWAS without collecting additional data. In contrast to the likelihood-based approaches, the proposed method adjusts for the effects of selection due to both stringent genome-wide thresholds and ranking of the association statistics over the genome. In addition, this method explicitly accounts for the effect of allele frequency because the expected bias is inversely related to power of the association test.

The method has been implemented to provide Bias-Reduced estimates via Bootstrap Re-sampling (BR-squared) for association studies of both disease status and quantitative traits, and applied in genome-wide association studies of Psoriasis and HbA1c. There is a greater than 50% reduction in the genetic-effect-size estimation for many associated SNPs, which translates into a greater than 4-fold increase in sample size requirements for replication studies. Thus, adjusting for the effects of the winner's curse is crucial for interpreting findings from genome-wide scans, and in planning replication studies, as well as attempts to translate findings into the clinical setting.

Mark Segal gave a talk on genomic applications of clustering with exclusion zones. Methods for formally evaluating the clustering of events in space or time, notably the scan statistic, have been richly developed and widely applied. In order to utilize the scan statistic and related approaches it is necessary to know the extent of the spatial or temporal domains wherein the events arise. Implicit in their usage is that these domains have no "holes" (or *exclusion zones*), regions in which events *a priori* cannot occur. However, in many contexts, this requirement is not met. When the exclusion zones are known it is straightforward to correct the scan statistic for their occurrence by simply adjusting the extent of the domain. He has tackled the more ambitious objective of formally evaluating clustering in the presence of *unknown* exclusion zones. By examining the behavior of *clumps* over the grid of putative cluster counts and lengths, he showed that the existence of exclusion zones manifests as a characteristic signature. This patterning is exploited to develop an algorithm for estimating total exclusion zone extent, the parameter needed to correct scan statistic based inference, with performance of the algorithm assessed via simulation study. Applications to genomic settings for differing marker (event) types are shown – *binding sites*, *housekeeping genes*, and *microRNAs* – wherein exclusion zones can arise through a variety of mechanisms. In several instances there are dramatic changes to unadjusted inference that does not accommodate exclusions.

Ingo Ruczinski discussed SNP association studies with case-parent trios. While at present most high-throughput SNP association studies are population-based, family-based designs also have some very attractive features. Case-parent trio designs in particular allow for the assessment of de-novo copy number variants, parent-of-origin effects, and transmission distortion. He discussed and demonstrated these via a genome-wide and a candidate gene association study that employ case-parent trios. The logic is also extended to regression methodology, originally developed for cohort and case-control studies, to detect SNP-SNP and SNP-environment interactions in studies of trios with affected probands. An efficient algorithm is derived to simulate case-parent trios where genetic risk is determined via epistatic interactions.

Houston Gilbert provided some results from a cross-platform evaluation study of reverse-phase protein microarray data. Reverse-phase protein microarrays (RPPMA) allow for the simultaneous detection of a single protein in complex analyte mixtures, such as those obtained from cell tissue culture or clinical sample protein lysate. To gain a better understanding of the RPPMA arena, he worked on an evaluation of three fee-for-service providers of this technology. Practical, statistical and biological results from the evaluation study have informed strategies for moving forward with RPPMA technology in research and development programs. The evaluation study has also highlighted areas for each of the companies to improve upon their own platforms.

From the Bench to the Clinic

Adam Olshen presented an overview of two projects involving high throughput data. One is more mature and concerns distinguishing primary tumors from metastases utilizing copy number data. The methodology was demonstrated on a lung cancer data set. The second is a work-in-progress involving methylation sequencing data. He discussed integrating multiple types of such data as well as methods for estimating copy number from it.

Mauro Delorenzi talked about translational studies for predictive and prognostic biomarkers in colon cancer, including of microsatellite instability by expression profiling in a clinical trial. Microsatellite instability (MSI) is the hallmark of a deficient mismatch repair system (MMR) in about 15% of colorectal cancers (CRC). Several studies confirm MSI as an independent prognostic marker associated with a better outcome in stage II and IIICRC. As MSI can be caused by different mechanisms, and dMMR leads to secondary oncogenic alterations, heterogeneity in the clinical and molecular features of MSI CRC is likely but not well understood. In this transcriptome expression study, his group explored which genes differentiate MSI from Microsatellite stable (MSS) tumors and looked for evidence of additional subclasses.

RNA extracted from formalin-fixed paraffin-embedded (FFPE) tissue blocks was used for expression profiling on the ALMAC platform SColorectal Cancer DSA Y T. Classifiers were constructed using AdaBoost and DLDA algorithms and assessed with area under the curve (AUC) by cross-validation. Survival analysis was based on Cox regression. Unsupervised methods allowed only weak separation of MSI and MSS specimen, despite 494 genes with significantly different expression (1% FDR), due to high variation in both groups. Gene expression differences were in agreement with results from reanalysis of three public datasets. Classifiers discriminated MSI and MSS with AUC of 0.96, using 40-80 selected genes. Prominent discriminatory genes include various pathways: Wnt (e.g. Axin2), MAPK (DUSP4); inflammation-immunity (REGs, STAT1), differentiation (TNNC2,mucins), metallothioneins. Association of these genes with RFS is heterogeneous.

Efficient discrimination of MSS and MSI in gene expression profiles can be obtained, with good quality FFPE material, using a multi-gene classifier. Inside both classes there is high residual heterogeneity. More samples are planned to be profiled in order to further define molecular subgroups and to search for prognostic genes. The ability to obtain reliable profiles form FFPE material implies that relevant information can be obtained from archival material stored in many biobanks.

Pete Haverty discussed the mutation spectrum revealed by paired genome sequences from a lung cancer patient. Previous studies have identified important common somatic mutations in lung cancers, but they have focused primarily on a limited set of genes and have thus provided a constrained view of the mutational spectrum. He presented results from the complete sequences of a primary lung tumour (60x coverage) and adjacent normal tissue (46x coverage). Comparing the two genomes, a wide variety of somatic variations were identified, including >50,000 high-confidence single nucleotide variants. 530 somatic single nucleotide variants in this tumour were validated, including one in the KRAS proto-oncogene and 391 others in coding regions, as well as 43 large-scale structural variations. These constitute a large set of new somatic mutations and yield an estimated 17.7 per megabase genome-wide somatic mutation rate. Notably, there is a distinct pattern of selection against mutations within expressed genes compared to non-expressed genes and in promoter regions up to 5 kilobases upstream of all protein-coding genes. Furthermore, a higher rate of amino acid-changing mutations is observed in kinase genes. He presented a comprehensive view of somatic alterations in a single lung tumour, and provided evidence of distinct selective pressures present within the tumour environment.

Donald Geman talked about several projects in expression-based biomarker discovery and pathway regulation, mainly focused on cancer. The driving application is translational medicine. He argued that rank-based statistics can account for combinatorial interactions among genes and gene products; accommodate variations in data normalization and limited sample sizes; and avoid the "black box" representations and decision rules generated by standard methods in computational learning. Applications using single or pairs of top-ranked genes were presented for several cancer studies.

Predictive Diagnostics and Designing Clinical Trials

Jane Fridlyand gave a talk on the design of proof of concept trials in oncology, focusing on speed, cost and trial success. With the cost of bringing a drug to market in the range of nearly a billion dollars, pharmaceutical companies are concerned with achieving proof of concept as early as possible in the clinical development process, so that decisions on further development can be made with minimal loss. The bulk of the talk was devoted to the explanation of industry constraints to academic researchers focused on prediction optimality.

Ru-Fang Yeh discussed some of the statistical challenges in the development of predictive biomarkers. It has been increasingly important to incorporate diagnostics in the drug development process to improve response to treatment and help Several statistical issues arise during the development of predictive biomarkers that aim to identify patients who will benefit from a particular treatment. Examples that highlight statistical challenges in biomarker discovery and clinical applications were presented, including threshold selection for continuous biomarkers and implmentation of complex predictors.

Venkat Seshan concluded the session with a talk on two-stage designs for gene-disease association studies. Gene-disease association studies based on case-control designs may often be used to identify candidate SNPs (markers) conferring disease risk. If a large number of markers are studied, genotyping all markers on all samples is inefficient in resource utilization. He proposed an alternative two-stage method to identify disease-susceptibility markers. In the first stage, all markers are evaluated on a fraction of the available subjects. The most promising markers are then evaluated on the remaining individuals in the second stage. This approach can be cost effective since markers unlikely to be associated with the disease can be eliminated in the first stage. He presented tables showing optimal allocations and cost savings/increases in power and efficiency.

Open Questions and Outlook for the Future

There remain several open areas of research in the domain of statistical problems in high-throughput biomedical studies; we outline some of these here.

Statistical Challenges of New High-Throughput Technologies

DNA sequence data are becoming more prominent in high-throughput biomedical studies, and will only gain in importance as sequencing technologies become more reliable and less expensive. The aim of sequencing is to determine the order of the nucleotide bases in a DNA molecule, even up to an entire genome. This knowledge can be used in a wide variety of important applications such as identification of new genes and alternative gene splicing, mutation mapping, polymorphism discovery, DNA-protein interaction, and personalized medicine.

The number of applications of new sequencing technologies is large and growing. Sequencing can be used to provide genome-wide measures of: transcription levels (mRNA-Chip/mRNA-Seq), alternative splicing, protein-nucleic acid interactions, e.g., transcription factor, binding sites (ChIP-Chip/ChIP-Seq), DNA methylation (methyl-Chip/methyl-Seq), DNA copy numbers (aCGH), genotypes, etc.

With the new sequencing technologies come new statistical issues at nearly every step of the experimental pipeline: experimental design; exploratory data analysis and quality assessment/control; pre-processing steps such as image analysis, base-calling, read-alignment/mapping, normalization and expression quantitation; downstream analyses such as identification of differential expression; and the overarching issue of reliable software implementing the best developed methodologies.

Many of the methods developed for analyzing microarray data do not carry over to sequence data. There are new issues: different technology-dependent biases, and at an even more fundamental level the data have a completely different quality (continuous measures of fluorescence intensity for microarray data versus discrete counts for sequence data).

In the realm of experimental design, some of the new problems are: choice of sequencing depth (sample size – number of input samples/lanes); allocation of input samples to library preparations/flow-cells/lanes; control lane for calibration in base-calling; type of read (Strandedness, length, single-end, paired-end, or strobed reads); library preparation (priming, fragmentation protocols).

As with microarray experiments, low-level analysis/pre-processing is required for any type of study and is highly-dependent on the sequencing platform. Preprocessing steps include image analysis, base-calling, and read mapping/alignment. Unlike microarray probe sequences, sequence clusters do not lie on a grid, complicating image analysis. The base-calling relies on a deconvolution of the base sequence from measured fluorescence intensities of the four nucleotides at each cycle, to yield base-level and read-level quality scores. Challenges include existence of cross-talk and machine cycle effect. The resulting reads must be assigned to positions in the genome, transcriptome, or other reference sequence.

Even older algorithms developed for earlier generations of sequencing data cannot be used "as is". Existing algorithms for alignment (read mapping) and sequence assembly of older (Sanger) sequence data cannot be used as-is, because of the much shorter reads generated by pyrosequencing (a few hundred nucleotides) – the algorithms do not scale to the increased data volume, and with shorter fragments there are in addition combinatorial complications. However, users are adopting the newer technologies due to their lower cost and higher throughput compared to Sanger sequencing. There is thus a need for new statistical models/frameworks and modified or novel scalable algorithms for processing and analyzing the vast amounts of deep sequencing data generated in a study.

Given base-level read counts, we need to derive expression measures for genomic regions of interest (e.g. exon, intron, splice junction, single-isoform gene, multiple isoforms from a given gene). Normalization requires adjustment of raw expression measures to ensure that observed differences in expression measures between lanes and/or between regions of interest are truly due to differential expression and not experimental artifacts (e.g., library preparation/flow-cell/lane effects, nucleotide composition). Other challenges include zero counts, heterogeneity of base-level counts, uncertainties in annotation, and alternative splicing.

Further investigation into a statistical framework is also needed. Of particular interest is the use of generalized linear models (GLM) and especially Poisson/log-linear regression, to evaluate and adjust for a variety of technical effects and to detect differential expression between regions of interest and/or input samples. Assessment of method performance on calibration/benchmark data sets, as has been done for microarrays, would provide researchers with valuable information on the reliability of existing and new methods.

Integration of High-Dimensional Heterogeneous Data

Meta-analytic methods have been applied in the genomic context for combining study results, often one gene at a time via estimated regression coefficients or p-values. Such cases typically combine results for the same data type (e.g. gene expression data), but perhaps generated by different technologies (e.g. single channel or dual channel microarrays). It seems clear, though, that meta-analysis is not straightforwardly applied to the problem of combining data of different types, the most obvious impediment being lack of a common parameter across data types. It may also be desired to combine data types that are not gene-based (e.g. gene expression and glycomic data). Approaches other than meta-analysis include Bayesian models as well as correlation-based, kernel, svd-type or distance-based methods. However, integrating multiple data types in an automated, quantitative manner remains a major challenge.

Moving beyond the single gene at a time framework would also be valuable. For example, it would be quite useful to be able to integrate data on sets of genes (rather than only individual genes), or for multi-dimensional/multi-type molecular "signataures" in human disease, such as cancer. Development of a comprehensive catalog of signatures for different disease processes would spur method development, leading to the potential to elucidate molecular mechanisms important in disease pathogenesis and progression.

Translational Research

Translation of genome findings in complex disease is a complex and challenging aim. Genomic discoveries for monogenic diseases have led to clinical tests but there are fewer applications for complex diseases. Assessing the validity and utility of genomic tests for specific diseases can be difficult.

There is substantial scope for statistical thinking and methodology to help achieve translational aims. There is already a vast body of basic research that needs to be harnessed in a reliable and efficient manner so that the important findings impact on treatment options to improve human health. With a massive expenditure of resources already consumed, it is vital to take advantage of the existing Genome Wide Association Studies (GWAS) by exploiting previously generated initial GWAS scans. Problems still exist in addressing the replication and continuation or combination of GWAS findings, and epidemiologic data must also be integrated. Biological studies carried out as complementary studies must also be integrated in a fundamentally sound way.

It would seem that, at least initially, very specific models will need to be created, reflecting the conditions of a particular set of studies (or study types). A major hope is that a flexible, encompassing framework will emerge that will facilitate translation of basic findings to clinical relevance.

A medical topic of increasing influence is the importance of *structural variation in human diseases* such as cancer and HIV/AIDS. Until now, most genome-wide association studies have focused only on SNPs, or single nucleotide polymorphisms. However, larger structural variation (for example, copy number variation, or CNV) is also highly abundant and is increasingly recognized as a substantial contributor to disease/phenotype variation. Deep sequencing technologies can be used to detect structural variation, allowing for systematic study on a whole genome level of genetic alterations. Such studies should lead to greater understanding of fundamental disease processes, and result in important implications in the prevention, detection, diagnosis, prognosis, and treatment of cancer and of HIV/AIDS.

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Chapter 29

Computational Complexity (10w5028)

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Organizer(s): Paul Beame (University of Washington) Stephen Cook (University of Toronto) Russell Impagliazzo (University of California, San Diego) Valentine Kabanets (Simon Fraser University) Avi Wigderson (Institute for Advanced Study)

Overview of the Field

Computational Complexity Theory is the field that studies the inherent costs of algorithms for solving mathematical problems. Its major goal is to identify the limits of what is efficiently computable in natural computational models. Computational complexity ranges from quantum computing to determining the minimum size of circuits that compute basic mathematical functions to the foundations of cryptography and security.

Computational complexity emerged from the combination of logic, combinatorics, information theory, and operations research. It coalesced around the central problem of ”P versus NP” (one of the seven open problems of the Clay Institute). While this problem remains open, the field has grown both in scope and sophistication. Currently, some of the most active research areas in computational complexity are

- the study of hardness of approximation of various optimization problems (using probabilistically checkable proofs), and the connections to coding theory,
- the study of the role of randomness in efficient computation, and explicit constructions of ”random-like” combinatorial objects,
- the study of the power of various proof systems of logic, and the connections with circuit complexity and search heuristics,
- the study of the power of quantum computation.

Recent Developments and Open Problems

The main focus of computational complexity is to understand *efficient* computation. One of the main open problems is the famous ”P versus NP” question which asks if there is an efficient algorithm for solving such problems as Satisfiability (SAT): Given a propositional formula in n variables, decide if there is a setting of the variables to the truth values (True and False) so that the formula on the assignment evaluates to True. This problem has been the driving force behind many developments in complexity theory, and continues to be such.

While the exact complexity of SAT remains unknown, researchers do come up with new results that shed more light on various aspects of this fundamental problem, and its counting version (given a propositional formula, count the number of its satisfying assignments). Some of these new developments were also reported at the workshop (see below).

Understanding the complexity of approximation problems (e.g., given a conjunction of constraints find an assignment that satisfies approximately the largest number of the constraints) is also one of the main tasks of complexity theory, and has been pursued since 1990's using the machinery of Probabilistically Checkable Proofs (PCPs). While the known PCP results imply tight inapproximability results (under the hypothesis that $P \neq NP$) for a number of approximation problems, there are a few important exceptions for which the currently known techniques seem powerless. This led to the formulation of a conjecture (Unique Games Conjecture) whose truth would imply inapproximability results for quite a few new problems. Whether this conjecture is true or false has become one of the main open problems in modern complexity theory, with no apparent consensus by the experts of what outcome is more likely. A number of discussions on this conjecture were also held at the workshop.

One of the main open problems in communication complexity is the Direct Sum Conjecture which basically says that the amount of communication needed to solve k instances of a given problem should be k times the amount of communication needed to solve a single instance of the problem. The conjecture is still open. However, some new ideas have been recently introduced that may eventually lead to the resolution of the conjecture, and already have provided some nontrivial weaker statements. These ideas are based on compressing the communication protocol between two parties, and very information-theoretic in nature. This problem has also been discussed at the workshop.

Understanding efficient computation also involves understanding the role of randomness in computation. In particular, one of the basic questions is to construct pseudorandom generators (PRGs) that are efficient algorithms stretching a short truly random input string into a much longer string that ”looks” random to a given class of observers. For the sufficiently general class of observers (say, when observers are themselves arbitrary efficient algorithms), no such construction is known (and it seems to be related to our lack of lower bounds for general models of computation). However, for sufficiently restricted classes of observers, some nontrivial PRG constructions are known. Some of the recent developments in the area have involved the class of polynomial threshold functions, showing that well-known constructions are actually pseudorandom for these functions, as well as giving new constructions of PRGs for these functions. Another important class of observers is the class of small-space algorithms, and is centered around the open problem of whether every small-space randomized algorithm can be made deterministic without increasing the space usage by more than a constant factor. While the general question remains open, some special cases have been recently solved. These PRG constructions have also been an important topic of discussion at the workshop.

Presentation Highlights

The Unique Games Conjecture

The famous result of Cook and Levin from 1970's introduced the important notion of NP-completeness. Many natural problems were later shown to be NP-complete, and hence unlikely to be efficiently solvable unless some well-studied hard problems (such as Satisfiability of propositional formulas, deciding if a graph has a large clique, and deciding if a graph is 3-colorable) are also efficiently solvable (in deterministic polynomial time).

The NP-completeness theory is applicable to the case of *exact* algorithms, which are required to compute the exact optimal solutions to a given NP-problem. The subsequently developed theory of Probabilistically Checkable Proofs managed to extend NP-hardness results to the case of *approximation* algorithms, where an algorithm is only required to obtain an approximately optimal solution (to within a certain approximation factor). A large number of optimization problems were shown NP-hard to approximate (to within certain approximation factors). This theory, developed starting from 1990's, has been extremely successful in classifying a large number of approximation problems, often establishing tight approximation factors (where the problem is NP-hard to approximate with a better factor, and on the other hand, there is an efficient algorithm approximating the problem with slightly worse factor).

Despite this success, some important approximation problems still escape such tight classification. One approach to deal with this was formulated by Khot, and is known as the "Unique Games Conjecture". The conjecture involves systems of linear equations over finite fields, where each equation is over 2 variables. Roughly, the conjecture states that it is NP-hard to distinguish the following two cases: (1) a system of such linear equations over a finite field (of appropriate size) where there is a vector that satisfies "many" equations, and (2) a system of such linear equations where no vector can satisfy more than "few" equations.

Lifting the restriction that each equation be over 2 variables to allow 3 variables per equation yields a well-known NP-hardness result due to Håstad. Khot conjectured that the same result is true even for 2 variables per equations, but this bold conjecture is still open.

At the workshop, there were a few discussions regarding the Unique Games Conjecture, attacking it from both sides: trying to prove it (see the talk by Moshkovitz), and trying to disprove it (see the talk by Steurer). There was also a talk describing interesting connections of the conjecture to the problem of expansion in graphs (see the talk by Raghavendra).

Below we list the abstracts of the relevant presentations.

P. Raghavendra *Approximating Graph Expansion: Connections, Algorithms and Reductions*

Approximating edge expansion, equivalently finding sparse cuts in graphs is a fundamental problem in combinatorial optimization that has received considerable attention in both theory and practice. Yet, the complexity of approximating edge expansion in graphs is poorly understood. Particularly, worse is the understanding of the approximability of the expansion of small sets in graphs. More formally, current algorithmic or hardness results do not settle the approximability of the following problem: Given a regular graph G and a very small constant c, find a set S of cn vertices in the graph such that minimum number of edges cross the set S. Recently it was shown that the complexity of this problem is closely tied to the Unique Games Conjecture. Furthermore, we show that the hardness of this problem is a natural assumption that generalizes the unique games conjecture, and yields hardness for problems like Balanced Separator and Minimum Linear arrangement.

D. Moshkovitz *Hardness of Approximately Solving Linear Equations Over Reals*

We consider the problem of approximately solving a system of homogeneous linear equations over reals, where each equation contains at most three variables. Since the all-zero assignment always satisfies all the equations exactly, we restrict the assignments to be "non-trivial". Here is an informal statement of our result: it is NP-hard to distinguish whether there is a non-trivial assignment that satisfies $1-\delta$ fraction of the equations or every non-trivial assignment fails to satisfy a constant fraction of the equations with a "margin" of $\Omega(\sqrt{\delta})$. Unlike the well-studied case of linear equations over finite fields, for equations over reals, the best approximation algorithm known (SDP-based) is the same no matter whether the number of variables per equation is two or three.

Our result is motivated by the following potential approach to proving The Unique Games Conjecture:

1. Prove the NP-hardness of solving approximate linear equations over reals, for the case of three variables per equation (we prove this result).

2. Prove the NP-hardness of the problem for the case of two variables per equation, possibly via a reduction from the three variable case.

3. Prove the Unique Games Conjecture.

An interesting feature of our result is that it shows NP-hardness result that matches the performance of a non-trivial SDP-algorithm. Indeed, the Unique Games Conjecture predicts that an SDP-based algorithm is optimal for a huge class of problems (e.g. all CSPs by Raghavendra's result). (Joint work with Subhash Khot)

D. Steurer *Subexponential Algorithms for Unique Games and Related Problems*

We give a subexponential time approximation algorithm for the Unique Games problem: Given a Unique Games instance with optimal value $1 - \epsilon^6$ and alphabet size k, our algorithm finds in time $exp(k \cdot n^\epsilon)$ a solution of value $1 - \epsilon$.

We also obtain subexponential algorithms with similar approximation guarantees for Small-Set Expansion and Multi Cut. For Max Cut, Sparsest Cut and Vertex Cover, our techniques lead to subexponential algorithms with improved approximation guarantees on subclasses of instances. Khot's Unique Games Conjecture (UGC) states that it is NP-hard to achieve approximation guarantees such as ours for Unique Games. While our result stops short of refuting the UGC, it does suggest that Unique Games is significantly easier than NP-hard problems such as Max 3-SAT, Label Cover and more, that are believed not to have subexponential algorithms achieving a non-trivial approximation ratio.

The main component in our algorithms is a new kind of graph decomposition that may have other applications: We show that by changing an ϵ fraction of its edges, any regular graph on n vertices can be broken into disjoint parts such that the stochastic adjacency matrix of each part has at most n^ϵ eigenvalues larger than $1 - \epsilon^6$. (Joint work with Sanjeev Arora and Boaz Barak.)

Complexity of Counting

In the pioneering work of from the late 1970s, Valiant studied the complexity of counting problems (such as #SAT: Given a propositional formula, compute the number of its satisfying assignments), and proved the computing the Permanent of a 0-1 matrix is a complete problem for this class of counting problems. It is widely believed that there is no efficient algorithm to solve such counting problems. However, in certain special cases (for restricted counting problems), it was observed that efficient algorithms are possible, and are essentially some determinant computations for appropriate matrices. Given such fairly non-intuitive efficient algorithms, one may ask what other counting problems can be efficiently solved via some kind of reduction to a problem solvable by these known algorithms. Recently, Valiant proposed a way to formalize such reductions, and defined the notion of ”Holographic algorithms”. Using this approach, he was able to solve efficiently some new counting problems which were not known efficiently solvable before. Naturally it is an important question to understand the limitations of this ”holographic method”, and this has been tackled in a number of recent papers by Valiant and other researchers.

At the workshop, Valiant gave a talk on the current status of holographic algorithms.

L. Valiant *Holographic Algorithms*

First we briefly review some recent dichotomy results, including some that strictly generalize constraint satisfaction problems, that showcase the power of the holographic method. We go on to define the notion of diversity for families of finite functions, and express the limitations of a class of holographic algorithms in terms of limitations on diversity. In particular, we show, by a new but very classical looking combination of counting and algebraic methods, that the class of elementary holographic algorithms, which has yielded novel polynomial time algorithms for such problems as special cases of Boolean Satisfiability, is insufficient for expressing general Boolean Satisfiability. We suggest that the question of how far this lower bound argument can be extended is of some general interest.

We go on to explore the power of nonelementary polynomial time holographic algorithms by describing such algorithms for certain parity problems for which no polynomial time algorithms were previously known. These algorithms compute the parity of the following quantities for degree three planar undirected graphs: the number of 3-colorings up to permutation of colors, the number of connected vertex covers, and the number of induced forests or feedback vertex sets. These holographic algorithms, besides being nonelementary, use bases of more than two components and thereby potentially evade the Cai-Lu Collapse Theorem.

Complexity of SAT

The problem SAT (satisfiability of a propositional formula) is one of the most famous NP-complete problems, and has been a popular problem to study for a long time. At the workshop, there were a couple of new results regarding the complexity of SAT for formulas (by Santhanam), as well as the impossibility of certain ”compression” of SAT (by van Melkebeek).

D. van Melkebeek *Satisfiability Allows No Nontrivial Sparsification Unless The Polynomial-Time Hierarchy Collapses*

Consider the following two-player communication process to decide a language L: The first player holds the entire input x but is polynomially bounded; the second player is computationally unbounded but does not know any part of x; their goal is to cooperatively decide whether x belongs to L at small cost, where the cost measure is the number of bits of communication from the first player to the second player.

For any integer $d \geq 3$ and positive real ϵ we show that if satisfiability for n-variable d-CNF formulas has a protocol of cost $O(n^{d-\epsilon})$ then coNP is in NP/poly, which implies that the polynomial-time hierarchy collapses to the third level. The result even holds for conondeterministic protocols, and is tight as there exists a trivial deterministic protocol for $\epsilon = 0$. Under the hypothesis that coNP is not in NP/poly, our result implies tight lower bounds for parameters of interest in several areas, including sparsification, probabilistically checkable proofs, instance compression, and kernelization in parameterized complexity.

By reduction similar results holds for other NP-complete problems. For the vertex-cover problem on n-vertex d-regular hypergraphs the above statement holds for any integer $d \geq 2$. The case $d = 2$ implies that no nontrivial parameterized vertex deletion problem on standard graphs can have kernels consisting of $O(k^{2-\epsilon})$ edges unless coNP is in NP/poly. Kernels consisting of $O(k^2)$ edges are known for several problems in the class, including vertex cover, bounded-degree deletion, and feedback vertex set.

Our approach refines the framework developed in recent papers showing that certain parameterized languages do not have protocols of cost bounded by any polynomial in the parameter unless coNP is in NP/poly. We study parameterized problems that do have protocols of polynomial cost, and show that no polynomial cost of lower degree than the current best is achievable unless coNP is in NP/poly. In order to obtain our tight bounds we exploit a result from additive combinatorics, namely the existence of high-density subsets of the integers without nontrivial arithmetic progressions of length three. (Joint work with Holger Dell.)

R. Santhanam *New and Improved Upper Bounds for Formula Satisfiability and TQBF*

I will describe what appears to be a new technique for bounding the running time of algorithms for satisfiability, based on proving concentration versions of results about random restrictions. I will show how this gives a running time upper bound of $2^{n-\Omega(n)}$ for a simple and natural algorithm for formula satisfiability on formulae of linear length, and explain how the technique also gives a strong average-case lower bound for Parity against linear-size formulae. I will pose some questions relevant to extending this line of research to satisfiability and lower bounds for polynomial-size constant- depth circuits. If time permits, I will also mention a memoization-based technique that beats brute force search for QBF satisfiability on formulae with a bounded number of variable occurrences.

Small-space computation

One of the basic open questions in computational complexity is whether every problem in P (solvable in polynomial time) can be solved also in small (logarithmic) space. In the complexity language, the question is whether $P = LOGSPACE$. Cook has recently launched a project trying to separate these two classes, by considering a very special problem in P (tree-evaluation problem), and trying to show that it cannot be solved by logspace-bounded algorithms. The final result seems still distant, but there has been some partial progress, which was reported by Wehr (a student of Cook).

D. Wehr *A lower bound for a restricted model of log-space computation*

I’ll show how to solve a problem posed in [Gal,Koucky,McKenzie ”Incremental branching programs”

2006] regarding a restricted model of small-space computation, tailored for solving the P-complete GEN problem. They define two variants of incremental branching programs, the syntactic variant defined by a restriction on the graph-theoretic paths in the program, and the more-general semantic variant in which the same restriction is enforced only on the consistent paths (those that are followed by at least one input). They used a lower bound for monotone circuits to show that exponential size is required for the syntactic variant, but left open the problem of superpolynomial lower bounds for the semantic variant. I'll give the main part of the proof of an exponential lower bound for the semantic variant; it is a generalization of a lower bound argument for a similar restricted model of computation tailored for solving the Tree Evaluation Problem, which appeared in [Braverman, Cook, McKenzie, Santhanam, Wehr "Fractional pebbling and thrifty branching programs" 09].

Oblivious computation

An oblivious algorithm is an algorithm whose "behavior" (say in terms of memory access) is independent of a given input (and so by observing the memory locations queried by the algorithm, one has no information about the input of the algorithm). There has been recently a renewed interest in efficient constructions of oblivious algorithms. At the workshop, Beame reported on the lower bound for making a given algorithm into an oblivious one.

P. Beame *Making RAMs Oblivious Requires Superlogarithmic Overhead*

We prove a time-space tradeoff lower bound of $T = \Omega(n \log(n/S) \log\log(n/S))$ for randomized oblivious branching programs to compute 1GAP, also known as the pointer jumping problem, a problem for which there is a simple deterministic time n and space $O(\log n)$ RAM (random access machine) algorithm. In a recent STOC paper, Ajtai derived simulations of general RAMs by randomized oblivious RAMs with only a polylogarithmic factor increase in time and space. Our lower bound implies that a superlogarithmic factor increase is indeed necessary in any such simulation. (Joint work with Widad Machmouchi.)

Quantum Computation

What is the power of quantum computation? Is there some problem that can be efficiently solved on a quantum computer (even with today's technology) but cannot be efficiently solved by classical computers? Aaronson addressed this question in his talk at the workshop.

In another talk, Umans considered a related question: Is quantum computation more powerful than what is captured by a classical complexity class PH (polynomial-time hierarchy)? No answer is known at the moment. Moreover, there is not even any evidence of the advantage of quantum computation over PH in the form of some relativized (oracle) construction. Umans discussed the problem of constructing such an oracle, and relates it some other interesting questions in classical complexity.

S. Aaronson *The Computational Complexity of Linear Optics*

We propose a linear-optics experiment that might be feasible with current technology, and argue that, if the experiment succeeded, it would provide evidence that at least some nontrivial quantum computation is possible in nature. The experiment involves generating reliable single-photon states, sending the photons through a random linear-optical network, and then reliably measuring the photon number in each mode. The resources that we consider are not known or believed to be universal for quantum computation; nevertheless, we show that they would allow the solution of certain sampling and relational problems that appear to be intractable for classical computers.

Our first result says that, if there exists a polynomial-time classical algorithm that samples from the same probability distribution as our optical experiment, then $P^{\#P} = BPP^{NP}$, and hence the polynomial hierarchy collapses to the third level. Unfortunately, this assumes an extremely reliable experiment. While that could in principle be arranged using quantum error correction, the question arises of whether a noisy experiment would already have interesting complexity consequences. To address this question, we formulate a so-called "Permanent-of-Gaussians Conjecture" (PGC), which says that it is $\#P$-hard to approximate the permanent of a matrix A of independent $N(0,1)$ Gaussian entries, with high probability over A; as well as a "Permanent Anti-Concentration Conjecture" (PACC), which says that $|Per(A)| >= sqrt(n!)/poly(n)$ with high probability over A. We then show that, assuming both the PGC and the PACC, polynomial-time classical simulation even of noisy linear-optics experiments would imply a collapse of the polynomial hierarchy. (Joint work with Alex Arkhipov)

C. Umans *Pseudorandom generators and the BQP vs. PH problem*

It is a longstanding open problem to devise an oracle relative to which BQP does not lie in the Polynomial-Time Hierarchy (PH). We advance a natural conjecture about the capacity of the Nisan- Wigderson pseudorandom generator [NW94] to fool AC^0, with MAJORITY as its hard function. Our conjecture is essentially that the loss due to the hybrid argument (which is a component of the standard proof from [NW94]) can be avoided in this setting. This is a question that has been asked previously in the pseudorandomness literature [BSW03]. We then show that our conjecture implies the existence of an oracle relative to which BQP is not in the PH. This entails giving an explicit construction of unitary matrices, realizable by small quantum circuits, whose row-supports are nearly-disjoint. Our framework generalizes the setting of [Aar09], and remains a viable approach to resolving the BQP vs. PH problem after the recent proof [Aar10] that the Generalized Linial-Nisan Conjecture of [Aar09] is false. (Joint work with Bill Fefferman)

Error-correcting codes

Error-correcting codes have become a central tool and an object of study in computational complexity. At the workshop, Dvir reported on an interesting connection between the classical complexity problem (on matrix rigidity) and certain (locally self-correctable) codes. In another talk, Guruswami showed a beautiful result establishing the tight list-decodability property of random linear codes, which shows that random linear codes achieve essentially the same list-decodability parameters (up to constant factors) as random non-linear codes.

Z. Dvir *On matrix rigidity and locally self-correctable codes*

We describe a new approach for the problem of finding rigid matrices, as posed by Valiant [Val77], by connecting it to the, seemingly unrelated, problem of proving lower bounds for locally selfcorrectable codes. This approach, if successful, could lead to a non-natural property (in the sense of Razborov and Rudich [RR97]) implying super-linear lower bounds for linear functions in the model of logarithmic-depth arithmetic circuits.

Our results are based on a lemma saying that, if the generating matrix of a locally decodable code is not rigid, then it defines a locally self-correctable code with rate close to one. Thus, showing that such codes cannot exist will prove that the generating matrix of any locally decodable code (and in particular Reed Muller codes) is rigid.

V. Guruswami *List decodability of random linear codes*

For every fixed finite field F_q, $0 < p < 1 - 1/q$, and $\epsilon > 0$, we prove that with high probability a random subspace C of F_q^n of dimension $(1-h_q(p)-\epsilon)n$ has the property that every Hamming ball of radius pn has at most $O(1/\epsilon)$ elements of C. (Here $h_q(x)$ is the q-ary entropy function.) This answers a basic open question concerning the list-decodability of linear codes, showing that a list size of $O(1/\epsilon)$ suffices to have rate within ϵ of the information-theoretic limit $1 - h_q(p)$. This matches up to constant factors the list-size achieved by general (non-linear) random codes, and gives an exponential improvement over the best previously known list-size bound of $q^{O(1/\epsilon)}$.

The main technical ingredient in our proof is a strong upper bound on the probability that m random vectors chosen from a Hamming ball centered at the origin have too many (more than $O(m)$) vectors from their linear span also belong to the ball. (Joint work with Johan Hastad (KTH) and Swastik Kopparty (MIT).)

Computational Learning

A basic task in computational learning is to ”learn” an object (say, a halfspace in a high-dimensional space) by having access to possibly noisy data (say, an oracle which answers if a given point is in the halfspace or not). Some of the main approaches to learning involve the algebraic techniques based on low-degree polynomial representations of the objects one needs to learn. While these techniques were successful for some classes of objects (e.g., halfspaces), they don't seem to help with others (e.g., intersections of halfspaces).

There were two talks at the workshop that addressed this issue. Sherstov explained his negative result (saying that low-degree techniques won't help for learning an intersection of two halfspaces). Klivans showed some new results on approximately representing intersections of ”regular” halfspaces (a special case of halfspaces), which in particular imply a new learning algorithm for intersections of such regular halfspaces.

A. Sherstov *Symmetrization Without Symmetries*

We prove that the intersection of two halfspaces on the n-cube cannot be sign-represented by a polynomial of degree less than $\Theta(n)$, which matches the trivial upper bound and solves an open problem due to Klivans (2002). This result shows that intersections of halfspaces are not amenable to learning by perceptron-based techniques, which have been successful in other cases (halfspaces, DNF formulas, read-once formulas). A mostly complete proof will be presented with emphasis on a key technical component, a method for symmetrizing a Boolean function f without any symmetries by averaging f over suitable sections over the n-cube.

A. Klivans *An Invariance Principle for Polytopes*

Let X be randomly chosen from $\{-1, 1\}^n$, and let Y be randomly chosen from a standard n-variate Gaussian. For any polytope P formed by the intersection of k halfspaces, we prove that $|Pr[X \in P] - Pr[Y \in P]| \leq polylog(k) \cdot \Delta$, where Δ is a parameter that is small for polytopes formed by the intersection of “regular” halfspaces (i.e., halfspaces with low influence). The novelty of our invariance principle is the polylogarithmic dependence on k. Previously, only bounds that were at least linear in k were known.

We give two important applications of our main result:

1. A bound of $polylog(k) \cdot \epsilon^{O(1)}$ on the noise sensitivity of intersections of k regular halfspaces (previous work gave bounds linear in k). This gives the first quasipolynomial-time algorithm for learning intersections of regular halfspaces.

2. The first pseudorandom generators (with polylogarithmic seed length) for regular polytopes. This gives an algorithm for approximately counting the number of solutions to a broad class of integer programs (including dense covering programs and contingency tables).

(This is joint work with Prahladh Harsha and Raghu Meka)

Communication Complexity

The communication complexity is concerned with the amount of communication (say, between two parties) needed for jointly solving a certain computational task (say, computing some function of two inputs, where one input is known to the first party, and the other input to the second party). There are various models of communication one can define, and a large number of lower and upper bound results are known. Still, a number of important questions remain open.

At the workshop, there were several discussions of different aspects of communication complexity. Regev showed a tight lower bound for a well-known problem of distinguishing two strings that are either close or far in the Hamming distance. Braverman discussed a new approach to an old problem in communication complexity (direct sum conjecture) via compressing a communication protocol so that the new compressed protocol uses the amount of communication that is closer to the information-theoretic lower bounds. Finally, Rao addressed an issue of error-correction in interactive communication.

O. Regev *Tight Bound for the Gap Hamming Distance Problem*

We consider the Gap Hamming Distance problem in communication complexity. Here, Alice receives an n-bit string x, and Bob receives an n-bit string y. They are promised that the Hamming distance between x and y is either at least $n/2 + \sqrt{n}$ or at most $n/2 - \sqrt{n}$, and their goal is to decide which is the case. The naive protocol requires n bits of communication and it was an open question whether this is optimal. This was shown in several special cases, e.g., when the communication is deterministic [Woodruff'07] or when the number of rounds of communication is limited [Indyk-Woodruff'03, Jayram-Kumar-Sivakumar'07, Brody-Chakrabarti'09, Brody-Chakrabarti-R-Vidick-deWolf'09]. Here we settle this question by showing a tight lower bound of $\Omega(n)$ on the randomized communication complexity of the problem. The bound is based on a new geometric statement regarding correlations in Gaussian space, related to a result of C. Borell from 1985, which is proven using properties of projections of sets in Gaussian space. (Partly based on a joint paper with Amit Chakrabarti.)

M. Braverman *Compression, information and direct sum for communication complexity*

We will present a tight three-way connection between three types of results related to the randomized two-party communication complexity of a problem:

1. Direct sum theorems, relating the communication complexity of computing many copies of a function to the complexity of computing one copy;
2. The information complexity of a problem, which is the smallest amount of information (as opposed to communication) the parties need to exchange to solve the problem; and
3. Compression theorems, which show how to convert two party communication protocols closer to the information-theoretically optimal bounds.

We will then use these connections along with new compression schemes to derive new results in communication complexity. Based on two joint works, one with [Boaz Barak, Xi Chen, and Anup Rao], and the second one with [Anup Rao].

A. Rao *Recovering from Maximal Errors in Interactive Communication*

We show that it is possible to encode any communication protocol between two parties so that the protocol succeeds even if a $(1/4 - \epsilon)$ fraction of all symbols transmitted by the parties are corrupted adversarially, at a cost of increasing the communication in the protocol by a constant factor (the constant depends on epsilon). No encoding can tolerate a 1/4 fraction of errors in the interactive setting, if the communication is to remain bounded in terms of the original communication of the protocol. This improves on an earlier result of Schulman, who showed how to recover when the fraction of errors is at most 1/240. (Joint work with M. Braverman)

Pseudorandom generators

Constructing pseudorandom generators is one of the basic tasks in computational complexity, and is an open problem for many models of computation. However, some progress has been made for certain restricted models.

Some recent such progress has been reported on by Zuckerman (for threshold functions), Lovett (for constant-depth modular circuits), Yehudayoff (for regular branching programs of constant width), and Pudlak (for group products). Also, Viola discussed the complexity of generating distributions of the form $h(x)$ for a random x, where h is some function from m to n bits, as well as some applications to succinct data structures and pseudorandom generators.

D. Zuckerman *Pseudorandom Generators for Polynomial Threshold Functions*

We study the natural question of constructing pseudorandom generators (PRGs) for low-degree polynomial threshold functions (PTFs). We give a PRG with seed-length $\log n/\epsilon^{O(d)}$ fooling degree d PTFs with error at most ϵ. Previously, no nontrivial constructions were known even for quadratic threshold functions and constant error ϵ. For the class of degree 1 threshold functions or halfspaces, we construct PRGs with much better dependence on the error parameter ϵ and obtain the following results.

1. A PRG with seed length $O(\log n \log(1/\epsilon))$ for $\epsilon > 1/poly(n)$.

2. A PRG with seed length $O(\log n)$ for $\epsilon > 1/poly(\log n)$. Previously, only PRGs with seed length $O(\log n \log^2(1/\epsilon)/\epsilon^2)$ were known for halfspaces. We also obtain PRGs with similar seed lengths for fooling halfspaces over the n-dimensional unit sphere.

The main theme of our constructions and analysis is the use of invariance principles to construct pseudo-random generators. We also introduce the notion of monotone read-once branching programs, which is key to improving the dependence on the error rate ϵ for halfspaces. These techniques may be of independent interest. (Joint work with R. Meka)

S. Lovett *Pseudorandom generators for $CC^0[p]$ and the Fourier spectrum of low-degree polynomials over finite fields*

In this paper we give the first construction of a pseudorandom generator with seed length $O(\log n)$, for $CC^0[p]$, the class of constant-depth circuits with unbounded fan-in MODp gates, for some prime p. More accurately, the seed length of our generator is $O(\log n)$ for any constant error $\epsilon > 0$. In fact, we obtain our generator by fooling distributions generated by low degree polynomials, over F_p, when evaluated on the Boolean cube. This result significantly extends previous constructions that either required a long seed [LVW93] or that could only fool the distribution generated by linear functions over F_p, when evaluated on the Boolean cube [LRTV09, MZ09]. Enroute of constructing our PRG, we prove two structural results for low degree polynomials over finite fields that can be of independent interest:

1. Let f be an n-variate degree d polynomial over F_p. Then, for every $\epsilon > 0$ there exists a subset S of variables of size depending only on d and ϵ, such that the total weight of the Fourier coefficients that do not involve any variable from S is at most ϵ.

2. Let f be an n-variate degree d polynomial over F_p. If the distribution of f when applied to uniform zero-one bits is ϵ-far (in statistical distance) from its distribution when applied to biased bits, then for every $\delta > 0$, f can be approximated over zero-one bits, up to error δ, by a function of a small number (depending only on ϵ, δ and d) of lower degree polynomials.

(Joint work with Partha Mukhopadhyay and Amir Shpilka.)

A. Yehudayoff *Pseudorandom generators for regular branching programs*

We give new pseudorandom generators for *regular* read-once branching programs of small width. A branching program is regular if the in-degree of every vertex in it is (0 or) 2. For every width d and length n, our pseudorandom generator uses a seed of length $O((\log(d) + \log\log(n) + \log(1/\epsilon))\log(n))$ to produce n bits that cannot be distinguished from a uniformly random string by any regular width d length n read-once branching program, except with probability ϵ. We also give a result for general read-once branching programs, in the case that there are no vertices that are reached with small probability. We show that if a (possibly non-regular) branching program of length n and width d has the property that every vertex in the program is traversed with probability at least p on a uniformly random input, then the error of the generator above is at most $2\epsilon/p^2$. (Joint work with Mark Braverman, Anup Rao, and Ran Raz)

P. Pudlak *Pseudorandom Generators for Group Products*

We will show that the pseudorandom generator introduced in [INW94] fools group products of a given finite group. The seed length is $O(\log n \log \frac{1}{\epsilon})$, where n the length of the word and ϵ is the precision. The result is equivalent to the statement that the pseudorandom generator fools read-once permutation branching programs of constant width. (Joint work with Michal Koucky and Prajakta Nimbhorkar.)

E. Viola *The complexity of distributions*

Complexity theory typically studies the complexity of computing a function $h(x) : \{0,1\}^m \to \{0,1\}^n$ of a given input x. We advocate the study of the complexity of generating the distribution $h(x)$ for uniform x, given random bits. We discuss recent work in this direction. This includes lower and upper bounds for various computational models (NC^0, decision trees, and AC^0) and the consequences of these bounds for succinct data structures and pseudorandom generators. (We expect the talk to be based on two papers ”The complexity of distributions” and ”Bounded-depth circuits cannot sample good codes,” the latter co-authored with Shachar Lovett.)

Social choice

Economics and social choice theory are becoming the objects of study by computer scientists, who bring the computational perspective on the old issued studied by economists and social scientists. One example of such interaction between social choice theory and computer science was given at the workshop in a talk by Kindler.

G. Kindler *A Quantitative Proof of the Gibbard-Satterthwaite Theorem*

A social choice function f with n voters and q alternatives, takes as input a tuple of n full rankings of the alternatives, supposedly corresponding to the preferences of the voters, and outputs the winner alternative. We say that f is manipulable at a given voting profile if a voter who knows the rankings given by the others can change her own ranking in a way that does not reflect her true preferences, but which leads to a winner that is more favorable to her.

Gibbard and Satterthwaite proved that any social choice function which attains three or more values, and which is not a dictatorship, must be manipulable. We show a quantitative version of the theorem in the case where f is neutral, showing that f must be manipulable at a uniformly chosen voting profile with probability bounded below by (the inverse of) a polynomial in n and q. Our results also imply that manipulations cannot be completely hidden by making them computationally hard to find: a voter can randomly try different permutations and find a useful manipulation with non-negligible probability.

Out results extend those of Friedgut, Kalai and Nisan, which worked only for the case of 3 alternatives. The methods we use are quite different though, using a canonical-paths style geometric argument.

Outcome of the Meeting

The meeting has brought together some of the best researchers actively working in various areas of complexity. The richness of the field of complexity theory has been reflected in the wide range of topics discussed at the meeting: from classical problems on the complexity of SAT, to communication complexity, learning, quantum algorithms, error-correcting codes, pseudorandomness, and even social choice theory. While seemingly different, many of these areas share ideas, and contribute techniques useful in other areas.

The workshop provided a valuable venue for exchange of ideas between researchers working in different areas, and stimulating discussions. Some new results have already been obtained thanks to such discussions at the workshop, and more are likely to follow. Even more importantly, the meeting has been a source of enthusiasm and encouragement for many young researchers who will be shaping complexity theory in the near future.

Participants

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Chapter 30

Multivariate Operator Theory (10w5081)

Aug 15 - Aug 20, 2010

Organizer(s): Ronald Douglas (Texas A & M University), Kenneth Davidson (University of Waterloo), Joerg Eschmeier (Universitat des Saarlandes), Mihai Putinar (University of California at Santa Barbara)

Overview of the Field

While the study of operator theory on Hilbert space has been underway for more than a hundred years, multivariate operator theory - the study of more than one operator at a tim - is of more recent origin. The study of self-adjoint algebras emerged in the late thirties in the works of Murray-von Neumann and Gelfand-Naimark. A couple of decades later, non self-adjoint algebras enjoyed considerable development in the sixties and seventies starting with the work of Kadison-Singer. Studies of multivariate operator theory which emphasized the analogues of analyticity, both commutative and non commutative, had to wait for the most part until the last couple of decades. Since then, however, this area has been pursued rather vigorously with some remarkable successes, both for its own sake and for its connections with other areas of mathematics such as complex and algebraic geometry. Moreover, the techniques and viewpoint from the multivariate case has enriched and contributed to the one variable theory. Although analyticity has played a key role in operator theory from the start, due in part to the analyticity of the resolvent, the algebraic and geometric underpinnings of function theory were less important in the one variable case. However, even natural examples in the multivariate case involve the framework of several complex variables in an essential way and depend on results from the theory of partial differential operators. One obstacle to the systematic development of this side of multivariate operator theory has been the development of an effective framework for the subject. Early researchers considered either n-tuples of operators or representations of algebras. Many researchers now have adopted the language of Hilbert modules.

A *Hilbert module* H over algebras of holomorphic functions such as the polynomials or entire functions depending on n (commuting) complex variables yields a variety of invariants, either with respect to topological isomorphism or the more rigid unitary equivalence. First, such a module defines a compact subset of $\mathbb{C}^n$, known as the Taylor joint spectrum. The Hochschild-type topological-homological localization encodes the refined structure of the joint spectrum with local invariants such as the Fredholm index, the local analytical K-theoretic index, a Hilbert-Samuel polynomial, or, on restricted subsets of the joint spectrum, a Hermitian holomorphic vector bundle with canonical connection and related curvature. All of these invariants, with pertinent examples and applications, were studied in the last two decades by (to name only a few) J. L. Taylor, F.-H. Vasilescu, R. Levi, X. Fang, K. Yan, G. Misra. W. B. Arveson and the four organizers of this workshop. Applications range from a novel proof of the Atiyah-Singer index theorem, of Grauert's finiteness theorem in complex analytic geometry, and to a classification of homogeneous Hermitian holomorphic vector bundles on classical domain of $\mathbb{C}^n$.

Many concrete Hilbert modules obtained by completing the polynomial algebra $A = \mathbb{C}[z_1, ..., z_n]$ with respect to an inner product are essentially reductive in the sense that all of the multiplication operators given by the module structure are essentially normal. Examples are the Hardy and Bergman spaces on the unit ball $\mathbb{B}^n$ in $\mathbb{C}^n$ as well as the symmetric Fock or n-shift space H^{2n}. In the case of the latter module, Arveson raised the question of whether this property is inherited by submodules $[I]$ (or, equivalently, the quotient $H/[I]$) obtained as the closure of a homogeneous ideal I in A and gave a positive answer for ideals generated by monomials. Arveson conjectured that the result was true in general and that, in fact, the cross-commutators were not only compact but were in the Schatten p-class for $p > n$. Arvesons conjecture was refined and extended by Douglas in two ways. First, he conjectured that for the cross-commutators of the operators defined on the quotient module were in fact in the Schatten p-class for p greater than the dimension of the zero variety, $Z(I)$, of I and established that was the case for ideals generated by monomials. Second, he observed that the quotient module defines an extension of the compact operators by $C(Z(I))$ and hence defines an element of the odd K-homology group for the intersection $Z(I)$ of $Z(I)$ with the unit sphere. Moreover, he conjectured that this element corresponds to the fundamental class determined by the almost complex structure on $Z(I)$. Such a result would yield a new kind of index theorem. (One can compare this conjectured result with the corresponding result for the K-homology class defined by a Dirac operator on a spinc-manifold.) Exciting progress has been made recently on these questions, mostly by Guo and Wang. In particular, they establish the original conjecture for all principal homogeneous ideals and for all homogeneous ideals for $n = 2, 3$. Moreover, they establish the refined conjecture involving the dimension of $Z(I)$ for $n = 2, 3$, and verify the index formula for $n = 2$. Finally, they show that the K-homology element is nontrivial for all proper ideals for $n = 3$. Principal tools, among other things, are the Hilbert-Samuel polynomial of M and techniques developed in the rigidity theory of analytic Hilbert modules. There should be interesting connections to recent results of X. Fang and J. Eschmeier on operator theoretic Samuel multiplicities and of Gleason-Richter-Sundberg on the index of invariant subspaces of analytic Hilbert modules. The above result on the essential normality of submodules and quotient modules are equivalent to compactness properties of commutators of the Bergman projector and multiplication by smooth functions in the case of certain weighted Bergman spaces, which, at present, cannot be obtained with the methods from PDE or SCV. In particular, there would seem to be implications from these results for global regularity for the $\overline{\partial}$-bar problem on such spaces over the unit ball. For these reasons and others, it would be extremely interesting to extend these results to higher dimensions or domains other than the unit ball. As one possible, quite fascinating application, one might hope to obtain operator theoretic invariants for the Brieskorn exotic spheres.

In addition to the specific problems described above, there are many basic questions in the field whose answers would have significant application to the general field as well as related areas. As was mentioned earlier, much of the progress which has been made has depended on the development of techniques which often arose in connection with similar basic questions. The rigidity theory developed to classify submodules defined by ideals and the Hilbert-Samuel polynomial used to classify certain Hilbert modules defined by isometries by Fang are two examples as is the functional calculus developed by Taylor and other researchers to define the joint spectrum. Among the basic questions for which there has been significant progress but for which many questions remain are interpolation and division. The seminal work connecting interpolation to operator theory is due to Sarason. His approach was absorbed into dilation theory and furthered the development by Sz.-Nagy and Foias of their canonical model for contraction operators. Work of Arveson extended dilation theory to a much more general context by showing that any (not necessarily commutative) operator algebra lives inside a canonical C*-algebra known as its C*-envelope. Interpolation problems can be reformulated in terms of calculating the C*-envelope of a quotient algebra of the space of analytic functions by the ideal of functions vanishing on the data set. Deep results of Agler for interpolation on an annulus make essential use of these operator theoretic ideas. Direct connections between interpolation and the Nevanlinna-Pick problem for the bidisk were obtained by Agler and McCarthy. More recent work of McCullough and Paulsen show in that for other domains, in both one and several variables, the C*- envelope of even three dimensional abelian quotients can be infinite dimensional and highly non commutative. These results illustrate a principle which is a second side of multivariate operator: understanding commutative phenomena often takes one naturally into the non commutative realm. Such lessons in classical algebraic geometry and theoretical physics are leading to the development of non commutative algebraic geometry in recent years. Connections between the work described in this overview and these latter developments seem likely.

The Sz.-Nagy-Foias machinery for studying a single operator has been extended to multivariate operator theory by Popescu, Davidson-Kribs-Shpigel and others based on the Frazho and Bunce dilation of a row contraction to a canonical model of m shifts on the full Fock space. Again, even when the operators all commute, the natural dilation theory leads to non-commutative C*-algebras. For example, if the model is of a row contraction, then one is lead to Drury's dilation theorem and the Arveson n-shift space mentioned earlier. Arveson showed that the C*-envelope is determined by representation by n-shifts on the symmetric Fock space. In general, calculating the C*-envelope is very difficult and only in the past decade have tools been developed to allow one to do this in general contexts. Muhly and Solel have a very general construction of C*-correspondences based on Pimsner's construction of a C*- algebra from a Hilbert C*-module. Many classical situations fit into this general framework. Nevertheless, explicit calculation of the C*-envelope in concrete situations such as interpolation makes a compelling connections between operator theory and function theory. Recent progress provides an opportunity to make real progress which holds the promise of significant applications to interpolation theory.

The interplay between the ideas and methods from operator theory and functional analysis with methods and ideas from function theory, commutative algebra and algebraic, analytic and complex geometry gives the field a strong interdisciplinary character. Moreover, the results obtained in operator theory have depended on extending and developing the techniques and ideas from the other fields. Further, the questions raised and results obtained in operator theory have cross-fertilized the other areas. Finally, in summary, the overwhelming goal for the workshop was to bring together leading researchers and young mathematicians from multivariate operator theory along with experts from related areas to survey, consolidate and extend the many advances of the past two decades.

Outline of the talks

Resolutions and quotients of Hilbert modules

The classical dilation theorem of Sz.-Nagy and Foias shows in particular that, for each contraction T of class $C_{0\cdot}$ on a complex Hilbert space H, there is a short exact sequence $0 \to H^2(\mathbb{D}, E) \xrightarrow{M_\theta} H^2(\mathbb{D}, E_*) \xrightarrow{q} H \to 0$ of $\mathbb{C}[z]$-module maps consisting of an isometric multiplier M_θ and a co-isometry q. Here the module action on H is given by the polynomial functional calculus of T. Using Arveson's model theory for row contractions and an extension of the classical Beurling-Lax-Halmos theorem due to McCullough and Trent to the case of Nevanlinna-Pick spaces one finds that, for every commuting pure row contraction, or equivalently, every pure co-spherically contractive Hilbert module $T \in L(H)^d$, there exists a resolution

$$(H_d^2 \otimes E_\bullet, M_{\theta_\bullet}) \xrightarrow{q} H \to 0$$

of $\mathbb{C}[z]$-module maps consisting of partially isometric multipliers $M_{\theta_i} : \; H_d^2 \otimes E_i \to H_d^2 \otimes E_{i-1}$ between vector-valued Drury-Arveson spaces and a co-isometry q. In his talk, Ronald Douglas gave a survey of this module theoretic approach to multivariate operator theory emphasizing in particular the differences between the single and multivariable case. The basic idea is to study general Hilbert modules over natural function algebras via resolutions by canonical modules. To give just one example, a recent result obtained in joint work of Douglas, Foias and Sarkar [4] shows that a pure co-spherically contractive Hilbert module H admits a finite partially isometric resolution of the above form only in the trivial case that H is isometrically isomorphic to $H_d^2 \otimes F$ for some Hilbert space F. A related problem is to find natural conditions under which quotient Hilbert modules are similar to free Hilbert modules of the form $H_d^2 \otimes F$. In addition Ronald Douglas described how one can reduce the structure of such quotient modules to the structure of an associated hermitian holomorphic bundle defined using the multiplier yielding the quotient module [5]. In the talk several problems of this type and their connection to complex analytic geometry were discussed.

Essential normality of homogeneous submodules

Let H_d^2 be the Drury-Arveson space on the open unit ball $\mathbb{B}$ in $\mathbb{C}^d$, that is, the analytic functional Hilbert space with reproducing kernel $K(z,w) = (1 - \langle z, w\rangle)^{-1}$. It is well known that the multiplication tuple $M_z = (M_{z_1}, \ldots M_{z_d}) \in L(H_d^2)^d$ consisting of the multiplication operators M_{z_i} with the coordinate functions is q-essentially normal for every $q > d$. Arveson conjectured that q-essential normality is inherited by every quotient tuple $S^M = M_z/M$ of M_z modulo a closed homogeneous submodule $M \subset H_d^2$, that is, modulo every closed subspace $M = \overline{(p)}$ arising as the closure of an ideal $(p) = (p_1, \ldots p_r) \subset \mathbb{C}[z]$ generated by finitely many homogeneous polynomials $p_1, \ldots, p_r$. A strengthening of the conjecture due to Douglas, supported by many typical examples, says that S^M should even be q-essentially normal for every q larger than the complex dimension of the zero variety $Z(I)$ of the underlying ideal.

Affirmative answers to these conjectures are expected to lead to interesting new connections between multivariate operator theory and complex geometry. A positive answer was given by Arveson for submodules generated by monomials. This result was extended by Douglas to more general classes of analytic Hilbert modules. Guo and Wang showed that the conjectures are true in dimension $d \leq 3$ and for all principal homogeneous submodules generated by a single homogeneous polynomial p. In his talk, Jörg Eschmeier showed that a modification of an operator inequality used by Guo and Wang in the case of principal homogeneous submodules is equivalent to the existence of factorizations of the form $[M_{z_j}^*, P_M] = (N+1)^{-\frac{1}{2}} A_j$, where N is the number operator on H_d^2, and therefore implies that the cross commutators $[S_j^{M*}, S_i^M]$ $(1 \leq i, j \leq d)$ factorize boundedly through $(N+1)^{-1}$. Using recent results on the Fredholm theory of graded Hilbert space tuples [8], one obtains that a proof of the above mentioned operator inequality would immediately yield positive answers to the conjectures of Arveson and Douglas. It turns out that in all cases in which the conjectures are known to be true, the inequality holds and leads to a unified proof of stronger results [7]. Whether the inequality is satisfied in general remains an intriguing open question at this moment. Recent work of Michael Wernet shows that all the results remain true on a much larger class of functional Hilbert spaces.

Operator algebraic geometry

For a homogeneous ideal $I \subset \mathbb{C}[z]$, let $F_I = H_d^2 \ominus I$ be the orthogonal complement of I in the Drury-Arveson space H_d^2, and let $A_I \subset L(F_I)$ be the norm-closed unital subalgebra generated by the compression S^I of the multiplication tuple $M_z = (M_{z_1}, \ldots, M_{z_d}) \in L(H_d^2)^d$ to F_I. According to Gelu Popescu, A_I is the universal operator algebra generated by a commuting row contraction T satisfying the relations $p(T) = 0$ for all $p \in I$. In his talk, Orr Shalit reported on joint results obtained with Ken Davidson and Christopher Ramsey which show that in quite general situations the operator algebras A_I can be classified in terms of the zero varieties $Z(I)$ of the underlying ideals. In this way intriguing analogues to the well-known classical correspondence between commutative algebra and geometry are obtained. For instance, if $I, J \subset \mathbb{C}[z]$ are radical homogeneous ideals, then A_I and A_j are isometrically isomorphic if and only if there is a unitary operator on $\mathbb{C}^d$ which maps $Z(I)$ onto $Z(J)$. Under suitable extra conditions, satisfied in many cases, A_I and A_J are shown to be isomorphic if and only if there is an invertible linear map A such that $AZ(J) = Z(I)$. It turns out that the complex geometry of the zero varieties of the underlying ideals is very rigid in the sense that in typical situations every biholomorphic map between $Z(I)$ and $Z(J)$ is automatically induced by a linear map.

Toeplitz quantization on symmetric domains

Let $D = G/K$ be an irreducible bounded symmetric domain in its Harish-Chandra realization, with G the connected component of the identity in the group of all biholomorphic self-maps of D and K the stabilizer of the origin. The unweighted Berman kernel on D is given by $K(x, y) = c\, h(x, y)^{-p}$, where c is a normalization constant, p is the genus and h denotes the Jordan determinant. The standard weighted Bergman spaces, that is, the subspaces consisting of all holomorphic functions in $L^2(D, \mu_\nu)$ with $\mu_\nu = c_\nu\, h(z, z)^{\nu-p}\, dz$, possess the reproducing kernels $K_\nu(z, w) = h(z, w)^{-\nu}$ for $\nu > p - 1$.

The asymptotic expansions of the Toeplitz star product $f \star g = \sum_{j=0}^{\infty} \nu^{-j} C_j(f, g)$, of the Berezin star product $f \odot g = \sum_{j=0}^{\infty} \nu^{-j} \tilde{C}_j(f, g)$ and the Berezin transform $B_\nu = \sum_{j=0}^{\infty} \nu^{-j} Q_j$ yield sequences of G-invariant (bi)-differential operators $C_j, \tilde{C}_j$ and Q_j. The Berezin transform is of central importance in the theory of deformation quantization of complex Kähler manifolds. Miroslav Englis indicated how a Peter-Weyl type decomposition for G-invariant differential operators can be used to obtain Peter-Weyl decompositions for the Berezin transform, the Berezin and the Toeplitz star product. For the Berezin transform, a result of this type was proved in a paper of Arazy and Orsted [1]. A corresponding expansion for the Berezin star product can be reduced to the the Arazy-Orsted expansion using suitable factorization properties of the star product $\odot$. A Peter-Weyl decomposition for the Toeplitz star product can be derived from a suitable expansion of the inverse Berezin transform B^{-1}. The resulting expansion for the Toeplitz star product $\star$ is new even in the simplest case of the unit disc. Analogous decompositions are also possible in the case of real bounded symmetric domains, where again there is a natural Berezin transform which is closely related to the well-known Segal-Bargmann transformations. The results presented in the talk have been obtained in joint work with Harald Upmeier [6].

In his lecture, Harald Upmeier reported on an extension of the above results, also obtained in collaboration with Miroslav Englis, concerning invariant operators and their asymptotic expansions in the case of compact symmetric spaces such as the Riemann sphere, the projective spaces or the Grassmann manifolds. Since in the compact case Bergman type spaces are finite dimensional, single Toeplitz operators have to be replaced by whole sequences of Toeplitz matrices in this case.

Classification of analytic Hilbert modules

Let $\Omega \subset \mathbb{C}^n$ be a bounded pseudoconvex domain and denote by $A(\Omega)$ the associated "disk algebra", that is the algebra of analytic functions in Ω which are continuous on $\overline{\Omega}$. The class of topological Hilbert modules H over the algebra $A(\Omega)$ comprises as particular cases all commutative n-tuples of operators with joint spectrum contained in Ω, and hence it is far from being classifiable in simple terms. Assume in addition that the fibers

$$H(\lambda) = H/\mathfrak{m}_\lambda H$$

are finite dimensional for all $\lambda \in \Omega$, where $\mathfrak{m}_\lambda \subset A(\Omega)$ stands for the maximal ideal at λ. If the function $\lambda \mapsto \dim H(\lambda)$ is locally constant and $\cap_{\lambda\in\Omega}\mathfrak{m}_\lambda H = 0$, then differential geometric constructions lead to curvature type invariants of H (modulo unitary, analytic equivalence). This dictionary and refined classification constitutes the heart of the famous Cowen-Douglas theory. The talk by Biswas focused on analytic Hilbert modules H with merely finite dimensional fibers $H(\lambda),\ \lambda \in \Omega$. Without aiming at obtaining complete unitary invariants, he has shown how methods of algebraic geometry and function theory of several complex variables naturally lead to higher curvature type invariants for H. His main idea was to adapt Grothendieck's duality between coherent analytic sheaves and families of linear subspaces of a vector space to the Hilbert space setting. The main technical difficulties being related to division problems with L^2-bounds, a well charted territory in several complex variables, see [2].

A related subject was exposed by Rongwei Yang in his lecture. He was dealing with analytic Hilbert submodules H of the Hardy space of a polydisk $\mathbb{D}^n$. By applying the classical one variable model theory (due to Sz.-Nagy and Foiaş) to the localization of H to the fibers of the canonical projection map $\mathbb{D}^n \longrightarrow \mathbb{D}^{n-1}$ he was able to obtained new unitary invariants for H. In particular, differential topology invariants were attached in this setting to the analytic submodule H, via the invertibility of the linear pencil $w_0 + w_1 M_1 + ... + w_n M_n$, where M_j denotes the multiplication with the coordinate function z_j on H.

A good portion of Marcus Carlsson's lecture was devoted to the classification of analytic submodules of finite codimension in a classical Hilbert space of vector valued analytic functions, such as the Bergman, Hardy or Dirichlet spaces. The quintessential example being a finite codimension submodule H of the Bergman space $L^2_a(\Omega)$ associated to a bounded, strictly pseudoconvex domain with smooth boundary. In which case $H = I \cdot L^2_a(\Omega)$, where $I \subset \mathcal{O}(\Omega)$ is an ideal of finite codimension, such that $\mathrm{supp}[\mathcal{O}(\Omega)/I] \subset \Omega$. This simple phenomenon was recently generalized by Carlsson to submodules of finite codimension of a vector valued Bergman space.

Applications of multivariate operator theory to function theory

One of the most interesting and rich component of the workshop was concerned with novel applications of multivariate operator theory to classical function theory. We include below details of three talks given during the workshop.

In his lecture, John McCarthy has presented new results, obtained jointly with Jim Agler and Nicholas Young, on matrix monotone functions. In 1934, K. Löwner published a very influential paper studying functions on an open interval $E \subseteq \mathbb{R}$ that are matrix monotone. That is functions f with the property that whenever S and T are self-adjoint matrices whose spectra are in E then

$$S \leq T \qquad \Rightarrow \qquad f(S) \leq f(T).$$

Roughly speaking, Löwner showed that if one fixes a dimension n and wants the inequality to hold for n-by-n self-adjoint matrices, then certain matrices derived from the values of f must all be positive semi-definite. As n increases, the conditions become more restrictive. In the limit as $n \to \infty$ (equivalently, if one passes to self-adjoint operators on an infinite dimensional Hilbert space), then a necessary and sufficient condition is that the function f must have an analytic continuation to a function F that maps the upper half-plane Π to itself.

McCarthy and collaborators have extended Löwner's results to functions of d variables applied to d-tuples of commuting self-adjoint operators. A few definitions are necessary for stating their main results. Given two d-tuples $S = (S^1, \ldots, S^d)$ and $T = (T^1, \ldots, T^d)$, we shall say that $S \leq T$ if and only if $S^r \leq T^r$ for every $1 \leq r \leq d$. We shall let $CSAM^d_n$ denote the set of d-tuples of commuting self-adjoint n-by-n matrices.

Definition: Let E be an open set in $\mathbb{R}^d$, and f be a real-valued C^1 function on E. We say f is locally M_n-monotone on E if, whenever S is in $CSAM^d_n$ with $\sigma(S) = \{x_1, \ldots, x_n\}$ consisting of n distinct points in E, and $S(t)$ is a C^1 curve in $CSAM^d_n$ with $S(0) = S$ and $\frac{d}{dt}S(t)|_{t=0} \geq 0$, then $\frac{d}{dt}f(S(t))|_{t=0}$ exists and is ≥ 0.

Definition: Let E be an open subset of $\mathbb{R}^d$. The set $Ł^d_n(E)$ consists of all real-valued C^1-functions on E that have the following property: whenever $\{x_1, \ldots, x_n\}$ are n distinct points in E, there exist positive semi-definite n-by-n matrices $A^1, \ldots, A^d$ so that

$$\begin{aligned} A^r(i,i) &= \left.\frac{\partial f}{\partial x^r}\right|_{x_i} \\ \text{and} \quad f(x_j) - f(x_i) &= \sum_{r=1}^{d} (x^r_j - x^r_i) A^r(i,j) \qquad \forall\, 1 \leq i,j \leq n. \end{aligned}$$

Theorem (Agler-McCarthy-Young) *Let E be an open set in $\mathbb{R}^d$, and f a real-valued C^1 function on E. Then f is locally M_n-monotone if and only if f is in $Ł^d_n(E)$.*

Theorem (Agler-McCarthy-Young) *Let E be an open set in $\mathbb{R}^2$, and f a real-valued C^1 function on E. Then f is locally operator monotone (i.e. M_n-monotone for all n) if and only if f has an analytic extension that maps Π^2 to Π.*

For rational functions, we can replace "local" by "global".

Theorem (Agler-McCarthy-Young) *Let F be a rational function of two variables. Let Γ be the zero-set of the denominator of F. Assume F is real-valued on $\mathbb{R}^2 \setminus \Gamma$. Let E be an open rectangle in $\mathbb{R}^2 \setminus \Gamma$. Then F is globally operator monotone on E if and only if F is in Ł(E).*

The lecture by Jim Agler aimed at generalizing a classical result of C. Carathéodory on analytic functions that map the disk to the disk. Let B_d be the open unit ball in $\mathbb{C}^d$. Assume that ϕ is an analytic function from B_d to the unit disk.

We shall say that ϕ has an angular gradient at a point $b \in \partial B$ if there exists $\omega \in \mathbb{C}$ and $\eta \in \mathbb{C}^d$ such that

$$n.t. \lim_{l \to b} \frac{f(l) - \omega - \eta \cdot (l - b)}{\|l - b\|} \;=\; 0,$$

where the left-hand side means that l tends to b non-tangentially from within B_d. We call ω the non-tangential gradient at b.

Theorem (Agler-McCarthy-Young) *If ϕ has a non-tangential gradient ω at b, then $n.t. \lim_{l \to b} \nabla \phi(l)$ exists and equals η.*

Theorem (Agler-McCarthy-Young) *If $b \in \partial B_d$ satisfies*

$$\liminf_{l \to b} \frac{1 - |\phi(l)|}{1 - \|l\|} \;<\; \infty,$$

then ϕ has a directional derivative at b in every direction that points into B_d.

In dimension $d = 1$, the hypothesis of the second theorem implies that of the first; but if $d \geq 2$, this no longer holds.

The talk by Brett Wick was focused on multivariate aspects of the Corona Problem on a Besov space. Quite specifically, the space $B_2^\sigma(\mathbb{B}_n)$ roughly consists of those analytic functions f whose derivatives of order $\frac{n}{2} - \sigma$ lie in the classical Hardy space $H^2(\mathbb{B}_n)$. More precisely, let $d\lambda_n(z) := (1 - |z|^2)^{-(n+1)} dV(z)$, with $dV(z)$ denoting the Lebesgue measure on the unit ball $\mathbb{B}_n$. For $0 \leq \sigma < \infty$, the Besov–Sobolev space $B_2^\sigma(\mathbb{B}_n)$ is the collection of functions that are analytic on $\mathbb{B}_n$ such that, for any integer $m \geq 0$, with $m + \sigma > \frac{n}{2}$, we have the following norm being finite:

$$\|f\|^2_{B_2^\sigma(\mathbb{B}_n)} := \sum_{j=0}^{m-1} |f^{(j)}(0)|^2 + \int_{\mathbb{B}_n} |(1 - |z|^2)^{m+\sigma} f^{(m)}(z)|^2 d\lambda_n(z).$$

The parameter σ recovers many of the important spaces in function and operator theory on the unit ball $\mathbb{B}_n$. When $\sigma = 0$, this corresponds to the Dirichlet space of analytic functions, the value $\sigma = \frac{n}{2}$ yields the classical Hardy space on the ball, and $\sigma = \frac{n+1}{2}$ yields the Bergman space.

When $\sigma = \frac{1}{2}$, $B_2^{\frac{1}{2}}(\mathbb{B}_n)$ is the celebrated Drury–Arveson space. In a sense, this space of analytic function is a universal space from the point of view of applications in operator theory. Using it, one can prove a generalization of the famous von Neumann Inequality for contractions, analogues of Beurling's Theorem on invariant subspaces, and Commutant Lifting Theorems for the multiplier algebra of this space. Surprisingly, many of the corresponding results for the spaces associated with $H^\infty(\mathbb{B}_n)$, the multiplier algebra of $H^2(\mathbb{B}_n)$, do *not* hold, placing the multiplier algebra of the Drury–Arveson space in a distinguished position. Thus, one can see that the Corona Theorems obtained in [3] are the proper generalization of Carleson's famous Theorem, to the unit ball $\mathbb{B}_n$.

For the Besov–Sobolev space $B_2^\sigma(\mathbb{B}_n)$, one defines the *multiplier algebra* $\mathcal{M}_2^\sigma(\mathbb{B}_n)$ as the collection of analytic functions φ that are pointwise multipliers of $B_2^\sigma(\mathbb{B}_n)$. Namely, $\varphi f \in B_2^\sigma(\mathbb{B}_n)$ for all $f \in B_2^\sigma(\mathbb{B}_n)$, and then norms $\mathcal{M}_2^\sigma(\mathbb{B}_n)$ by

$$\|\varphi\|_{\mathcal{M}_2^\sigma(\mathbb{B}_n)} := \sup_{f \in B_2^\sigma(\mathbb{B}_n)} \frac{\|\varphi f\|_{B_2^\sigma(\mathbb{B}_n)}}{\|f\|_{B_2^\sigma(\mathbb{B}_n)}}.$$

Theorem (Ş. Costea, E. Sawyer, Wick, [3]) *Let* $\sigma \geq 0$ *and* $1 < p < \infty$*. Given* $g_1, \ldots, g_N$ *in* $\mathcal{M}_p^\sigma(\mathbb{B}_n)$ *satisfying*

$$1 \geq \sum_{j=1}^{N} |g_j(z)|^2 \geq \delta > 0 \quad \forall z \in \mathbb{B}_n,$$

there is a constant $C_{n,\sigma,p,\delta}$ *such that for each* $h \in B_p^\sigma(\mathbb{B}_n)$*, there are* $f_1, \ldots, f_N$ *in* $B_p^\sigma(\mathbb{B}_n)$ *satisfying*

$$\sum_{j=1}^{N} \|f_j\|_{B_p^\sigma(\mathbb{B}_n)}^p \leq C_{n,\sigma,p,\delta} \|h\|_{B_p^\sigma(\mathbb{B}_n)}^p \quad \text{and} \quad \sum_{j=1}^{N} g_j(z) f_j(z) = h(z) \quad \forall z \in \mathbb{B}_n.$$

When $0 \leq \sigma \leq \frac{1}{2}$ and $p = 2$, these spaces of analytic functions have a complete Nevanlinna–Pick kernel, following the terminology of Agler and McCarthy. Consequently, this Hilbert space result for $B_2^\sigma(\mathbb{B}_n)$ can be lifted to the corresponding result for the multiplier algebra $\mathcal{M}_2^\sigma(\mathbb{B}_n)$. This leads to the following theorem giving the first positive (non-trivial) Corona result for multiplier algebras in several complex variables.

Theorem (Ş. Costea, E. Sawyer, Wick, [3]) *Let* $0 \leq \sigma \leq \frac{1}{2}$*. Given* $g_1, \ldots, g_N$ *in* $\mathcal{M}_2^\sigma(\mathbb{B}_n)$ *satisfying*

$$1 \geq \sum_{j=1}^{N} |g_j(z)|^2 \geq \delta > 0 \quad \forall z \in \mathbb{B}_n,$$

there is a constant $C_{n,\sigma,\delta}$ *and there are functions* $f_1, \ldots, f_N$ *in* $\mathcal{M}_2^\sigma(\mathbb{B}_n)$ *satisfying*

$$\sum_{j=1}^{N} \|f_j\|_{\mathcal{M}_2^\sigma(\mathbb{B}_n)} \leq C_{n,\sigma,\delta} \quad \text{and} \quad \sum_{j=1}^{N} g_j(z) f_j(z) = 1 \quad \forall z \in \mathbb{B}_n.$$

The above theorem is also true in the case of matrix-valued Corona Data, though for convenience, only the scalar case is stated. Namely, the constant $C_{n,\sigma,\delta}$ is *independent* of N (as listed). When $\sigma = \frac{1}{2}$, the space $B_2^{\frac{1}{2}}(\mathbb{B}_n)$ is the Drury–Arveson space, and we obtain the Corona Theorem for its multiplier algebra of analytic functions on $\mathbb{B}_n$.

In the case of one complex variable, $n = 1$, some related results were known. In particular, Carleson's famous Corona Theorem is the case $\sigma = \frac{1}{2}$. Tolokonnikov obtained the result for $0 \leq \sigma < \frac{1}{2}$. And recent work by Trent gave another proof of $\sigma = 0$, [9]. The results in [3] not only give new proofs of these results, but also addresses the situation $n > 1$. These new results are a significant breakthrough in the study of multivariable Corona Problems.

Multivariate moment problems

The transition from one to several variables in moment problems is not smooth. Due to the fact that not all positive polynomials on $\mathbb{R}^n, n > 1$, are sums of squares, there is no effective way of solving a full or truncated moment problem for positive measures. One venue, preferred by physicists and statisticians, is to add to the moment constraints the maximum entropy assumption. This selects among all solutions the most unbiased one, in a precise sense. The talk by Calin Ambrozie was focused on the theoretical aspects of maximal entropy solutions to truncated moment problems. His main techniques were derived from infinite dimensional duality between convex cones (the so-called Fenchel duality), obtaining in this way exponential of polynomials as solutions. A more constructive approach to truncated moment problems, in a more restrictive setting, made the subject of Florian-Horia Vasilescu's talk. He focused on flat (i.e. constant rank) extensions of Hankel type matrices of moments, reflecting in their structure the condition that the unknown measure/distribution is supported by an algebraic curve in $\mathbb{R}^2$. A great deal of his theory extends to the non-commutative, free-* setting.

Non-commutative operator theory

Operators generally do not commute, and there is a lot of recent work on multivariate operator theory where the algebras studied are not abelian.

Gelu Popescu spoke about part of his program to develop the theory of holomorphic functions on a domain consisting of n-tuples of operators on Hilbert space. His early work concentrated on the analogue of the n-ball, the set of all row contractions. Many theorems about analytic functions on the ball in $\mathbb{C}^n$ have natural analogues for power series in indeterminates lying in this non-commutative ball. In his talk at BIRS, Popescu defined a family of domains that have rotational symmetry like the Reinhardt domains, but here they are defined in terms of completely positive maps. He was particularly interested in questions of isomorphism of the operator algebras of all operator holomorphic functions on these domains. He obtained a rigidity theorem based on Cartan's theorem in several complex variables. (Shalit had a similar result in the commutative context mentioned earlier.) This led to an analogue of Thulen's theorem, showing that the list of domains with non-trivial automorphisms is limited to a small list. The final results showed that isomorphism of the algebras is determined by biholomorphic equivalence of the underlying operator domains.

Paul Muhly reported on work with Baruch Solel. Inspired by an old paper of Joseph Taylor on general functional calculus in several variables, and recent work of Dan Voiculescu on what he calls free analysis, Muhly considers these questions in the context of Hardy algebras of C*-correspondences. Like Popescu's work, these are algebras of operators that are non-commutative analogues of $H^\infty(\mathbb{D})$. He considers elements of these algebras as functions on a non-commutative ball, and asks about the structure of the ball and these functions. One of their results is the existence of a completely positive definite Szego kernel on the ball, forming a non-commutative reproducing kernel Hilbert space.

We give below more details about Muhly's talk, as it also naturally interacts with the talk of Vinnikov. *Fully matricial sets and functions* arise quite naturally when one tries to build a complex function theory based on free algebras of various sorts. This was recognized first by J. Taylor (Adv. Math. **3** (1972). See section 6.) and has arisen anew in the work of Voiculescu on free analysis questions. He coined the terms "fully matricial sets and functions". But they are implicit in a lot of other work that has been evolving in recent years and they are becoming more and more explicitly studied. (See, in particular, the recent work by Helton, McCullough, Klepp, Putinar, Vinnikov and others on dimension free linear matrix inequalities and the work of Ball, Davidson, Katsoulis, Pitts, Popescu and others on free holomorphic functions.) Muhly's talk focused on sets and functions that arise as follows: Let E be a W^*-correspondence over a W^*-algebra M and let $H^\infty(E)$ be the Hardy algebra we build from (E, M) as described in Math. Ann. **330** (2004). Then for each normal representation σ of M on a Hilbert space H_σ there is a natural W^*-correspondence over $\sigma(M)'$, called the *σ-dual correspondence of E,* and denoted E^σ. This is a space of intertwining operators between σ and the representation induced by E in the sense of Rieffel, $\sigma^E \circ \varphi$, where φ gives the left action of M on E. The unit ball in the space of adjoints of E^σ, $\mathbf{D}(E^\sigma)^*$, is part of a fully matricial family of sets. This is because $E^{n\sigma}$ is in a very natural way $M_n(E^\sigma)$ for each positive integer n. The importance of $\mathbf{D}(E^\sigma)^*$ lies in the fact that as σ runs over the space of normal representations of M, the points in $\mathbf{D}(E^\sigma)^*$ label (most of) the ultra-weakly continuous, completely contractive representations of $H^\infty(E)$ in $B(H_\sigma)$. For $\eta^* \in \mathbf{D}(E^\sigma)^*$, $\eta^* \times \sigma$ denotes the representation of $H^\infty(E)$ determined by η^*. Each each element $F \in H^\infty(E)$ gives rise to a function $\widehat{F}_\sigma : \mathbf{D}(E^\sigma)^* \to B(H_\sigma)$ defined by $\widehat{F}_\sigma(\eta^*) := (\eta^* \times \sigma)(F)$. It is an easy calculation to see that for each σ, the collection $\{\widehat{F}_{n\sigma}\}_{n\geq 1}$ forms a fully matricial function on the fully matricial set $\{\mathbf{D}(E^{n\sigma})^*\}_{n\geq 1}$.

When $M = \mathbf{C}$, $E = \mathbf{C}^d$ and σ is the one dimensional representation of $\mathbf{C}$, then $H^\infty(E)$ is the free semigroup algebra $\mathcal{L}_d$ and $\mathbf{D}(E^{n\sigma})^*$ is the space of row contractions of d $n \times n$ matrices. An $F \in H^\infty(E)$ has a representation in terms of a series indexed by the free semigroup on d generators, and the function $\widehat{F}_{n\sigma}$ is obtained by replacing the d generators by the d components of a row contraction. Thus $\widehat{F}_{n\sigma}$ lies in a certain completion of the algebra of d generic $n \times n$ matrices.

The basic question addressed by Muhly and Solel is: Given a family of functions $\{\Phi_\sigma\}$, where σ runs over all the normal representations of M and where $\Phi_\sigma : \mathbf{D}(E^\sigma)^* \to B(H_\sigma)$, when does there exist an element $F \in H^\infty(E)$ so that $\widehat{F}_\sigma = \Phi_\sigma$ for all σ. One solution is formulated in terms of certain intertwining spaces and is connected to Taylor's original analysis, as well as to recent work by D. Kalyuzhnyĭ-Verbovetzkiĭ and V. Vinnikov. The second solution is based on their generalization of the Nevannlina-Pick Theorem and Lyapunov analysis.

Although the results of Muhly and Solel are formulated in terms of general W^*-algebras, W^*-correspondences and normal representations, they contain the situations when M and E are finite dimensional and σ is finite dimenionsional as special cases. These cases yield very interesting finite dimensional matrix balls expressed as $\mathbf{D}(E^\sigma)^*$. The functions we study lie in completions of spaces of polynomial maps studied in invariant theory.

Elias Katsoulis discussed joint work with E. Kakariadis. He considered the action of an isometric automorphism on the tensorr algebra associated to C*-correspondence. When the automorphism is the restriction of a $*$-automorphism of the enveloping C*-algebra, there is an associated semicrossed product sitting inside the semicrossed product of the C*-algebra. The study of such semicrossed products goes back to work of Arveson, and later to the universal construction of Peters, in the case of a single self map on a compact space. The associated algebras were eventually shown to be (algebraically) isomorphic if and only if the two maps are topologically conjugate by Davidson and Katsoulis [5]. More recent work has dealt with families of maps and endomorphisms of nonself-adjoint operatopr algebras. Arveson's famous work reshaping dilation theory [2] suggests that one should identify the C*-envelope, the minimal C*-algebra containing a nonself-adjoint algebra. Katsoulis and Kakariadis identify this C*-envelope for the semicrossed product of a tensor algebra by a $*$-extendable endomorphism.

Wing Suet Li talked about Horn's conjecture. For complex selfadjoint $n \times n$ matrices A, B, C, with $A + B + C = 0$, A. Horn conjectured in 1962 a set of inequalities that would characterize the possible eigenvalues of these matrices. The conjecture was proved to be correct by A. Klyachko and A. Knutson and T. Tao in the late 1990s, using techniques from algebraic geometry, representation theory and very intricate combinatorics. One of the key ingredients to show that these inequalities are necessary is to establish that the intersection of certain Schubert varieties is nonempty. Recently, W.-S. Li, H. Bercovici, B. Collins, K. Dykema, and D. Timotin were able to construct an explicit element in the intersection of three given Schubert varieties when the intersection contains a unique element. This element is constructed generically as the result of a (finite) sequence of lattice operations. This sequence of operations can be applied to appropriately defined analogous of Schubert varieties in the Grassmannian, associated with a finite von Neumann algebra. The arguments requires a good understanding of a combinatorial structure that is closely related to the honeycombs, developed by A. Knutson and T. Tao. Earlier work of W.-S. Li with H. Bercovici showed that the eigenvalues of selfadjoint elements a, b, c with $a + b + c = 0$ in the factor $\mathcal{R}^\omega$ are characterized by a system of inequalities analogous to the classical Horn inequalities, as one would naturally expect. The present result shows that these inequalities are also true for an arbitrary finite factor. In particular, if x, y, z are selfadjoint elements of a finite factor and $x + y + z = 0$, then there exist selfadjoint $a, b, c \in \mathcal{R}^\omega$ such that $a + b + c = 0$ and a (resp. b, c) has the same eigenvalues as x (resp. y, z).

Victor Vinnikov's talk was focused on his recent work with Dmitry S. Kaliuzhnyi-Verbovetskyi on rational functions over free variables, their difference-differential calculus and realization formulas as determinants of linear pencils of matrices. Their approach complements that of Muhly-Solel, and it is pertinent to recent advances in free probability theory.

Outcome of the Meeting

As was perhaps suggested in the Overview section of the report, Multivariate Operator Theory (MVOT) is less a community than a collection of several sub communities, each focused on topics in which algebras of Hilbert space operators occur either concretely or as part of the framework for the research. In most instances the goals of the various groups are quite distinct and the techniques and conceptual templates may have little, if any, overlap. In many instances the other communities, such as several complex variables, harmonic analysis to name just two, have been around for almost a century, which is the case also for single operator theory.

As the subject of MVOT has matured, techniques and ideas from one part can and should enrich and leaven others. Considerable progress at accomplishing this goal was realized at the meeting as was detailed in the previous section on talks. Moreover, people working on similar problems but in different communities got to meet and know each other. One can expect rich collaborations to flow from these events.

As was pointed out in the overview, one could divide MVOT into the commutative and non-commutative areas and to too large an extent these two communities have remained apart. However, researchers have begun to realize deep, non obvious connections between the two. In a fascinating juxtaposition of talks, three approaches to the concept of functions of non commuting variables were given starting with the obvious notion of polynomials in non-commuting variables. A clearer understanding of this notion should have applications in free probability theory and theoretical physics. Moreover, there could be some surprising insights gained into ordinary algebraic geometry.

In a similar vein, ideas from classical interpolation theory lead to new results in the extension of functions as well as abstract frameworks in the context of non selfadjoint and C*-algebras. Several talks explored these connections and generalizations. Related to these questions are problems and structures which arise in the single operator theory motivated by systems theory. Looking at these matters in the context of MVOT provides new insights as well as frames questions about the extension of these questions to the context of several variables.

As was pointed out in the overview section, concepts and techniques from complex geometry enter the picture naturally in the MVOT context even showing that geometrical notions went unnoticed in the single variable case. One situation in which this has become apparent is in the efforts related to the corona problem.

All in all, the most recent results in the subject were reviewed among the varied groups of researchers which is expected to result in considerable cross-fertilization and adoption of a broader set of tools and methods in exploring the topic and its connections with other areas.

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Chapter 31

Extreme events in climate and weather an interdisciplinary workshop (10w5016)

Aug 22 - Aug 27, 2010

Organizer(s): Peter Guttorp (University of Washington), Montserrat Fuentes (North Carolina State University)

August 22-27 an interdisciplinary workshop was held at the Banff International Research Station on Extreme events in climate and weather. The workshop had 32 participants from 7 countries. The goal of the workshop was to set a research agenda for statistical analysis of extreme climate events. The format was two lectures in the mornings, and group discussions in the afternoons. The lectures and posters, as well as a list of the participants, are available at the meeting website http://temple.birs.ca/ 10w5016

This document contains an overview of the lectures (section 1) and a summary of the discussions of research directions held at the workshop (sections 2-6). Each research direction has some concrete needs in boldface.

Lectures

Introduction

In the opening lecture Peter Guttorp described how general circulation models work, going from a simple energy balance model to the modern gridded solutions to a system of partial differential equations. He discussed the various sources of uncertainty in climate analysis, including uncertainties in forcings and data, and how well the models cope with features such as El Niño. The downscaling of global models to regional ones was demonstrated, and a comparison of data to a regional model was illustrated.

The second lecture of the first day was given by Eric GIlleland, who demonstrated the different scales of extreme weather events. He described the various definitions of droughts and heat waves, and illustrated some analyses based on extreme value theory. Analyses based on global models benefit from developing large-scale indicators of extreme weather, such as the product of maximum wind speed and wind shear, illustrated with various approaches to analysis and forecasting/projection.

Time series extremes

On the second day, Georg Lindgren posed the question whether a fixed seasonal model is adequate for analysis of weather related extremes in the presence of strong seasonal effects, and demonstrated in a simulation study that high quantiles may be underestimated by a factor of 2-3. He also discussed peaks over threshold analysis, and the effect of a temporal trend in the seasonal amplitude, suggesting use of nonparametric quantile regression in the latter case.

In the second lecture RIck Katz described how to use extreme value theory to model nonstationary weather phenomena. The effect of scaling and aggregation was illustrated. For clustered events, such as heat spells, he suggested modeling the clustering, rather than the common declustering approach. Models of damage from extreme weather events were presented and related to insurance issues. He closed with a discussion of risk communication under climate change, suggesting that we stop using the return level terminology under a changing climate, and rather use a probabilistic language.

Spatial extremes

Zhenyung Zhan opened the third day by presenting an analysis of US precipitation, with the emphasis on tail dependency between spatial pairs of stations. The main tool for testing for tail dependency was the tail quotient correlation coefficient with random thresholds, for which asymptotic theory was developed and checked using simulation studies. Strong tail dependency was found in many cases between stations quite far apart,

Dan Cooley gave the second lecture, making a distinction between weather and climate in the context of spatial dependence, where climate effects are changes of marginal distribution by location, while weather effects is the joint behavior of multiple locations. He suggested to replace he classical regional frequency analysis from hydrology with a Bayesian hierarchical model. The relatively standard conditional independence assumption made in such models was shown not to hold because of weather effects. The statistical difficulties with max-stable processes casts some doubt over whether this is the right approach. He showed an attempt to make approximate Bayesian inference using composite likelihood replacing the (uncomputable) real likelihood, showing improvement over the conditional independence model.

Forests and observing networks

Charmaine Dean described a mixture-modeling approach to Canadian forest fires, where the probability of a fire in a given location is a mixture of normal, extreme, and zero-heavy components. The question of interest is trends in this type of model, where the trend is both in the parameters of the different components and in the mixing proportions. The results show a movement from zero-heavy to normal risk, while the probability of the extreme component is relatively stable. She discussed data issues, such as changing detection efficiency and fire management strategies.

In the final lecture, Paul Whitfield illustrated the usefulness of networks of stations to study precipitation patterns as well as extreme precipitation (defined as at least one station in the network having extreme precipitation). The Pineapple Express, delivering moisture from the Pacific to the northwestern Americas, was used as a particularly interesting illustration. The effect of climate change on jet stream paths is still somewhat uncertain.

Climate models and extremes

Climate models and regional models produce outputs for several meteorological variables at predetermined spatial scale in terms of averages over a grid cell or areas over a grid cell. An interesting area of research is to develop models to downscale the outputs of such models to point level, or even to develop models to downscale predictions for extremes obtained from climate or regional models (Mannshardt-Shamseldin et al., 2010). Adapting to climate models methods already adopted to downscale outputs from air quality models, a possible approach would use historical station data and regress it on the regional model output for the grid cell where the meteorological station lies using coefficients that vary in space and time (Berrocal et al., 2011). The coefficients would then be in turn modeled using appropriate statistical models. Possibilities include Gaussian processes, appropriate transformation of Gaussian processes, Gaussian copulas, or Dirichlet processes, all with an autoregressive structure in time.

Output from climate models at different scales can be used to generate testable hypotheses about changes in weather.

There is a need to develop models to downscale the outputs of such models to point level, or even to develop models to downscale predictions for extremes obtained from climate or regional models.

Comparison of regional models to data

The interpretation of a grid square value depends on several factors, such as the numerical solution scheme, the boundary values and forcings chosen, etc. In fact, a regional model value may be a better descriptor of the area around the grid square than the precise grid square itself. To accommodate the fact that the output of a regional and a climate model really refers to a neighborhood of a grid cell, it might be more appropriate to actually regress the historical station data on the regional/climate model output at neighboring grid cells to the one where the meteorological station lies.

The distribution of observed (or reanalyzed) weather needs to be compared to distributions from the climate model. One can borrow spatial strength from nearby stations to predict grid square observation, or use spatial regression tools to predict station observations from model output. Statistical issues here include developing tools for multivariate two-sample comparisons,

Seasonal-to-decadal predictions (10-30yr) form an active field of research in the course of CMIP5 (Coupled Model Intercomparison Project 5). Decision makers that need to account for climate change adaptation and mitigation measures are particularly interested in these predictions, especially in terms of extreme climate events. The potential for skillful decadal predictions depends largely on the initialization of the GCM1 (Global Climate Model) runs and whether the GCMs simulate sufficient decadal climate variability, both in magnitude and structure (Meehl et al. 2009). It is, in this context, very important to investigate GCM ensembles since multiple initial conditions with contrasting parameter values and model structure are needed in order to capture extreme events in transient systems.

There is a need to develop more appropriate methods for validating the representation of extreme events in models.

Skill scores for climate models

With the new CMIP5 database becoming available in the next years, we will have multiple decadal model predictions available, for which we have to find appropriate statistical methods to analyze various aspects regarding extreme values. These include (1) skill assessment of the GCM predictions, (2) comparison of multi-model ensemble distributions to observations, and (3) determination of uncertainties in the predictions.

Concerning the skill assessment of GCMs, it will be important to first identify mechanisms (climate and/or weather patterns such as El Nino and atmospheric blocking, topography, etc.) that contribute to the occurrence of extreme events but can also be well captured with the available model resolution. Based on that knowledge we need to extend the current practice (i.e. described in Tebaldi and Knutti. 2007; Ferr0, 2007) and develop objective skill measures, that could be region specific, to rank GCMs within the multi-model ensemble. Numerous methods have been proposed in the forecasting literature to spatially verify weather forecasts on small scales, see Gilleland et al. (2009) and Gilleland et al. (2010). To be used in the current context, these methods need to be adapted both to account for the large scale of the GCMs and to focus on the specific mechanisms of interest.

Once a ranking of the multi-model GCM ensemble has been established, it can be used to obtain a probabilistic distribution from the appropriately weighted ensemble members (Friedrichs and Hense, 2007). Further statistical tools are then needed to evaluate the skill of the probabilistic distribution obtained from the weighted ensemble as compared to observations/reality. Such tools should also involve the estimation of the uncertainties (e.g. model based, scenario based) in the predictions. The usefulness of commonly applied skill measures including correlation coefficients or MSE (Kharin et al. 2009) should be analyzed in this context. To ensure propriety in the evaluation, the procedure should be based on proper scoring rules for probability distributions, such as the logarithmic score or the continuous rank probability score (Gneiting and Raftery, 2007; Stephenson et al., 2008).

There is a need for appropriate statistical methods to analyze various aspects regarding extreme values. These include (1) skill assessment of the GCM predictions, (2) comparison of multi-model ensemble distributions to observations, and (3) determination of uncertainties in the predictions

Multivariate extreme value tools

It would be desirable to have a peaks-over-threshold approach for multivariate extreme values. One possible approach would be to use the point process representation of max-stable processes to develop more tractable multivariate extremes models. We also need tools for dealing with extremes in vector block extremes that occur at different times during the block.

There is a need for appropriate statistical methods to analyze time series of multivariate extreme values.

Spatial and space-time models for extreme values

Tractable spatial models

The max-stable processes, while mathematically seemingly well suited to the analysis of spatial extremes, are statistically not very tractable, and only ad hoc approaches to their statistical inference are currently available.

Another approach to temporal extremes of space-time processes is to assign a spatial prior for the GEV-parameters for annual or seasonal extremes over a network of station while treating the stations as conditionally independent. However, considering, for example, temperature data, it is quite common in upper latitudes for extremely cold weather to arise from Arctic air masses in a high pressure situation. Hence there is a tendency for annual minima to appear simultaneously at several stations. The appropriate likelihood (as long as separated minima can be considered independent) would be the product of conditional densities of the nonextreme sites, given the values at the extreme sites. Calculating these densities can of course be a daunting task in itself, but the approximation due to Heffernan and Tawn (2004), appropriately extended to the situation at hand, would be a possibility.

There is a need for methods that are well suited to the analysis of spatial extremes and that are statistically tractable.

Temporal nonstationarity

It seems that the most usual approach to deal with 'non-stationarities' in extremes is to allow for parametric changes in time for a GEV distribution. Linear trends on GEV parameters are a first step and had shown practical use to assess long term changes in climate/weather extremes. On the other hand, there has been some work in using Generalized Additive Models and state-space models to accommodate smooth/non-linear parameter change (Davison and Ramesh, 2000; Yee and Stephenson, 2007). An interesting idea is to apply Hidden Markov Models to represent change points in time and cluster structure. A state-space model can account for seasonalities with time-varying amplitudes. In general, it is unclear that in analyzing time series of extremes that arise in weather and climate, these perhaps more flexible models are more useful than simple linear trends. What model comparison tools are available to learn about this?

There is a need for models with distributional changes and in particular with different shape parameters, but one has to be careful about estimating this shape parameter. It was recommended to first model changes in location, then location/scale, and finally consider location/scale/shape. Beyond parameter changes, we may also need to consider temporal dependence in extremes.

One main problem with nonstationarity of extreme data is our poor understanding of natural low frequency climate oscillations. For instance, the Atlantic Multi-Decadal Oscillation (AMO), arising from the slow oscillation in the strength of the North Atlantic thermohaline circulation, has a period of about 70 years, with a profound effect on the number and strength of Atlantic hurricanes. Our short climate records make it difficult to detect/understand very low frequency climate oscillations, and their contribution to nonstationarity in our relatively short records of extreme data.

There is a need for methods that are suitable for series that are non-stationary, whether that non-stationarity is in location, distribution, etc., and such methods need to be able to address the connection to climate time series.

Climate and weather extremes

Heat waves

Heat waves are a complex form of extreme climate event with substantial health impacts. Yet extreme value theory has rarely been applied. Challenges include how to model the temporal clustering of temperatures at high levels and whether multivariate extreme value theory can be used to model climate variables that can contribute to heat waves (e.g., maximum and minimum temperature, dew point or humidity, wind speed, cloud cover) (Coles et al.,1994; Smith et al., 1997; Meehl and Tibaldi, 2004; Furrer et al., 2010). Such a research effort is needed to compare the statistics of observed heat waves (frequency, duration, severity) with those simulated by climate models, as well as to detect trends in heat wave statistics.

There is a need to improve the statistical modelling used for heat waves and other meteorological extremes.

Forest fires

One specific application area considered at the workshop was the analysis of fire events with a view to detecting trends in extremes. Spatio-temporal methods for this important application area have not utilized methodology from extreme value theory. In the forest fire context, increasing temperatures could lead to an increase in the number of ignitions, an increase in the length of the fire season, and an increase in the amount of severe fire weather (Schoenberg et al., 2003). Some additional challenges with quantifying extremes in this context is the need for homogenization of data from long records, incorporating information about changes in suppression activities, and fire management strategies. Given the challenges with climate predictions, it is also unclear what is the best way to accommodate weather variables to evaluate impacts under future climate scenarios; a sensible approach may be to focus on accessing how large a change in weather would lead to specific forestry vulnerabilities.

There is a need for methods that allow reconstruction, restoration, infilling of incomplete records.

There is a need for more robust methods to detect changes in environmental time series that are rich in zeros such as forest fires and ephemeral streamflows.

Extreme events that are not modeled by extreme value theory

Not all extreme climate events are extreme in the statistical sense. For example, Heavy rain on frozen ground can lead to severe flooding, or high winds following heavy snow and temperatures just around freezing can lead to severe forest destruction. One may be able to use climate model output to get an idea of future frequencies of particularly dangerous combination of factors, not all of which need to be extreme. From a modeling point of view it would be important to estimate conditional joint distributions of variables, given that one is extreme (Heffernan and Tawn, 2004), is one approach to this. Quantities such as trends in the onset of frost appear not directly amenable to extreme value theory, but would rather need nonstationary time series tools for directional data.

There is a need for robust methods that allow the separation of extreme events in relation to the generating processes. Floods being one example of an event with multiple generating mechanisms.

Index numbers

Climate and environmental indices need to be [1] robust, [2] specific, [3] relevant, and [4] comparable. There are many indices that may be useful in reducing the dimensions of climate and ecological studies, but many of them are problematic; some such as those that attempt to define the end of drought or the start and end of floods are particularly difficult in practice. Others such as FRICH for comparing global models may be more useful in the model comparison perspective than as test of reality. Indices may be more valuable when considering a change in the index as opposed to its absolute value.

Technically one can view indices as exceedances outside convex manifolds, and perhaps develop functionals that assess the degree of severity of the exceedance.

Water supply forecast models share many of the characteristics of indices as they are generally linear functions of several environmental variables. However, their output is either an estimate of future flow volumes or of their distribution function. Water supply forecasts are only of great importance for low values. EVT may be able to contribute to more rigorous forecasts of low flows which may occur due to the interaction of non-minimal variables. EVT may also be able to quantify the additional uncertainty of low flow volumes due to non-stationarity.

There is a need for methodology that can be used to assess properties of environmental indices, and determine if the are robust, specific, and comparable.

Further, the potential for indices that are not linear combinations, but of non-linear combinations would be useful in filed such as hydrology and climatology where non-linear processes are common, should be explored.

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Chapter 32

Rate-independent systems: Modeling, Analysis, and Computations (10w5075)

Aug 29 - Sep 03, 2010

Organizer(s): Giuseppe Savare (University of Pavia (Italy)) Ulisse Stefanelli (Istituto di Matematica Applicata e Tecnologie Informatiche del CNR)

Introduction

The mathematical treatment of rate-independent systems has recently attracted an increasing deal of attention. For this 5-days meeting at BIRS in Banff we have succeeded in gathering some of the most active researchers in the field. Their presentations (recorded below) are documenting some of the current investigation lines for this community. We hope that this short informal report would help in order to document the current standpoint and outlook into some near-future research lines.

We take this opportunity in order to acknowledge the very kind hospitality of the BIRS and friendliness and effectiveness of its staff. The success of this meeting has been clearly linked to the delightful atmosphere of the Center.

An informal introduction to rate-independent systems

We shall present here some very introductory material. Our aim is that of introducing some basic keywords for this field in a sufficiently informal way so that to possibly be of use also for the non-specialist. Moreover, we will take the occasion to record some relevant references.

Basics

The term *rate-independent* is usually referred to time-dependent processes which are invariant under time rescaling. More precisely, assume to be given a process that maps a given time-dependent input function $t \in [0,T] \mapsto \ell(t)$ into a time-dependent output $t \in [0,T] \mapsto q(t)$. We say that the mapping $\ell \mapsto q$ is *rate-independent* if, given a sufficiently smooth time-reparametrization $s : [0,T] \to [0,T]$ we have that

$$\ell \mapsto q \quad \Longleftrightarrow \quad \ell \circ s \mapsto q \circ s.$$

This feature is responsible of the appearance of so-called *hysteresis*. In particular, it gives the right to illustrate the complex time-dependent mapping $\ell \mapsto q$ by identifying curves on the (ℓ, q)-plane which are then followed during the evolution, *independently from the rate at which the input changes* (= *rate-independently*).

The hysteretic behavior of physical systems is of a great importance, particularly in Mechanics. Examples of rate-independent systems are friction, damage, crack propagation, plasticity, delamination, solid-solid phase change, ferromagnetism, ferroelectricity, just to mention a few. The ubiquitous emergence of rate-independent behaviors in applications has triggered an intense mathematical research which has to be traced back at to the work by KRASNOSELŠKIĬ & A. V. POKROVSKIĬ which has been then formalized into the first monograph on this subject [23]. Reference monographs on the mathematical treatment of rate-independent evolutions are also those by MAYERGOYZ [33], VISINTIN [76], BROKATE & SPREKELS [7], and KREJČÍ [25]. The non-strictly-mathematical literature on hysteresis is obviously huge.

A toy rate-independent system

Let us illustrate here the easiest possible of such an examples: friction. Assume to be interested in sliding a heavy block on a rough surface by pulling it by means of a linearly elastic rope. The input of the system is the position $\ell(t)$ at time t of the free end of the linearly elastic rope within some given 1D frame whereas $q(t)$ is the position of the block (the insertion point of the rope, say). The roughness of the surface is such that the block will not move until the force exerted by the rope is (in modulus) less than some critical activation threshold $\tau > 0$. Above this threshold, the block slides rigidly with ℓ. In particular, no inertial effects are to be considered. By assuming that the tension of the rope equals $k(\ell - q)$ (with $k > 0$), the evolution of this system can described by the system of relations

$$|k(\ell - q)| \leq \tau, \qquad \dot{q}(f - k(\ell - q)) \leq 0 \quad \text{for every } f \in [-\tau, \tau]. \tag{32.1}$$

The first relation asserts that the tension of the rope is always below the threshold τ. The second relation says that if the tension is in modulus strictly less than τ then $\dot{q} = 0$ and the block does not move. If the tension is exactly at the threshold, then $\ell - q$ is constant. It is immediate to check that the latter system is rate-independent: by doubling the speed at which ℓ moves the effect on q is doubled in speed.

Rate-independent processes are indeed very common and often arise as limiting situations in cases when the relevant time scale of the input ℓ is much longer with respect to the intrinsic time scales in the system. This happens quite classically when *inertial* effects turn out to be negligible. In the latter example the inertia of the block has been neglected.

Energetic solutions

In the last ten years the mathematical theory of rate-independent systems has progressively grown as an effect of the new concept of *energetic solutions* introduced by MIELKE, THEIL, & LEVITAS [54, 55]. Assume to be given a system defined by its *state* $q(t) \in Q$ as a function of time where Q is some given state-space ($Q = \mathbb{R}^d$, for instance). We shall describe the evolution of the system by providing a time-dependent *energy* functional $E(t, \cdot) : Q \to \mathbb{R} \cup \{+\infty\}$ and a *dissipation* potential $D : TQ \to [0, +\infty]$ and imposing the relation

$$\partial D(\dot{q}(t)) + \partial_q E(t, q(t)) \ni 0 \quad t > 0, \qquad q(0) = q^0. \tag{32.2}$$

Here, q^0 is some initial state and the latter relation (settled in the cotangent space $T^*Q = (TQ)^*$) represents the balance of the system of conservative actions $\partial_q E(t, q(t))$ and that of dissipative actions $\partial D(\dot{q}(t))$. The symbol ∂ stands for some kind of differential, possibly suitably generalized for non-smooth situations: in this case on the left of (32.2) we might have a set and this justifies the inclusion notation. Note that, whenever the potential D is assumed to *positively* 1-*homogeneous*, the resulting differential problem (32.2) turns out to be rate-independent. Namely, if q solves (32.2) then $q \circ s$ solves (32.2) with $E(s, \cdot)$ instead of $E(t, \cdot)$.

The differential problem (32.2) is the reference for rate-independent systems: it appears quite naturally in all the above mentioned applications, in both the finite and infinite-dimensional setting. The toy situation of Subsection 32 can be included in the general frame of (32.2) by letting $Q = \mathbb{R}$, $E(t,q) = kq^2/2 - k\ell(t)q$, $D(\dot{q}) = \tau|\dot{q}|$. Indeed, in this case we have that relation (32.2) reads $\tau\partial|\dot{q}| + k(q-\ell) \ni 0$ which can be equivalently rewritten as

$$\dot{q} \in N(k(\ell - q)) \quad t > 0, \qquad q(0) = q^0$$

where $N(r) : \mathbb{R} \to 2^{\mathbb{R}}$ is the (necessarily multivalued) normal cone to the interval $[-\tau, \tau]$ at point r. The latter relation can be equivalently rewritten in form of a variational inequality as in (32.1).

Problem (32.2) is quite non-smooth and very often fails to admit strong solutions. Hence, some kind of weak solution notion has to be advanced. Energetic solutions respond quite effectively to this demand. An energetic solution $t \mapsto q(t) \in Q$ is an everywhere-defined function such that $q(0) = q^0$, $t \mapsto \partial_t E(t, q(t)) \in L^1(0,T)$, and, for all $t \in [0,T]$,

$$E(t, q(t)) \leq E(t, \hat{q}) + D(\hat{q} - q(t)) \quad \forall \hat{q} \in Q, \tag{32.3}$$

$$E(t, q(t)) + \int_0^t D(\dot{q}) \mathrm{d}s = E(0, q^0) + \int_0^t \partial_t E(s, q(s)) \mathrm{d}s. \tag{32.4}$$

These two relations are referred to as *global stability* (32.3) and *energy balance* (32.4). The global stability condition says that the state $q(t)$ is such that no competitor state $\hat{q}$ can be preferred in terms of energy gain vs. dissipation. The energy balance just reflects the belief that the energy at time t plus the energy dissipated in the time interval $[0,t]$ (the sum in the left-hand side of (32.4)) equal the initial energy plus the work supplied by external actions (the right-hand side of (32.4)).

In case the energy E is strictly convex with respect to q, the energetic formulation (32.3)-(32.4) and the differential formulation (32.2) are equivalent. This is particularly the case of the above toy problem. The energetic formulation is however more general as it is directly adapted to the case of non-smooth potentials (no differentiation of potentials actually shows up in (32.3)-(32.4)) and could be modified in order to encompass non-smooth in time evolutions $t \mapsto q(t)$. Moreover, it allows a very robust existence and approximation theory [36]. In particular, even in the non-convex energy frame, limits of time-discretized solutions are energetic solutions.

These desirable features have attracted a lot of attention and existence results in the energetic frame have been obtained for elasto-plasticity [24, 9, 29, 34, 32, 73, 52], damage [5, 37, 48], brittle fractures [12, 21], delamination [22, 67], ferro-electricity [56], shape-memory alloys [53, 41, 39, 47, 65, 1], materials models [19, 66, 4, 3, 30, 14, 71], and vortex pinning in superconductors [68]. Moreover, an extensive attention has been devoted to the extension of this concept to non-linear state-space settings [17, 31, 43], non-smooth evolutions [44], homogenization [57], optimal control [61, 62], approximation [42, 40, 49, 50], and variational characterization [28, 38, 51, 69, 70].

Beyond energetic solutions

Despite of its recent success, the concept of energetic solution seems nowadays not completely satisfactory out of the realm of convex energies. The crucial point is that global stability (32.3) turns out to be an excessively strong constraint for evolution. Indeed, when E is not convex it may happen that (32.2) admits a strong solution which is not an energetic solution.

This remark is not at all new and evidence of the unsatisfactory behavior of energetic solutions has been provided in [34, Ex. 6.1], [20, Ex. 6.3], [44, Ex. 7.1]. The global minimality in (32.3) is a central issue in the variational theory of fracture propagation and an example of some non-physical evolution via global minimization has to be traced back to BRAIDES, DAL MASO, & GARRONI [6]. More recently, local instead of global minimization in (32.3) has been considered by NEGRI & ORTNER [59], KNEES, MIELKE, & ZANINI [20], and TOADER & ZANINI [74]. See also the comparative analysis in NEGRI [58]. A second example in the frame of associative (linearized) elasto-plasticity with softening is due to DAL MASO, DESIMONE, MORA, & MORINI [10]: by requiring global stability (32.3), no softening actually occurs. Some additional 1D discussion on this topic is in [64, 70].

There is a general belief that a possible tool in order to move beyond energetic solutions is that of considering so-called *vanishing viscosity solutions*. In particular, these are small-viscosity limits $\epsilon \to 0$ of solutions q_ϵ to (compare with (32.2))

$$\epsilon A\dot{q}_\epsilon(t) + \partial D(\dot{q}_\epsilon(t)) + \partial_q E(t, q_\epsilon(t)) \ni 0 \quad t > 0, \qquad q_\epsilon(0) = q^0 \tag{32.5}$$

where A is a given linear operator (viscosity matrix). Solutions to (32.5) are better behaved than those of (32.2) and have been proved to exists and admit limits in many different concrete cases [8, 11, 15, 20, 74] as well as some abstract context [13, 44, 45, 46]. Note however that the vanishing-viscosity approach features the introduction of some additional *modeling* for the viscous behavior of the system. This choice is safe in the scalar case but it influences the vanishing-viscosity limit already in two dimensions [70, 45].

Let us mention that alternative (in some sense intermediate) ideas in order to *localize* stability are that of MIELKE [35] and LARSEN (see [27]). Both these approaches are intended to restrict minimization to neighboring states with respect to dissipation (the former) or smaller in energy up to a positive tolerance (the latter, in the frame of brittle fractures). Even more recent are the attempts to define rate-independent evolution by passing to the limit into a dynamic regularization.

Energetic formulations are specifically tailored for the weak solution of the differential system (32.2). Although the system (32.2) is quite general, it is far from encompassing *all* rate-independent evolutions. Results aimed at extending (and often suitably modifying) the energetic viewpoint to more general situations (non-associative plasticity, thermo-mechanics, magneto-mechanics, for instance) are currently in progress [2, 60, 63, 75].

Current research

The arguments of the conferences in our meeting were quite focused on the current trends in the mathematical research on rate-independent systems. As such, by recording here some keywords of what has been presented during the workshop we believe that we are indeed providing some reliable portrait of actual research as well.

The talks have been basically focusing on these main themes:

- Plasticity theories (5 presentations)
- Damage and crack propagation (10 presentations)
- Shape memory alloys (6 presentations)
- General/abstract results (5 presentations)

We shall devote separate subsections to these areas, with the understanding that this distinction is sometimes rather weak and basically motivated by the sake of presentation.

Plasticity

The effective description and prediction of the material behavior in presence of plastic evolution is clearly of extraordinary applicative interest. As such, the mathematical treatment of always refined plastic theories is constantly attracting attention.

A first result on plasticity was presented by G. Francfort in collaboration with F. Babadjian and M. G. Mora. The authors have considered some non-associative plasticity case. By passing to the limit in a viscous regularization of the problem, they proved the existence of suitably behaved solutions to the full 3D quasi-static evolution problem.

The presentation by D. Reddy has been focused on the variational analysis of so-called strain-gradient linearized elasto-plasticity. The second-order nature of strain-gradient plasticity allows for the inclusion of moderate softening behavior. Time-discretizations have also been commented.

G. Dolzmann presented a result in collaboration with S. Müller and C. Kreisbeck and a simple yet critical model for hardening effect in crystal plasticity. The idea here was to focus directly on some incremental energy minimization encoding the compatibility geometric requirements and pass then to a relevant Γ-limit.

The talk by B. Schweizer was targeting stochastic homogenization issues in dynamic plasticity and porous media. This talk has been slightly paralleled by the presentation by M. Veneroni who presented a periodic-homogenization result for classical Prandtl-Reuss plasticity including linear kinematic hardening effects.

The talk by P. Dondl in collaboration with N. Dirr and M. Scheutzow was focused on the emergence of rate-independent dynamics as an effect of the motion of a material interface through a lattice with defects. The related results might be related to material interfaces moving in materials.

Damage and crack propagation

These themes attracted the largest number of contributions to our workshop. The non-linear evolution of cracks in brittle material is not only a crucial applicative issue but also a quite demanding test-case for variational and non-variational functional methods. To some extent, damage theories represent a possible phase-filed-like view at the sharp-interface crack problem and are often more amenable for mathematical discussion, especially in combination with other complex materials behaviors. A direct connection between damage and brittle fracture via a scaling limit has been provided by M. Thomas in collaboration with A. Mielke and T. Roubíček.

A. Fiaschi presented some existence results in collaboration with D. Knees and U. Stefanelli for the case of non-regularized in space damage. Lacking a compactifying effect in space, the damage parameter is here allowed to develop as a Young measure [16].

In the talk presented by J. Zeman in collaboration with P. Gruber, some analysis and simulations for the mixed-mode evolution in delamination situation has been discussed. The case of mixed-mode crack propagation via approximate stress-intensity factors has then be analyzed by M. Negri. Some phase-field and adaptive finite-element methods for the prediction of crack growth have been presented by C. Ortner in collaboration with S. Burke and E. Süli.

G. Lazzaroni has presented an existence result for the finite-strain Griffith-crack propagation with non-interpenetration constraints (in collaboration with G. Dal Maso) and R. Toader reported on her work with G. Lazzaroni on the viscous approximation in the frame of crack growth. Finally, D. Knees presented some numerical convergence analysis for a vanishing viscosity approach to fracture.

Thermal effect in materials have also be mentioned in the presentations. In particular, a thermo-visco-elastic model in case of contact with adhesion friction has been presented by E. Bonetti in collaboration with G. Bonfanti and R. Rossi. Moreover, T. Roubíček in collaboration with S. Bartels presented the analysis of a Kelvin-Voigt visco-elastic model with internal variables (plastic, damage).

Shape memory alloys

A good deal of attention has been focused on the description of the complex thermomechanical behavior of shape memory alloys (SMAs) [18]. We had talks ranging from the more applied/experimental to the more analytic. We shall follow this path also here.

P. Šittner has reported on an extended experimental campaign targeting the complex thermomechanical evolution of microstructures in amorphous NiTi alloy wires and relating these microstructures with resistance to fatigue. Then a new plate finite tailored to the celebrated SMA model by Souza-Auricchio has been presented by E. Artioli in collaboration with S. Marfia, E. Sacco, and R.L. Taylor. Some numerical experiments on a finite-strain version of the Souza-Auricchio model have been illustrated by A. Reali with J. Arghavani, F.

Auricchio, R. Naghdabadi. A general result on error-control for full space-time discretization of the Souza-Auricchio model by implicit-Euler in time and conformal finite-elements in space has been presented by A. Petrov with A. Mielke, L. Paoli, and U. Stefanelli [40]. J. Zimmer with M. Kružík advanced and analyze a model including both SMA and plastic behavior whereas J. Kopfová, in collaboration with M. Eleuteri and P. Krejčí, presented a novel modeling view at Thermomechanics based on a suitable use of Preisach-type hysteretic operators.

Abstract theory

A miscellanea of novel results at the abstract level have been presented. All of these basically tackle the understanding of rate-independent evolution and the outreach of the current theory in the direction of non-smooth, non-convex, or non-deterministic scenarios.

In collaboration with A. Mielke and G. Savaré, R. Rossi has presented a quite general result on convergence and characterization of the limit of viscous regularizations of rate-independent evolutions in the frame of Banach spaces [45]. With the same aim of overcoming the restrictive global minimality conditions in (32.3), C. Larsen presented his notion of ϵ-stability and applied it to Griffith-crack evolution. M. Liero presented his result with P. Krejčí[26] on rate-independent evolution in the frame of regulated (non-smooth) functions via Kurzweil integration and V. Recupero outlined his analysis on the possible extension of some rate-independent operators (including the sweeping process) from Lipschitz to discontinuous inputs.

Finally, T. Sullivan illustrated his results with M. Koslowski. M. Ortiz, and F. Theil on the effect of an heat bath on a rate-independent system. This *thermalization* of the system is actually interacting with the evolution and destroying the rate-independent character of the systems around equilibrium. This observations are connected with the so-called Andrade creep effect [72].

Outcome of the Meeting

Let us express again our gratitude to the BIRS for supporting this workshop, which all participants found very interesting and productive. Indeed, the familiar atmosphere at Corbett Hall has, we believe, facilitated the interaction of this small but highly focused community of researchers. Scientific relations have been boosted not only by the possibility of informally interacting during the scientific part of the meeting but also by some very rewarding (and in some sense inspirational) excursions in the stunning surroundings of the Centre. It was a real privilege for us to hold our meeting at BIRS.

To our view, a very nice first outcome of the meeting was a clear picture of future research lines for the rate-independent community. In particular, the interplay between a more theoretic/variational point of view with the exciting challenges coming from the applications in plasticity, shape-memory alloys and fracture will be a main trend of the future research and constitutes one of the strength point of the workshop, with the interaction of many specialists of the field and young promising researchers. In this respect, we regard the possibility of sketching this informal report as very appropriate in view of reporting on the current standpoint in this field.

Some collaborations have been initiated or renewed at the meeting and new results have already been obtained thanks to discussions at BIRS. Some of the presentations have been invited for publication in a special issue of the journal *Discrete and Continuous Dynamical Systems - Series S* edited by G. Dal Maso. A. Mielke, and U. Stefanelli. This issue, entitled *Rate-independent evolution*, should appear during 2012.

Plans for gathering the rate-independent community have been made at the BIRS. An important occasion will be the workshop on *Variational methods for evolution* at the *Mathematishes Forschungsinstitut Oberwolfach* in December 2011, which will offer the possibility of interaction with different kinds of evolutionary problems and variational techniques.

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Chapter 33

Test problems for the theory of finite dimensional algebras (10w5069)

Sep 12 - Sep 17, 2010

Organizer(s): Vlastimil Dlab (Carleton University), Jose Antonio de la Pena (Universidad Nacional Autonoma de Mexico), Helmut Lenzing (University of Paderborn), Claus Michael Ringel (Universitaet Bielefeld)

Overview of the Field

The roots of representation theory go far back into the history of mathematics: the study of symmetry, starting with the Platonic solids and the development of group theory; the study of matrices and the representation theory of groups by Klein, Schur and others which led to the development of the concepts of rings, ideals and modules; the study of normal forms in analysis, in the work of Weierstrass, Jordan and Kronecker, among others; the development of Lie theory. Some of the famous Hilbert's problems relate representation theory with fundamental geometric concepts.

Starting in the middle 60's of last century, the 'modern' Representation Theory of finite dimensional algebras had a very fast start with three main driving forces: The categorical point of view, represented by Maurice Auslander and his school, leading to the concepts of almost-split sequences, Auslander-Reiten duality, and Auslander-Reiten quivers. The introduction of the concept of quiver representations by Pierre Gabriel, which is now a main tool in the analysis of the representation theory of finite dimensional algebras. The reformulation of problems from representation theory as matrix problems, associated to the Ukrainian school of A. Roiter lead to classification results in certain representation-infinite situations and the conceptual dichotomy of algebras according to their representation type as tame (including representation-finite) or wild.

This 'modern' Representation Theory of finite dimensional algebras, typically over an algebraically closed field, is thus characterized in its early stages by the dominance of linear methods, functor categories and homological theory. A specific flavor, in that form not present in any other subject, is constituted by Auslander-Reiten theory (almost-split sequences, Auslander-Reiten quivers, Auslander-Reiten duality), an aspect reflecting a deep combinatorial structure of homological nature. The area has by now reached a highly mature stage, leaving behind the original motivation of determining (if possible) all the indecomposable representations relating to the concepts of representation-finite, tame and wild type, respectively. The present situation is best described by strong interactions of representation theory with other mathematical subjects, like Graph Theory, Combinatorics, Lie Theory, Algebraic and Differential Geometry, Singularity Theory, Quantum Groups, and Mathematical Physics. Moreover, as reflected by conferences like the biannual series of ICRAs (International Conferences on the representations of algebras and related topics), the vitality of the subject is characterized by continuously conquering new topics of neighboring areas.

Recent Developments and Open Problems

In a sketchy fashion we list some important recent developments and open problems:

Cluster algebras and categories.

Cluster algebras were introduced by S. Fomin and A. Zelevinski [18, 19] at the start of this decade by formalizing the concept of *mutations*. Cluster algebras are interesting and difficult subalgebras of rational function fields reflecting deep combinatorial properties; correspondingly they enjoy a ubiquitous appearance in mathematics. By work of A. Buan, R. Marsh, M. Reineke, I. Reiten, and T. Todorov [8], finite dimensional representation theory enters the scene by achieving a categorification (of central classes) of cluster algebras through the *cluster category* of a finite quiver Q, interpreting mutations as (generalized) reflections, a subject closely related to tilting theory. The cluster category $\mathcal{C}$ is constructed as the orbit category of the derived category $D^b(\mathrm{kQ})$ of the path algebra of Q, more generally of a hereditary category. By a central result of B. Keller [31] the cluster category is itself triangulated. Much recent work has been invested by C. Amiot, O. Iyama, B. Keller, I. Reiten and collaborators in extending the context in various directions (a) by forming cluster categories for finite dimensional algebras of global dimension two [1], (b) by introducing and investigating cluster mutations for 2-Calabi-Yau categories [1], (c) by developing 'higher' cluster categories, see [28, 2], (c) introducing a categorification for quivers with potential [1]. In this Workshop the lectures by B. Keller, see section 33, and O. Iyama, see section 33, dealt with aspects of cluster and higher cluster theory.

Higher Auslander-Reiten and higher cluster theory.

This topic has some overlap with the previous one, but has a different and wider scope. A major recent development is O. Iyama's re-investigation of Auslander-Reiten theory, see [27], leading to what is now called *higher Auslander-Reiten theory*, see also [26, 28, 2]. We thus have n-almost-split sequences, n-representation-finiteness, n-preprojective algebras, n-Calabi-Yau triangulated categories, n-cluster categories etc., where the case $n = 2$ corresponds to the 'classical' situation. For instance, a triangulated category is called n-Calabi-Yau if there are functorial isomorphisms $\mathrm{Hom}(X, Y) = \mathrm{D}\mathrm{Hom}(Y, X[n])$ where D stands for the formation of the dual vector space. The subject is judged to have a high mathematical potential, correspondingly we expect it to have a large impact on the further development of representation theory. O. Iyama's Workshop lecture was about joint work with C. Amiot and I. Reiten [2] with the focus on stable categories of n-Cohen-Macaulay modules. Interpreting higher preprojective algebras as coordinate algebras of non-commutative projective schemes, the subject also produces challenging examples for non-commutative algebraic geometry, see section 33.

Wild algebras, and link to Algebraic Geometry.

Wild algebras, roughly speaking, don't allow an *explicit* classification of all their indecomposable modules. Though, much information (for instance growth behavior, shape of Auslander-Reiten quivers, certain aspects of module varieties) is now available for many classes of wild algebras, additional structural information on the set of all (or suitable families of) representations is missing, though in some cases moduli spaces for small dimension vectors have been studied successfully. Clearly the matter is geometric in spirit, and conjecturally related to non-commutative algebraic geometry. In the Workshop the matter was addressed in sections 33 and 33 for the class of wild hereditary algebras, yielding significant progress but leaving major questions still open.

Existence of tilting objects in triangulated categories.

This is a vast subject with many open problems, where only partial results are known, the initial results mainly due to work of Russian mathematicians, for instance A. Rudakov and collaborators. One fundamental question is: '*Which smooth projective varieties (stacks, orbifolds) admit a tilting object, more generally a full exceptional sequence for their derived category of coherent sheaves?*. At the Workshop significant progress in the surface case was reported by L. Hille and K. Ueda, see section 33 for further details. Another instance of the problem is the existence of tilting objects (full exceptional sequences) in the singularity category à la Buchweitz and Orlov [9, 45]. For Kleinian and Fuchsian singularities this has been solved by work of H. Kajiura, K. Saito, A. Takahashi [29, 30] or Lenzing, de la Peña [40]. For triangle singularities there are independent solutions by A. Takahashi and D. Kussin, H. Meltzer and H. Lenzing [36], respectively. The subject is still a matter of much current research. For further aspects we refer to sections 33 and 33.

Homological techniques and conjectures.

During the last 10 to 15 years finite dimensional representation theory experienced an important shift in emphasis. Instead of module categories their bounded derived categories have moved into the center of interest, allowing to prove that many representation theoretic concepts are actually invariant under derived equivalence.

It is customary to claim that triangulated categories are the natural framework for homological techniques. To confirm this claim still a lot of fundamental work has to be done. As an example we mention *Hochschild cohomology* another is the (graded) center of a triangulated category. By results of B. Keller one knows that the Hochschild cohomology of a finite dimensional algebra A is a derived invariant, hence only depends on the derived category $D^b(\mathrm{mod}(A))$. However, a direct interpretation of Hochschild cohomology for a triangulated category is missing, though in case of a tilting object T, one can use Keller's result resorting to the Hochschild cohomology of the endomorphism ring of T. The Hochschild cohomology ring is an essential tool, for instance to investigate *support varieties* for suitable classes of finite dimensional algebra. This approach, yielding a geometric insight for modules follows the group-theoretic example by L. Evens and J.F. Carlson and is the basis of much recent work by Ø. Solberg, K. Erdmann, N. Snashall, and Benson-Iyengar-Krause [5].

Typically, important homological conjectures for representations of a finite dimensional algebra A are still unsolved, though being around for several decades and being verified in many special cases. Here, we just mention the *Auslander conjecture*, dealing with bounds on the vanishing of $\mathrm{Ext}^n(X, -)$, the (generalized) *Nakayama conjecture* dealing with the structure of the minimal injective resolution of the regular A-module A, and the *finitistic dimension conjecture* which asks whether a bound of the finite projective dimensions of (finite dimensional) A-modules exists.

An exception to this general rule is M. Auslander's question on the possible values for the *representation dimension* which measures how far a finite dimensional algebra is from being representation-finite. Here, O. Iyama's proof [25] that this dimension is always finite came as a surprise and stimulated a lot of still ongoing activity to determine the exact value for special classes of algebras. (It is meanwhile known that this dimension can get arbitrarily large, a non-trivial fact, whose proof involves significant input from algebraic geometry.)

Presentation Highlights

The following two Workshop talks were video-taped.

Quantum Dilogarithm identities from quiver mutations

A highlight of the Workshop, yielding substantial mathematical progress, was the talk by B. Keller *Quantum Dilogarithm identities from quiver mutations*. Such identities for the quantum dilogarithm first occurred in work of Faddeev-Kashaev [17]; they were generalized by Kontsevich-Soibelman [34] and Reineke [47] using ideas from algebraic geometry, for instance stability structures and Donaldson-Thomas type invariants. The Faddeev-Kashaev identities and their generalizations imply corresponding identities for the classical dilogarithm, a fact relevant to number theory. Another application is to discrete dynamical systems with applications to mathematical physics.

In his talk, Keller presented a transparent and systematic method to derive a whole bunch of such identities from the theory of cluster algebras and categories by using sequences of socalled 'green quiver mutations'. Assume that the quiver Q in question is "good"; for instance Dynkin quivers or box products of two Dynkin quivers (corresponding to the tensor product of their path algebras) are good. First, one forms an enlargement $\tilde{Q}$ of Q by adding to each vertex v of Q a new vertex v' together with a new arrow $v \to v'$. The new vertices are considered to be frozen: it is not allowed to mutate there. Each time two such mutation sequences for $\tilde{Q}$ yield isomorphic quivers (the isomorphisms need to fix the frozen vertices), there results a quantum dilogarithm identity where two products of quantum dilogarithms turn out to be equal. The number of factors on each side of the identity equals the length of the corresponding mutation sequence, yielding new non-trivial identities. Moreover, the two sides may have different numbers of factors. The Faddeev-Kashaev identity corresponds that way to the Dynkin quiver A_2. Since for more complicated (good) quivers the combinatorics of quiver mutations is quite delicate, Keller has enhanced his Java applet for quiver mutations (obtainable from `www.math.jussieu.fr/ keller/quivermutation/`) to deal with this specific application of cluster theory. The Dynkin quiver $Q_1 = E_6$, the box product $Q_2 = A_5 \Box A_2$ of two Dynkin quivers, and the corresponding identities, were presented in detail. Since diagrams like Q_1 and Q_2 play a prominent role in singularity theory, this potential relationship needs to investigated further.

Summary: Cluster mutations, more generally cluster algebras and categories, are a powerful mathematical tool related to many mathematical subjects. We should expect to see further instances of spectacular applications of cluster techniques to many mathematical questions.

Sequences of triangulated categories

H. Lenzing's talk *Sequences of triangulated categories with focus on ADE-chains* did address two of the Workshop's main objectives, viz. the two test problems *Sequences of algebras* and *Nilpotent operators*.

There is much experimental evidence that sequences (A_n) of finite dimensional algebras obeying the 'same building law', enjoy a close relationship between representation-theoretic properties of their bounded derived categories $D^b(A_n)$ and the spectral properties of A_n (Coxeter transformation, Coxeter polynomial, etc.). An attempt to formalize 'nice' building laws is the concept of sequences (A_n) of *accessible algebras* [42] which are obtained from the base field by forming successive 1-point-extension by exceptional modules. An important example is formed by the Nakayama algebras $A(n,r)$, given by the linear quiver $1 \to 2 \to 3 \cdots \to n-1 \to n$ with n vertices, where the composition of any r consecutive arrows is assumed to be zero. Note that D. Happel and U. Seidel [21] determined all such algebras which are piecewise hereditary, i.e. derived equivalent to the path algebra of a finite acyclic quiver.

Of particular importance is the sequence $A_n = A(n,3)$ since it 'extends' the derived types of the Dynkin diagrams E_6, E_7 and E_8. (We say that the sequence (A_n) forms an ADE-chain.) A workshop at Bielefeld University, directed by C.M. Ringel, October 31-November 1, 2008 on the "ADE-chain problem" dealt with the ubiquity (and surprising similarity) of such ADE-chains arising in many different mathematical subjects, among others in

1. the *bounded derived category* of the Nakayama algebras $A(2(n-1),3)$,

2. the triangulated *singularity category* à la Orlov [45] and Buchweitz [9] of the triangle singularity $f_n =$

$x^2 + y^3 + z^n$. This category has alternative incarnations as *stable category of vector bundles* $\underline{\mathrm{vect}}(\mathbb{X})$ on the weighted projective line $\mathbb{X}(2,3,n)$, or as the *stable category of CM-modules* (graded sense) over $S = k[x,y,z]/(f_n)$ or, alternatively, as the (stable) category of matrix factorizations of f_n.

3. The triangulated category of *invariant subspaces of nilpotent operators* of nilpotency degree n (graded sense) of Ringel-Schmidmeier [52].

It came as a surprise [35], see also [10], that the problems, listed above, yield identical triangulated categories: notation $\mathcal{T}_{2(n-1)}$, 'showing' a remarkable uniqueness of such ADE-chains. Major features of the category $\mathcal{T} = \mathcal{T}_{2(n-1)}$ are:

1. $\mathcal{T}$ has 'natural' tilting objects T_1, T_2 whose endomorphism rings are, respectively, the Nakayama algebra $A(2(n-1),3)$ or the tensor product $k\vec{A}_2 \otimes k\vec{A}_{n-1}$ of two linear Dynkin quivers. (There is related work of Ladkani [37]).

2. The category $\mathcal{T}$ is fractionally Calabi-Yau of CY-dimension $1 - 2\chi_{\mathbb{X}}$, where $\chi_{\mathbb{X}}$ is the (orbifold) Euler characteristic of the weighted projective line $\mathbb{X}(2,3,n)$. (It then follows that the Coxeter transformation is periodic, typically of period $\mathrm{lcm}(3,n)$), and the Coxeter polynomial factors into cyclotomic polynomials.

The matter — in a more general setting — is taken up again in the Workshop lecture of D. Kussin, see section 33; additional aspects are treated in the Workshop lecture of A. Takahashi, see section 33.

Summary. The talk reported on significant recent progress on ADE-chains, and further sequences of algebras and triangulated categories, revealing surprising links between representation theory, singularity theory and operator theory. Arising Calabi-Yau properties, existence and shape of tilting objects were highlighted.

Scientific Progress Made

Varieties with a tilting object

The two lectures by L. Hille on *"Tilting Bundles on Rational Surfaces and Quasi-Hereditary Algebras"* and K. Ueda on *"Dimer models, exceptional collections, and non-commutative crepant resolutions"* dealt with similar questions from a somewhat orthogonal perspective. They constitute significant progress and, potentially, allow the representation theory of finite dimensional algebras to deal with specific three-dimensional singularities. (Sofar, the link to singularity theory is mainly in dimensions one and two).

The existence of tilting objects (in different terminology, of full strong exceptional sequences/collections) in derived categories of coherent sheaves over a smooth projective variety (more generally in a weighted, or stacks, or orbifold version) is central for linking finite dimensional representation theory, algebraic geometry and singularity theory. Concerning the link to singularity theory, the introduction of Orlov's singularity category [45], see also former work by R. Buchweitz [9], has given the subject a strong additional momentum.

Categories of coherent sheaves $coh(X)$ on a smooth projective variety X share many important properties with categories $mod(A)$ of finite dimensional representations over a finite dimensional algebra A (of finite global dimension): they are abelian categories whose homomorphism and extension spaces are finite dimensional over the base field k (mostly assumed to be algebraically closed). Moreover, the bounded derived categories $D^b(X)$ and $D^b(A)$ satisfy Serre duality, and consequently admit Auslander-Reiten theory, thus enabling to speak of their Auslander-Reiten quiver and Auslander-Reiten components. While this analogy is merely on the formal level, it gets very specific once the (derived) category of coherent sheaves on X admits a *tilting object*, that is, an object T without self-extensions and generating the derived category: In this case $D^b(X)$ and $D^b(A)$ are actually equivalent, thus allowing a direct comparison of complexes of modules or sheaves, and establishing the endomorphism ring of T as a kind of coordinate system for the category $D^b(X)$. Since the first appearance of this effect in work of Beilinson's influential paper [4], there has been much interest in the question for which smooth projective varieties/schemes/stacks the derived category has a tilting object. For a one-dimensional variety, Riemann-Roch implies that this occurs only for the projective line (if the base field k is algebraically closed). This result extends to a weighted (=stacks, orbifold) setting: only the weighted projective lines allow a tilting object, see [39] and [49].

Passing to projective varieties X of higher dimension, the question of the existence of a tilting object (more generally, of a full exceptional sequence) constitutes a severe restriction since it forces the Grothendieck group to be finitely generated free. And the existence problem constitutes an open problem: While it is frequently possible to disprove the existence of full exceptional sequences by general arguments (for instance, in case of big size or the existence of non-trivial torsion for the Grothendieck group, or by the non-existence of any exceptional objects for Calabi-Yau varieties), any existence proof affords an explicit construction and thus a highly explicit understanding of the (derived) category of coherent sheaves and its exceptional objects. The conjecture has been around for about 20 years that such tilting objects (resp. full exceptional sequences) exist exactly for rational varieties (always assumed to be smooth projective). While there had not been much progress in this matter for a long time, recent development did create a strong momentum: In 1997, A. D. King [33] conjectured that any complete smooth toric variety has a tilting sheaf which is a direct sum of line bundles. In this form, the conjecture has been disproved by L. Hille and M. Perling [22] already for (Hirzebruch) surfaces; but with a proper modification King's conjecture is basically correct, as was reported in L. Hille's Workshop talk *Tilting Bundles on Rational Surfaces and Quasi-Hereditary Algebras*. Based on previous work [23], Hille and Perling (2010) have shown how to construct tilting bundles for any rational surface X: They first construct a full exceptional sequence E of line bundles; in a second step, by killing higher extensions through *universal extensions* they obtain a *tilting bundle* T which, in general, is no longer a direct sum of line bundles and such that, moreover, the endomorphism algebra of T is *quasi-hereditary*. (Quasi-hereditary algebras are of finite global dimension with significant extra structure; their main structural properties have been established by V. Dlab and C.M. Ringel, see for instance [14]).

In dimension two, the weighted (stack, orbifold) version still remains open, however important results exist. K. Ueda in his Workshop talk "*Dimer models, exceptional collections, and non-commutative crepant resolutions*" reported on joint work [24] with A. Ishii using *dimer models*. A dimer model is a bicolored graph on a real two-torus which encodes the information of a quiver with relation. Ueda showed how to use dimer models to establish a *cyclic* tilting object of line bundles for two-dimensional weak Fano stacks, thus establishing King's conjecture for such stacks, a result also proved by Borisov and Hua [7] by different methods. The significant improvement by Ueda and Ishii concerns the combinatorial strategy to use dimer models in constructing tilting objects of a special kind.

Summary: The new and significant results reported by Hille and Ueda constitute a breakthrough and provide substantial additional insight. Moreover, they pave the way for a representation-theoretic treatment of three-dimensional singularities. (Two-dimensional singularities are related to the weighted projective curves.)

Nilpotent operators

This topic constitutes one of the test problems of the Workshop. As mentioned in section 33 it is related to the test problem on sequences of algebras and deals with the classification of invariant subspaces of nilpotent operators (on finite dimensional vector spaces). This problem has a long history that can be traced back to Birkhoff's problem [6], dealing with the classification of subgroups of finite abelian p-groups. Despite earlier work by D. Simson [54], the major breakthrough was was through recent work by Ringel and Schmidmeier [52]. Their work includes an explicit classification for nilpotency degree six, yielding *tubular type*, related to the representation theory of tubular algebras, a problem initiated and accomplished by Ringel in [51].

The three Workshop lectures

1. C.M. Ringel: *What is known about invariant subspaces of nilpotent operators? A survey. I*
2. M. Schmidmeier: *What is known about invariant subspaces of nilpotent operators? A survey. II*

3. M. Schmidmeier: *Three slides.*

reported the current status of the invariant subspace problem for nilpotent operators. Then D. Kussin: *The two-flag invariant subspace problem for nilpotent operators.* reported on the link to singularities and generalizations to more complicated systems of invariant subspaces, yielding interesting new classes of exact categories and triangulated categories.

For this test problem representation theory has passed the test: It was already mentioned in Lenzing's lecture that the invariant subspace problem is related to the investigation of triangle singularities of type $(2, 3, n)$ and the stable categories of vector bundles on a weighted projective line of the same type. Kussin, reporting on unpublished joint work with Lenzing and Meltzer, described an even more general setting, constituting substantial progress: Given a triple (a_1, a_2, b) of integers ≥ 2, the invariant two-flag problem of nilpotency degree b (graded version) with flag lengths $a_1 - 1$ and $a_2 - 1$ yields an exact category which is *almost Frobenius*, in general no longer Frobenius, whose associated stable category is equivalent to the triangulated category of stable vector bundles on a weighted projective line $\mathbb{X}$ with weight triple (a_1, a_2, b). This way, a complete classification for the indecomposables for Euler characteristic $\chi_{\mathbb{X}} \geq 0$ is achieved. In general, these triangulated categories are all fractional Calabi-Yau (of CY-dimension $1 - 2\chi_{\mathbb{X}}$) and all have tilting objects whose endomorphism rings are arising in singularity theory. This last issue is also related to A. Takahashi's Workshop talk and work by Xiao-Wu Chen [10]. Despite this enormous progress, new problems pop up: Schmidmeier reported on the interesting concept of *curvature* for the Frobenius categories of invariant subspaces (of fixed nilpotency degree), a concept, needing further clarification: in particular it's relationship to the curvature (orbifold sense) of the corresponding weighted projective line is presently unclear. Schmidmeier compared subspace problems for growing nilpotency degree, thus raising the question about the nature of the (direct) limit of the subspace categories.

Summary: The representation theory has passed the test concerning the test problem *Nilpotent operators*. Substantial, and in this form unexpected, progress was achieved. As a result a firm link between the topics representation theory, singularity theory and operator theory was established. New, and probably important, questions about the shape of corresponding limit categories did evolve.

Sequences of finite dimensional algebras, ADE-chain problem

The test problem "*Sequences of finite dimensional algebras*" was somehow the core of the meeting; a large number of Workshop contributions was devoted to this topic. For the general scope we refer to section 33, for further aspects to section 33. By the cumulative efforts of Workshop participants, significant progress could be achieved, and a large number of aspects has now been clarified. The main achievements are:

1. A firm link has been established between finite dimensional representation theory, singularity theory and operator theory,

2. The role of ADE-chains, in relationship to Nakayama algebras, weighted projective lines, matrix factorizations, singularities, and nilpotent operators has obtained much clearer contours,

3. The central role of being *fractional Calabi-Yau* for the sequence problem has been recognized.

4. As a new problem, the formation of limits of triangulated categories, determined by a sequence (A_n) of finite dimensional algebras, has emerged.

In addition to the lectures mentioned in sections 33 and 33 the following ones concern fundamental aspects of the sequence problem: J.A. de la Peña: "*Accessible algebras*" dealt with the spectral properties of accessible towers algebras. D. Happel: "*Piecewise hereditary Nakayama algebras* reported on general properties of the algebras $A(n, r)$, see [21], in particular settled the question when such an algebra is piecewise hereditary, i.e. derived-equivalent to a hereditary category. S. Oppermann: "*Implications of fractional Calabi-Yau for derived categories*" and S. Ladkani: "*On fractional Calabi-Yau algebras*" collected important evidence that

Calabi-Yau properties are essential for the sequences problem. Moreover, Ladkani did present an impressive list of examples. H. Krause: "*Expansions of abelian categories*" reported on joint work with Xiao-Wu Chen [11] to construct sequences of abelian categories by insertion of new simple objects. This was to some extent continued by Chen: "*Recollement of vector bundles and homomorphism chains*" by studying sequences of categories of coherent sheaves on weighted projective lines by changing a single weight and investigating the effect on their categories of vector bundles (resp. stable categories of vector bundles). A.D. King: "Observations on Grassmannian cluster algebras" presented a conjectural relationship between the series $D_5, E_6, E_7, E_8, ...$ and $A_2, D_4, E_6, E_8, ...$ that arises in the context of Grassmannian cluster algebras, and further is related to the study of frieze categories.

Summary: In all respects, the represenation theory has passed the test concerning the test problem *Sequences of finite dimensional algebras*. Because its relationship to many other subjects (singularity theory, matrix factorizations, operator theory, non-commutative algebraic geometry) it is fair to predict that it has a large potential to further influence developments in representation theory. A particular promising topic is the formation of limit categories suggested by the Workshop.

Kerner's exotic space, and link to non-commutative algebraic geometry

A main objective of the Workshop was to explore "Kerner's exotic space" $\Omega(A)$, a hypothetical mathematical structure parametrizing the Auslander-Reiten components for a wild hereditary algebra A. We always assume A to be finite dimensional and connected, defined over an algebraically closed field; such that we may restrict to the case where A is the path algebra kQ of a finite wild connected quiver Q. A particular aim was to understand $\Omega(A)$ as an object of non-commutative Algebraic Geometry (NCAG for short), and to identify its 'geometric' properties. There were four talks specifically addressing this topic.

1. O. Kerner: *The category of regular modules over wild hereditary algebras*,
2. H. Minamoto: *Ampleness of two-sided tilting complexes*,
3. I. Mori : *Quantum Beilinson algebras*,
4. P. Smith : *Non-commutative spaces and finite dimensional algebras*.

Kerner's talk was introductory, and addressed also to non-experts of representation theory. In the focus of his talk was the surprising existence of 'natural bijections' between any two such 'spaces' $\Omega(A)$, for A a wild, hereditary as above, see [32, 12] The talks by Minamoto and Mori formed a unit. H. Minamoto's talk based on [43, 44] mainly attacked Kerner's exotic spaces by analyzing the projective spectrum of the graded *preprojective algebra* $\Pi(A)$ of a wild hereditary algebra A and of the graded noncommutative *Beilinson algebra* $k\langle x_1, \ldots, x_r\rangle/(\sum_{i=1}^r x_i^2)$; he further presented basic features of *Fano algebras*, a new and promising class of finite dimensional algebras inspired from the homological properties of Fano varieties. I. Mori extended the setting by investigating *quantum Beilinson algebras* and their attached projective spectrum. He then continued the investigation of Fano algebras and their NCAG, started by Minamoto. It was very interesting to observe that the *higher preprojective algebras*, as introduced by Iyama, enter the scene, thus creating a new contact surface between NCAG and the representation theory for finite dimensional algebras A of finite global dimension $d \geq 2$. (In the follow-up it was considered very important thus to wave the initial restriction to hereditary algebras). P. Smith finally gave an overview of core techniques of NCAG in a talk specifically addressed to representation theorists. Smith also raised a test problem for NCAG: "*Can NCAG help us to understand finite dimensional algebras?*", a question including the Kerner space test problem. Smith further discussed challenging examples of NCAG, some very remote from classical algebraic geometry. In some detail he treated the projective spectrum of a free non-commutative algebra as a 'baby example' for exotic properties of NCAG.

We now describe the consequences for Kerner's exotic space(s) $\Omega(A)$ as they result from these talks and corresponding follow-up discussions. Let A be a wild hereditary algebra as above. Up to Morita-equivalence

A is the path algebra kQ of a finite, connected, wild quiver Q. Typical examples of wild quivers are the r-Kronecker quiver $\circ \Rrightarrow \circ$, $r \geq 3$ arrows, and a wild hereditary star $[p_1, p_2, \dots, p_t]$ with t branches of lengths $p_1, \dots, p_t$ and such that $2 - \sum_{i=1}^{t}(1 - 1/p_i)$ is < 0. Then $\Omega(A)$ is a virtual 'space' which parametrizes the set of all Auslander-Reiten components of (indecomposable) regular A-modules. Recall for that purpose that the indecomposable representations of a wild hereditary algebra $A = kQ$ as above are either preprojective, preinjective or regular. The preprojective (resp. preinjective) modules have a somewhat discrete flavor, and each form a single Auslander-Reiten component. By contrast, the regular modules are arranged in a 'continuous' family Auslander-Reiten components. By a fundamental result of C.M. Ringel all these components have shape $\mathbb{Z}A_\infty$, see [50]. For a wild hereditary algebra let $\Omega(A)$ be the set of its regular Auslander-Reiten components. Let A and A' be two wild, connected, hereditary, finite dimensional algebras over an algebraically closed field k. By a surprising result of O. Kerner [32, 12] there exist unexpected 'natural' bijection between the sets $\Omega(A)$ and $\Omega(A')$. In his talk, Kerner included the remarkable result of his student J.C. Reinhold, see [48], who established another bijection extending the setup of the Crawley-Boevey-Kerner result, crossing the border between hereditary algebras and coherent sheaves on a weighted projective line. Let $\mathbb{X}$ be a weighted projective line [20] of wild type $(p_1, \dots, p_t)$, and let L be any line bundle in $\mathrm{coh}\mathbb{X}$. Then the perpendicular category $L^\perp$ is naturally equivalent to the category $\mathrm{mod}(C)$, where C is the path algebra of the star $[p_1, \dots, p_t]$ with standard orientation. Let E be the Auslander bundle given as the extension term of the almost-split sequence $0 \to \tau L \to E \to L \to 0$. Then Reinhold shows that the factor category $\mathrm{reg}(C)/[\tau^{\mathbb{Z}}E]$ is equivalent to $\mathrm{vect}\mathbb{X}$, and hence inducing a natural bijection between $\Omega(C)$ and the set of AR-components of $\mathrm{vect}\mathbb{X}$. [Note in this context that 'stabilization' from $\mathrm{reg}C$ to $\mathrm{vect}\mathbb{X}$ leaves the Auslander-Reiten components almost intact, but changes the category structure drastically since it reduces exponential growth for $\mathrm{reg}C$, see [13], to linear growth for $\mathrm{vect}\mathbb{X}$, see [41], when dealing with the sequences $\dim_k \mathrm{Hom}(X, \tau^n Y)$.]

The existence of Kerner bijections raises some obvious questions:

1. What is the *mathematical nature* of the hypothetical 'spaces' $\Omega(A)$ parametrizing the regular components for wild hereditary algebras? Are they objects of NCAG?
2. Should we think of just one (universal) space Ω or of several spaces $\Omega(A)$, linked by Kerner bijections, and then all having a comparable structure?

As an outcome of the workshop, the answer to the first question is 'yes', more specifically $\Omega(A)$ *should be viewed as an exotic curve whose category of coherent sheaves is derived equivalent to the category of finite dimensional representations of* A. Concerning the second question, the idea to have a single universal space was refuted; from the structural point of view, the relationship between the various $\Omega(A)$, however, still needs clarification. In more detail, $\Omega(A)$ should be the virtual non-commutative space, whose category of coherent sheaves is the projective spectrum of the (graded) preprojective algebra $\Pi(A)$: Let A be a representation-infinite, hereditary, connected finite dimensional algebra. The *preprojective algebra* $\Pi(A)$, which has infinite k-dimension, has a simple combinatorial definition in terms of the quiver of A due to I.M. Gelfand and V.A. Ponomarev. For the present purpose, however, the following two $\mathbb{Z}$-graded (isomorphic) incarnations of $\Pi(A)$ are relevant, see [3]. Namely, $\Pi(A)$ can be considered as the *tensor algebra* $\mathbb{T}(M)$ of the (A, A)-bimodule $M = \mathrm{Tr}\mathrm{D}A = \mathrm{Ext}^1_A(DA, A)$ or alternatively as the *orbit algebra* of $\tau_A^{-1} = \mathrm{TrD}$, where TrD is Auslander's transpose-dual, that is, $\Pi(A) = \bigoplus_{n \geq 0} \mathrm{Hom}_A(A, \tau^{-n} A)$. Applying *Serre's construction* [53] to $\Pi(A)$ yields a category $\mathcal{H}(A) = \mathrm{mod}^{\mathbb{Z}}\Pi(A)/\mathrm{mod}_0^{\mathbb{Z}}\Pi(A)$ with the following properties, independently due to several authors: [38, 3, 43, 44]: (1) $\mathcal{H}(A)$ is abelian, Hom-finite, and hereditary. (2) $\mathcal{H}(A)$ admits *Serre duality* in the form $\mathrm{DExt}^1(X, Y) = \mathrm{Hom}(Y, \tau X)$ for an auto-equivalence τ of $\mathcal{H}(A)$, resembling Serre duality for smooth projective curves. (3) By means of the decomposition $\mathrm{mod}(A) = \mathrm{preproj}(A) \vee \mathrm{reg}(A) \vee \mathrm{preinj}(A)$ into preprojective, regular, resp. preinjective modules, we have

$$\mathcal{H}(A) = (\mathrm{preinj}(A)[-1] \vee \mathrm{prepr}(A)) \vee \mathrm{reg}(A),$$

viewed as a full subcategory of the bounded derived category $D^b(\mathrm{mod}(A))$. We write $\mathcal{H}_l$ for $(\mathrm{preinj}(A)[-1] \vee \mathrm{prepr}(A))$ and $\mathcal{H}_r$ for $\mathrm{reg}(A)$ such that $\mathcal{H}(A) = \mathcal{H}_l \vee \mathcal{H}_r$. (4) $\mathcal{H}_l(A)$ is equivalent to the category $\mathrm{proj}^{\mathbb{Z}}$ of finitely generated projective graded $\Pi(A)$-modules. (5) $\mathcal{H}(A)$ has a tilting object T with endomorphism ring A. (6) $\mathcal{H}(A)$ has no simple objects.

Note that $\operatorname{mod}^{\mathbb{Z}}\Pi(A)$ denotes the category of all *finitely presented*, $\mathbb{Z}$-graded right $\Pi(A)$-modules. Due to coherence of $\Pi(A)$ this category is abelian. The subscript 0 then refers to the full subcategory of finite length modules. It offers more flexibility to interpret $\operatorname{mod}^{\mathbb{Z}}\Pi(A)$, like in [38], as the category of finitely presented abelian-group valued functors on the category $\operatorname{prepr}(A)$ of preprojective A-modules. This also shows that for A the r-Kronecker algebra, $r \geq 3$ we may replace $\Pi(A)$ by the (graded) generalized Beilinson algebra $k\langle x_1, \ldots, x_r\rangle/(\sum_{i=1}^{r} x_i^2)$ without changing the projective spectrum. Further relevant research includes J.J. Zhang's classification of Artin-Schelter regular algebras of dimension two [55], D. Piantkovski [46], and most specifically H. Minamoto [43, 44]. That $\mathcal{H}(\mathcal{A})$ has no simple objects, is an obstacle to understand the geometry of $\Omega(A)$. This absence of simples suggests the following interpretation. In the category of coherent sheaves $\mathcal{H}(A)$ on $\Omega(A)$ we don't see the points of $\Omega(A)$. Simple objects, and then points, will however exist in the category of quasi-coherent sheaves, to be thought of as the closure of $\mathcal{H}(A)$ under direct limits. It affords further research to clarify how such 'points' relate to the regular Auslander-Reiten components of A.

There is a lot of evidence that Kerner's exotic spaces classify the set of Auslander-Reiten components in many further instances and thus play a role also in singularity and operator theory.

Summary: (1) Many aspects of Kerner's exotic spaces $\Omega(A)$ could be clarified during the Workshop. By the properties of their categories of coherent sheaves it is reasonable to consider them as *non-commutative projective non-noetherian (exotic) curves*. (2) A good knowledge of $\Omega(A)$ is of relevance for many problems in Representation Theory or Singularity Theory. (3) The relationship between 'virtual' points of $\Omega(A)$ and regular Auslander-Reiten components of A still needs clarification by further research. In particular, such a study has to invoke the category of quasi-coherent sheaves. (4) It is desirable to extend the range of the theory to finite dimensional algebras A of higher global dimension ≥ 2 by means of Iyama's construction of higher preprojective algebras, that is, the tensor algebras of higher extension spaces $\operatorname{Ext}_A^d(DA, A)$, $d \geq 2$. For the particular situation that A is Fano, interesting new results are expected, yielding higher dimensional (exotic) spaces.

Strange duality and mirror symmetry

This topic concerns the talks by A. Takahashi "*Mirror symmetry, strange duality and matrix factorization*" and W. Ebeling "*Strange duality and monodromy*". The two talks concern recent results based on their joint paper [16] and additional collaboration between Ebeling and Gusein-Zade [15]. These investigations were motivated in part by the outcome of the BIRS Workshop "*Spectral Methods in Representation Theory of Algebras and Applications to the Study of Rings of Singularities* (08w5060)", where a successful interaction between representation theory and singularity theory was initiated.

Mirror symmetry is now understood as a categorical duality between algebraic geometry and symplectic geometry. Takahashi and Ebeling apply ideas of mirror symmetry to singularity theory in order to understand various mysterious correspondences among isolated singularities, root systems, Weyl groups, Lie algebras, discrete groups, finite dimensional algebras and so on. In the two talks they generalize Arnold's strange duality for the 14 exceptional unimodal singularities to a specific class of weighted homogeneous polynomials in three variables called *invertible polynomials*.

For the base field of complex numbers, Ebeling and Takahashi obtain a complete classification of such invertible polynomials. In a condensed form, the main result of Ebeling and Takahashi, explaining strange duality, states the following. Let $f = f(x, y, z)$ be such an invertible, weighted homogeneous polynomial, and let f^t denote its Berglund-Hübsch transpose. Then (1) If $R_f = \mathbb{C}[x, y, z]/(f)$ equipped with the maximal L_f-grading, then the projective spectrum of R_f, obtained by Serre construction [53], is a weighted projective line $\mathbb{X}$ with three weights, and whose weight triple $(\alpha_1, \alpha_2, \alpha_3)$ yields the *Dolgachev numbers* for the pair (f, L_f). (2) $f^t(x, y, z)$ deforms into the cusp singularity $T_{\gamma_1,\gamma_2,\gamma_3} = (x')^{\gamma_1} + (y')^{\gamma_2} + (z')^{\gamma_3} - x'y'z'$. (3) The *Gabrielov numbers* $(\gamma_1, \gamma_2, \gamma_3)$ for f^t coincide with the Dolgachev numbers of f. (4) The singularity category $D^{L_f}_{Sg}(R_f)$ in the sense of [45, 9] admits a semi-orthogonal decomposition into the derived category $D^b(\mathrm{coh}\mathbb{X})$ and the derived category of a representation-finite quiver. (5) The singularity category is *fractional Calabi-Yau*, and has a *tilting object*.

The above properties of the singularity category $D^{L_f}_{Sg}(R_f)$ are related to, and for the case $f = x^{\alpha_1}+y^{\alpha_2}+z^{\alpha_3}$ indeed identical to, results obtained by Kussin-Meltzer-Lenzing [35]. They are thus directly related to the discussion on sequences of triangulated categories in section 33. W. Ebeling, in his talk, additionally gave a crash-course how to obtain the Coxeter-Dynkin diagram of an isolated singularity f by morsification of f, and to get hold of its monodromy (Coxeter transformation). He also included an account on the spectral properties (Poincaré series, Coxeter polynomials, and zeta functions) and the monodromy of weighted homogeneous polynomials.

Summary: The approach by Ebeling-Takahashi embeds Arnold's strange duality, which is initially an isolated phenomenon dealing with 17 cases, into a larger mathematical set-up, where 'strange duality' finds a natural explanation. It is, moreover, satisfying to witness in this case a particularly high degree of interaction between representation theory and singularity theory with significant impact on a main objective of the Workshop (sequences of algebras and triangulated categories).

Higher Auslander-Reiten theory, higher cluster categories

In his Workshop lecture "*Stable categories of Cohen-Macaulay modules and cluster algebras*" O. Iyama reported on joint work with C. Amiot and I. Reiten on certain aspects of higher Auslander-Reiten theory and higher cluster theory with the focus on the higher theory of Cohen-Macaulay modules.

A very important recent development is O. Iyama's re-investigation of Auslander-Reiten theory, see [27], leading to what is now called *higher* Auslander-Reiten theory, see also [26, 28, 2]. We thus have n-almost-split sequences, n-representation-finiteness, n-preprojective algebras, n-Calabi-Yau triangulated categories, n-cluster categories etc., where the case $n = 2$ corresponds to the 'classical' situation. For instance, a triangulated category is called n-Calabi-Yau if there are functorial isomorphisms $\mathrm{Hom}(X, Y) = \mathrm{DHom}(Y, X[n])$. The subject is judged to have a high mathematical potential, correspondingly the organizers expect it to have a major impact on the further development of representation theory. O. Iyama's Workshop lecture was about joint work with C. Amiot and I. Reiten [2] with the focus on stable categories of n-Cohen-Macaulay modules. Interpreting higher preprojective algebras as coordinate algebras of non-commutative projective schemes, the subject also produces challenging examples for non-commutative algebraic geometry.

In a certain degree related to the topic was the lecture by R. Takahashi "*Some classifications of resolving subcategories*" dealing, in particular, with aspects of Cohen-Macaulay modules.

Summary: This subject will certainly have a major influence on the further development of representation theory. A particular promising aspect is the *interplay with non-commutative algebraic geometry* through the concept of higher preprojective algebras, as subject, still in its early stages.

Covering theory

Inclusion of this subject into the Workshop was motivated by the objective to get more insight in the representation theory of wild Kronecker algebras. Covering theory is an essential tool to classify indecomposable situations explicitly, and to determine the representation type. This works well in 'good' situations (always representation-finite or tame) but has a major disadvantage that it does not coexist with degenerations of algebras, another useful tool in determining representation types. There were two related talks on the subject, one by A. Hajduk on "*On the different types of degenerations for algebras*" the other by P. Dowbor on "*Coverings and degenerations*". All these methods are geometric in spirit. Hajduk presented a new type of degenerations, called GCB-degenerations, allowing dimension change during degeneration. Hajduk showed a remarkably complete theory. His main result is that the representation type of a GCB-degeneration is at least as complicated as the representation type of the original algebra. In his subsequent talk, P. Dowbor did introduce degenerations of covering functors and related 'covering degenerations of algebras', thus extending the range of classical covering methods by Bongartz-Gabriel.

Summary: In itself, these investigations constitute a significant progress. The hope, however, using covering theory to obtain a better understanding of the representations of wild Kronecker quivers did not materialize. It seems that further new ideas are necessary to obtain progress in this direction.

Outcome of the Meeting

The mere formulation of the test problems for the Workshop has triggered a lot of exciting development, much of it already happening before the Workshop even started. In the judgement of the organizers this fact, and the corresponding success of the Workshop, is due to a clear and predefined focus of workshop topics where, on the other hand, the central workshop topics (Test Problems)

1. The representation theory of wild Kronecker algebras,
2. The unknown nature of Kerner's exotic space,
3. Sequences of algebras,
4. Nilpotent operators,

were sufficiently open to encourage leading experts to participate and contribute. As in the previous BIRS Workshop *Spectral Methods in Representation Theory of Algebras and Applications to the Study of Rings of Singularities (08w5060)* the Workshop was supported by a careful composition of experts, coming from different areas, able and interested to work together across mathematical boundaries. From our point of view, this particular scheme has proven to be incredibly successful; accordingly the response of participants to such a specific setup was very positive, sometimes even enthusiastic.

A workshop at Bielefeld University, directed by C.M. Ringel, October 31-November 1, 2008, was instrumental in sharpening the focus: as reported in section 33, it there became clear — still on a conjectural level — that test problems 3. and 4. should be very closely related through the concept of an ADE-chain. The conjectured links are meanwhile mathematical theorems that were reported at the BIRS Workshop, see sections 33 and 33. As an outcome of problems discussed at this Workshop, C.M. Ringel organized a further workshop at Bielefeld University with the title *Projective dimension two* on October 8-9, 2010, for details see the web-site http://www.math.uni-bielefeld.de/ sek/dim2/.

The status achieved with test problems 3 and 4 has been spectacular, in particular the established link between singularity theory and nilpotent operators was originally absolutely unexpected. For the specific achievements see sections 33, 33 and 33; the shape and the completeness of the results and corresponding completion of research by Ringel and Schmidmeier, see section 33, exploiting the tool of weighted projective lines by Kussin-Lenzing-Meltzer, see sections 33 and 33 was not be expected at all when the organizers did propose the Workshop scheme. It is satisfying, in particular, that through these studies the link between representation theory and singularity theory has gotten very strong; the explanation of Arnold's strange duality by Ebeling and Takahashi, see section 33, through invertible polynomials was another highlight of the meeting. It was also satisfying to see an emerging strong cooperation between representation theory and noncommutative algebraic geometry, a link, very worthwhile to be continued.

Concerning test problem 1 the expected progress on representations of wild Kronecker quivers via covering theory did not materialize. Apparently new techniques and insights are needed. On the other hand, a new conceptual understanding of the representation theory of wild Kronecker (and other wild) quivers via methods of noncommutative algebraic geometry (cf. test problem 2, section 33) appears to be quite promising; but still much work has to be done there.

Another promising subject emerged with links to the other topics discussed: the higher Auslander-Reiten theory developed by O. Iyama and collaborators, see sections 33 and 33. Its apparent links to cluster categories (also in a higher version) and noncommutative algebraic geometry makes it particularly challenging.

Though originally not triggered by the particular scope of the meeting, the contribution by B. Keller on dilogarithm identities was another instance of an unexpected and indeed, very powerful, application of representation theory (quiver mutations) to problems outside representation theory. On a similar level, the breakthrough by L. Hille and K. Ueda on the existence and construction of tilting objects could not be expected beforehand, though they were perfectly fitting in the general scheme of the Workshop by enforcing existing links to singularity theory, and pointing to new directions of research.

Summary: The organizers are very happy with the outcome of a meeting that met standards much above our original (high) expectations. The scientific progress achieved through the meeting itself and the preparations in front of the meeting are significant and partly even spectacular. In particular, the organizers feel confirmed and encouraged by the very positive, partly even enthusiastic, response from participants of the meeting.

Participants

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Chen, Xueqing (University of Wisconsin-Whitewater)
Chen, Xiao-Wu (University of Paderborn)
de la Pena, Jose Antonio (Universidad Nacional Autonoma de Mexico)
Dlab, Vlastimil (Carleton University)
Dowbor, Piotr (Nicolaus Copernicus University)
Ebeling, Wolfgang (Leibniz Universität Hannover)
Hajduk, Adam (Nicolaus Copernicus University)
Happel, Dieter (Technische Universität Chemnitz)
Hille, Lutz (University Münster)
Iyama, Osamu (Nagoya University)
Keller, Bernhard (University Paris Diderot - Paris 7)
Kerner, Otto (University of Duesseldorf)
King, Alastair (University of Bath)
Kleiner, Mark (Syracuse University)
Krause, Henning (University of Bielefeld)
Kussin, Dirk (Universitaet Bielefeld)
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Oppermann, Steffen (Norwegian University of Science and Technology)
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Chapter 34

Classification of amenable C*-algebras (10w5092)

Sep 19 - Sep 24, 2010

Organizer(s): Marius Dadarlat (Purdue University) Soren Eilers (University of Copenhagen) George Elliott (University of Toronto) Mikael Rordam (University of Copenhagen) Andrew Toms (Purdue University)

CLASSIFICATION OF AMENABLE C*-ALGEBRAS

Final Report

Introduction

The conference brought together leading researchers and young mathematiciansworking on the classification theory of amenable C*-algebras. The talks surveyed some of the very recentbreakthroughs and offered a chart for future expected developments. This led to a consolidation of our understanding of the open problems and some of the promising ideas in the classification theory.From the point of view of the organizers, what was particularly satisfactory for this conference was the timeliness with which it was held, allowing us to draw on the insight gained through many recently announced deep results, and to stimulate the future work in the area by bringing together influential (established as well as beginning) researchers. Since it is well established that operator algebra theory thrives in frequent and diverse interaction with other mathematical subjects the program contained not only talks relating to the core of classification theory, but also presenting interesting applications of results or methods from other areas to ours, or from ours to other areas. All of these efforts are naturally interwoven with ties in many directions represented mainly by scientific collaborations among their proponents, but to organize this report we will attempt a taxonomy as follows:

1. Dimension theory, regularity properties and classification of amenable C*-algebras
2. Computations of the Cuntz semigroup
3. Invariants of non-simple C*-algebrasand applications to graph C*-algebras
4. Classification of dynamical systems and group actions on amenable C *-algebras
5. General theory

For each of these areas we shall attempt below a brief overview of what the conference talks and the general discussion seemed to indicate about the status quo and the direction of future work.

Dimension theory, regularity properties and classification of amenable C^*-algebras

Talks

George Elliott

Inductive limits of matrix algebras over the circle

Guihua Gong

ASH-inductive limits: Approximation by Elliott-Thomsen building blocks

Huaxin Lin

Unitaries in simple C^*-algebras of tracial rank one and homomorphisms into simple $\mathcal{Z}$-stable C^*-algebras

Zhuang Niu

A remark on AH algebras with diagonal maps

Leonel Robert

Classification of inductive limits of 1-dimensional NCCW-complexes

Karen Strung

A technique to show certain C^*-algebras are TAI after tensoring with a UHF algebra.

Wilhelm Winter

Dimension, $\mathcal{Z}$-stability, and classification, ofnuclear C^*-algebras

Discussion

In the past five years the state of knowledge around Elliott's conjecture for simple C^*-algebras has advanced rapidly, particularly in the case that the projections of the algebra separate its tracial functionals. For instance, we now know by ground-breaking work of Toms and Winter that the C^*-algebras associated to minimal uniquely ergodic dynamics on finite-dimensional spaces are determined up to isomorphism by their graded ordered K-theory, as outlined in the talk given by Winter. At the centre of these developments are the Jiang-Su algebra $\mathcal{Z}$ and the attendant property of $\mathcal{Z}$-stability (a C^*-algebra A is $\mathcal{Z}$-stable if $A \cong A \otimes \mathcal{Z}$). This sort of tensorial absorption property is ubiquitous in operator algebra classification: Connes's proof that an amenable II_1 factor $\mathcal{M}$ with separable predual is the hyperfinite factor $\mathcal{R}$ proceeded by showing first that $\mathcal{M}\bar{\otimes}\mathcal{R} \cong \mathcal{M}$; the Kirchberg-Phillips classification of simple purely infinite C^*-algebras relies heavily on the fact that any such algebra A satisfies $A \cong A \otimes \mathcal{O}_\infty$ for the Cuntz algebra $\mathcal{O}_\infty$. But not all simple separable nuclear C^*-algebras are $\mathcal{Z}$-stable, in contrast with the tensorial absorption properties of factors and purely infinite algebras. Why so? Very roughly, the latter two classes of algebras are non-commutative generalizations of low-dimensional spaces, while general C^*-algebras may exhibit characteristics of higher-, even infinite-dimensional topological spaces. Here as in the classical case, one expects many strong theorems to hold only for C*-algebras which are finite-dimensional in a suitable sense. One is hence drawn to the conjecture that for A a unital simple separable nuclear C*-algebra, the following properties are equivalent:

(i) A has finite nuclear dimension;

(ii) $A \otimes \mathcal{Z} \cong A$;

(iii) A has strict comparison.

A detailed exposition of properties (i) and (iii) is beyond the scope of this report; let us mention only that nuclear dimension generalizes the classical covering dimension of a space to the realm of C*-algebras, and that strict comparison means, roughly, that the pre-order on Hilbert modules over A given by inclusion up to isomorphism is determined by the rank of the modules as measured by traces. The implications $\mathrm{(i)} \Rightarrow \mathrm{(ii)} \Rightarrow \mathrm{(iii)}$ are known, and $\mathrm{(iii)} \Rightarrow \mathrm{(ii)}$ holds under some additional conditions. The implication $\mathrm{(ii)} \Rightarrow \mathrm{(i)}$ is only known for classes where Elliott's classification conjecture holds, so that Elliott's program is a central facet of the conjecture. The equivalence of $\mathrm{(ii)}$ and $mathrm(iii)$ would represent a broad generalization of Kirchberg's celebrated $\mathcal{O}_\infty$ stability theorem for nuclear simple separable purely infinite C*-algebras. A lot of focus in the field, and at the workshop in particular, is aimed at resolving this conjecture, relating $\mathcal{Z}$-stability to topological and homological notions of finite-dimensionality for C*-algebras, and understanding how these notions may be used to delimit the universe of classifiable simple C*-algebras in a useful way. The conjecture was addressed directly in the talks by Lin and Winter. It has proven fruitful to revisit some of the classes of simple C*-algebras given as inductive limit of building blocks in the light of recently acquired insight, and indeed five of the talks (by Elliott, Gong, Niu, Robert and Strung) were drawing on knowledge from the initial stages of the Elliott program to shed light on these issues, and address key aspects of the central conjecture mentioned above.semigroup and comparison of open projections

Francesc Perera

Semigroup valued lower semicontinuous functions (with applications to theCuntz semigroup)

Discussion

Cuntz introduced his semigroup in 1978 to study traces and their generalizations, but only in recent years has it been realized that this object is a fruitful vessel also for classification theory. The semigroup is related to the K_0-group, but instead of recording the structure of finitely generated projective modules over a C*-algebra, it records the structure of its countably generated modules. Whereas it was recognized early that this object carried a lot of the information of the underlying C*-algebra, for many years it was thought that it would be too difficult to compute to be of theoretical or practical use in classification theory.The examples given by Villadsen, Rørdam and Toms have established that the classical invariants based on K-theory and traces, shown to be complete by Elliott in a multitude of important cases, do not suffice in general, and since the Cuntz semigroup was used to establish the existence of such examples in Toms's work there has been intense interest in understanding how to compute or describe it, and how to derive and improve known classification results using this object. A key result was obtained by Perera and Toms to the effect that when a C*-algebra is "nice" in the sense of being $\mathcal{Z}$-stable, then the Cuntz semigroup is determined by the non-stable K-theory and the trace space of the C*-algebra in question.Recently, a lot of work has gone into the analysis of the Cuntz semigroup of a C*-algebra of the form $\mathrm{C}(X, A)$ and talks both by Perera and Tikuisis reported on progress in this direction, in the first case obtained in joint work with Antoine and Santiago. Also, Ortega in his talk explored the possibilities for understanding or computing the Cuntz semigroup by means of the concept of open projections studied by Akemann and Pedersen.reas the classification theory for non-simple **stably finite** C*-algebras was developed in parallel with the simple case, and by use of more or less the same type of invariants, completely new ideas go into the case of non-simple **purely infinite** C*-algebras. The early breakthroughs of Kirchberg, who defined and employed ideal-related KK-theory to attack these types of problems, gave access to profound isomorphism results and complete classification for $\mathcal{O}_2$-stable nuclear C^*-algebras by means of their primitive ideal space, but is has been a great challenge to complement Kirchberg's theory by finding the K-theoretical invariants which lead to ideal-related KK-isomorphism in Kirchberg's sense. Asking that the ideal lattice be finite is natural in this context, but many fundamental questions remain open even for very small such lattices.Work of Meyer and Nest (outlined in Meyer's talk) represented the next big breakthrough in this area, and was the main suject of discussion in this particular section of the conference. Fixing a finite ideal lattice, Meyer and Nest provide a machinery for analyzing whether or not the family of K-groups associated to subquotients (along with the natural maps between them) allow the establishing of a universal coefficient theorem which may then in combination with Kirchberg's result lead to classification. Meyer and Nest proved that in the linear case, this is always the case, but also gave examples to show that for other ideal lattices, these invariants are not enough. As Meyer reported, Bentmann and Köhler have characterized precisely which spaces share this property with the linear case, and further studied Meyer and Nest's analysis which leads to positive results when one adds more groups to the invariant. Also, work by Arklint, Restorff, and Ruiz (reported in Arklint's talk) has demonstrated than in some cases where classification by the natural invariant is known to fail in general, one still gets a complete invariant in the real rank zero case.In a parallel effort, much recent work has gone into the classification theory for non-simple graph C^*-algebras. This well-studied class of C^*-algebras cuts across the traditional boundaries of classification theory in the non-simple case, since some simple subquotients may be AF and others purely infinite, but nevertheless work by Eilers and Tomforde showed that classification was possible also here, employing the Corona Factorization Property and ideas by Rørdam, refined in a paper by Eilers, Restorff, and Ruiz. The talks of Ruiz and Tomforde outlined recent progress in this area of research which apart from its applications to graph algebra theory seems to carry a lot of insight into the boundaries of non-simple classification theory away from the stably finite case. Also, the question of which invariants may be used in this special case were discussed in Arklint's talk in the context of the results outlined in the previous paragraph.The classification theory for non-simple C^*-algebras does not as yet come equipped with as precise range results as those which have been known for decades in the simple case. Most notably, the class of (non-Hausdorff) spaces which may occur as the primitive ideal space of a C^*-algebra remains unknown, but recent work reported at the workshop by Kirchberg has remedied the situation under the natural restriction of amenability. Also, Tomforde reported on range results in the context of the classification of graph C^*-algebras, obtained in joint work with Eilers, Katsura and West.On the one hand, operator algebras associated to dynamical systems have proved to be extremely important and challenging examples which have inspired much deep work and lead to beautiful results, and on the other hand, results and invariants obtained in the context of operator algebras have proved to be useful at the core of the theory of ergodic theory and dynamical systems.The backdrop for our workshop in this particular context was two very satisfactory, and in some sense final, results pointing mainly in the aforementioned direction. Firstly, the results by Toms and Winter (also mentioned above) had established (by an inventive reinterpretation of an idea of Putnam) that crossed products given by minimal $\mathbb{Z}$-actions on spaces with finite dimension were, in fact, classifiable by the Elliott invariant, by invoking many of the most important recent additions to classification theory: the nuclear dimension of Kirchberg, Winter, and Zacharias the theory of recursively subhomogeneous algebras of Phillips, the tracial rank zero classification by Lin, and the notion of $\mathcal{Z}$-stability. And secondly, the results by Giordano, Matui, Putnam, and Skau had finally established that any minimal $\mathbb{Z}^n$-action on a Cantor set was in fact strongly orbit equivalent to an action of $\mathbb{Z}$ (just as in the measurable case), thus reducing the classification of $\mathbb{Z}^n$-actions up to this equivalence relation, and the classification of the associated crossed products, to the fundamental case resolved by Giordano, Putnam, and Skau.With these long-standing open problems resolved, it is natural to break new ground and study to what extent the methods developed may carry over to higher generality. The talks of Matui and Phillips presented quite complete results on classifying actions on simple purely infinite C^*-algebras by $\mathbb{Z}^n$ and by finite groups, respectively, refining the notion of Rohlin property and leading to algebraic challenges related to those described in the previous section. Hirshberg presented joint work with Winter and Zacharias showing the preservation of the – for classification – key property of finite nuclear dimension under passage to certain crossed products. And Sierakowski described joint work with Rørdam explaining when thecrossed product of a C^*-algebra by an exact discrete group is purely infinite (simple or non-simple). There is some hope that these results may combine with classification theory for non-simple C^*-algebras as mentioned above.

General theory

Talks

Bruce Blackadar

On the work of Simon Wassermann

Ilijas Farah

Classification of C^*-algebras and descriptive set theory

Thierry Giordano

A generalization of the Voiculescu-Weyl-von Neumann theorem

Ian Putnam

Relative K-theory of some groupoid C^*-algebras

Iain Raeburn

C^*-algebras related to dilation matrices

Hannes Thiel

A characterization of semiprojectivity for commutative C^*-algebras

Simon Wassermann

Simple non-amenable C^*-algebras with no proper tensor factorisations

Stuart White

Near inclusions of C^*-algebras

Discussion

A number of talks were presented w hich in a multitude of ways stressed the interrelation between classification theory and other parts of operator algebras or indeed other areas of mathematics. An entire afternoon was committed to the celebration of Simon Wassermann's sixtieth birthday and his work of which the emphasis on tensor products and exactness has played an important role in the development of classification, as manifestly present in the idea of $\mathcal{Z}$-stability. Wassermann himself presented new results on the class of C^*-algebras which are prime in the sense that they can not be written as a tensor product of other C^*-algebras, and Blackadar gave an overview of Wassermann's work and its impact.In recent years, ties between operator algebras and descriptive set theory have been found and developed in the work of Akemann, Farah, and Weaver, and as an exciting development this venture has been taken into the realm of classification by work of Farah, Toms, and Törnquist. Farah reported on this in his talk.The notion of semiprojectivity, coined by Blackadar in 1985, has played an important role in classification theory and is known to hold for a large class of household C^*-algebras. However, much has been unclear regarding the exact boundaries of the class of semiprojective C^*-algebras until recently, when a number of questions have been resolved in the aftermath of a conference in Copenhagen. Thiel reported on his solution with Sørensen of the old problem of deciding precisely which spaces X give a semiprojective C^*-algebra $C(X)$.When two C^*-algebras A and B on the same Hilbert space are contained in each other up to a fixed error ϵ, must they then be the same or at least share properties as ϵ tends to zero? This is a classical question in C^*-algebra theory which has seen a renaissance recently by joint work of Christensen, Sinclair, Smith, White, and Winter. Although the final resolution of a main problem in this area reported on in White's talk does not use classification results, the use of classification theory (and in particular the Elliott intertwining argument) was instrumental in reaching these results.The talks of Putnam and Raeburn in different ways addressed the problem of applying methods from classification to understanding the structure of KMS states on certain C^*-algebras, and in Giordano's talk the question of finding "localized" versions of the classical Voiculescu-Weyl-von Neumann theorem by, e.g., specializing the targets was discussed.

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Chapter 35

Linking neural dynamics and coding: correlations, synchrony, and information (10w5102)

Oct 03 - Oct 08, 2010

Organizer(s): Eric Shea-Brown (University of Washington), Brent Doiron (University of Pittsburgh), Kresimir Josic (University of Houston), Nancy Kopell (Boston University), Andre Longtin (University of Ottawa), Alex Reyes (New York University)

Overview

Understanding the mechanisms by which the nervous system represents and processes information is a fundamental challenge for mathematical neuroscience. It has long been known that information is carried in the intensity of *individual* neurons' responses to stimuli. As a consequence, many mathematical tools have been developed to describe populations of statistically independent neurons. However, new experimental techniques show the prominence of correlations and synchrony in neural activity – and understanding whether and how these *collective* dynamics encode information has become a major challenge for mathematical neuroscience.

This question was the focus of our workshop. We brought together international experts working in network dynamics and network information theory to forge new connections between underlying biological mechanisms and their consequences. Thus, the week was spent seeking bridges among three mathematical disciplines: (1) dynamical systems, (2) statistical mechanics, and (3) probability and information theory. These three branches of the mathematical sciences coincide with three central sub-disciplines in theoretical neuroscience whose focus is the study of collective nervous system activity. The first two concern how correlations and synchrony develop through network interactions, and the third seeks to quantify their information-theoretic impact on the neural code:

1. **Dynamical systems and network oscillations:** Recurrently (feedforward-feedback) coupled networks of spiking neurons often show synchronous activity. Mathematical analysis has revealed the mechanisms by which asynchronous activity loses stability and synchronous population rhythms arise. These mechanisms – and the specific patterns of synchronous rhythms that emerge – depend on rich interactions between network structure, coupling type, and single-oscillator dynamics. Moreover, recent

research has shown that rhythms with distinct frequencies appear to interact. Unraveling the dynamical mechanisms of such interactions poses a new set of challenges that are only beginning to be addressed. How synchronous patterns are modified, created, and destroyed when networks are driven by external stimuli (e.g., sensory inputs) is another essential question that is being addressed using these mathematical tools.

2. **Statistical mechanics of network correlations:** Correlations can develop due to overlapping input in purely feedforward networks with irregular, stochastic activity. This is of particular importance for *layered* network architectures ubiquitous in neuroscience, where the propagation and amplification of correlated activity has been studied in systems ranging from cultured neural circuits to intact brains. Here, mathematical analysis seeks to quantify how correlated activity – modeled via multivariate point processes – is transferred among layers. This is a critical challenge; while it is evident from neural recordings that weak correlations are often present and presumably play an important part in normal brain function, excessive correlations are associated with neurological diseases, such as Parkinson's disease and epilepsy. Other current challenges focus on higher-order (beyond pairwise) correlations, and on how these correlation patterns depend on the spatiotemporal structure of stimuli.

3. **Information theory of network coding:** Neuroscience observations from high density electrode arrays are becoming more prevalent, posing the challenge of interpreting data recorded simultaneously from approximately 100 spatial locations. At the same time, results from information theory show that even weak correlations and synchrony can have strong effects on stimulus coding. However, whether these effects improve or degrade coding depends on the spatiotemporal structure of the collective activity. The primary challenge is to develop a systematic framework that predicts the impact of correlations in specific cases, and generalizes to allow an intuitive understanding of the underlying mechanisms of information encoding and decoding.

The experimental neuroscientists attending the workshop have been selected, in part, because of their collaborations with theorists. Their input was essential in guiding our discussion.
The question that unites these three areas is:

> **What are the information-theoretic consequences of the correlation and synchrony patterns that arise through the dynamics of prototypical neural circuits?**

Below, we report on progress toward the answer that was covered at our meeting.

Integration of graduate students and postdocs: A number of graduate students and postdoctoral fellows participated in the meeting. Nearly all of these participants also gave talks during the meeting. It is important to note that, while many of these students came from either side of the mathematics/neuroscience divide, they had no trouble in communicating their ideas to the diverse audience attending the workshop. All talks contained non-trivial mathematics, but presented in a way understandable to the participating experimentalists (admittedly, a selected group). We also observed, that while some of the presented research made use of fairly sophisticated mathematical ideas, all of it was well motivated by questions pertinent to neuroscientists.

Mathematical and scientific content of the meeting

The lectures and discussions at our meeting fell into four main themes:

1. Linking oscillations and signal processing

2. Correlations in specific circuit architectures
3. Defining useful metrics for encoding and decoding collective network dynamics
4. Linking feedforward and recurrent mechanisms for collective network activity

We next give a brief discussion of each, together with selected abstracts contributed by participants after the meeting that summarize the thrust of their talks (in some cases these were also edited by the organizers).

Linking oscillations and signal processing

There is increasing evidence that synchronous oscillatory activity is controlled by both stimulus characteristics and the specific context of the recordings, e.g. during sleep vs. tasks requiring attention. While the mechanisms that underly oscillatory activity in the brain are being uncovered, little is known about the impact that oscillations have on the processing of sensory inputs. An especially challenging, and fascinating, question is: how does the brain make use of coexistent, multi-frequency, interacting rhythms? Especially intriguing are opportunities to apply information theoretic metrics to network models on either side of the transition from asynchronous behavior to different patterns of synchronous oscillations, as one step toward linking oscillations and neural coding.

Jonathan Rubin: Rhythms in central pattern generators

Central pattern generators (CPGs) drive rhythmic movements such as respiration and locomotion. CPG outputs are rhythmic and repetitive, featuring multiple phases of activity with abrupt transitions between phases. Many different sets of intrinsic dynamics and connections between neurons can yield similar rhythms, yet these may involve different phase transition mechanisms. Although these transition mechanisms may not be discernible from direct examination of CPG output patterns, which mechanisms are present can have significant implications for CPG responses to external perturbations. In this talk, Rubin presented some theoretical analysis of this principle in an abstract, simplified rhythmic circuit. He subsequently illustrates the implications of transition mechanisms in several particular computational CPG models. In particular, analysis of transition mechanisms can be used to predict changes in respiratory phase durations in response to changes in particular external drives, to explain phase invariance of inspiration under hypercapnic conditions, and to explain differences between locomotor CPG rhythms with and without feedback from muscle afferents. More generally, transition mechanisms in CPG rhythms may play key roles in feedback control of CPG outputs.

Ryan Canolty: Role of patterns of oscillatory local field potential (LFP) phase coupling in regulating spiking activity

Hebb proposed that cell assemblies anatomically-dispersed but functionally integrated groups of neurons – are critical for effective perception, cognition, and action. However, evidence for brain mechanisms that coordinate multiple coactive assemblies remains lacking. Neuronal oscillations have been suggested as one possible mechanism for cell assembly coordination. In *Role of patterns of oscillatory local field potential (LFP) phase coupling in regulating spiking activity*, Ryan Canolty presented both experimental evidence and an associated dynamical model that investigate this issue.

Prior studies have shown that spike timing depends upon local field potential (LFP) phase proximal to the cell body, but few studies have examined the dependence of spiking on distal LFP phases in other brain areas far from the neuron, or the influence of LFP-LFP phase coupling between distal areas on spiking. Canolty and colleagues investigated these interactions by recording LFPs and single unit activity using multiple microelectrode arrays in several brain areas, and then used a probabilistic multivariate phase distribution to model the dependence of spike timing on the full pattern of proximal LFP phases, distal LFP phases, and LFP-LFP phase coupling between electrodes.

The results show that spiking activity in single neurons and neuronal ensembles depends on dynamic patterns of oscillatory phase coupling between multiple brain areas, in addition to the effects of proximal LFP phase. Neurons that prefer similar patterns of phase coupling exhibit similar changes in spike rates, while neurons with different preferences show divergent responses providing a basic mechanism to bind different neurons together into coordinated cell assemblies. Surprisingly, phase-coupling-based rate correlations are independent of inter-neuron distance. Phase-coupling preferences correlate with behavior and neural function, and remain stable over multiple days. These findings suggest that neuronal oscillations enable selective and dynamic control of distributed functional cell assemblies.

Chris Pack: Encoding of sensory stimuli by local field potentials in macaque visual cortex

Local field potentials (LFPs) are low-frequency fluctuations in electrical activity that are found throughout the brain. Because they correlate well with electroencephalography and fMRI BOLD signals, LFPs are critical to the study of brain function. In *Encoding of sensory stimuli by local field potentials in macaque visual cortex*, Christopher Pack presented experimental data from primate visual recordings suggesting a surprisingly strong link between the sensory tuning of low-frequency cortical LFPs and afferent inputs, with important implications for the interpretation of imaging studies and for models of cortical function.

Mark Kramer: Network oscillations in epilepsy, and beyond

During seizure, the aggregate voltage activity of neural populations often exhibits stereotypical rhythmic patterns, typically dominated by large amplitude voltage oscillations observable at the scalp or cortical surface. These rhythmic activities recorded from separate brain areas often exhibit correlations that also evolve in characteristic ways. In this *Network oscillations in epilepsy, and beyond*, Mark Kramer described correlation patterns observed in invasive voltage recordings from a population of human subjects with epilepsy. He showed that correlations increase at seizure onset and termination compared to pre-seizure intervals, suggesting the surprising result that macroscopic cortical areas decorrelate during the middle intervals of the seizure. Kramer also characterized other network properties during the seizure, including their coalescence and fragmentation. Finally, he applied these analyses to non-seizure recording intervals and to examine the common network structures that emerge.

Leslie Kay: Complementary functional and behavioral roles for olfactory beta and gamma oscillations

In *Complementary functional and behavioral roles for olfactory beta and gamma oscillations*, Leslie Kay presented a complementary view on the role of correlated dynamics on coding in olfactory discrimination tasks. Here, the correlations took the role of coordinated, rhythmic spiking across a neural population.

Moving beyond the anatomy or input wiring, Kay discussed a broad range of dynamic processes in the olfactory bulb, the first central and cortical stage of olfactory processing. She showed that olfactory bulb gamma oscillations (40-100 Hz oscillations of the local field potential), representing the precision of the underlying neural population, increase when rats learn to discriminate highly overlapping input patterns in a 2-alternative choice task. The mechanism for producing these oscillations is known to be the reciprocal dendrodendritic synapse between glutamatergic mitral cells and GABAergic granule cells.

Intriguingly, when rats were trained in a similar go/no-go task, gamma oscillations were not enhanced, and beta oscillations (20 Hz) instead predominated. These oscillations are not just a different frequency, but they rely on a different network. When centrifugal input to the olfactory bulb is ablated, gamma oscillations increase and beta oscillations disappear. However, the results are not quite as dichotomous as they might seem, because coherence patterns point to an underlying beta oscillation network in the distributed olfactory system in both tasks.

Correlations in specific circuit architectures

Given that subtle differences in spatiotemporal correlations can have a major impact on encoded information, networks that have even small differences in their architectures may encode stimuli in substantially different ways. A mechanistic theory that connects patterns of neural correlation to network architectures needs to be based on a small family of prototypical circuits. But which should be chosen to best represent signal encoding in the brain? Interaction with experimental neuroscientists such as Alex Reyes (NYU) on cortical circuits and Leonard Maler (U. Ottawa) on sensory circuits that have evolved for different information processing tasks framed many of our discussions of these topics.

Valentin Dragoi, Adam Kohn and Andreas Tolias: Correlated variability in laminar cortical circuits

Valentin Dragoi, Andreas Tolias and Adam Kohn, all researchers working with multi-electrode recordings in primates, gave a joint presentation about the impact of correlated variability in cortical circuits. This is a topic of much current interest. These participants are in the forefront of the field, and each has contributed fundamental results.

All participants agreed that the amount of information encoded by cortical circuits depends critically on the capacity of nearby neurons to exhibit correlations in their responses. Despite the fact that strong trial-by-trial correlated variability in response strength has been reported in many cortical areas, Andreas Tolias suggested that neuronal correlations may be much lower than previously thought. He started with the observation that many cortical areas are organized into functional columns, in which neurons are believed to be densely connected and share common input. Many numerous studies report a high degree of correlated variability between nearby cells. He described the work of his group on the development of chronically implanted multi-tetrode arrays offering unprecedented recording quality to re-examine this question in primary visual cortex of awake macaques. They found that even nearby neurons with similar orientation tuning show virtually no correlated variability. These findings suggest a refinement of current models of cortical microcircuit architecture and function: either adjacent neurons share only a few percent of their inputs or, alternatively, their activity is actively decorrelated.

In response Valentin Dragoi presented his work with laminar probes to revisit the issue of correlated variability in primary visual cortical (V1) circuits. Dragoi found that correlations between neurons depend strongly on local network context - whereas neurons in the input (granular) layer of V1 showed virtually no correlated variability, neurons in the output layers (supragranular and infragranular) exhibited strong response correlations. He showed how to use a linear decoder to demonstrate that, contrary to expectation that the output cortical layers would encode stimulus information most accurately, the input network encodes more information and offers superior discrimination performance compared to the output networks. He noted that laminar dependence of spike count correlations is consistent with recurrent models in which neurons in the middle (granular) layer receive intracortical inputs mainly from nearby cells, whereas neurons in superficial (supragranular) and deep (infragranular) layers receive inputs over larger cortical distances.

Similarly, Adam Kohn reviewed the mounting evidence that suggests that determining how neuronal populations encode information and perform computations will require understanding correlations between neurons, as well as the stimulus and behavioral conditions that modify them. His lab is taking advantage of the recent advent in recording techniques such as multielectrode arrays and two-photon imaging has made it easier to measure correlations, opening the door to detailed exploration of their properties and contributions to cortical processing. He noted a number of participants at the workshop reported discrepant findings, providing a confusing picture about the level and import of correlations in neuronal networks. He reviewed a selection of these studies and presented simulations to explore the influence of several experimental and physiological factors that affect the measurement of correlations. Differences in response strength, the time window over which spikes are counted, internal states, and spike sorting conventions can all dramatically affect measured correlations and systematically bias estimates. He concluded by offering guidelines for measuring and interpreting correlation data.

Marlene Cohen: A link between gains, correlations, and behavior

Attention allows observers to focus on a small subset of a cluttered scene and improves perception of attended locations or features. Both spatial and feature attention multiplicatively scale the firing rates of sensory neurons: typically, attending to a location that is close to a neurons spatial receptive field or to a feature that matches its stimulus preference increases sensory responses. We also showed previously that spatial attention tends to decrease correlations between the trial-to-trial fluctuations in the responses of nearby neurons (Cohen and Maunsell, 2009; see also Mitchell et al, 2009). To directly compare the effects of feature and spatial attention on neuronal populations, we recorded simultaneously from dozens of V4 neurons in both hemispheres while animals performed a change detection task in which we varied spatial and feature attention. We found that like spatial attention, feature attention modulates both firing rates and correlations. We found a strong inverse relationship between modulation of rate and correlation for both types of attention: when gains are increased, correlations decrease. While spatial attention increases the firing rates of most neurons, feature attention can either increase or decrease firing rates, depending on the similarity between a neurons tuning and the attended feature. There is an inverse relationship between rate and correlation modulation for cells whose gains decreased as well: feature attention increases the correlations between these neurons. Furthermore, on behavioral trials in which the animal made an error, the correlation structure looks like the correlation structure in the opposite feature and spatial attention condition, suggesting that the animal made an error because attention was misallocated. Together, our results suggest that a single mechanism accounts for the changes in firing rates and spike count correlation caused by any type of attention.

Bruno Averbeck: Dopamine, dynamics and information in the basal ganglia

Bruno Averbeck is a researcher at the NIH, and described a problem related to the work of other meeting participants, but of significant importance in medical research: Dopamine depletion in cortical-basal ganglia circuits in Parkinsons disease (PD) grossly disturbs movement and cognition. Classic models relate Parkinsonian dysfunction to changes in firing rates of basal ganglia neurons. Taking both inappropriate firing rates and other dynamics into account, and determining how changes in the properties of these neural circuits that occur during PD impact on information coding, is thus important.

Averbeck described *in vivo* network dynamics in the external globus pallidus (GPe) of rats before and after chronic dopamine depletion. He showed that dopamine depletion leads to decreases in the firing rates of GPe neurons and increases in synchronized network oscillations in the beta frequency (13-30 Hz) band. Using logistic regression models he showed the combined and separate impacts of these factors on network entropy, a measure of the upper bound of information coding capacity. Importantly, changes in these features in dopamine-depleted rats lead to a significant decrease in GPe network entropy. Changes in firing rates have the largest impact on entropy, with changes in synchrony also decreasing entropy at the network level. Changes in autocorrelations tended to off-set these effects as auto-correlations decreased entropy more in the control animals. Thus, it is possible that reduced information coding capacity within basal ganglia networks may contribute to the behavioral deficits accompanying PD.

Complementary to the GPe work his group also examined GPe, STN interactions by analyzing neurons recorded simultaneously from these nucleiin dopamine lesioned and healthy control rats. Both nuclei display a pronounced increase of beta frequency (20 Hz) oscillations in the lesioned state. Additionally, analyses of the information transfer between nuclei show that the transfer was significantly increased in the lesioned state. Furthermore, the temporal profile of the information transfer matches well the known neurochemistry of the nuclei, being inhibitory from the GPe to the STN and excitatory from the STN to the GPe and the dynamics of this interaction match well previously published estimates of the dynamics seen in Parkinsons patients.

Overall, these results showed that data analysis inspired by deep mathematical concepts can be used to provide evidence of specific changes in the functional connectivity between basal ganglia nuclei in the dopamine lesioned state.

Jeremie Lefebvre: Driven networks of ON and OFF cells with recurrent feedback

The origin of gamma oscillations in sensory networks continues to attract a lot of attention. Such oscillations are known to occur in the electrosensory system when stimuli have a large spatial extent. These past studies have modeled this phenomenon using a population of ON cells receiving spatio-temporal noise as its input, and with delayed feedback in its network topology. Jeremie Lefebvre presented results on how the presence of ON and OFF cells embedded in such a delayed feedback network influences the genesis of gamma oscillations. He illustrated the responses of neural populations to spatio-temporal forcing, mimicking those found in most sensory systems. ON pyramidal cells received sensory inputs directly, while OFF cells received a mirror image of the stimuli via an interneuron, inverting their response. The connectivity was determined solely by global inhibitory recurrent connections. Using a combination of neural field theory and numerical simulations, he showed that input-induced Andronov-Hopf bifurcations can occur; the stability of oscillations is determined by the spatial features of the input. He also showed how the network can double the frequency of an input in its firing activity. This is a consequence of rectification in the feedback network. He finally showed how adaptation can enhance gamma oscillations in such circuits.

Alex Pouget and Jeff Beck: Insights from a simple expression for linear Fisher information in a recurrently connected population of spiking neurons / Neural basis of perceptual basis

Alex Pouget and Jeff Beck presented joint talks. First, in *Insights from a simple expression for linear Fisher information in a recurrently connected population of spiking neurons*, they gave a simple expression for a lower bound of Fisher information for a network of recurrently connected spiking neurons which have been driven to a noise-perturbed steady state. This lower bound is called linear Fisher information, as it corresponds to the Fisher information thatcan be recovered by a locally optimal linear estimator. Unlike recent similar calculations, the approach used here includes the effects of non-linear gain functions and correlated input noise, and yields a surprisingly simple and intuitive expression that allows for substantial insight into the sources of information degradation across successive layers of a neural network. Here, this expression is used to (1) compute the optimal (i.e., information maximizing) firing rate of a neuron, (2) demonstrate why sharpening tuning curves by either thresholding or via the action of recurrent connectivity is generally a bad idea, (3) show how a single cortical expansion is sufficient to instantiate a redundant population code which can propagate across multiple cortical layers with minimal information loss, and (4) show that optimal recurrent connectivity strongly depends upon the covariance structure of the inputs to the network.

Next, these results found application in *Neural basis of perceptual basis*. The motivation was from cognitive neuroscience: extensive training on simple tasks results in large improvements in performance, a form of learning known as perceptual learning. Previous neural models have argued that perceptual learning is the result of sharpening and amplification of tuning curves in early visual areas. However, these models are at odds with the conclusions of psychophysical experiments manipulating external noise, which argue for improved decision making, presumably in later visual areas. Here, Pouget and Beck explore the possibility that perceptual learning for fine orientation discrimination is due to improved probabilistic inference in early visual areas. This mechanism captures both the changes in response properties observed in early visual areas and the changes in performance observed in psychophysical experiments. The modeling also suggests that sharpening and amplification of tuning curves may play only a minor role in improving performance, in comparison to the role played by the reshaping of inter-neuronal correlations.

Maurice Chacron Neural variability and contrast coding by correlations

Understanding how populations of neurons encode sensory information is of critical importance. Correlations between the activities of neurons are ubiquitous in the central nervous system and, although their implications for encoding and decoding of sensory information has been the subject of arduous debates, there is a general consensus that their effects can be significant. As such, there is great interest in understanding how correlated activity can be regulated. Recent experimental evidence has shown that correlated activity amongst pyramidal cells within the electrosensory lateral line lobe (ELL) of weakly electric fish can be regulated based on the behavioral context: these cells modulate their correlated activity depending on whether the fish is performing electrolocation or communication tasks without changing the mean firing rate of their response. Moreover, it was shown in the same study that the changes in correlated activity were correlated with changes in bursting dynamics. In this work we explore the role of intrinsic bursting dynamics on the correlated activity of ELL pyramidal neurons. We use a combination of mathematical modeling as well as in vivo and in vitro electrophysiology to show that bursting dynamics can significantly alter the ability of neuronal populations to be correlated by common input. In particular, our model predicts that the ratio of output to input correlations (i.e. the correlation susceptibility) is largely independent of stimulus amplitude when neurons are in the tonic firing model. In contrast, we find that the correlation susceptibility increases with stimulus amplitude when the neurons are in the bursting mode. We then performed in vivo and in vitro experiments to verify this prediction. Our results show that intrinsic dynamics have important consequences on correlated activity and have further revealed a potential coding mechanism for stimulus amplitude through correlated activity.

Michael Graupner Correlations in the auditory cortex during spontaneous activity

Spiking correlations between neurons have been found in many regions of the cortex and under multiple experimental conditions. Despite their importance consequences for neural population coding, the origin and the magnitude of such correlations remain a highly debated issue. Potential sources of correlations include shared presynaptic input. However, theoretical investigations have shown that shared inputs do not necessarily lead to correlations. Instead, active decorrelation occurs provided that the neurons are tightly coupled in a balanced configuration of excitation and inhibition. In support of these results, recent experiments measure virtually no correlations. However, those findings are in contrast to a large body of prevalent results suggesting strong correlations. We examine to which extent spontaneously active cortical networks meet the conditions of a balanced, decorrelated activity regime.

To investigate synaptic input, membrane potential and spike-output correlations between pairs of neurons, we perform simultaneous whole-cell recordings from pairs of pyramidal neurons in thalamocortical slices from young mice (P14-18).

We find correlated excitatory as well as inhibitory input to pairs of cortical cells during spontaneous activity. Interestingly, excitatory and inhibitory inputs are anticorrelated leading to cancellation of correlations at intermediate membrane potentials. We furthermore measure weak spike-count correlations between neurons (0.01). Together, our results show that nearby (100 m) cortical neurons receive correlated synaptic input. However, spiking correlations are suppressed due to negative correlations between excitatory and inhibitory inputs. Our results suggest that cortical networks are structured to actively suppress correlations and thereby increase their information coding capacities.

Defining useful metrics for encoding and decoding collective network dynamics

The standard metrics used to asses encoding of sensory information in spike trains are Fisher and Mutual Information. The former quantifies the accuracy with which sensory stimuli can be estimated from (stochastic) patterns of spikes, and the latter measures the reduction in uncertainty about a stimulus from observations of the response. These metrics can be made mathematically precise yet often assume system optimality, and are not necessarily motivated by the biophysical constraints present in the brain. They also require the specification of the neural 'response', a matter of much debate among experimentalists and theorists. Using mechanistic models of neural response will prompt a principled exploration of these areas, specifically of how correlations shape the neural code. An issue of special focus is models that address emerging large datasets from many simultaneously recorded neurons.

Andrea Barreiro: When are microcircuits well-modeled by pairwise maximum entropy methods?

The conference theme was that collective activity is widespread in the nervous system and has important implications for functionality. When can we represent such activity by lower dimensional models, and how does our ability to do so depend on basic circuit properties such as input statistics, internal dynamics and network connectivity – such as the descriptions in wide use at the conference, where only pairwise spike correlations were considered? In *When are microcircuits well-modeled by pairwise maximum entropy methods?*, Andrea Barreiro took some first steps toward answering this question by studying the ability of maximum entropy models to characterize the spiking activity of networks modeled on retinal circuitry.

She first considered systems of N=3 spiking cells, driven by a common fluctuating input against independent background noise. She probed this circuit over a wide variety of operating regimes and input correlation structures, assessing the efficacy of the PME model by calculating the KL-divergence between the observed and PME distributions. Using a novel visualization method she showed that bimodal inputs generate spiking distributions that break the PME. Barreiro gave an analytical justification of these findings: in the small parameter describing the strength of common inputs to the circuit, D_{KL} is at least an order (often more) smaller for unimodal vs. bimodal inputs. This persists for larger N.

Barreiro then constructed a biophysical model constrained by intracellular recordings of primate parasol RGCs. She exposed a triplet of such cells to stimuli at a wide variety of spatial and temporal scales. Even in the presence of highly correlated inputs, and significant cell-to-cell heterogeneity (induced by blocky spatial patterns of comparable size to the cell receptive fields), spiking outputs are well fit by the PME model. This surprising result explains previous experimental results, and leads to predictions for stimuli and RGC classes that will lead produce departures from PME responses. Preliminary results indicate that the feedforward structure of these circuits is highly significant in achieving the above results; introducing recurrence into this circuit can increase higher-order correlations by a factor of 20.

Liam Paninski: Coding and Computation by Neural Ensembles in the Primate Retina

The neural coding problem — deciding which stimuli will cause a given neuron to spike, and with what probability — is a fundamental question in systems neuroscience. We apply statistical modeling methods to analyze data recorded from a complete mosaic of macaque parasol retinal ganglion cells in a small region of visual space. We find that a surprisingly simple model with functional coupling between neurons captures both the stimulus dependence and the detailed spatiotemporal correlation structure of multi-neuronal responses; in addition, ongoing network activity in the retina accounts for a significant portion of the trial-to-trial variability in a neuron's response. We assess the significance of correlated spiking by performing optimal Bayesian decoding of the population spike responses. Finally, we discuss work in progress on the following questions: how much temporal precision is necessary to capture the neural code in the retina? How can we adapt our optimal decoding methods to estimate behaviorally relevant signals such as image velocity? How do we perceive stable images when the retina must contend with the constant motion due to small random eye movements? Finally, what can statistical spike-train analysis methods tell us about the underlying circuitry of the retina?

Jean-Philippe Thivierge: The Creative Nature of Neurons: How Heterogeneous Networks Provide a Rich Repertoire of Brain Activity

The brain is a creative organ it never responds to the same sounds and sights in exactly the same way twice. Jean-Philippe Thivierge's work on modeling brain responses across time sheds new light on the origins of this variability. Neurons of the brain are heterogeneous, meaning that they each possess slightly different characteristics that make them unique. According to his new theory, this property gives rise to a rich repertoire of possible brain states, and prevents the brain from getting ?stuck? in certain patterns of activity. Despite this wealth of possible states, neurons can also fine tune their interactions in order to reproduce rhythmic patterns beyond their time of presentation. He argued how this may explain the formation of short-term perceptual memories, as well as persistent rhythms of activity in neuropathological conditions. This presentation elicited a lot of questions about the interplay of fine tuning and network heterogeneity.

Don Katz: Modeling the impact of attention on coherent cortical ensembles: decreasing temporal coding variability by increasing noise

In interpreting neural activity, it is often assumed that information available in single-neuron responses is of primary importance: many theoretical models of population function take as their input highly preprocessed characterizations of single-neuron responses (i. e., response magnitudes, collapsed across trials and post-stimulus time), and many discussions of between-neuron correlations center on the concern that any overlap in the information available in each of two single-neuron responses reduces the information available in the population (i. e., "redundancy").

In *Modeling the impact of attention on coherent cortical ensembles: decreasing temporal coding variability by increasing noise*, Don Katz presented an alternative view. His group approaches the population coding of taste from a different angle, restricting our analysis to simultaneously-recorded ensembles of neurons and characterizing activity in single trials, without averaging across within- or between-trial timescales. The data is interpreted the information available in single neurons only in light of a primary population-level characterization, rather than vice-versa, and thus a clearer picture of the true dynamics of the system in action may be appreciated. Specifically, he observes cortical and amygdalar ensembles progressing through a sequence of coherent, nonlinear (attractor-like) firing-rate transitions; the sequences are reliable and stimulus-specific, but the timing of these transitions is highly variable from trial to trial–that is, much of the seeming "correlated noise" in the single-neuron responses reflect important aspects of the population dynamics. We argue that averaging single-neuron activity across time (and collapsing neurons that were collected non-simultaneously into single ensembles) obscures critical aspects of the population dynamics.

Ila Fiete: Beyond classical population coding for nearly exact estimation in the brain

The brain represents and transforms external variables to perform computations and achieve goals. Representation and transformation are inherently noisy when performed by neurons. One way to extract a less noisy estimate of the encoded variable is by averaging over large neural populations. Classical population codes, as seen in the sensory and motor peripheries, lead to only modest (polynomial, or N) improvements in inverse squared error with increasing neuron number (N).

In *Beyond classical population coding for nearly exact estimation in the brain*, Ila Fiete explored an intriguing alternative. She showed that the entorhinal grid cell code for animal location is in a qualitatively different performance class than classical population codes. It allows unprecedented accuracy, enabling nearly exact removal of noise from noisy neural representations, with inverse squared error that improves exponentially ($\sim e^{aN}$ for some $a > 0$) with population size. The noise removal is enabled by the peculiar structure of the grid code, and does not rely on the existence of external cues. Moreover, a simple neural network model, similar to the hippocampus, can decode the grid represenation to take advantage of its error-control properties. This raises the possibility that the grid code is not unique, and that the brain could contain numerous examples of strong error-correcting codes for computing with analog variables.

Tatyana Sharpee: Maximally informative irregularities in neural circuits.

In *Maximally informative irregularities in neural circuits* Tatyana Sharpee explored the possibility that irregularities in neural circuits serve a useful computational function. To answer this question she and her colleagues focused on the retina, a well-studied circuit where many aspects of its average organization were previously found to be in good agreement with optimization principles. Previous experimental work has demonstrated the presence of fine scale irregularities in the shapes of individual receptive fields. Sharpee found that, in the presence of lattice irregularities, the irregular receptive field shapes increase the spatial resolution from 60% to 92% of that possible for a perfect lattice. Optimization of receptive field boundaries around their fixed center positions reproduced experimental observations on a neuron-by-neuron basis. These results suggest that lattice irregularities determine the shapes of retinal receptive fields and similar algorithms may improve the performance of the retinal prosthetics where substantial irregularities arise at their interface with the neural tissue. Taken more broadly, the results contribute to the emerging theme that irregularities in the organization of the nervous system are key to achieving its near optimal performance.

John Beggs: Information flow in networks of cortical neurons

John Beggs addressed the problem of information flow in networks of cortical neurons. Understanding this question would help us see how the brain integrates information across its different parts – a fundamental problem in neuroscience. Beggs noted that the average pyramidal neuron in cortex makes and receives approximately 7,000 synaptic contacts, suggesting that local cortical networks are connected in a fairly equal manner. The pattern of information flow in such networks, however, is poorly understood and can not be inferred from anatomy alone. Theory indicates that an unequal distribution of flows can actually contribute to network efficiency and robustness.

Beggs' group sought to examine the distribution of information flow in recordings from cortical slice cultures ($n = 6$) and monkey motor cortex ($n = 1$) containing 100 ± 25 identified neurons. They used transfer entropy to quantify information flow, as validation tests revealed that this measure could reliably distinguish true from spurious flows in a variety of realistic conditions. Beggs showed that information flow was distributed significantly more unevenly in the networks extracted from the data than in random control networks. This was evident in the distribution of information flow strengths, the distribution of total information flow into and out of each neuron, and in the distribution of connections with significant information flow per neuron. Simulations indicated the observed cortical information flow networks were significantly more efficient in routing signals, could form significantly more combinations among inputs per node, and were significantly more robust than random control networks. This is the first study of information flow in local cortical networks.

Beggs ended with an intriguing conclusion: The highly unequal distribution of information flow among cortical neurons contributes to the efficiency and robustness of information processing in cortex.

Ruben Moreno Bote: Weak synchrony in networks with finite input information

Neurons in cortex are correlated, but the functional role of these correlations remains elusive. It has been proposed that neuronal networks work in the so-called asynchronous state where correlations between pairs of neurons become vanishingly small for large networks. In such networks, the dynamics effectively decorrelates neurons firing, a process which is thought to improve coding because the percentage of input information conveyed by the output of the network increases with network size. However, these studies tacitly assume that the input information also increases without bounds with the network size, which is unrealistic. In contrast, we analyzed the dynamics of neuronal networks with finite input information. We find that with finite input information, and dominant inhibition, neuronal networks of integrate-and-fire neurons spontaneously settle down in a state of weak but not vanishingly weak- correlations, despite the dense connectivity, and despite the strong shared noise induced by the finite input information constraint. Moreover, and quite surprisingly, the finite information conveyed by the inputs is completely recoverable from the output spike counts of the network. We also show that excitation-dominated networks generate strong correlations but still preserve the input information in the output spike counts. In other words, whether the network decorrelates or not, there is no change in the amount of information transmitted. This challenges the notion that decorrelation is a universal mechanism for improving the quality of neural code. Moreover, given the relatively small correlation values observed in cortex, we propose that cortical networks are in a weakly synchronous state where inhibition dominates over excitation.

Linking feedforward and recurrent mechanisms for collective network activity

Feedforward and recurrent networks both generate correlated activity. However, the mechanisms by which this is achieved are distinct. Real neural circuitry has aspects of both architectures, and it

remains to be understood how the development of correlation in mixed feedforward and recurrent networks occurs. A fundamental piece of this puzzle is understanding the genesis of neural correlations in simple pairs of cells with different intrinsic dynamics; the meeting featured several discussions of this unresolved issue as well.

Duane Nykamp: When feedforward intuition deceives: the influence of connectivity motifs on synchronization in recurrent networks

The synchronizability of a network captures how network structure can influence the tendency for a network to synchronize, independent of the dynamical model for each node. I demonstrate a synchronizability analysis that takes advantage of the framework of second order networks, which defines four second order connectivity statistics based on the relative frequency of two-edge network motifs. This analysis allows one to parametrically vary the amount of common input in a recurrent network in order to analyze the intuition from feedforward networks that common input is an important source of correlations and synchrony. In contrast to this intuition, the analysis determines that common input has little influence on synchrony in recurrent networks. Instead, the frequency of two-edge chains in the network plays a critical role, as synchrony increases dramatically with these chains. This dependence of synchrony on chains and not common input holds for a wide variety of neuron models.

Ashok Kumar: Shaping magnitude and timescale of correlations with state dependent synaptic input

Spike trains produced by sensory neurons often exhibit correlations that vary depending on neural state and stimulus properties. However, the circuit mechanisms responsible for changing the degree and timescale of pairwise correlated activity remain elusive. In contrast, many well-studied biophysical mechanisms have been shown to modulate single neuron response properties, such as firing rate gain. If these single neuron properties also shape correlations, then mechanisms of single neuron modulation may explain the shifts in correlation observed in sensory systems. We first study this possibility with simplified neuron models receiving varying levels of balanced, conductance-based synaptic input. This input modulates single neuron gain by changing membrane potential variability and conductance, and we show how this mechanism also shapes the timescale of correlation of neuron pairs. Next, we model and analyze data from the electrosensory system of weakly electric fish, in which recruitment of slow inhibitory feedback yields a reduction in single neuron transfer of low-frequency stimuli. We show that this effect also leads to a reduction in long timescale correlations between pairs of electrosensory neurons. These two studies demonstrate that modulatory synaptic input to neuron pairs can differentially shape precise spike time synchrony and average spike rate correlations. The results have consequences for state-dependent processing and propagation of neural activity.

Robert Rosenbaum: Using simplified integrate-and-fire models to understand how correlations propagate in neuronal networks

Robert Rosenbaum, a mathematics graduate student at the University of Houston, presented his work on the use of simplified integrate-and-fire models to understand how correlations propagate in neuronal networks. He observed that overlapping afferent populations and correlations between presynaptic spike trains can introduce correlations between the inputs to downstream cells. While in several other talks about the impact of correlations, participants have considered more detailed models, or larger networks, Robert described how simplified models can help us develop an intuitive and mechanistic description of the dominant mechanisms that control how correlations propagate. He showed several new results that proved that the degree to which input correlations are preserved is strongly modulated by cellular dynamics and also by synaptic variability. Both of these factors are frequently ignored in computational studies. He also demonstrated that correlations within an afferent population are significantly amplified by synaptic convergence. This amplification of correlations is the primary mechanism responsible for the synchronization of feedforward chains, a simple observation that did not seem to be widely known.

Bard Ermentrout: Correlation transfer by heterogeneous oscillators

Neurons are heterogeneous in many ways and this affects how they respond to inputs. In particular, identical inputs going into heterogeneous neurons will produce different outputs. There are many sources of heterogeneity including different channel distributions, different mean firing rates, and different noisy synaptic inputs. By considering the neurons as oscillators, we can write down equations for the phase of the oscillators as a function of the inputs. Using correlated white noise inputs, it is possible to compute the phases for a pair of heterogenous oscillators. The variance of these and the covariance allows us to compute the output correlation as a function of the input correlation. We derive formulae for the spike-count correlation for short windows (near synchrony) and find that neural oscillators that have a phase-resetting curve which has a nearly zero mean will maximize the transfer of correlation. For long time windows, the flatter is the PRC, the better the transfer of correlation. We combine these results with numerics to complete the picture of correlation transfer in long and short windows. We close by providing analytic approximations for the phase differences between two oscillators that have different frequencies and or differently shaped PRCs.

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Chapter 36

New Perspectives in Univariate and Multivariate Orthogonal Polynomials (10w5061)

Oct 10 - Oct 15, 2010

Organizer(s): Plamen Iliev (Georgia Institute of Technology), Edward Saff (Vanderbilt University), Tom Bloom (University of Toronto), Jeffrey Geronimo (Georgia Institute of Technology), Doron Lubinsky (Georgia Institute of Technology)

Overview of the Field

Given a finite positive measure μ on the real line, with infinitely many points in its support, we can define orthonormal polynomials $\{p_n\}_{n=0}^{\infty}$ satisfying, for all $m, n \geq 0$,

$$\int p_n p_m d\mu = \delta_{mn}.$$

Here

$$p_n(x) = \gamma_n x^n + ..., \gamma_n > 0,$$

is a polynomial of degree n, with positive leading coefficient γ_n. The $\{p_n\}$ may be generated by the Gram-Schmidt process, applied to the monomials $1, x, x^2, ...$ with inner product

$$(f, g) = \int fg \, d\mu.$$

Orthonormal polynomials have been the subject of investigation for over 150 years. They have applications in areas ranging from statistical physics to combinatorics to signal processing. There are obvious links to special functions and harmonic and numerical analysis.

The notion of an orthogonal polynomial has been greatly generalized in recent decades. While the extension to measures on the plane is obvious, multivariate analogues already present the problem of how to order monomials in higher dimensions. Then there are important generalizations to the case where a single orthogonality relation is replaced by one involving more than one measure, or more than one polynomial.

Active intrinsic topics of study include analytic and algebraic aspects, and asymptotics. Applications to areas like random matrices and numerical analysis have given new insight into orthogonal polynomials, and their generalizations. Some key references are [14], [16], [18], [26], [39], [40], [41], [43].

Topics Covered by the Workshop

Measures on the Real Line

A classical result of Szegő asserts that when μ is an absolutely continuous measure supported on $[-1,1]$, with

$$\int_{-1}^{1} \frac{\log \mu'(x)}{\sqrt{1-x^2}} dx > -\infty,$$

then

$$\lim_{n\to\infty} \frac{p_n(z)}{\left(z+\sqrt{z^2-1}\right)^n} = D(z),$$

uniformly for z in closed subsets of $\mathbb{C}\setminus[-1,1]$. Here $z+\sqrt{z^2-1}$ is the conformal map of $\mathbb{C}\setminus[-1,1]$ onto $\mathbb{C}\setminus\{z : |z| \leq 1\}$, and $D(z)$ is the Szegő function for μ. The case where $[-1,1]$ is replaced by finitely many intervals was considered by Harold Widom in a celebrated paper [45]. The case of infinitely many intervals (and more general sets of homogeneous type) was considered more recently by Peherstorffer, Sodin, and Yuditskii. At the workshop, Jacob Christiansen presented asymptotics, and related conjectures, for the case where the support is still more general than a set of homogeneous type.

Lilian Manwah Wong discussed the problem of adding point masses to a given measure on the real line, and comparing the asymptotics of the new orthogonal polynomials, and related quantities, to those for the original measure. Christian Remling discussed reflectionless measures, with applications to extensions of the Denisov-Rakhmanov Theorem relating recurrence coefficients of orthogonal polynomials, and the support of the measure. Vilmos Totik presented new methods for establishing asymptotics for Christoffel functions on the real line (which also work over arcs in the plane), and consequences in approximation theory. Avram Sidi presented asymptotics for coefficients in Legendre expansions, and related quadrature errors, when the underlying functions have certain types of singularities.

Sasha Aptekarev showed how to use sophisticated analysis of recurrence relations, to derive specific types of Plancherel-Rotach asymptotics for discrete orthogonal polynomials such as Meixner polynomials. As a consequence, the local behavior of the reproducing kernels is obtained. Mourad Ismail discussed the J-Matrix method introduced in the 70's to study the spectrum on Schrödinger operators in physics. It is a tridiagonalization technique and Ismail [19] discussed how to make the technique rigorous and apply it to study orthogonal polynomials.

Orthogonal Relations in the Complex Plane

Weighted Bergman polynomials involve an orthogonality relation against an area measure, rather than an arc. Let G be a bounded simply-connected domain in the complex plane $\mathbb{C}$, whose boundary is a Jordan curve, let w be a function positive on G, and define $\{p_n\}$ by the Hermitian relation

$$\int_G p_n(z)\overline{p_m(z)}w(z)\,dA(z) = \delta_{mn},$$

where A stands for area measure. The classical Bergman case is the unweighted case $w = 1$. There are many unresolved questions concerning the behavior of the polynomials and their zeros, for example, when the boundary of G is not a smooth curve. Laurent Baratchart presented asymptotics for $\{p_n\}$ when G is the unit disk when weak assumptions are made about w, involving its behavior on the circle $|z| = r$ as $r \to 1-$. Erwin Miña-Diaz considered the case where G is the disk, and $w = |h|^2$, for some polynomial h.

Nikos Stylianopoulos discussed the case $w = 1$, for domains with piecewise analytic boundary - but without cusps. An especially interesting case with cusps is the hypocycloid. Nikos presented joint work with Ed Saff for this region, showing how certain Hessenberg matrices approach Toeplitz matrices associated with Faber polynomials. He also presented a very interesting application to the Arnoldi process for numerical calculation of orthogonal polynomials, showing its stability in comparison to the classical Gram-Schmidt process. A further conclusion is that ”finite term” recurrence relations for Bergman polynomials do not hold, except in the essentially ”trivial” case where the region is bounded by an ellipse. Thus for most regions, the associated Hessenberg matrices are not banded.

There is a close connection between Padé approximation and orthogonal polynomials. Let $f(z)$ be a function admitting an expansion about ∞ in negative powers of z:

$$f(z)=\sum_{j=1}^{\infty} f_j z^{-j}$$

The $(n-1,n)$ Padé approximant to f is a rational function π_n of type $(n-1,n)$ satisfying, as $z\to\infty$,

$$f(z)-\pi_n(z)=O\left(z^{-2n}\right).$$

In the case where f is a Markov function, the denominator polynomial in π_n is an orthogonal polynomial. In the general case, the denominator still satisfies a non-Hermitian orthogonality relation, arising from the matching condition. Maxim Yattselev presented asymptotics for the Padé approximants associated with certain types of elliptic functions,

$$f(z)=\frac{1}{i\pi}\int_{\Delta}\frac{h(t)}{t-z}\frac{dt}{\sqrt{(t-a_0)(t-a_1)(t-a_2)(t-a_3)}_+}.$$

Here Δ is a collection of three arcs joining the point a_0 to the non-collinear points a_1, a_2, a_3, taken to have minimal capacity, and h satisfies a suitable Dini condition. Riemann-Hilbert techniques are used to obtain the asymptotics.

Of course, Padé approximants are a special type of rational approximation. Vasiliy Prokhorov discussed results on best rational approximation, derived via elaborations and extensions of the Adamjov-Arov-Krein theory.

Potential Theory in One and More Variables

The link between polynomials and potentials is easily seen from the relation

$$\frac{1}{n}\log\left|\prod_{j=1}^{n}(z-z_j)\right|=\int\log|z-t|\,d\nu(t), \tag{36.1}$$

where ν places mass $\frac{1}{n}$ at each of the z_j. The function

$$U^{\nu}(z)=\int\log|z-t|^{-1}\,d\nu(t)$$

is the potential associated with the measure ν.

Joe Ullman was a pioneer in using potential theory to analyze asymptotics of orthogonal polynomials for compactly supported measures. It was Hrushikesh Mhaskar, Evgenii Rakhmanov, and Ed Saff who developed its use for the case of measures with non-compact support, and for varying measures [36]. Thus if $d\mu(x)=e^{-x^2}dx$ is the Hermite weight, one looks for a probability measure ν with compact support, such that

$$U^{\nu}(x)=-x^2+\text{constant},\ x\in\text{supp}[\nu].$$

More generally, if the field x^2 is replaced by $Q(x)$, one replaces x^2 by $Q(x)$ in this last identity. The measure ν is called an equilibrium measure for the external field Q. The support of Q, and the properties of ν, are crucial in analyzing orthogonal polynomials. At the conference, Benko and Dragnev gave new conditions for convexity of ν' using an elaboration of the iterated balayage algorithm, which they call ping pong balayage.

Another powerful application of potential theory was given by Igor Pritsker. He derived discrepancy estimates, in the spirit of the Erd́os-Turán theorem, but instead involving discrete energies. As a consequence a classic problem of means of zeros of integer polynomials was analyzed, and surprising restrictions were given for growth of integer polynomials in the disk.

Potential theory in the multivariate case is far more challenging than the univariate case. There is no longer such a simple relationship between polynomials and potentials like (1). A fascinating account of recent developments was given by Norman Levenberg [25]. He showed how the complex Monge-Ampere operator arises in both weighted and non-weighted multivariate potential theory. Concepts of weighted transfinite diameter, and Fekete points, and L_2 approximations to equilibrium measures were discussed. Using deep recent results of Berman and Boucksom [3], [4] from a more abstract setting, it was shown that appropriate discrete approximations to equilibrium measures converge weakly, as the number of points grows to infinity. In particular, this is the case for Fekete points.

Tom Bloom showed how the same tools of pluripotential theory can be applied to discuss large deviations for random matrices, and give alternative tools and insights to those typically used in the theory of random matrices.

Universality Limits and Riemann-Hilbert Problems

It was the physicist Eugene Wigner who in the 1950's first used eigenvalues of random matrices to model the interactions of neutrons for heavy nuclei. One classical setting can be described as follows: let $\mathcal{M}(n)$ denote the space of n by n Hermitian matrices $M = (m_{ij})_{1\leq i,j\leq n}$. Consider a probability distribution on $\mathcal{M}(n)$,

$$P^{(n)}(M) = cw(M)\left(\prod\nolimits_{j=1}^{n} dm_{jj}\right)\left(\prod\nolimits_{j<k} d(Re\, m_{jk})\, d(Im m_{jk})\right).$$

Here $w(M)$ is a function defined on $\mathcal{M}(n)$, and c is a normalizing constant. One important case is $w(M) = \exp(-2n \text{ tr } Q(M))$, involving the trace tr, for appropriate functions Q defined on $\mathcal{M}(n)$. In particular, the choice $Q(M) = M^2$, leads to the Gaussian unitary ensemble, apart from scaling, that was considered by Wigner. One may identify $P^{(n)}$ above with a probability density on the eigenvalues $x_1 \leq x_2 \leq ... \leq x_n$ of M,

$$P^{(n)}(x_1, x_2, ..., x_n) = c\left(\prod_{j=1}^{m} w(x_j)\right)\left(\prod\nolimits_{i<j}(x_i - x_j)^2\right).$$

See [10, p. 102 ff.]. Again, c is a normalizing constant.

It is at this stage that orthogonal polynomials arise [10]. Let μ and $\{p_n\}$ be as above. The nth normalized reproducing kernel for μ is

$$\widetilde{K}_n(x,y) = \mu'(x)^{1/2}\mu'(y)^{1/2}\sum_{j=0}^{n-1} p_j(x)\, p_j(y).$$

When $\mu'(x) = e^{-2nQ(x)}dx$, there is the basic formula for the probability distribution $P^{(n)}$ [10, p.112]:

$$P^{(n)}(x_1, x_2, ..., x_n) = \frac{1}{n!}\det\left(\tilde{K}_n(x_i, x_j)\right)_{1\leq i,j\leq n}.$$

One may use this to compute a host of statistical quantities - for example the $m-$point correlation function for $M(n)$ [10, p. 112]:

$$\begin{aligned} R_m(x_1, x_2, .., x_m) &= \frac{n!}{(n-m)!}\int ... \int P^{(n)}(x_1, x_2, ..., x_n)\, dx_{m+1}\, dx_{m+2} ... dx_n \\ &= \det\left(\tilde{K}_n(x_i, x_j)\right)_{1\leq i,j\leq m}. \end{aligned}$$

The *universality limit in the bulk* asserts that for fixed $m \geq 2$, and ξ in the interior of the support of $\{\mu\}$, and real $a_1, a_2, ..., a_m$, we have

$$\begin{aligned} &\lim_{n\to\infty} \frac{1}{\tilde{K}_n(\xi,\xi)^m} R_m\left(\xi + \frac{a_1}{\tilde{K}_n(\xi,\xi)}, \xi + \frac{a_2}{\tilde{K}_n(\xi,\xi)}, ..., \xi + \frac{a_m}{\tilde{K}_n(\xi,\xi)}\right) \\ = \ & \det\left(\frac{\sin\pi(a_i - a_j)}{\pi(a_i - a_j)}\right)_{1\leq i,j\leq m}. \end{aligned}$$

Of course, when $a_i = a_j$, we interpret $\frac{\sin\pi(a_i-a_j)}{\pi(a_i-a_j)}$ as 1. Because m is fixed in this limit, this reduces to the case $m = 2$, namely

$$\lim_{n\to\infty} \frac{\tilde{K}_n\left(\xi + \frac{a}{\tilde{K}_n(\xi,\xi)}, \xi + \frac{b}{\tilde{K}_n(\xi,\xi)}\right)}{\tilde{K}_n(\xi,\xi)} = \frac{\sin\pi(a-b)}{\pi(a-b)}. \tag{36.2}$$

There are a variety of methods to establish (2). The deepest methods are the Riemann-Hilbert methods, which yield far more than universality [10], [11]. The whole topic of universality limits was dramatically advanced by Riemann-Hilbert experts, and they also communicated the topic to others, including those using more classical techniques to analyze orthogonal polynomials. We note that there are several settings, other than that described above, for universality limits for random matrices [42].

How general is (2), that is what restrictions are need on μ? Here is a

Conjecture
Let μ be a measure with compact support. Then for a.e. $\xi \in \{\mu' > 0\}$, we have (2).

Here, of course, $\{\mu' > 0\} = \{\xi : \mu'(\xi) > 0\}$. The most general pointwise result to date towards this conjecture is due to Vili Totik [44]. He showed that if μ is a regular (in the sense of Ullman, Stahl, and Totik) measure with compact support, and (c, d) is an interval such that

$$\int_c^d \log\mu' > -\infty,$$

then, indeed, (2) holds for a.e. $\xi \in (c, d)$. Barry Simon established a similar result when the support has finitely many intervals. Another recent development, presented by Doron Lubinsky at the workshop [28], is that without local or global regularity, universality holds in measure.

One cannot in general expect that universality with the sinc kernel holds at points where $\mu'(x) = 0$. For example, at the edges of the support of μ, when the support consists of finitely many intervals, one instead obtains the Bessel kernel. At interior points where μ' has a jump discontinuity, Martinez et al discovered that one obtains a new, non-classical kernel. This suggests that universality with the since kernel is associated with points where μ' exists and is positive. A very interesting result of Breuer, presented for the first time at the Banff conference, was that there are measures μ with support $[-1, 1]$, that are purely singularly continuous, and yet universality with the sinc kernel holds at each point of $(-1, 1)$. This surprising result is obtained by sparsely perturbing the recursion relation of classical Chebyshev polynomials.

Of course universality goes way beyond measures with compact support, or even varying measures. This was powerfully illustrated by the talk of Arno Kuijlaars. In modelling the Brownian motion of particles that start at time $t = 0$ from a finite number of given points, and end at time $t = 1$ at a finite number of points, while following non-intersecting paths, one is led to mixed type multiple orthogonal polynomials. In analyzing the asymptotics of these, one use Riemann-Hilbert problems of larger size, such as 4×4 matrices for the case of two start and end points. In contrast, classical orthogonal polynomials require only 2×2 matrices. Kuijlaars illustrated the depth of techniques required for the analysis, and the new universality phenomena that arise, often described using solutions of Painlevé equations.

Sobolev Orthogonal Polynomials

Sobolev orthogonal polynomials are polynomials whose orthogonality relation involves derivatives. Thus we might search for polynomials $\{p_n\}$ that satisfy, for example,

$$\int p_n(x)\,p_m(x)\,d\mu(x) + \int p_n'(x)\,p_m'(x)\,d\nu(x) = \delta_{mn},$$

where μ and ν are positive measures. Higher derivatives could also be involved. They arise in a number of applications, and have received substantial attention in recent decades [1], [30]. An obvious question is how the measures μ and ν interact. In many standard cases, the dominant term is provided by the derivative term, and p_n' behaves roughly like an orthogonal polynomial for the measure ν. In other cases, however, there is interaction between the two terms.

At the workshop, Paco Marcellan considered the case when μ has unbounded support, while ν is a Dirac delta, or sum thereof. Issues such as zeros, asymptotics, comparison to the compact case were considered. A multivariate version of these was discussed by Miguel Pinar, with the derivative being replaced by a gradient.

Multiple Orthogonal Polynomials

Given measures $\{\mu_j\}_{j=1}^p$ on the real line, and a p-tuple of integers $(n_1, n_2, ..., n_p)$, the type II multiple orthogonal polynomial P is a monic polynomial of degree $n_1 + n_2 + ... + n_p$ such that for $j = 1, 2, ..., p$, and $0 \leq k \leq n_j - 1$,

$$\int P(x)\,x^k d\mu_j(x) = 0.$$

The dual type I polynomials $A_1, A_2, ..., A_p$ are determined by the conditions

$$\int x^k \left(\sum_{j=1}^{p} A_j d\mu_j(x) \right) = 0,$$

for $0 \leq k \leq n_1 + n_2 + ... + n_p - 2$, with degree$(A_j) \leq n_j - 1$.

Multiple orthogonal polynomials have connections to rational approximation in the complex plane, to diophantine approximation in number theory, and to random matrix ensembles. Bill Lopez presented powerful results on Nikishin systems for two intervals, finding probability measures, and associated multiple orthogonal polynomials that satisfy a recurrence relation of order 4. Walter Van Assche showed how potential theory, Riemann-Hilbert (and other) methods can be used to analyze asymptotics of multiple orthogonal polynomials. Arno Kuijlaars exhibited the use of multiple orthogonal polynomials in non-intersecting Brownian motions.

Multivariate polynomials

From the orthogonality relation it follows that any family of orthogonal polynomials on the real line satisfies a three term recurrence relation:

$$a_n p_{n+1}(x) + b_n p_n(x) + a_{n-1} p_{n-1}(x) = x p_n(x).$$

The classical orthogonal polynomials (Jacobi, Hermite, Laguerre, Bessel) which appear in numerous applications in mathematics and physics are characterized by the fact that they are eigenfunctions of a differential operator, which is independent of the degree n. In other words the classical orthogonal polynomials are characterized by a bispectral problem [13] since they satisfy a second-order difference equation in the degree variable n and a differential equation in the variable x. The construction of bispectral orthogonal polynomials in higher dimensions brought different new tools from combinatorics, representation theory and integrable systems into this old classical area.

Orthogonal polynomials associated with root systems

One possible extension of the above theory to orthogonal polynomials of more than one variable is related to the theory of symmetric functions and the corresponding Macdonald-Koornwinder polynomials [29, 22]. These polynomials were introduced as the unique eigenfunctions of certain remarkable commuting symmetric difference operators. Each family depends on a root system and several free parameters. Special cases lead to classical families of symmetric functions such as Schur functions and characters of corresponding Lie groups, Hall-Littlewood functions, Jack polynomials, or more generally, the multivariate Jacobi polynomials due to Heckman and Opdam [17]. The bispectrality in this case is closely related to the Macdonald conjectures which were established with the theory of double affine Hecke algebras [8]. Recently, there has been a major development in this field leading to biorthogonal elliptic functions generalizing Macdonald-Koorwinder polynomials [33]. In particular, one needs to work with generalized eigenvalue problems which require several new techniques. The latest progress in this beautiful theory was described by Eric Rains who outlined the main ingredients of the construction and the crucial properties. Tom Koornwinder studied the nonsymmetric Askey-Wilson polynomials as vector-valued polynomials. As a particular new result made possible by this approach he obtained positive definiteness of the inner product in the orthogonality relations, under certain constraints on the parameters.

Orthogonal polynomials in $\mathbb{R}^d$

Yuan Xu discussed a discrete Fourier analysis on the fundamental domain of A_d lattice that tiles the Euclidean space by translation [27]. In particular, Chebyshev polynomials can be defined using symmetric and antisymmetric sums of exponentials. One of the interesting outcomes of this theory is the construction of Gaussian cubatures, which exist very rarely in higher dimension.

Bispectral properties of orthogonal polynomials within the usual framework [14] of orthogonal polynomials in $\mathbb{R}^d$ attracted a lot of attention recently. Interesting examples of such polynomials go back to the multivariate Hahn and Krawtchouk polynomials in the pioneering works of Karlin and McGregor [20] and Milch [31] related to growth birth and death processes. A probabilistic model that involves cumulative Bernoulli trials led Hoare and Rahman to a new family of 2D Krawtchouk polynomials. In his talk, Mizan Rahman derived a 5-term recurrence relation, thus showing that these polynomials possess the bispectral property. He also indicated possible extensions to 3 or more variables. Paul Terwilliger explained how the recurrence formulas for the same polynomials can be derived using the Lie algebra $\mathfrak{sl}_3$. George Gasper considered general methods for the derivation of second-order partial difference equations. Alberto Grünbaum illustrated with examples the interaction between orthogonal polynomials and random walks. Plamen Iliev discussed a new characterization of the commutative algebras of ordinary differential operators that have orthogonal polynomials as eigenfunctions, which leads to multivariate extensions. Luc Vinet showed that the d-orthogonal Charlier and Hermite polynomials appear naturally as matrix elements of nonunitary transformations corresponding to automorphisms of the Heisenberg-Weyl algebra, thus establishing duality, recurrence, and difference equations.

Greg Knese described recent results [21] on polynomials orthogonal on the bi and poly circle and their relation to bounded analytic functions on the polydisk. Important in this work is a Christoffel-Darboux like formula which in the bivariate case can be related to stable polynomials, Bernstein-Szeǵo measures and gives a new proof of Ando's celebrated theorem in operator theory. Geronimo [6] discussed a new proof of Gasper's theorem on the positivity of sums of triple products on Jacobi polynomials. This theorem plays an important role in setting up a convolution structure for Jacobi polynomials. The new techniques are based on a correlation operator which was discovered by Carlen, Carvahlo, and Loss in their solution of the spectral gap problem in the Kac model. The correlation operator is an operator on the N-sphere looking for its eigenfunction expansion in various angular momentum sectors leads to Gasper's Theorem and to the Koornwinder-Schwartz product formulas for the biangle This is an extension of Gasper's theorem to the bivariate case.

Connections with integrable systems and algebraic geometry

One of the landmarks in the modern theory of integrable systems is the work of Sato-Sato [37] which assigns a solution to the Kadomtsev-Petviashvili (KP) hierarchy to each point of a certain infinite dimensional Grassmannian. The construction uses the so called τ-function, which defines a Baker-Akhiezer function via the formula:

$$\psi(t,z) = \frac{\tau(t_1 - \frac{1}{z}, t_2 - \frac{1}{2z^2}, \dots)}{\tau(t)} \exp\left(\sum_{k=1}^{\infty} t_k z^k\right),$$

where $t = (t_1, t_2, \dots)$ are the KP flows. Important examples of τ-functions are the Schur functions, the Riemann θ-function (appropriately evaluated and multiplied by a quadratic exponential factor in the time variables) and the partition function of the two-dimensional gravity [23, 38, 46]. John Harnad reviewed this construction with an emphasis on the algebro-geometric solutions of Krichever [24]. He discussed the subtle question of determining the Plücker coordinates appearing in the expansion of the τ-function as an infinite linear combination of Schur functions.

An interesting link between Krichever's work and the polynomials associated with root systems was discovered in [7], by constructing a mutivariate Baker-Akhiezer function for specific values of the free parameters in the Macdonald-Koornwinder operators. In particular, this approach can be used to prove the bispectrality uniformly for all root systems as well as for certain deformations where other techniques (e.g. Hecke algebras) do not seem to be applicable. Oleg Chalykh explained the main ingredients of this connection and derived new orthogonality relations for the Baker-Akhiezer functions.

Outcome of the Meeting

The conference led to several unusual interactions: between researchers in the abstract special function side, and those on the analysis side; between those studying orthogonal polynomials of a single variable, and those studying many variables; between those studying multivariate polynomials from a real angle, and those studying from a multivariate complex angle; and between those applying potential theory in one variable, and practitioners of the multivariate theory. In addition, there were numerous interactions within individual topics.

Several recent doctorates expressed the belief that their research horizons expanded. Participants agreed that they learnt a lot about the broader field. This was especially the case for univariate researchers, who learnt a lot about multivariate potential theory, and the general multivariate settings.

Participants

Aptekarev, Alexander (Keldysh Institute Applied Mathematics)
Baratchart, Laurent (INRIA-Sophia-Antipolis)
Benko, David (University of South Alabama)
Bloom, Tom (University of Toronto)
Breuer, Jonathan (Hebrew University of Jerusalem)
Chalykh, Oleg (University of Leeds)
Christiansen, Jacob (University of Copenhagen)
Dragnev, Peter (Indiana-Purdue)
Gasper, George (Northwestern University)
Geronimo, Jeffrey (Georgia Institute of Technology)
Grunbaum, F. Alberto (University of California Berkeley)
Hardin, Douglas (Vanderbilt University)
Harnad, John (Concordia University and Centre de Recherche Mathematique)

Iliev, Plamen (Georgia Institute of Technology)
Ismail, Mourad (City University of Hong Kong and King Saud University)
Knese, Gregory (University of California at Irvine)
Koornwinder, Tom (KdV Institute for Mathematics, University of Amsterdam)
Kuijlaars, Arno (Katholieke Universiteit Leuven)
Levenberg, Norm (Indiana University)
Levin, Eli (Open University of Israel)
Lubinsky, Doron (Georgia Institute of Technology)
Marcellan, Francisco (Universidad Carlos III de Madrid)
Mina-Diaz, Erwin (University of Mississippi)
Pinar, Miguel (Universidad de Granada)
Pritsker, Igor (Oklahoma State University)
Prokhorov, Vasiliy (University of South Alabama)
Rahman, Mizan (Carleton University)
Rains, Eric (California Institute of Technology)
Remling, Christian (University of Oklahoma)
Saff, Edward (Vanderbilt University)
Sidi, Avram (Technion-Israel Institute of Technology)
Stylianopoulos, Nikos (University of Cyprus)
Terwilliger, Paul (University of Wisconsin)
Totik, Vilmos (University of Szeged and University of South Florida)
Van Assche, Walter (Katholieke Universiteit Leuven)
Vinet, Luc (Universite de Montreal)
Wang, Xiang-Sheng (York University)
Wong, Manwah (Georgia Tech)
Xu, Yuan (University of Oregon)
Yattselev, Maxim (University of Oregon)

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Chapter 37

Front propagation in heterogeneous media: mathematical, numerical, and statistical issues in modelling a forest fire front (10w5077)

Oct 17 - Oct 22, 2010

Organizer(s): Chris Bose (University of Victoria) Anne Bourlioux (Universite de Montreal) John (Willard) Braun (University of Western Ontario)

Overview of the Field

The main objective of this workshop was to bring together applied mathematicians, statisticians, and forest fire researchers and managers to discuss key issues relating to numerical algorithms, physical modelling and mathematical/statistical analysis relevant to the simulation of a propagating forest fire front.

Numerical Algorithms

The most popular wildfire spread simulators used in Canada and the United States are PROMETHEUS (Tymstra, 2005) and FARSITE (Finney, 2004). Both of these simulators are based on a marker method solution of a Lagrangian form of partial differential equations which describe the evolving fire front (for example, Richards, 1990). The principal difference between the two simulators lies in the manner in which the input parameters are determined. Inputs are derived from fuel type (i.e. type, density and characteristics of vegetation), weather (wind speed and direction, relative humidity, temperature, and precipitation), and topography (i.e. elevation, slope and aspect). In Canada, an empirical modelling approach (based on observations on a large inventory of experimental and well-documented wildfires) has been employed in order to relate the partial differential equation parameters to these inputs, while in the United States, a physical process approach (based on extensive laboratory experimentation) has been employed. Remarkably (or perhaps because of the robustness of the equation solutions), the two approaches often yield similar results.

However, because of the highly spatially heterogeneous nature of the media through which wildfires often burn, there is potential for much less smoothness than postulated by the original equations of Richards. Thus, there are a number of numerical issues that have arisen in association with this marker solution. Most notable among these issues is the frequent production of tangles in the numerical modelled fire front. Among the solutions that have been proposed in the past is a turning point algorithm. Unfortunately, such solutions have not always been successful in removing complicated tangles. Furthermore, these algorithms add to the computational complexity of the algorithm and slow the simulator down. Thus, there has been a perceived need for improved methods for handling tangles.

Another issue is the need for stochasticity. Prometheus and Farsite are deterministic, but fire managers would benefit from burn probability maps, since there is much uncertainty associated with the outcome of a given fire ignition. Many of the current methods for generating such maps rely on repeated runs of the deterministic simulator on randomized weather streams. An example is Burn-P3 (Parisien et al., 2005) which is based on Prometheus. In order for burn probability maps to be produced in real time, there is a need for improvements in the computational speed of the solution algorithm.

Modelling Issues

Forest wildfire behaviour is strongly related to weather conditions, particularly wind. Some progress has been achieved in including qualitative predictions of micro-weather conditions but there is much left to be done in formulating fully coupled models. Particularly challenging is the issue of how to include small-scale intermittent effects on the effective propagation of the front, even if one limits oneself to the class of models considered in this workshop where the fire is represented as an infinitesimally thin interface.

Another challenging modelling issue is formulation of a probabilistic model to describe the process by which a fire can “jump” over an obstacle or can be ignited by firebrands at remote locations ahead of the front, so-called fire-spotting.

Mathematical/Statistical Issues

Even though the phenomenon being modelled is that of a deterministic spread, for all practical purposes, the significant small scales fluctuations in the various parameters affecting the burning rate lead to a very noisy process and very noisy predictions, best interpreted in a probabilistic sense. Statisticians approach this by relying on stochastic process models, such as cellular automata.

On the other hand, applied mathematicians have formulated idealized advection-reaction-diffusion models to analyse the effective propagation of fronts in heterogeneous or even random media as needed in turbulent combustion for instance (although the models typically considered would not apply to the type of solid, immobile fuel we are talking about here).

Presentation Highlights

Many of the issues discussed in the overview were reviewed and discussed in the initial presentations given by Mark Finney, John Braun, Robert Bryce and Chris Bose. Finney reviewed the history of fire growth modelling, while Braun and Bryce focussed their attention on the Prometheus fire growth model.

Finney’s talk also included an extensive discussion of the fire risk assessment modelling program being carried out in the United States. Assessments are being done at various scales from the level of a single project to the level of the entire nation. Finney reaffirmed the generally held belief that weather is the principal driver behind the uncertainty in fire behaviour, and by randomizing weather streams, one can generate realistic burn probability maps using deterministic simulators. Thus, FARSITE is used to study the problem of a single fire under a single weather scenario, FSPro is used to study the risk due to a single fire under an all-weather scenario, FlamMap is used to study large-scale fire risk under a single weather scenario, and FSim is used for large scale fire risk under an all-weather scenario. Because of the importance of the weather, some time was devoted to the problem of generating realistic weather scenarios, recognizing that only about 20-30 years of high quality weather data is available across the United States. The current approach is to use linear methods to model and simulate a fire moisture code. Even with this relatively simple method, Finney observed that the methods yield a “pretty good correlation” between fires by size class with simulated fires by size class, thus concluding that the resulting burn probability maps are reasonably realistic.

Braun’s description of Prometheus was designed so that mathematicians and statisticians could see precisely how weather, fuel and topographic data are assimilated. The latter part of his talk focussed on some of the shortcomings of the modelling approach used and described how forecast uncertainty, diurnal variation in wind speed and rate of spread variability are not properly accounted for.

Robert Bryce, the chief Prometheus programmer, gave an overview of recent developments in the Prometheus simulator, highlighting the implementation of a new untangler. Chris Bose described the new untangler in detail in his presentation. The theoretical basis for this untangler lies in a two-colour theorem, and the resulting algorithm has proved to be much faster while at the same time handling more artifacts correctly compared to previously implemented untanglers.

Burn Probability Mapping and Stochastic Models

David Martell discussed the production of burn probability maps from a fire management perspective. Accurate maps will facilitate best practices in the scheduling of timber harvesting. Part of his presentation focussed on a case study based in northeastern Ontario for which a contagion type fire spread model was coupled with climate and historic ignition data to predict burn probabilities.

Kerry Anderson continued the theme of producing burn probability maps. Anderson considered multiple time scales as well as multiple spatial scales in his treatment of the problem. Satellite data was combined with Environment Canada weather data to calibrate a simple model for fire spread which was then applied to ensembles of simulated weather series. Validation studies indicated some issues for the short-range and medium-range model, but the long-range model appears to be reasonably accurate.

Jonathan Lee described a case study conducted in the Muskoka District in which Burn-P3 was used to obtain a burn probability map. Model assessment was undertaken by comparing the fire size distribution in the simulations with the historic fire size distribution. Part of this study involved field work in which it was found that substantial portions of the most recent fuel map were inaccurate.

Reg Kulperger presented an interacting particle system model for fire spread as an alternative to the more popular deterministic front propagation methods. The advantages of interacting model is that it is stochastic and it is raster based. The latter characteristic leads to realizations which do not have tangles.

Hao Yu discussed parallel computing approaches to fire spread modelling. This approach may be necessary to reduce the amount of time required to do repeated simulations in fire risk assessment studies.

Rob Deardon applied an Ising-type model to some particular fire burn patterns using Bayesian MCMC methods. The models have previously been successfully applied to the spread of infectious disease and this led naturally to the question of whether the spread of fire follows an analogous mechanism.

Fluid Dynamics, Eulerian and Reaction-Diffusion-Advection Approaches

Mary Ann Jenkins discussed her work with large eddy simulators, focussing on the behaviour of fire as it travels up hill under variable winds. A particular challenge for this type of modelling is the wide multi-scale nature of the process, with length scales ranging from millimeters (detailed combustion processes) to kilometers (weather inputs).

Alexandre Desfosses-Foucault described the level-set approach to the fire front propagation problem. This approach has several theoretical and computational advantages over the marker approach, largely avoiding the issues connected with tangling.

Thomas Hillen discussed existence and uniqueness of travelling wave solutions to semi-physical combustion models for wind driven fires. In some specific situations, rather surprisingly, there can exist multiple (slow and fast) propagation fronts.

Anne Bourlioux discussed the use of *homogenization* in the modelling of front propagation in heterogeneous environments (such as patchy fuel loads) and the effects of wind gustiness on the rate of spread of fire.

Petro Babak derived a probabilistic model for fire propagation using coupled parabolic differential equations (containing the diffusion, advection and reaction components) together with an ordinary differential equation (which specifies the cumulative probability distribution of the fire). The advantage of this kind of approach is that confidence bands for the fire perimeter can be derived without resorting to lengthy simulations.

Jonathan Martin discussed the problem of fire-spotting, by deriving the landing distribution, given the lofting height distribution for burning firebrands. He considered several special cases.

Statistical Approaches: Fire Weather Index and Ignitions

Sylvia Esterby discussed statistical models for the Forest Fire Weather Index (FWI) which gives a numeric rating of fire intensity. The focus was on British Columbia data, and the objective was to model the index temporally, taking into account spatial location. This theme was followed up later by Lengyi Han, who described some time series models for the FWI.

Doug Woolford discussed models for wildfire ignitions in Ontario, taking into account possible effects due to climate change.

Ed Johnson presented his work on process models for moisture in the duff layer and the effects of fire on soil erosion.

The Banff Prescribed Burn Program

Ian Pengelly (Parks Canada) gave a presentation on prescribed burns which highlighted the unpredictability of fire, and how prescribed burns can sometimes run out of control. Of particular interest was his description of a fire which spread surprisingly fast under winter conditions.

Following his presentation, Pengelly led the group on a bus tour of prescribed burns in Banff National Park and described the FireSmart program followed in the park. This experience occurred early on in the week and provided participants with an opportunity to see firsthand the effects of wildfire on surface and canopy fuels.

Poster Session

A number of posters were presented on one of the evenings. Sean Michaletz, a graduate student in ecology at the University of Calgary, presented some of his work on process models for tree mortality. Lengyi Han, a graduate student at the University of Western Ontario, presented work on a new empirical model for the rate of spread in jack pine fuels, and showed how the estimated variance of the error for this model could be used to model the uncertainty in the input parameters in a deterministic simulator such as Prometheus. Jonathan Lee, also of Western, provided more details on his risk assessment of the Muskoka District based on Burn-P3.

Open Problems

Although much progress has been made in the numerical and statistical modelling of fire fronts, a large number of issues remain unresolved. The problem of fire-spotting remains largely unsolved. Certain aspects of the problem have been addressed as discussed in the presentations of Mary Anne Jenkins and Jonathan Martin. However, much work remains to be done: spotting frequency distributions are completely unknown, and lofting height distributions are still not well understood.

The problem of ignition prediction plays a key role in fire risk assessment. For this purpose, basic stochastic models are now available. For the purpose of predicting particular fire flaps, there are currently no adequate models.

Extinguishment also remains a largely unsolved problem. When will a fire stop spreading? Under certain weather conditions and when fire suppression activities are effective, a fire will be extinguished, but a completely specified model for extinguishment remains to be developed.

Roundtable

Thursday afternoon was devoted to a roundtable discussion for all participants. The session began with a review of the somewhat different needs and perspectives of the (roughly) two groups of scientists represented at the meeting.

Fire Scientists (mostly industry and government scientists):

NEEDS	RESOURCES
access to students	scientific expertise and experience
new methods of solution	a historical context
	data/brains
	choice of relevant problems
	critique of mathematical approaches
	database of historical fire size/shape
	avenue for real fire experience for students/researchers
	ability to host academic visitors
	Modus hot spot data
	infrared image library

Mathematical and Statistical Scientists (mostly university academics):

NEEDS	RESOURCES
access to fire scientists	student manpower
real data	expertise and novel techniques
relevant problems	knowledge of useful approaches from other modelling fields
critique of approaches	model validation
broader prespective (ecosystem, water etc)	willingness to solve toy problems requiring new approaches
spotting data	
knowledge of sources of data	
lines of communication on the subject	
participation in experiments (students and researchers)	

The participants observed that there appear to exist many opportunities to match needs and resources between the two groups. Some specific ideas were:

- joint publications
- co-supervision of HQP
- research collaboration
- MITACS/NSERC internships

- joint conferences

There also appear to be opportunities for NSERC Industrial postdoc and MITACS internship placements at CFS and other government labs. These need an academic and industrial supervisor in collaboration.

Promising new directions for research

The original PROMETHEUS development committee proposed a large number of projects – only some of these have been addressed to date. A (partial) list of topics still needing attention was collected:

- spotting experiments
- improved spread algorithms
- incorporating spotting into spread (models?)
- incorporation of realistic diurnal weather data
- models of extinguishment
- FBP fuel parameters
- spatial weather (wind!) modelling at many scales.
- suppression models
- operations research
- resource management approaches
- fire occurrence prediction
- ignition models (physical or semi-physical)

It was observed that some of these items are already under consideration by various groups in the fire modelling community (for example, see the Open Problems section above)

There was a general discussion about the process by which mathematical ideas and models become developed and accepted by the fire scientists, and if possible, implemented in the field (the latter is of course a serious but realistic challenge). It was felt that one mechanism to encourage this would be to get mathematical scientists (and/or their students) into the field to meet the managers, firefighters and if possible observe real fires. There are obvious administrative barriers to this (safety, security. . .).

Further observations on spotting: there is very little data from large-scale experimental burns and not likely to be more in the near future. Lofting data from wind tunnel experiments may continue to appear, and detailed studies of ignition processes could be done. Both of these would be aimed at understanding sub-processes in the spotting model.

Realistic Coupled Wind models: A simulation was presented at the workshop based on a real fire. Video images from the real fire are available on You Tube. The presenter pointed out that while the fire was lit in calm conditions, there was considerable wind involvement once the fire got started. This points to the large effect that thermally generated ’wind’ contributes. This needs to be incorporated into realistic models.

Data Gathering Exercises known to be ongoing:

- Modus hotspot data. (NOAA data also)
- Weather Data
- Fire size/shape data

Upcoming Meetings/SummerSchools:

- Fire and Forest Meteorology New Mexico FAll 2011 (AMS)
- Wildland Fire Canada 2012, Calgary (Tymstra and McAlpine)
- Western Region Fire Research Ctr (UofA)(Mike Flannigan head)

Conclusions

As had been proposed, the workshop did bring together a wide range of perspectives on forest fire modelling. It attracted participants from both government and academia, the latter including graduate students and postdoctoral researchers. Both mathematical and statistical approaches to a range of common problems were treated in depth during the workshop and both theoretical and applied aspects were represented. The conference was attended by Canadian and US Fire Scientists, some of whom had not had a chance to interact before.

Participants

Anderson, Kerry (Natural Resources Canada)
Babak, Petro (University of Alberta)
Bose, Chris (University of Victoria)
Bourlioux, Anne (Université de Montréal)
Braun, John (Willard) (University of Western Ontario)
Bryce, Robert (Brandon University)
Dean, Charmaine (University of Western Ontario)
Deardon, Rob (Guelph)
Desfosses Foucault, Alexandre (Université de Montréal)
El-Shaarawi, Abdel (Canada Centre for Inland Waters)
Esterby, Sylvia (University of British Columbia Okanagan)
Finney, Mark (USDA Forest Service - Missoula)
Francis, Michael (University of Victoria)
Han, Lengyi (University of Western Ontario)
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Chapter 38

Control and Optimization with Differential-Algebraic Constraints (10w5029)

Oct 24 - Oct 29, 2010

Organizer(s): Stephen Campbell (North Carolina State University), Larry Biegler (Carnegie Mellon), Volker Mehrmann (Technische Universität Berlin)

Overview of the Field

Differential Algebraic Equations (DAEs) are mixed systems of differential and algebraic equations. It has been recognized for some time now that they have great potential both theoretically and in applications. DAEs form one of the most elegant and simple ways to model a physical system because they allow for the creation of separate models for subcomponents that can then be pasted together via a network. As a consequence, this concept is used in many modern CAD/modeling systems like SIMULINK, Scicos and DYMOLA, although most software packages cannot fully exploit the full potential of DAE models.

But this nice feature of DAEs for modeling has also a disadvantage, since it shifts all of the difficulties of a system onto the analysis and the numerical methods. For this reason in recent years much effort has been spent to analyze general DAEs and to derive suitable numerical methods either for general DAEs, see e.g. [9, 19, 18, 20, 29, 38] or for special DAEs arising in applications, see e.g. [6, 12, 28, 37].

This analytical and numerical work so far has been primarily driven by the simulation community, where the desire was to simulate the behavior of a complex system which could be electrical, mechanical, chemical, or all three. Due to the ever growing complexity of models which pose new challenges, the field is developing rather rapidly including now also hybrid [2, 3, 4, 11, 21, 31, 39] and delay systems [16, 17, 25, 26, 27].

Once a system can be modeled and simulated, there arises the need to control the process or optimize its performance. The control of physical processes is an important task in many applications and over the last two decades there have been tremendous advances in the theory and applications of control in almost all disciplines of science and technologies. Note that this includes not only the obvious applications such as designing a more efficient process, but also determining what are the control mechanisms inherent in complex biological systems and fitting models to data.

Recent Developments and Open Problems

As the two topics, simulation of DAEs and control/optimization, have evolved in recent years, there has been a growing awareness of interconnections which arise in a number of ways. One obvious way is the control of DAE modeled systems. Optimality conditions and a maximum principle for general DAEs have only recently been obtained [30] and the results are far from complete. But there are other more subtle connections in that the necessary conditions for an optimal control problem typically form a DAE and the solution of some control problems in the presence of constraints or invariants also involve DAEs. An *open problem* is in particular the analysis and numerical solution of the resulting optimality system and its proper regularization in the case of singular control.

Another important topic in which recently breakthroughs have been made is the stability analysis for DAEs, including the computation of Lyapunov exponents and Sacker-Sell spectra [32, 33]. Here an *open problem* is the extension of these results to fully nonlinear systems as well as the development of improved computational methods for large scale problems.

It is clear that another limiting factor is the growing size of DAE problems in application, ranging from several thousands in chemical engineering to billions of equations in circuit simulation. So in order to apply control and optimization methods, model reduction becomes an essential issue. However, classical approaches for model reduction lead to enormous difficulties when considering DAEs. This is mainly due to the fact that the constraints and physical properties, like stability and passivity, must be respected in the approximated model to achieve physically meaningful results [1, 35]. On the other hand the approximated model must be efficiently computable. To resolve this conflict is an open problem in many areas, which can only be resolved by efficiently exploiting the structure or by making compromises.

Another recent connection between DAEs and control are hybrid systems of DAEs, where different DAE models are chosen depending on some switching function. Important applications are chemical engineering systems, mechanical systems with friction, or electronic circuits, where depending on the frequency different circuits are used in the simulation and control [4, 5].

In addition, there are strong synergies on the proper modeling and formulation of DAE-constrained optimization problems and their solution with recently developed algorithms for nonlinear programming and mixed integer nonlinear programming.

Due to the many connections, some researchers in the numerical DAE community have begun to consider control/optimization issues while at the same time some from the control/optimization community have begun to examine DAE issues [7, 8, 10, 13, 14, 15, 22, 23, 34, 36].

With these new developments and more and more applications emerging, and with the increasing complexity of problems it was absolutely essential to bring the different communities working in these areas together. In spite of this natural interest on both sides, this was the first workshop ever devoted to control/optimization and DAEs. It brought together the widely scattered researchers from a number of disciplines in academia and from industry, and we believe that is was a milestone in the move to the next major advances to occur in this fundamentally important field. There were participants from chemical engineering, aerospace engineering, and electrical engineering. It is absolutely clear that further advances require the intensive interdisciplinary cooperation for the solution of fundamental mathematical, numerical, and algorithmic concerns and to attack the challenges that arise in many applications.

Presentation Highlights

The workshop featured 30 one-hour talks and it was decided that each speaker should make a strong effort to integrate the different (numerical analysis, control, optimization and engineering) communities in the discussion. In most talks this was really achieved, and was documented by the intensive discussion during and after each talk. Almost all talks were of extremely high quality.

It would be difficult to list all the highlights during the week, so we just mention a few. The chosen examples represent several of the key application areas of optimization of DAE based systems, namely mechanics, chemical engineering, and electrical systems.

Thanos Antoulas presented a concept of generating system models in a very simple way by not insisting that the resulting model is a regular model. This again is an interesting approach which allows simpler modeling put puts a large burden on the analytic and numerical treatment afterwards. This approach fits in well with the DAE modeling philosophy of working with relationship models. Immediate discussions started right after the talk how to integrate current methods for staircase computation with this new modeling approach.

Roland Freund presented a new approach for model reduction for super-large DAEs arising in circuit simulation. He emphasized that it is essential to guarantee that system properties like stability and passivity must be preserved. He then presented a new method, which is proven to achieve this goal without sacrificing the approximation accuracy. Model reduction is important any time large models are involved.

Francisco Borelli discussed new approaches to model predictive control. He, in particular, presented the need for new methods to control in real-time complex systems. As an example he used driver support systems in cars and trucks which support the interaction of the human driver, the vehicle and the environment. Another example concerned the optimal heating/cooling of buildings. He then suggested new approaches using robust control invariant sets and showed how these can be used efficiently.

Paul Barton, motivated by large complex problems in chemical engineering, discussed approaches for global optimization techniques with differential-algebraic constraints. He suggested a new approach for the relaxation and convexification of DAE constraints and how to put the constraints into interval boundaries. He demonstrated the approach for several applications using interval Newton-type methods.

Peter Kunkel presented a global optimality result for general nonlinear DAE optimal control problems and suggested several state-or-the-art developments. In particular he showed that the standard naive approach may lead to wrong results. He showed that it is possible to remodel the current model in what is called a strangeness-free formulation, that allows one to apply classical results for constrained optimization of optimal control problems with DAE constraints.

Serkan Gugercin showed that interpolation based model reduction methods can be constructed that directly work on higher order models or parametric models. The features of the new approach were demonstrated via several examples and it was shown that this new approach is very flexible towards different properties of the system.

Matthias Gerdts presented new results on local and global minimum principles for optimal control problems with mechanical DAE constraints. He demonstrated the quality of the results and their implementation via several examples from multibody dynamics.

Scientific Progress Made

Several research collaborations were started during the meeting and are continued afterwards. During every break and every night, several groups of people met for intense discussions, to work on new research projects or to discuss the talks of the previous sessions.

Many new collaborations were started and existing cooperations were refreshed.

To name a few examples, Tatjana Stykel and Serkan Gugercin worked almost every evening on new developments for model reduction of higher order and parametric systems.

Steve Campbell, Peter Kunkel, and Volker Mehrmann were able to carry out initial discussions on an examination of general regularization procedures for optimal control methods for general DAEs. Peter Kunkel's presentation served as the starting point for their discussions. Plans were made for further meetings over the next year and the framework for a paper giving a new general approach synthesizing several ideas presented at the workshop was developed.

Steve Campbell and John Betts had worked before. At the workshop a new collaboration was begun with Karmethia Thompson on direct transcription optimal control software for DAEs with delays. Their discussions at the workshop were especially stimulated by discussions with Larry Biegler about alternative collocation schemes for control problems and the handling of discontinuities which can occur with delays, with Bill Hager on the convergence of discretizations on optimal control problems solved by direct transcription, with Ray Spiteri who has used direct transcription software, and with Enright who has developed a number of delay numerical solvers. Ray Spiteri may also become involved in this collaboration.

Motivated by excitement generated at the workshop, the three organizers Larry Biegler, Steve Campbell, and Volker Mehrmann began a collaborative effort to produce a volume based on the workshop. This volume will be more than just a collection of talks but will also include a major introductory survey that the organizers will write. Initial reviews have been very favorable to the proposal. Both publishers that were given the proposal have expressed strong interest and a book contract is expected by early February. This volume is discussed more fully in the next section.

Outcome of the Meeting

The meeting was very intense and the efforts made by the speakers to integrate the different communities led to intensive discussions and cooperations.

With the intense interaction between the different groups, it was felt that a research monograph with surveys on the state-of-the-art of the research in this field would be an essential accelerator for future research work. Too often, new results appear as focused research publications in specialized journals and do not get to other disciplines. Instead, to reach a wider audience, the participants decided to produce a monograph by summarizing selected topics from the workshop and making them accessible to the different communities. Most of the speakers have volunteered to write survey articles of an expository nature, that provide essential review material but especially also present new research directions and challenges. The volume will also include a major introductory survey by the organizers.

All the talks presented are publically available at the conference website.

Participants

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Chapter 39

Integrable and stochastic Laplacian growth in modern mathematical physics (10w5019)

Oct 31 - Nov 05, 2010

Organizer(s): Darren Crowdy (Imperial College London) Bjorn Gustafsson (Royal Institute of Technology, Stockholm) John Harnad (Centre de Recherche Mathematique, Université de Montréal) Mark Mineev (Max Planck Institute for the Physics of Complex Systems) Mihai Putinar (University of California, Santa Barbara)

This workshop took place Oct 31–Nov 5 2010 and consisted of approximately 35 participants representing a broad spectrum of scientific disciplines, from pure and applied mathematicians to physicists. The central topic was Laplacian growth and its various manifestations in different scientific and mathematical areas. The event was a natural sequel to the earlier BIRS worskshop:

July 15th-20th 2007: Workshop on "Quadrature domains and Laplacian growth in modern physics", Banff International Research Station (Pacific Institute for Mathematical Sciences), Banff, Canada.

In the 2010 workshop, several new ideas and theoretical connections which became apparent during the 2007 workshop were explored and developed. The emphasis in the 2010 workshop was in many ways complementary to the earlier workshop; in 2010, more emphasis was placed on the mathematical connection of Laplacian growth and potential theory with stochastic growth problems. This has already led to ongoing collaborations and new ideas.

Among the participants were several PhD students, most of whom were invited to give shorter 30 minute presentations as part of our program.

The following pages include extended abstracts describing the content of the program of talks and presentations that took place during the workshop.

Integrable structures in the relativistic theory of extended objects

Jens Hoppe

A dynamical symmetry, as well as special diffeomorphism algebras generalizing the Witt-Virasoro algebra, related to Poincare-invariance and crucial with regard to quantisation, questions of integrability, and M(atrix) theory, were recently found to exist in the theory of relativistic extended objects of any dimension (and have been presented in my talk).

In a second part of my talk, I discussed the singularity formation for strings moving in a plane. Self-similar string solutions in a graph representation were presented, near the point of singularity formation.

Computation and calculation of some free boundary Hele-Shaw flows

N. Robb McDonald

The time-dependent evolution of source-driven Hele-Shaw free boundary flows in the presence of an obstacle are computed numerically. The Baiocchi transformation is used to convert the Hele-Shaw Laplacian growth problem into a free boundary problem for a streamfunction-like variable $u(x, y, t)$ governed by Poisson's equation (with constant right hand side) with the source becoming a point vortex of strength linearly dependent on time. On the free boundary both u and its normal derivative vanishes, and on the obstacle the normal derivative of u vanishes. Interpreting u as a streamfunction, at a given time the problem becomes that of finding a steady patch of uniform vorticity enclosing a point vortex of given strength such that the velocity vanishes on the free boundary and the tangential velocity vanishes on the obstacle. A combination of contour dynamics and Newton's method is used to compute such equilibria. By varying the strength of the point vortex these equilibria represent a sequence of source-driven growing blobs of fluid in a Hele-Shaw cell.

The practicality and accuracy of the method is demonstrated by computing the evolution of Hele-Shaw flow driven by a source near a plane wall; a case for which there is a known exact solution. Other obstacles for which there are no known exact solutions are also considered, including a source both inside and outside a circular boundary, a source near a finite-length plate and the interaction of an infinite free boundary impinging on a circular disc.

An equation governing the evolution of a Hele-Shaw free boundary flow in the presence of an arbitrary external potential–generalized Hele-Shaw flow–is derived in terms of the Schwarz function $g(z, t)$ of the free boundary. This generalizes the well-known equation $\partial g/\partial t = 2\partial w/\partial z$, where w is the complex potential, which has been successfully employed in constructing many exact solutions in the absence of external potentials.

The new equation is used to re-derive some known explicit solutions for equilibrium and time-dependent free boundary flows in the presence of external potentials including those with singular potential fields, uniform gravity and centrifugal forces.

Some new solutions are also constructed which variously describe equilibrium flows with higher-order hydrodynamic singularities in the presence of electric point sources, unsteady solutions describing bubbles under the combined influence of strain and centrifugal potential.

Random normal matrices by Riemann-Hilbert problem

Seung-Yeop Lee

Consider an ensemble of normal matrices with a certain prescribed probability distribution. We study the induced distribution of the eigenvalues as the size of the matrices gets large. It has been known that the eigenvalues behave like the 2 dimensional Coulomb gas subject to a certain external potential. In this correspondence, the size of the matrix becomes the number of Coulomb particles, and one may consider the scaling limit where the number of particles grows with the strength of the external potential, linearly with a given ratio, say t. In this limit, the limiting density of the particles tends to be supported uniformly on a finite domain $D \in \mathbb{C}$, and D behaves like the non-viscous domain in ideal Hele-Shaw flow when one considers t as the Hele-Shaw time.

The above particle system is known to be a determinantal point process, and the system is closely related to the orthogonal polynomial with respect to an area integral (Weighted Bergman polynomial). Especially, all the probabilistic information is expressed in terms of the reproducing kernel, that can be obtained from the orthogonal polynomial. Therefore, we set our primary goal to obtaining the asymptotic information about the orthogonal polynomial.

A well-known technique for orthogonal polynomial on the real line (or any contour) is the nonlinear steepest descent analysis of the corresponding Riemann-Hilbert problem by Deift-Kricherbauer-McLaughlin-Venakides-Zhou. To apply this technique we redefine the orthogonal polynomial over area integral, in terms of a line integral over some contour. Then the standard technique applies to produce the strong asymptotics for the orthogonal polynomial.

To demonstrate the technique, we consider a specific toy model that has one logarithmic singularity in the external potential. This produces Joukowsky map for the domain D. This toy model, though very simple, contains the critical moment where the topology of the domain D changes. We showed that such criticality is described by a special solution of Painlevé II equation (as expected in literature). Along with the strong asymptotics for the orthogonal polynomial, we have confirmed the theorem by Ameur-Hakan-Makarov that the norm of the orthogonal polynomial is asymptotically related to the harmonic measure on $\mathbb{C} \setminus D$.

Unlike the orthogonal polynomial on the real line, the Christoffel-Darboux identity (that allows one to write the kernel in terms of only "a few" orthogonal polynomials) is more complicated to write down. In our toy model, we have written down the identity, and obtained some preliminary result on the spectral density (i.e. density of the Coulomb particles).

This project is a work in progress with Ferenc Balogh, Marco Bertola and Kenneth McLaughlin.

Asymptotics of the interface of Laplacian growth with multiple point sources

Michiaki Onodera (National Taiwan University)

We study the asymptotic behavior of the interface of a Hele-Shaw ow produced by the injection of fluid from

infinitely many points at different speeds. We prove that, as time tends to infinity, the interface approaches the circle centered at the barycenter of the injection points with weights proportional to the injection rates. The distances from the barycenter to the boundary points are estimated both from above and below. The proof is based on a precise estimate of quadrature domains on the measure $\alpha\delta_i + \beta\delta_{-i}$ in the case where $\alpha, \beta > 0$ and $\alpha + \beta$ is sufficiently large. Hence $\delta_{\pm i}$ denote the Dirac measures at $\pm$i respectively. Combining an induction argument with the estimate yields the result.

Large-time behavior of multi-cut solutions to Hele-Shaw flows

Yu-Lin Lin

In the case of zero surface tension Hele-Shaw flows driven by injection, it is found that there is a large set of functions which can give rise to global solutions to the Polubarinova-Galin equation driven by injection. In this talk, we assume solutions are global and hence obtain a most precise way of describing rescaling behavior in terms of some conserved quantities. These conserved quantities are called Richardson's complex moments. In this talk, we focus on the special set of solutions which are called multi-cut solutions and this set of solutions are the combination of rational functions and logarithmic functions.

In this talk, we first look at the polynomial solution case and show how each coefficient of these multi-cut solutions decays in terms of Richardson's complex moments and hence obtain large-time behavior of multi-cut solutions $f(\zeta, t)$ in terms of these conserved quantities. Next, we show that all global multi-cut solutions behave like polynomials and hence obtain similar results to polynomial cases. From this talk, we can see that this method is the most precise way of describing large-time boundary behavior to Hele-Shaw flows. One of the important step of the proof is to formulate ODEs for poles and branch points of $f(\zeta, t)$. Part of this talk is joint-work with B. Gustafsson.

Structure theorems on quadrature domains for subharmonic functions

Makoto Sakai

For a positive Radon measure on the Euclidean space having a compact support, we assign a positive measure called a partial balayage. By using the measure, we obtain the existence and nonexistence theorems on quadrature domains of the given measure for subharmonic functions with finite volume. We describe all quadrature domains with finite volume by using two open sets determined by the measure. As a measure, a quadrature domain with finite volume is uniquely determined.
We also discuss a positive Radon measure whose support may not be compact. In this case, a large number of quadrature domains for subharmonic functions are possible. We introduce the generalized Newtonian potential of the measure and define the partial balayage of the measure replacing the Newtonian potential of a measure with compact support by the generalized Newtonian potential of the measure. Every quadrature domain can be describe by using the partial measure of a measure which is different from the given measure.

Schwarz symmetry principle and dynamical mother bodies

Tatiana Savin(a)

The talk consists of two separate parts which however have some connections from both mathematical and physical viewpoints. Both considered problems can be thought as applications of the Schwarz function.

First part is devoted to generalizations of the celebrated, point-to-point, Schwarz symmetry principle. This principle serves as a convenient tools in analysis and mathematical physics and its development has been attracting attention of many mathematicians. From the viewpoint of applications it is important to have an explicit reflection formula for every specific problem. One of the open questions is the following: for what partial differential equations, boundary conditions and spatial dimensions such a formula exists and what is the structure of this formula, in other words, whether it is a point to point formula or it has a more complicated structure, for example, a point to a finite set or a point to a continuous set.

It turns out that unfortunately the point-to-point reflection, holding for harmonic functions subject to the Dirichlet or Neumann conditions on a real-analytic curve in the plane, almost always fails for solutions to more general elliptic equations. We will discuss non-local, point-to-compact set, reflection operators for different elliptic equations subject to different boundary conditions.

The second part of the talk is a joint project with Alexander Nepomnyashchy (Technion). We will introduce dynamical mother bodies arising in an attempt to answer the question: what distribution of sinks allows the complete removal of a droplet with an algebraic boundary from a Hele-Shaw cell.

Indeed, it is well-known that in the framework of the internal Hele-Shaw problem the fluid can not be fully removed through a single sink because of the cusp formation before the moving boundary reaches the sink unless the initial domain is a circle with the sink located in its center. We give a definition of a dynamical mother body and use it for developing an algorithm of complete removal of a fluid droplet having algebraic boundary. To illustrate our theory we consider examples, where fluid can be completely removed through the sinks distributed along arcs of curves and/or points.

Originally, the concept of a (static) mother body was introduced by D. Zidarov, who studied gravitational potential of a family of heavy bodies producing the same gravitational field. His starting point was as follows: a sphere uniformly filled by masses generates the same gravitational field as the point mass of the same magnitude placed at the center of the sphere. Thus, this point mass is a minimal element of the infinite family of concentric balls, each member of which generates the same gravitational field outside of the biggest one. Using Poincare sweeping method one may start from an arbitrary body with a smooth boundary and try to construct the family of graviequivalent bodies. The minimal element for the family is called a mother body. It was considered by Gustafsson, Sakai and others (including the author). Here we specify and use the concept of a dynamical, time dependent, mother body for the internal Hele-Shaw problem.

Parametrization of the Loewner-Kufarev evolution in Sato's Grassmannian

Irina Markina and Alexander Vasil'ev

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The Virasoro algebra $\mathfrak{vir}$ plays a prominent role in modern mathematical physics, both in field theories and solvable models. It appears in physics literature as an algebra obeyed by the stress-energy tensor and as a Lie algebra of the conformal group, called the Virasoro-Bott group Vir, of the worldsheet in two dimensions. It is a unique central extension of the Lie algebra $\mathfrak{diff}S^1 \simeq VectS^1$ for the Lie-Fréchet group $\mathcal{D}iffS^1$ of sense-preserving diffeomorphisms of the unit circle S^1, and it is an infinite-dimensional real vector space. The group $\mathcal{D}iffS^1$ can be thought of as a group of reparametrizations of a closed string. The exponential map from the Lie algebra $\mathfrak{diff}S^1$ to the Lie-Fréchet group $\mathcal{D}iffS^1$ is neither injective nor surjective. However Kirillov and Yuriev in 1986 proposed to consider a Fréchet homogeneous manifold $\mathcal{D}iffS^1/S^1$ and proved that there exists a local bijective exponential map $\exp\colon Vect_0S^1 \to \mathcal{D}iffS^1/S^1$, where $Vect_0S^1 = VectS^1/\text{const}$.

Our main objects of interest will be the complexification of $\mathcal{D}iffS^1/S^1$ and $\mathcal{D}iffS^1$ given as

- $(\mathcal{D}iffS^1, H^{(1,0)})$, where $H^{(1,0)} \oplus H^{(0,1)} = \text{corank}_1(VectS^1 \otimes \mathbb{C})$;
- $(\mathcal{D}iffS^1/S^1, T^{(1,0)})$, where $T^{(1,0)} \oplus T^{(0,1)} = Vect_0S^1 \otimes \mathbb{C}$.

An important fact is the following relation of these complexified objects to analytic functions. Let us denote by $\mathcal{F}$ the class of all smooth univalent functions in the unit disk $\mathbb{D}$, $f(z) = z(a_0 + a_1z + \dots)$, by $\mathcal{F}_1$ its subclass defined by the normalization of the conformal radius of $f(\mathbb{D})$ to be 1, and we denote by $\mathcal{F}_0$ the subclass of $\mathcal{F}_1$ of normalized univalent functions in $\mathbb{D}$, $f(z) = z(1 + c_1z + \dots)$. Then there is the biholomorphic equivalence.

- $(\mathcal{D}iffS^1/S^1, T^{(1,0)}) \leftrightarrow \mathcal{F}_0$,

and the bijective Cauchy-Riemann map

- $(\mathcal{D}iffS^1, H^{(1,0)}) \leftrightarrow \mathcal{F}_1$;

The Fourier basis vectors $v_n = -ie^{in\theta}\frac{d}{d\theta}$ in $Vect_0S^1 \otimes \mathbb{C}$, therefore, are mapped onto the vectors $L_n[f](z)$ of the tangent space $T_f\mathcal{F}_0$, $n \in \mathbb{Z}$. The vectors $L_n[f](z)$ are simple for $n > 0$, $L_n[f](z) = z^{n+1}f'(z)$, and for $n = 0$, $L_0[f](z) = zf'(z) - f(z)$. In the first canonical quantization they are the Virasoro generators

$$L_n = \partial_n + \sum_{k=1}^{\infty}(k+1)c_k\partial_{n+k},$$

where $\partial_k = \partial/\partial c_k$, for $n > 0$, and $L_0 = \sum\limits_{k=1}^{\infty} kc_k\partial_k$.

The next part of our research deals with the Löwner-Kufarev evolution given as an infinite-dimensional control system. Any univalent function $f : U \to \Omega$, $f(z) = z + c_1z^2 + \dots$ (from the class $Sb \supset \mathcal{F}_0$)

can be represented as the limit $f(z) = \lim_{t\to\infty} e^t w(z,t)$. The function $\zeta = w(z,t)$ normalized as $w(z,t) = e^{-t} z \left(1 + \sum_{n=1}^{\infty} c_n(t) z^n\right)$, satisfies the Löwner-Kufarev equation

$$\frac{dw}{dt} = -wp(w,t),$$

with the initial condition $w(z,0) = z$. The control function $p(z,t) = 1 + u_1 z + \dots$ is measurable in $t \in [0,\infty)$ for every $z \in \mathbb{D}$, analytic in $\mathbb{D}$ for almost all $t \in [0,\infty)$, and has positive real part in $\mathbb{D}$. We shall consider the functions p which are integrable in $t \in [0,\infty)$ and smooth on S^1. Then the contour evolution given by the curve $f(z,t) = e^t w(z,t)$ in $\mathcal{F}_0$ generates an evolution of smooth contours $f(S^1,t)$.

Theorem. *Consider the Hamiltonian function on the cotangent bundle to $\mathcal{F}_0$*

$$H(f,\psi) = \int_{z\in S^1} f(z,t)\big(1 - p(e^{-t} f(z,t),t)\big)\bar{\psi}(z,t)\frac{dz}{iz}, \quad f \in \mathcal{F}_0, \ \ \psi \in T^*\mathcal{F}_0.$$

Then the conserved quantities of the Löwner-Kufarev evolution defined by H, in their first quantizations coincide with the Virasoro generators $L_n[f]$.

The final part is devoted to a parametrization of the Löwner-Kufarev evolution in Sato's Grassmannian. The idea consists of considering a trivial bundle of smooth Grassmannians Gr_∞ over the cotangent bundle $T^*\mathcal{F}_0$ to $\mathcal{F}_0$. Inside each Grassmannian we construct special points which form a principal bundle $\mathfrak{E} = (\mathcal{F}_0, \mathfrak{W})$ over $\mathcal{F}_0$ with fiber $\mathfrak{W}$ which is a countable family $\mathfrak{W} = \{W^{(-n)}\}_{n=0}^{\infty}$ of linear subspaces of a Hilbert space $L^2(S^1 \to \mathbb{C}) \cap C^\infty$. These special points $W^{(-n)}$ are graphs of rapidly decaying Hilbert-Schmidt operators. The graphs are defined by the Virasoro generators L_{-n}, $n \geq 0$. Making use of the standard basis $\{z^k\}_{k=-\infty}^{+\infty}$ of $L^2(S^1 \to \mathbb{C})$ we consider the polarization

$$\begin{aligned} \mathcal{H}_+ &= spn_{\mathbb{C}}\{z, z^2, z^3, \dots\}, \\ \mathcal{H}_- &= spn_{\mathbb{C}}\{1, z^{-1}, z^{-2}, \dots\}. \end{aligned}$$

Theorem. *The Löwner-Kufarev evolution in $\mathcal{F}_0$ gives a curve in the principal bundle $\mathfrak{E}$, such that it traces sections in each connected component $U_{\mathcal{H}_+}^{(-n)}$ of the neighbourhood $U_{\mathcal{H}_+}$ of the point $\mathcal{H}_+ \in Gr_\infty$.*

"Fingerprints" of the Two Dimensional Shapes and Lemniscates

Dmitry Khavinson

The newly emerging field of vision and pattern recognition often focuses on the study of two dimensional "shapes", i.e. simple, closed smooth curves. A common approach to describing shapes consists in defining a "natural" embedding of the space of curves into a metric space and studying the mathematical structure of the latter. Another idea that has been pioneered by Kirillov and developed recently among others by Mumford and Sharon consists of representing each shape by its "fingerprint", a diffeomorphism of the unit circle. Kirillov's theorem states that the correspondence between shapes and fingerprints is a bijection modulo conformal automorphisms of the disk. In this talk we discuss the recent joint work with P. Ebenfelt and Harold S. Shapiro outlining an alternative interpretation of the problem of shapes and Kirillov's theorem based on finding a set of natural and simple fingerprints that is dense in the space of all diffeomorphisms of the unit circle. This approach is inspired by the celebrated theorem of Hilbert regarding approximation of smooth curves by lemniscates. We shall outline proofs of the main results and discuss some interesting function-theoretic ramifications and open questions regarding possibilities of numerical applications of this idea (joint with Peter Ebenfelt and Harold S. Shapiro).

Non-univalent solutions of the Polubarinova-Galin equation

Björn Gustafsson

We discuss solutions of the Polubarinova-Galin (PG)

$$\mathrm{Re}\,[\dot{f}(\zeta,t)\overline{\zeta f'(\zeta,t)}] = q(t) \quad (|\zeta| = 1),$$

and Löwner-Kufarev (LK)

$$\dot{f}(\zeta,t) = \zeta f'(\zeta,t) P_f(\zeta,t) \quad (|\zeta| < 1),$$

equations in the case that the "mapping" function $f(\zeta,t)$ from the unit disk to the fluid domain of a Hele-Shaw blob, subject to injection ($q(t) > 0$) or suction ($q(t) < 0$) at the origin, is no longer univalent. Here $P_f(\zeta,t)$ denotes the Poisson-Schwarz integral of $q(t)|f'(\zeta,t)|^{-2}$. Of special interest is the "Abelian" case, i.e., when

$$f'(\zeta,t) = b(t)\frac{\prod_{k=0}^{m}(\zeta - \omega_k(t))}{\prod_{j=0}^{n}(\zeta - \zeta_k(t))}$$

($m \geq n$), in other words, when $f(\zeta,t)$ is an Abelian integral on the Riemann sphere.

When f is univalent, or locally univalent, the PG and LK equations are equivalent. However, when f' has zeros inside the unit disk LK is strictly stronger than PG, in fact LK is equivalent to PG plus the additional condition that the functions $f(\cdot,t)$ make up a subordination chain, equivalently lift to a fixed (independent of t) Riemann surface R over $\mathbb{C}$. On R, which inherits a Riemannian metric from $\mathbb{C}$, the variational inequality weak solution (see reference below) makes sense. By exploiting this solution we are able to show, in the injection case, that the LK equation has a global in time solution in the appropriate weak sense. The main difficulty lies in the fact that the Riemann surface R does not exist in advance, but has to be constructed along with the solution. It has to be continuously enlarged, and every time a zero of f' reaches the unit circle it has to be updated with new branch points in order to prevent the solution domain to become multiply connected, and then outside the scope of the LK equation. In particular, the weak solution will not be smooth when zeros of f' cross the unit circle (as can also be realized directly from the PG and LK equations).

Abelian solutions remain Abelian for all time, but the structure may change during the evolution, namely when zeros $\omega_k(t)$ cross the unit circle. The process is not fully understood at present, but the examples we have been able to elaborate give the impression that the appearence of a new branch point on R is accompanied by the creation of a pair of a zero and a pole of f'.

The talk is based on joint work with Yu-Lin Lin, Taipei.

Reference: B. Gustafsson, A. Vasilév, *Conformal and Potential Analysis in Hele-Shaw Cells*, Birkhäuser, 2006.

Topological recursion, β-ensembles and quantum algebraic geometry

Marchal Olivier

During this talk, I presented the topological recursion recently developped by Eynard and Orantin to solve the general expansion of matrix models. In particular, I reviewed the method in the case of the one-matrix model where I presented first the general recursion scheme and then an application on a example given during a previous talk by P. Bleher, namely, the case where the potential is cubic: $V(x) = \frac{x^2}{2} - ux^3$. In this case, when the parameter u is close to zero, the spectral curve obtained is of genus 0 and I showed how the topological recursion could be easily implemented concretely. Then I naturally switched to the case of the two-matrix model, gave the general stting and made the connection with Laplacian growth. In particular, since some cases of Laplacian growth can be modeled by a formal two-normal matrix model, I presented the way to derive the spectral curve in this context, by application of the Eyanrd Orantin formula. In order to illustrate this setting, I gave the spectral curve corresponding to the simple case presented earlier during the week by Seung Lee and given by $V(z) = -c\ln(z-a)$. In this example, getting the boundary of the fluid is trivial and I showed on a picture of such aircraft wings contours.

Then I switched to the second part of my talk which consisted in the generalization of the topological recursion scheme in the case of β-ensemble. First I recalled to the audience the definition of the model, which can be viewed as an extension of the traditionnal hermitian matrix model. Then I gave the so-called loop equations in that case and presented a method to solve them. In this context, the loop equations are no longer algebraic, but diffential. Therefore, the solution implies the introduction of a "quantum" Riemann surface and to generalize in this context all standard tool of algebraic geometry. Hence I presented the links between Stokes phenomenon, subdominant solutions and the way to define: genus, cycles, holomorphic differentials, third kind differential, Bergman kernel in the context of a "quantum" curve. Eventually, I gave the generalization of the topological recursion scheme for β ensemble providing a solution to the loop equations for β-ensembles. To conclude, I gave some unsolved problems that still miss to have a complete understanding of β ensmbles.

An assembly of steadily translating bubbles in a Hele-Shaw channel

Christopher Green

New solutions for any finite number of steadily translating bubbles in a Hele–Shaw channel were presented. The problem in consideration is a paradigmatic example of a Laplacian growth process and can be shown to be a special type of Riemann-Hilbert problem on a multiply-connected circular domain. The solutions can be written down explicitly, and elegantly, in terms of a special transcendental function known as the SchottkyKlein prime function. In doing so, our solutions generalize exact single bubble solutions found first by Taylor & Saffman, Tanveer, and Vasconcelos and Crowdy (references below).

We presented various plots showing different bubble configurations at some prescribed speed. We qualitatively observe the interaction effects of the bubbles and also how the configuration adjusts due to the effects from the two channel sidewalls. As a check on these solutions, we verified the Taylor-Saffman limit by measuring the aspect ratios for our small bubbles and we found that they are indeed in agreement with Taylor and Saffman's result.

This work has a number of important aspects. We have solved another version of a classical Laplacian growth nonlinear free boundary value problem and therefore adds to the body of prior work on bubbles in Hele–Shaw channels and cells. Our problem formulation makes no *a priori* assumptions on the geometrical arrangement of the bubbles, and is therefore very general. Our solution is neatly expressed in terms of the Schottky-Klein prime function which is both mathematically concise and also convenient for computational purposes, particularly now that software is freely available for its computation (reference to website below) [joint work with D. Crowdy].

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Laplacian growth, elliptic growth, and singularities of the Schwarz potential

Erik Lundberg

The Schwarz function has played an elegant role in understanding and in generating new examples of exact solutions to the Laplacian growth (or "Hele-Shaw") problem in the plane. The guiding principle in this connection is the fact that "non-physical" singularities in the "oil domain" of the Schwarz function are stationary, and the "physical" singularities obey simple dynamics.

This talk discussed the same principle for Laplacian growth in higher dimensions and in a non-homogeneous environment ("elliptic growth"), Each case has simple dynamics of singularities of the *Schwarz potential*, a generalization of the Schwarz function introduced by D. Khavinson and H.S. Shapiro,

Given a domain Ω bounded by a non-singular, algebraic hypersurface Γ, the *Schwarz potential* is the unique solution to the following Cauchy problem for Laplace's equation:

$$\begin{cases} \Delta w = 0 \text{ near } \Gamma \\ w|_\Gamma = \frac{1}{2}||\mathbf{x}||^2 \\ \nabla w|_\Gamma = \mathbf{x}, \end{cases}$$

Based on this connection new exact solutions were described for both cases: the higher-dimensional Laplacian growth and the case of Elliptic growth. $\mathbb{C}^n$-techniques for holomorphic PDEs were presented as an important means of locating singularities of the Schwarz potential.

Participants

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Chapter 40

Nonstandard Discretizations for Fluid Flows (10w5041)

Nov 21 - Nov 26, 2010

Organizer(s): Peter Minev (University of Alberta), Vivette Girault (University of Paris VI), Jean-Luc Guermond (Laboratoire d'Informatique pour la Mecanique et les Sciences de l'Ingenieur), Guido Kanschat (Texas A&M University)

Overview of the Field

Computational Fluid Dynamics is a field on the interface between Numerical Analysis, Computational Science, Physics and Engineering. It underwent an intensive development primarily because of the needs of aeronautics, nuclear physics and engineering, geophysics, chemical and automotive engineering etc., and the rapid development of fast computers. The major efforts are concentrated on the efficient numerical approximation of the solution of the incompressible, quasi-compressible and compressible Navier-Stokes or Euler equations, sometimes in conjunction with additional advection-diffusion systems for transport of heat or substances. Relatively recently, the scope of problems was widened by considering fluid structure interaction, MHD and non-Newtonian fluids, which introduced some major new challenges. In addition, the development of models for multiphase flows, biofluids, micro/nanofluids is a challenge by itself, and it is far from being completed yet. The focus of this workshop was on the development and analysis of new algorithms as well as the practical solution of some very challenging physical problems (which themselves require some non-standard thinking even if more classical techniques are used).

The common ground for all these models is that they comprise nonlinear advection-diffusion(-reaction) equations with linear constraints. Depending on the parameters of the system, they can exhibit the whole scale from a predominantly parabolic/elliptic behaviour (low Reynolds number flows) up to a predominantly hyperbolic behaviour (the Euler system). Other challenges are the (sometimes very strong) non-linearity of the problems, the presence of constraints which necessarily lead to saddle point systems, the appearance of more than one spatial and/or temporal scale, etc. All these make the development of a universal and optimal algorithm impossible and stimulated the development of various methods for the various classes of problems.

Several major classical discretization techniques have been developed, based on finite difference, finite element, finite volume and spectral methods. More recently, we witnessed the development of some new interesting techniques like the hp finite elements, discontinuous Galerkin methods and other non-conforming or div-conforming methods, unstructured finite volumes, domain decomposition and mortar techniques. In case of advection-dominated flows, these techniques are combined with various stabilization mechanisms: edge stabilization; residual- and entropy-based viscosity; and special fluxes for discontinuous Galerkin schemes. These are closely related to some recent approaches for turbulence modelling like subgrid viscosity, variational multiscale methods and large eddy simulation. A major development in all these areas was the idea for a posteriori error estimation and nonlinear adaptivity. The discretization of time dependent problems triggered the development of various operator splitting and projection techniques as well as time adaptive schemes.

Finally, distributed parallel computers with fast interconnect and a massive number of processors added a new challenge which triggered the development of highly parallelizable solution methods for linear systems based on domain decomposition or multigrid. Actually, currently one of the most important characteristic of any solution method is its performance when implemented in parallel. This led to the rediscovery and further development of some methods dating from the dawn of numerical analysis, like fictitious domain/penalty methods and direction splitting methods.

CFD being too vast of a field to be dealt with at one single workshop, the workshop was mainly focused on solution methods for incompressible and quasi-incompressible flow problems in the context of advanced applications. These included in particular multiphysics problems like magneto-hydrodynamics, combustion, fluid-structure interaction, mixtures, and of multiscale problems like turbulent flows, particle flows and sedimentation.

Recent Developments and Open Problems

Several open problems were discussed during the workshop and we are summarizing below some of them.

A lot of effort has been spent toward the development of parameter-free or almost parameter-free stabilization techniques for the Euler and Navier-Stokes equations. These are often combined with a posteriori estimation and adaptivity. There is also a clear link between those stabilization techniques and the various LES turbulence models developed by the physics community.

In multicomponent fluids and the treatment of contact lines, the quest for an efficient and optimal method is still open. A new development is the so-called phase-field method and several presentations were focussed on its development. Some recent results on the analysis of the immersed boundary methods were also shown. The treatment of contact lines is in general quite open too.

The development of optimal methods for multiphysics problems, for instance fluid-structure interaction or the coupling of Stokes and Darcy or Stokes and Brinkman models, is a very active research area with competing models and methods. Interesting results on the integration of observation and modelling were presented.

Another area which is quite open from both, modelling and analysis points of view, is the non-Newtonian fluid mechanics. Some new models and particularly their numerical analysis and the development of optimal solution methods were discussed in several presentations. Some interesting results on the non-Newtonian behaviour of blood even in the largest vessels were presented.

Finally, new developments of massively parallel algorithms for the incompressible Navier-Stokes equations were discussed, for instance a very recent new development is based on a direction splitting algorithm which allows for extremely efficient parallelization and highly accurate discretization.

Presentation Highlights and Scientific Progress

Stabilization techniques and Discontinuous Galerkin (DG) methods

When the Reynolds number is high the standard Galerkin method may fail to produce the expected optimal error reduction under refinement even for smooth flows. Regardless of whether or not some turbulence model is used, stabilized methods are therefore a mandatory tool if computations are to be performed without resolving the viscous scales of the flow. To illustrate this, some simple examples of the failure of the standard Galerkin method were discussed and compared with a stabilized method. Then the ideal properties of the stabilized method were discussed and theoretical or computational results in the literature, either for the full Navier-Stokes' equation or for simpler model problems, were recalled, indicating the possibility of designing methods with the desired properties [1, 2, 3, 5].

Modeling of high Reynolds number turbulent fluid flow based on computational solution of the Navier-Stokes equations (NSE) poses a number of challenges related to stability, accuracy and resolution of the turbulent scales in the problem. Finite element (FE) methods produce approximate weak solutions to NSE. If not all scales in the flow are resolved by the computational mesh, a stabilized discretization is needed. One can show that certain FE approximations satisfy a local energy equation, with dissipation of kinetic energy from the numerical stabilization. A numerical stabilization, based on the residual of NSE, is active mainly where the method is unable to approximate the NSE on the given mesh, typically near shocks, boundary layers or turbulence, which are parts of the flow where also high physical dissipation takes place. J. Hoffman presented an investigation of the dissipative effect from numerical stabilization, focussed on incompressible turbulent flow and modeling of turbulent boundary layers. This problem was studied in the context of adaptive FE methods for turbulent flow, and a posteriori error estimation of mean value output from the computation.

With respect to the time-discretization methods, it is important to distinguish between Petrov-Galerkin methods, such as the SUPG method or the PSPG method, and the more recently introduced symmetric stabilization methods. In the latter case time-discretization is relatively straightforward and some results both for stabilization of dominant convection and for the pressure-velocity coupling of the Stokes' problem were presented. Then these results were compared with recent results for the respective Petrov-Galerkin methods [4, 6]. The solution of fluid flows may lead to numerical instabilities due to the incompressibility restriction, and also to dominating operator terms such as convection, Coriolis force, among others. These stability restrictions are treated by bounding a convenient range of high-frequency components of the terms to be stabilized. This is achieved either by enriching the velocity discretization space (Mixed methods), or by adding specific terms to the standard Galerkin discretizations (Stabilized methods). Both procedures turn out to be essentially equivalent, as this second procedure may be interpreted as an augmented mixed method constructed with an enriched velocity space, via bubble finite element functions (Cf. [7]). Mixed methods include stabilizing degrees of freedom that do not yield accuracy, so becoming more costly than stabilized methods. The talk of E. Burman was focussed on high-order stabilized methods, due to their reduced computational cost and high accuracy. On one hand, high-order penalty methods are considered, which are an extension of the well-known Brezzi-Pitkäranta method. These methods provide low-cost solvers with high accuracy. On another hand, the Orthogonal Sub-Scale (OSS) method is considered, which is a residual-based stabilized method that introduces a minimal level of numerical diffusion (Cf. [8]). In both methods the stabilizing terms are filtered by projection operators, in such a way that only the high-frequency components that are not representable in the discretization space are stabilized.

The talk of A. Ern considered discontinuous Galerkin (DG) methods for the steady incompressible Navier–Stokes equations. It focused on stabilized versions with equal-order approximations for velocity and pressure; other choices can be considered as well. A crucial issue is the design of a suitable discrete trilinear form for the convective term that does not modify the kinetic energy balance. This feature allows both to reduce numerical dissipation and to infer an existence result for the discrete problem under very mild assumptions. Two choices were discussed, one based on Temam's device and the other which is fully conservative and requires a nonstandard modification of the pressure hinted to in [10]. The main result, see [11], is the existence of a solution for the discrete problem and the convergence of (a subsequence of) discrete solutions to a solution of the continuous problem without any smallness assumption on the data and with the minimal regularity requirement on the exact solution. The convergence proof, inspired by [12], relies on new discrete functional analysis tools in broken polynomial spaces, namely discrete Sobolev embeddings and a compactness result for discrete gradients. Examples illustrating the theory and numerically delivering convergence rates were presented. Finally, it briefly addressed the unsteady case by discussing a projection method originally proposed in [9] and showing some numerical results on 2D and 3D problems. The primary focus was on the ability of the method to deal with convection-dominated problems. Different choices for the approximation of the pressure were also investigated.

Stabilized finite element methods for convection-dominated problems require the choice of appropriate stabilization parameters. From numerical analysis, often only their asymptotic values are known. The talk of V. John presented a general framework for optimizing the stabilization parameters with respect to the minimization of a target functional. Exemplarily, this framework was applied to the SUPG finite element method, see [13], and spurious oscillations at layers diminishing (SOLD) schemes. The minimization of different target functionals, e.g. residual-based error estimators and error indicators, was considered. Benefits of this approach were shown and further improvements were discussed.

A variational multiscale method for Large-Eddy simulation of turbulent incompressible flows based on a general proposal in [14] was considered in the talk of G. Lube. More precisely, the approach relies on local projection of the velocity deformation tensor and grad-div stabilization of the divergence-free constraint, see [15]. An a priori error estimate with rather general nonlinear and piecewise constant coefficients of the subgrid models for the unresolved scales of velocity and pressure is derived in the case of inf-sup stable approximation of velocity and pressure. An extension of the approach to the incompressible Navier-Stokes/ Fourier model can be found in [16]. The talk also discussed preliminary numerical simulations for basic benchmark problems like decaying homogeneous isotropic turbulence, channel flow and natural convection in a differentially heated cavity. The efficient solution of the arising discrete problems relies on a flexible GMRES method with a robust preconditioner for the generalized Oseen problem together with parallel computation [17].

The talk of G. Matthies considered finite element discretizations of the Oseen problem by inf-sup stable finite element spaces. In contrast to standard equal order interpolation, no pressure stabilization is needed. However, the Galerkin method still suffers in general from spurious oscillations in the velocity which are caused by the dominating convection. To handle this instability, the local projection stabilization is used. Originally, the local projection technique was proposed as a two-level method where the projection space is defined on a coarser mesh. Unfortunately, this approach leads to an increased discretization stencil. The main objective is to analyze the convergence properties of the one-level approach of the local projection stabilization applied to inf-sup stable discretizations of the Oseen problem. Moreover, new inf-sup stable finite element pairs approximating both velocity and pressure by elements of order r with respect to the H^1-norm were proposed. In contrast to the 'classical' equal order interpolation, the velocity components and the pressure were discretized by different elements. For these pairs of finite element spaces it was shown an error estimate of order $r + 1/2$ in the convection dominated case $\nu < h$.

The objective of the talk of R. Codina is to present a framework for the finite element approximation of elliptic problems in which the unknown is split into two parts, the first corresponding to a continuous approximation and the second to a discontinuous one. A hybrid formulation is used for the discontinuous part, using as unknowns the field in the interior of the elements of the finite element partition and the fluxes and traces on the boundaries. Thus, the resulting formulation involves four unknowns, namely, the continuous part and the three fields coming from the hybrid formulation of the discontinuous part. A general result stating well–posedness of this problem is presented. The key assumptions are an appropriate minimum angle condition between the spaces for the continuous and discontinuous components of the unknown and inf-sup conditions between the spaces for fluxes and bulk field of the discontinuous part as well as between the spaces for traces and bulk field of this discontinuous part. Different applications of the framework presented are discussed. First, it is shown that classical discontinuous Galerkin methods can be derived by deleting the continuous component of the approximation and taking appropriate closed form expressions for the traces and fluxes of the discontinuous component. In particular, it is shown that if fluxes are approximated using classical finite difference approximations and the traces are determined by imposing continuity of fluxes, generalized versions of the interior penalty discontinuous Galerkin method are recovered, including in particular the treatment of discontinuous coefficients. As a second application, stabilized finite element methods for the convection-diffusion and the Stokes problems are presented. The unknown in this case is split into a resolvable continuous component and a so-called subgrid scale part which is taken as discontinuous, and for which the hybrid formulation described before is employed. Closed-form expressions are proposed for the three fields associated to the discontinuous part. The result is a stabilized formulation that accounts for boundary contributions of the subgrid scales [46]. In the case of domain interaction problems, the ideas described above allow one to design iterative algorithms with enhanced convergence properties. In the case of homogeneous domain interaction, better enforcement of transmission conditions between subdomains is achieved, whereas in heterogeneous domain interaction, such as fluid-structure interaction problems, convergence of iterative schemes is improved. In particular, this alleviates the so called added mass effect found when fluid and solid densities are similar [47].

D. Schoetzau presented a new class of discontinuous Galerkin (DG) methods for the numerical discretization of incompressible flow problems that yield exactly divergence-free velocity approximations [26]. Exact incompressibility is achieved by using divergence-conforming finite element spaces for the velocities and suitably matched discontinuous spaces for the pressures. The H^1-continuity of the velocities is enforced through a discontinuous Galerkin approach. He then presented extensions to hp-version DG methods on geometrically and anisotropically refined meshes in three dimensions. In particular, it was shown that the discrete inf-sup constants are independent of the elemental aspect ratios, and depend only very weakly on the polynomial degrees. Finally, the application of exactly divergence-free methods to an incompressible magneto-hydrodynamics problem [27] was demonstrated. All theoretical findings were illustrated and verified in numerical experiments.

Free boundary flows

The accurate numerical computation of two-phase flows is a challenging task, in particular if <u>surf</u>ace <u>act</u>ive <u>ag</u>e<u>nt</u>s are present which lower the surface tension on the interface. Nonuniform distributions of surfactants on the interface induce Marangoni forces. Adsorption and desorption of surfactants between the interface and the bulk phase may take place in the soluble surfactant case. Thus, the presence of surfactants influences strongly the dynamics of the moving interface. The talk of L. Tobiska considered a mathematical model for two-phase flows consisting of the incompressible Navier-Stokes equations, a transport equation for the surfactant concentration in the outer phase, and a surface transport equation for the surfactant concentration on the interface. The Navier-Stokes equations are solved together with the bulk and interface concentration equations using the coupled ALE-Lagrangian method in 3D-axisymmetric configuration [19]. The surface force can be directly incorporated due to the resolution of the interface by the moving mesh. The curvature in the surface force is replaced by the Laplace-Beltrami operator and an integration by parts is applied to reduce the order of differentiation [20]. Continuous, piecewise polynomials of second order enriched by cubic bubble functions and discontinuous, piecewise polynomials of first order (P_2^b/P_1^{disc}) for the discretization of the velocity and pressure, respectively, are used. The bulk and interface concentrations are approximated by continuous, piecewise polynomials of second order (P_2). A fractional step-ϑ scheme has been used for the temporal discretization. To handle the moving mesh, the elastic-solid technique has been applied [18]. The numerical scheme has been validated for surface flows with insoluble surfactants in [19] and for interfacial flows with soluble surfactants in [21]. Several examples of numerical tests were presented.

The talk of P. Quintela focussed on the movement of two fluids, one of them being a gas bubble immersed in a liquid, considering the surface tension effects. Using an Eulerian methodology to simulate the transport of the bubble, a velocity-pressure mixed formulation was proposed to solve the hydrodynamic equations, combined with a level set method to characterize the position of each fluid. In order to improve the approximation of the pressure when there is a severe discontinuity in the interface, the finite element space is enriched on the elements being cut by the interface. Besides, the static condensation technique in the bubble components on the enriched elements has been developed. In order to evaluate the elemental matrices on the elements crossed by the interface and their neighbours, a suitable quadrature rule has to be chosen, since a classical one cannot be applied to discontinuous functions. It is usual to overcome these difficulties by splitting the elements into subelements where the integrands are continuous. The description of the interface considered allows to automatically split a simplex into several sub-simplices and to construct a new quadrature formula for the element avoiding a casuistic analysis. The partitioning is done for numerical quadrature purpose only and it does not modify the approximation properties of the finite elements in a direct way. Numerical results for academic examples were presented for large ratios of density and viscosity. A laboratory experiment was also numerically reproduced and a benchmark example shown.

The no-slip boundary condition is usually regarded as a cornerstone in fluid dynamics, and its applicability has been proven for diverse fluid flow problems. However, when dealing with two-phase flows it is of importance to accurately describe the displacement of the so-called contact line, that is, the points which are at the intersection of the solid boundary of the domain and the interface separating the two fluids. In this case, contrary to what is seen in experiments, the no-slip condition implies that the contact line does not move. This is known as the contact line problem (paradox) and it has recently been the subject of intense research and debate (see [29, 32] for more details). On the basis of molecular dynamics simulations, Qian *et. al.* have proposed (c.f. [32]) the so-called generalized Navier-slip boundary condition, which aims at resolving the contact line problem. Later ([33]), the same authors derived this condition from thermodynamical principles. The first objective of the talk of A. Salgado was to introduce the generalized Navier-slip boundary condition and show that the obtained initial boundary value problem, which consists of a Cahn-Hilliard Navier-Stokes system with non-local boundary conditions, has an energy law. After that it presented a discretization of this problem which is based on an operator splitting approach for the Cahn-Hilliard part, much similar to the ones existing in the literature. For the Navier-Stokes part, the scheme consist of fractional time-stepping based on penalization of the divergence, in the spirit of [30, 31] and [34]. It was shown that this scheme satisfies a discrete energy law similar to the one obtained in the continuous case.

The talk of J. Shen presented a new phase-field model for the incompressible two-phase flows with variable density which admits an energy law. It also utilized weakly coupled time discretization schemes that are energy stable. Efficient numerical implementations of these schemes were also presented. The model and the corresponding numerical schemes are particularly suited for incompressible flows with large density ratios. Ample numerical experiments are carried out to validate the robustness of these schemes and their accuracy.

Non-Newtonian Fluid Mechanics

Motivated by live experiments, the talk of A. Bonito presented an algorithm for Oldroyd-B viscoelastic fluids with complex free surfaces in three space dimensions. A splitting method is used for the time discretization and two different grids are used for the space discretization in order to separate the advection terms from the others. The advection problems are solved on a fixed, structured grid made out of small cubic cells, using a forward characteristic method. The viscoelastic flow problem without advection is solved using continuous, piecewise linear stabilized finite elements on a fixed, unstructured mesh of tetrahedra. Numerical results are provided for the buckling of a jet and for the stretching of a filament where finger instabilities are observed. In the second part of the talk, a new stochastic model based on a reflected diffusion process is proposed. Its advantages together with different possible numerical approximations were discussed.

Owens [43] introduced a new haemorheological model accounting for the contribution of the red blood cells to the Cauchy stress. In this model the local shear viscosity is determined in terms of both the local shear rate and the average rouleau size, with the latter being the solution of an advection-reaction equation. The model describes the viscoelastic, shear-thinning and hysteresis behavior of flowing blood, and includes non-local effects in the determination of the blood viscosity and stresses. This is done through an advection-reaction equation for the extra-stresses, in the spirit of Oldroyd-B viscoelastic models. In the talk of Y. Bourgault, this rheological model was first briefly derived. A stabilized finite element method was next presented, extending the Discrete Elastic Viscous Split Stress (DEVSS) method of Fortin et al. [44] to the solution of this Oldroyd-B type model but with a non-constant Deborah number. A streamline upwind Petrov-Galerkin approach is also adopted in the discretization of the constitutive equation and the microstructure evolution equation. Test cases were next presented to assess the accuracy and computational requirements of the finite element method. The results show that the passage from a constant to a non-constant Deborah number in the Oldroyd-B model has a strong impact on the convergence of the method. Numerical challenges related to the solution of this rheological model were covered. The need for efficient FEM will be highlighted using a test case in an aneurytic channel under both steady and pulsatile flow conditions. Comparisons are made with the results from an equivalent Newtonian fluid. This choice of material parameters leads to only weakly elastic effects but noticeable differences are seen between the Newtonian and non-Newtonian flows, especially in the pulsating case.

Mathematical models for non-Newtonian fluid flows typically involve a system coupling the Navier-Stokes equations with other equations describing the mechanical behaviour of the material which are termed as constitutive equations. Numerical simulations can then be performed by judiciously choosing established discretizations of the Navier-Stokes equations and coupling them with adequate discretizations of the constitutive equations. Yet, the picture may not be so simple and years of computational rheology have indeed shown that intuitively good discretizations can be unstable. For viscoelastic fluids, this was often referred to as the High-Weissenberg Number Problem (HWNP). the talk of S. Boyaval discussed discretizations of the Oldroyd-B equation preserving a physical quantity that is also a Lyapunov functional for the Dirichlet problem, the so-called free energy. Another question of interest for these ”multiscale” systems of equations is how to reduce the computational effort needed by numerical simulations, even in simple geometries.

Multiphysics Techniques

The Immersed Boundary Method (IBM) has been designed by Peskin for the modeling and the numerical approximation of fluid-structure interaction problems and it has been successfully applied to several systems, including the simulation of the blood dynamics in the heart; see [35]. In the IBM, the Navier-Stokes equations are considered everywhere and the presence of the structure is taken into account by means of a source term which depends on the unknown position of the structure. These equations are coupled with the condition that the structure moves at the same velocity as the underlying fluid. Recently, a finite element version of the IBM has been developed, which offers interesting features for both the analysis of the problem under consideration and the robustness and flexibility of the numerical scheme; see [36, 37, 38]. The numerical procedure is based on a semi-implicit scheme for which we performed a stability analysis showing that the time-step and the discretization parameters are linked by a CFL condition, independently of the ratio between the fluid and solid densities. The mass conservation of the IBM is strictly related to the discrete incompressibility of the scheme used for the approximation of the fluid.

Data assimilation of distributed mechanical systems – i.e. estimation of uncertain physical parameters from a set of available measurements – can be performed through a variational approach, i.e. minimizing a least square criterion which includes observation error and regularization. One of the main difficulties of this approach lies in the iterative evaluation of the criterion and its gradient, often based on adjoint problem. In the work of J.F. Gerbeau another family of methods is considered: the sequential filtering. The model prediction is improved at every time step by means of the statistical information from observations and model output. Classical Kalman filtering is not tractable for distributed systems, but some effective sequential procedures were introduced recently for mechanical systems in [40] and are the basis of the proposed approach [39]. The resulting algorithm can easily be run in parallel, making the total time needed for the estimation similar to the duration of a sequential direct computation. Preliminary results were shown for blood flows in large arteries.

The talk of B. Fabreges presented a method to solve elliptic problems in domains with holes, in particular those which arise in fluid-rigid bodies simulations. It considered the system of the Stokes equations and the rigid body motion condition. To solve this system a fictitious domain method is used. In order to preserve optimality of the finite element approximation, a control approach is utilized (in the spirit of [41] and [42]) to build an H^2 extension, within the inclusions, of the solution. Thus, it uses a non-physical extension in the whole domain of the right-hand side of the Stokes equations as a control to enforce the rigid body motion. The idea is to find an extension of the right-hand side which leads to a solution of the Stokes equations that satisfies the rigid body motion condition. First of all it was proved that there exists such a right-hand side. Second the algorithm used to find an optimal control has the following features: It consists in minimizing a cost functional with a conjugate gradient method. The gradient of this functional is the solution of a Stokes problem, with Neumann boundary conditions, set within the inclusions. These Neumann problems are solved using fictitious domain methods around each particles which leads to the resolution of problems where the right-hand side is a single layer distribution on the boundary of the particles. One way to discretize these problems is to approximate the single layer distributions by a sum of Dirac functions. Rigorous numerical analysis of this method was also presented.

Y. Yotov discussed numerical modeling of Stokes-Darcy flow based on Beavers-Joseph-Saffman interface conditions. The domain is decomposed into a series of small subdomains (coarse grid) of either Stokes or Darcy type. The subdomains are discretized by appropriate Stokes or Darcy finite elements. The solution is resolved locally (in each coarse element) on a fine grid, allowing for non-matching grids across subdomain interfaces. Coarse scale mortar finite elements are introduced on the interfaces to approximate the normal stress and impose weakly continuity of the velocity. Stability and a priori error analysis is presented for fairly general grid configurations. By eliminating the subdomain unknowns the global fine scale problem is reduced to a coarse scale interface problem, which is solved using an iterative method. A multiscale flux basis is precomputed, solving a fixed number of fine scale subdomain problems for each coarse scale mortar degree of freedom, on each subdomain independently. Taking linear combinations of the multiscale flux basis functions replaces the need to solve any subdomain problems during the interface iteration. Numerical results for coupling Taylor-Hood Stokes elements with Raviart-Thomas Darcy elements were presented.

Massive Parallel Algorithms

The simulation of incompressible flows on very large unstructured meshes, that is up to billions of cells, leads to the important issue of solving the Pressure-Poisson equation on supercomputers grouping up to tens of thousands of cores. As the cost of this solving tends to be the largest part of the computational costs of the simulation, the issue of implementing as fast a parallel linear solver as possible becomes primordial. Multigrid methods, widely used on structured meshes, become more challenging to implement efficiently on unstructured grids ; whether geometric or algebraic multigrid methods are used, they actually require to refine the grid, which presents great difficulties for unstructured meshes. This seems to be a sufficient reason that deflation methods are preferred in this case. Many solvers used nowadays start by grouping cells from the fine mesh in order to create a coarse one, thus creating a ”two-level hierarchy of grids” on which a deflated solver is implemented (see e.g. [48] and [49]). In order to accelerate the convergence of the Pressure-Poisson equation solver, a deflation-based Preconditioned Conjugate Gradient solver has been implemented in Yales2 that benefits from a geometric multigrid-approach, that is : a three-level hierarchy of grids is created, so that the solution on the fine grid is computed thanks to a deflated solver, in which the solution on the coarse grid is computed thanks to a deflation on an even coarser grid. The whole program is stabilized thanks to the A-DEF2 algorithm described and tested by Tang et al. in [50]. As the number of iterations of the fine grid solver remains the same, the number of iterations of the coarse grid solver is dramatically reduced at every call by the deflation applied to it. Therefore, computational times for the Pressure-Poisson solver in parallel are reduced by up to 15 percent compared to the usual two-level deflated solver, which has to be confirmed by further testing for massively parallel use.

The talk of P. Minev discussed a new direction-splitting-based fractional time stepping for solving the incompressible Navier-Stokes equations. The main originality of the method is that the pressure correction is computed by solving a sequence of one one-dimensional elliptic problem in each spatial direction (see [51]). The method is unconditionally stable, very simple to implement in parallel, very fast, and has exactly the same convergence properties as the Poisson-based pressure-correction technique, either in standard or rotational form. The one-dimensional problems are discretized using central difference schemes which yield tri-diagonal systems. However, other more accurate discretizations can be applied as well. The method is validated on the lid-driven cavity problem showing an excellent parallel efficiency on up to 1024 processors.

Finite Volume Methods on Unstructured Grids

The talk of R. Eymard proposed an extension for the MAC scheme to any nonstructured nonconforming grid in 2D or 3D. This extension, dedicated to the approximation of the incompressible Navier-Stokes equations, is based on the following principles:

1. the degrees of freedom for the pressure are the values in the grid blocks of the mesh; they are associated to the discrete conservation of the fluid mass in each grid block;
2. the degrees of freedom for the velocity are the normal components to the faces of the mesh;
3. an interpolator is defined for reconstructing second order velocity at the faces of the mesh;
4. a finite volume operator is used for computing the viscous terms in a variational formulation;
5. the nonlinear term is discretized in such a way that it involves at most a positive contribution in the kinetics energy balance, in the case of the upstream weighting scheme.

It was shown that this scheme converges to a continuous solution of the Navier-Stokes equations, thanks to discrete analysis tools developped for the diffusion equation.

R. Herbin presented the study of numerical schemes for the simulation of the flow of compressible fluids, for which little is known up to now. It considered the "classical" Marker and Cell (MAC) scheme for the discretization of a "toy" problem, that is the steady state compressible Stokes equations, on two or three dimensional Cartesian grids. The discrete unknowns are the pressure located at the cell centers and the normal components of the velocity located at the barycenters of the interfaces of the pressure grid cells. Existence of a solution to the scheme is proven, followed by estimates on the obtained approximate solutions, which yield the convergence of the approximate solutions, up to a subsequence, and in an appropriate sense. Then it was proven that the limit of the approximate solutions satisfies the mass and momentum balance equations, as well as the equation of state: the passage to the limit in the EOS is the main difficulty of this study.

Outcome of the Meeting

The following important directions for further research were clearly identified:

- The phase field method possesses good potential for simulation of flows with free boundaries. Its mathematical theory requires further development. Some discretization issues around the interface are still open.
- Clearly one of the main challenges at present is the development of models and appropriate numerical methods for multiphysics problems. Significant progress was made in the coupling of porous media to Stokes flows. Fluid-structure interaction, however, requires a lot more attention. Its numerical analysis is still in its infancy and the numerical algorithms are expensive. The models used so far are mostly qualitative. Some important areas of applications like biological flows will require the integration of actual data in the simulations.
- Although the stabilization techniques are a focus of the community for many years, the progress is very slow. One very encouraging development is the combination with a posteriori based adaptivity which allows to minimize the effect of stabilization on the results and simulate complex phenomena like turbulent boundary layers for example.

- The appearance of powerful parallel computers clearly redefines the requirements to the numerical algorithms making their parallel performance one of the most important features. A new development is based on the direction-splitting techniques which allows to develop stable algorithms with a complexity similar to fully explicit methods.

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Two-day Workshop Reports

Chapter 41

Cascades topology (10w2165)

Apr 09 - Apr 11, 2010

Organizer(s): Veronique Godin (University of Calgary), Kristine Bauer (University of Calgary), Jens von Bergmann (University of Calgary), Peter Zvengrowski (University of Calgary)

The Cascade Topology Seminar was started in the early 90s by Steven Bleiler (Portland State Univ.), Douglas Ravanel (Univ. of Washington), and Dale Rolfsen (Univ. of British Columbia). It has continued since that time as a very successful biannual topology meeting for the Pacific Northwest region, although the original geographic terminology representing the Cascade Mountains of Oregon, Washington, and British Columbia has been broadened to include meetings in California, Nevada, Idaho, and Alberta. The CTS has also been run under the auspices of PIMS for the past half dozen years or so. The current meeting was the second to be held in Alberta, both taking place at BIRS. Very aptly, one can look out of the rooms at BIRS and have a striking view of nearby Cascade Mountain.

The influence of the original three founders was quite apparent at this meeting. Steven Bleiler was present and one of the talks, as well as a talk given a day before the meeting at the Univ. of Calgary (by Stanislav Jabuka), was related to his work. Dale Rolfsen has attended most of the meetings but this time he was well represented by his former graduate student Adam Clay, who gave the second lecture. Doug Ravanel, the third founder, moved to Rochester a number of years ago but his recent work with Hopkins and Hill was represented by the final talk of the meeting, given by Mike Hill.

Since the list of talks and participants is available to BIRS, we will just give a brief demographical summary in this paragraph. In total there were 26 participants. The 12 from the US came from California, Illinois, Indiana, Michigan, Nevada, New York, New Mexico, Oregon and Virginia. The 14 from Canada included 8 from Alberta, 4 from British Columbia, and 2 from Ontario. We have not listed the individual universities, but it is worth noting that for the first time a topologist (Ryan Budney) from Univ. of Victoria participated, a very welcome addition to the list of universities in the area that are active in topology. Indeed, the 45th Cascade Topology Seminar is already planned for Spring 2011 in Victoria. In total, there were 16 faculty members, 4 postdoctoral fellows and 6 graduate students in attendance.

Before turning to a brief description of the material covered in the lectures, here is a quote from an email of one of the participants, Rustam Sadykov, who is from Moscow State University, then spent two years in Japan, and currently is a postdoc at the Univ. of Toronto.

“The conference was very enjoyable and the organization was superb. To begin with the talks were interesting and well presented. I think the speakers did a superb job. Of course I was happy to finally meet you (the conference was a nice opportunity) and it was nice that we had time for a discussion. I hope that we will continue our cooperation.

As for the place of the meeting, it's perfect! Nature, hiking, nice food - all these also create a friendly atmosphere. I hope to participate in subsequent meetings as well. I also hope to have a chance to present my work at one of these wonderful meetings."

To obtain some perspective on the content of the lectures, let us go back to the CRG (Collaborative Research Group) that took place under the auspices of PIMS in 2003-2005. This CRG was divided into two halves, the first year concentrating on low dimensional topology and the second year on geometric topology and homotopy theory. Of course topology has grown during the 20th Century into an enormous subject, but it is probably safe to say that these two concentrations of the CRG represent the most important current trends and developments. One can easily make a strong case that topology has experienced the most significant growth of any branch of mathematics in the first decade of the 21st century, due to the solution of two outstanding conjectures in the subject. The first is the Poincaré Conjecture, which has received the most publicity (as one of the seven Millenium Problems). The second and more recent is the solution of the Kervaire Conjecture (also called the Arf Invariant One Conjecture), by Mike Hill, Mike Hopkins, and Doug Ravanel. In the author's view this is even more important than the Poincaré Conjecture, since it is not only basic to our understanding of space through the theory of manifolds, but is also fundamental to the understanding of stable homotopy theory (of course not everyone will agree with this view). In any case, having Mike Hill speak on this breakthrough as the final talk of the meeting was a very exciting and fitting conclusion to the meeting.

Indeed, each of the six talks represented significant new progress in various areas of topology as well as the closely related area of algebraic K-theory. The first two talks, given by Matthew Hedden (Michigan State Univ.) and Adam Clay (Univ. of British Columbia), were in the general area of low dimensional topology. Both of these talks were related to knot theory, but to different aspects of it. Hedden's talk dealt with the knot concordance group, the smooth version being denoted $\mathcal{C}$ and the topological version $\mathcal{C}_{top}$. There are some subtle differences between the two and the talk described significant progress in understanding this. Clay's talk dealt with a subject very dear to his supervisor, ordered groups. The first half of the talk gave a clear introduction to this topic and dealt mainly with algebraic questions. In the second half interesting topological applications were made, in particular to knot theory.

The next two talks, given by Eric Malm and Ralph Cohen (both from Stanford Univ.) came under the general heading of string topology. Cohen is an acclaimed authority in this area, and the main organizer of the meeting, Veronique Godin, was a student of his. The first talk emphasized some of the algebraic aspects of string topology arising from the celebrated Chas-Sullivan Theorem, with close connexions and analogies to Hochschild homology and non-commutative geometry. The second talk went more into some of the categorical aspects and the connexions with topological field theory.

The second last talk, by Teena Gerhardt of Indiana Univ., was mainly about algebraic K-theory as mentioned above. Computations in this subject are few and notoriously difficult, but she has succeeded in a few interesting examples. As one example,

$$K_{2i-1}(\mathbb{Z}[X]/(X^m),\ X) \approx \mathbb{Z}^{m-1},$$

while K_{2i} is not fully computed here but is known to have finite order $(mi)!(i!)^{m-2}$. We have already discussed the final talk by Mike Hill.

All these talks were presented using chalk and blackboard only, a most impressive achievement for the speakers and a most pleasant experience for the listeners, I believe, in this day and age of power point presentations that are nearly always so rapid as to be incomprehensible and often hardly even worth attending. To conclude, many thanks to the main organizer Veronique Godin, and the other organizers were Kristine Bauer, Jens von Bergmann, and myself, all from the Univ. of Calgary.

Participants

Bauer, Kristine (University of Calgary)
Bleiler, Steven (Portland State University)
Budney, Ryan (University of Victoria)
Clay, Adam (University of British Columbia)
Cockett, Robin (University of Calgary)
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Eldred, Rosona (University of Illinois at Urbana-Champaign)
Gerhardt, Teena (Michigan State University)
Godin, Veronique (University of Calgary)
Gomez, Jose (University of British Columbia)
Hedden, Matthew (Michigan State University)
Hill, Mike (University of Virginia)
Isaacson, Samuel (University of Western Ontario)
Jabuka, Stanislav (University of Nevada-Reno)
Johnson, Brenda (Union College)
Lam, Kee Yuen (University of British Columbia)
Malm, Eric (Stanford University)
Naik, Swatee (University of Nevada at Reno)
Peschke, George (University of Alberta)
Powell, Beth (University of Alberta)
Rahmati, Saeed (University of Alberta)
Ramras, Daniel (New Mexico State University)
Sadofsky, Hal (University of Oregon)
Sadykov, Rustam (University of Toronto)
von Bergmann, Jens (University of Calgary)
Zvengrowski, Peter (University of Calgary)

Chapter 42

Ted Lewis Workshop on SNAP Math Fairs in 2010 (10w2161)

Apr 23 - Apr 25, 2010

Organizer(s): Tiina Hohn (Grant MacEwan University), Ted Lewis (University of Alberta), Andy Liu (University of Alberta)

This was the eighth BIRS math fair workshop, named as The Ted Lewis Workshop on SNAP Math Fairs, which is becoming a popular annual event. The participants came from elementary schools, junior-high and high schools, from independent organizations, and from universities and colleges. The twenty participants at this year's workshop in are educators of all types, from teachers to grad students to expert puzzle and game designers.

The purpose of the workshop was to bring together educators who are interested in using our particular type of math fair, called a SNAP math fair, to enhance the mathematics curriculum. (The name SNAP is an acronym for the guiding principles of this unconventional type of math fair: It is student-centered, non-competitive, all- inclusive, and problem-based.) The projects at a SNAP math fair are problems that the students present to the visitors. In preparation, the students will have solved chosen problems, rewritten them in their own words, and created hands-on models for the visitors. At a SNAP math fair, all the students participate, and the students are the facilitators who help the visitors solve the problems. This process of involving students in fun, rich mathematics is the underlying vision that makes the SNAP program so unique and effective. No first prize! No arguments about judging! Everyone is a winner!".

At the BIRS workshop, the participants learn about and try math-based puzzles and games that they can use in the classroom. They have a chance to see how other teachers have organized math fairs at their schools, how the SNAP math fair fits the curriculum, and what some schools have done for follow-ups. And then they go back to their schools and change the culture of mathematics in their class-room.

This year we enjoyed several samples of math fair puzzles prepared by the students of St. Marys University in Calgary. The grad students from University of Alberta told us what they are doing in visiting schools in Edmonton area. We learned how to put on a math fair, shared some experiences from different schools all the way from Ontario with some of our participants. One of the highlights and talks that teachers specially found interesting was the talk by Dr. Elaine Beltaos about how the trends in the research of todays world of advanced algebra directly relates to the basic shapes and methods in an elementary classroom topic of triangles and groups. And of course we tried our hands on new puzzles presented by Dr Andy Liu .

The BIRS math fair workshops have contributed greatly to the proliferation and popularization of the SNAP math fair. In some places, the use of a SNAP math fair to change children's attitudes about mathematics has almost become a ”grass-roots” movement, and so it is difficult to pin down exactly how many schools are now doing them. We have a fair idea about the numbers in Edmonton and Calgary - for example over 60 percent of the elementary schools in the Edmonton catholic system now hold regular math fairs, and as far as we can gauge, the numbers are high in the public system as well. GENA reports similar figures for the Calgary area.

SNAP and CMS are also providing some support for the launch of a similar math fair workshop in the Fields institute in Toronto, and PIMS is providing math fair booklets for the participants. The Fields workshop is being organized by Tanya Thompson who has been a valuable participant at past BIRS workshops. Altogether, the BIRS math fair workshops are having a noticeable impact on mathematics education.

Regards,

Ted Lewis, Department of Mathematical and Statistical Sciences, The University of Alberta

Tiina Hohn Mathematics Department Grant MacEwan University

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Harris, Tara (Edmonton Schools)
Harris, Jessica (University of Alberta)
Hoffman, Janice (Edmonton Public Schools)
Hohn, Tiina (Grant MacEwan University)
Jacobs, Rebecca (St. Mary’s University College)
Leiser, Estee (St. Mary’s University)
Lewis, Ted (University of Alberta)
Liu, Andy (University of Alberta)
Marinova, Rossitza (Concordia University College of Alberta)
Mckenzie, Hannah (University of Alberta)
Nichols, Ryan (Edmonton Schools)
Pasanen, Trevor (University of Alberta)
Rainsong, Kathleen (St. Mary’s University College)
Rioux-Wilson, Judith (St.Catherine School)
Semenko, Svitlana (Edmonton Schools)
Wheeler, Jeanette (University of Alberta)

Chapter 43

Alberta Number Theory Days – L-functions (10w2162)

Apr 30 - May 02, 2010

Organizer(s): Paul Buckingham (University of Alberta), Matthew Greenberg (University of Calgary)

Overview

Alberta Number Theory Days fell at the very start of the newly formed PIMS CRG in Number Theory, and was thus an excellent opportunity to kickstart interactions between three of the participating institutions, the universities of Alberta, Calgary and Lethbridge. A broad range of topics in number theory were featured, but almost all talks were in areas motivated by the understanding of L-functions. Indeed, two key frameworks in which L-functions are viewed were addressed during the weekend, each forming a core of talks.

The first framework is the analytic study of L-functions with the view to deriving properties of prime numbers. This included a reformulation of the generalized Riemann hypothesis by Brandon Fodden in terms of a decidable property of the natural numbers, thus giving a new insight into this most important of conjectures. In a related direction, Amir Akbary (discussing joint work with Brandon Fodden) gave improved bounds on the power moments of L-functions in the Selberg class, with applications to principal automorphic L-functions and Artin L-functions. Kaneenika Sinha's presentation also concerned bounds, but this time bounds on the analytic rank of Jacobians of modular curves, an area of study with links to the famous conjecture of Birch and Swinnerton-Dyer.

The second framework is the overarching Langlands programme, one of whose principal goals is to equate L-functions of Galois representations, important objects associated with the absolute Galois group of $\mathbb{Q}$, with L-functions of automorphic representations. The talks of Clifton Cunningham, Vinayak Vatsal and Jeremy Sylvestre can be viewed under the umbrella of the Langlands programme, and a particular highlight was Cunningham's criterion for when a certain L-packet arising from an elliptic curve was infinite, a criterion given in terms of the set of supersingular primes of the elliptic curve.

It was also a delight to observe Dustin Moody's talk on a novel way to count isogenies between elliptic curves over finite fields via isogeny volcanoes. The closing talk of the conference, by Matthew Greenberg, demonstrated the impressive contribution that Dembélé, Greenberg and Voight have made towards the verification of a conjecture of Gross, with only one case remaining.

The context for the talks will be described more fully in Section 43.

Conference themes in more detail

Analytic number theory

One of the main principles in studying the analytic behaviour of L-functions is to be able to infer properties of the prime numbers. For example, the biggest open problem in this direction is the Riemann hypothesis, whose assertion is that the non-trivial zeroes of the Riemann ζ-function should all have real part $1/2$. The most important arithmetic consequence of this is a very precise description of the distribution of the primes in terms of the logarithmic integral Li. In the words of Enrico Bombieri, “In the opinion of many mathematicians, the Riemann hypothesis, and its extension to general classes of L-functions, is probably the most important open problem in pure mathematics today.”

Related to the Riemann hypothesis (a consequence, in fact, in the case of the Riemann ζ-function) is the Lindelöf hypothesis, which makes a prediction concerning the clustering of the zeroes of the ζ-function around the line $\mathrm{Re}(s) = 1/2$. It implies, in particular, a bound on the difference between consecutive primes.

Both of the above conjectures were featured in Alberta Number Theory Days. In the first case, it is known that the Riemann hypothesis is equivalent to a statement of the form $\forall n, P(n)$, where $P(n)$ is a decidable property of the natural numbers; this goes back to Kreisel. A property $P(n)$ which is more amenable to study was found by Davis, Matiyasevich, Robinson and Shapiro in 1976. **Brandon Fodden** discussed work in which he generalized this idea to the Selberg class, a class of Dirichlet L-functions proposed by Selberg [9] which satisfy certain standard expected properties of L-functions that arise in arithmetic contexts. More precisely, if f is a member of the Selberg class, then Fodden gives an explicit property $P(n)$ for natural numbers n such that the generalized Riemann hypothesis for f holds if and only if $P(n)$ is true for all n. As an application, he showed that when f is the L-function of an elliptic curve over $\mathbb{Q}$ – an archetypal member of the Selberg class – the property $P(n)$ is indeed decidable. By the work of Davis, Matiysevich and Robinson on Hilbert’s tenth problem, this therefore implies that the generalized Riemann hypothesis for f is equivalent to the insolvability of a Diophantine equation.

Now to turn to another problem associated with the Selberg class. The Lindelöf hypothesis for a member of the Selberg class can be reformulated in terms of the power moments of that series, which are integrals of powers of the given series along partial segments of a vertical line in the critical strip. Ramachandra showed that in the case of the Riemann ζ-function, the kth power moment is bounded below in terms of $T(\log T)^{k^2}$ under the assumption of the Riemann hypothesis, with Heath-Brown [5] removing that assumption a year later in 1981, at the cost of restricting attention to rational k rather than real k.

In the past five years, Laurincikas et al have succeeded in obtaining similar results for power moments of other Dirichlet series, inspired by Heath-Brown’s method. Principally they dealt with kth power moments where k is the reciprocal of an integer greater than 2. As discussed in his talk, **Amir Akbary**, together with Brandon Fodden, has obtained a quite general result on a class of Dirichlet L-series that can be specialized to include principal automorphic L-functions and Artin L-functions. In the former case, Akbary and Fodden’s result generalizes the aforementioned result of Laurincikas et al to rational k. In the Artin case, the lower bound given by Akbary and Fodden is $T(\log T)^{(\|\chi\|k)^2}$, where $\|\chi\|$ is the norm of the given character χ. This specializes, in the case of the Dedekind ζ-function of a Galois extension of $\mathbb{Q}$ of degree n, to the lower bound $T(\log T)^{nk^2}$, improving on a lower bound of Ramachandra.

A particular kind of L-function that is at the forefront of the geometric side of number theory is the L-function associated to some arithmetically defined abelian variety. Such an L-function is expected to hold important information about the arithmetic of the variety. For example, the order of vanishing of the L-function at 1, called the analytic rank, is conjectured by Birch and Swinnerton-Dyer (original form found in [1]) to be the rank of the group of rational points on the variety, also known as the algebraic rank. This conjecture on the analytic and algebraic ranks of an abelian variety over a number field is still only known in restricted cases.

In her talk, **Kaneenika Sinha** described how one can obtain upper bounds on the analytic rank of the new part of the Jacobian of the modular curve $X_0(N)$, at least when averaging over a sequence of consecutive values of N. More precisely, this bound is given in terms of the average of the dimensions of the spaces of new forms of level N and weight 2 for the same consecutive integers N.

The Langlands programme

Class field theory, the framework in which one aims to survey all abelian extensions of a given number field, could be said to have had its origins in the Kronecker–Weber Theorem, which asserts that every abelian extension of $\mathbb{Q}$ is contained in a cyclotomic field. One way to prove this theorem is via the information which goes into constructing L-functions associated with $\mathbb{Q}$. On the one hand, there are Artin L-functions for abelian Artin representations of $\mathbb{Q}$, and on the other hand there are Dirichlet L-functions for Dirichlet characters arising from the Artin representations. It turns out that the information that the latter gives about the former says enough about the splitting of primes in a given abelian extension of $\mathbb{Q}$ to establish that it must lie in a cyclotomic field.

The Langlands programme can be seen as a large-scale generalization of this phenomenon. Dirichlet characters are replaced by automorphic representations of the adelic points of a connected reductive algebraic group, and Artin representations by Galois representations into the Langlands "dual group" ${}^LG$. The philosophy is that there should be a way of assigning the latter to the former in a precise way, but in particular so that L-functions are preserved. If the programme is successful, the applications to L-functions, and number theory more generally, will be significant. Indeed, L-functions of Galois representations are in themselves difficult to study, but if we knew that they were equal to L-functions of automorphic representations, which are simpler to understand, a host of expected properties of the Galois L-functions would be confirmed.

When the algebraic group in question is GL_n, this assignment is expected to be bijective. However, in general this need not be the case, and the potential failure of injectivity gave rise to the notion of L-packets. These are defined to be the fibres of the assignment taking automorphic representations of G to Galois representations into ${}^LG$. In the local version of the conjectures, L-packets are finite, but this is not always the case in the global setting.

The infinitude of L-packets in the global setting was a point of commonality of the talks of **Clifton Cunningham** and **Vinayak Vatsal**. A highlight of Cunningham's talk was a characterisation of when a particular L-packet arising naturally from an arithmetic situation would be infinite. More precisely, if one considers the automorphic representation of GL_2 arising from an elliptic curve, then although the corresponding L-packet is a singleton, the L-packet once we pass by functoriality to SL_2 need not be. Indeed, as described by Cunningham, the L-packet of SL_2 is infinite if and only if the elliptic curve admits infinitely many supersingular primes. Note that this L-packet is therefore necessarily infinite for elliptic curves defined over a number field of odd absolute degree, thanks to Elkies' proof of the infinitude of the set of supersingular primes of such an elliptic curve [3]. Vatsal's talk also addressed differences between representations of GL_2 and SL_2, with emphasis on the effects on the non-vanishing of L-functions.

Also viewable in the context of the Langland's programme, the talk by **Jeremy Sylvestre** discussed depth-zero representations of GL_n of a local field, and θ-twists of these. The main aims of the talk were to show that the character of the twist satisfies a Harish-Chandra type integral formula, and to provide an equation for the character in terms of characters of depth-zero supercuspidal representations.

Volcanoes

in 1985, René Schoof [8] proposed an algorithm, later improved by Elkies and Atkin, for computing the number of points on an elliptic curve over a finite field, a key ingredient in the definition of the L-function of an elliptic curve over a global field. Some variations of this algorithm, known as the SEA algorithm after the principal contributers, employ so-called *isogeny volcanoes* as a way of organising the information about isogenies between elliptic curves. Constructing isogeny volcanoes is something of an ad hoc process. In his very illuminative talk, **Dustin Moody** outlined some improvements on algorithms for constructing isogeny volcanoes, with the aim of improving the efficiency. Applications of the method include identifying m-isogenies with m a prime or a product of two primes (not necessarily distinct).

Positive solutions to cases of a conjecture of Gross

Controlling ramification in extensions of number fields is not a straightforward process. In particular, the number of primes that ramify can be large, and demanding that only one prime ramify imposes significant restrictions. For abelian extensions of $\mathbb{Q}$, finding examples where only one prime ramifies is classical: one can just take cyclotomic extensions obtained by adjoining a root of unity of prime-power order, taking the maximal real subfield if one further wishes the infinite place to split completely. However, for non-solvable Galois extensions of $\mathbb{Q}$, the problem is still not entirely complete.

In [4], Gross conjectured that for each prime p, there should be a real non-solvable Galois extension of $\mathbb{Q}$ ramified only at p. (Note: In our present formulation of the conjecture, we opt to use Neukirch's convention on the terminology for the splitting of infinite primes [7, p.184]. Namely, infinite primes are always declared unramified, but are either split completely or not split completely. Thus in the above formulation of the conjecture, it is necessary under this convention to include the word "real", since "unramified outside p" does not capture this.) For $p \geq 11$, Gross' Conjecture is a consequence of the work of Khare and Wintenberger [6] on Serre's Modularity Conjecture, but for the primes 2, 3, 5 and 7, Gross' Conjecture saw no further progress until Dembélé's discovery [2] of a real non-solvable Galois extension of $\mathbb{Q}$ ramified only at 2.

In a very interesting talk discussing joint work with Dembélé and Voight, **Matthew Greenberg** revealed examples giving a positive solution to the conjecture for the primes 3 and 5. Building on the method of Dembélé for $p = 2$, the strategy of Dembélé, Greenberg and Voight used Hilbert modular forms to obtain systems of Hecke eigenvalues in the cohomology of a Shimura curve. The computations themselves are also impressive, exhibiting examples of fields with approximate absolute degrees of as much as $3 \cdot 10^{52}$. The case $p = 7$ of Gross' Conjecture is now the remaining unsolved case.

Concluding remarks

A number of participants commented on how much they enjoyed the conference, with particular reference to the high quality of the talks. The success of the weekend increases the likelihood that Alberta Number Theory Days, previously a one-day meeting, will remain a two-day event in subsequent years.

The organizers would like to thank BIRS and the Banff Centre for their hospitality and helpful staff, greatly adding to the enjoyment of the weekend. We would also like to thank the speakers for their hard work, and to acknowledge the generous support from PIMS and the universities of Alberta and Calgary.

Participants

Akbary, Amir (University of Lethbridge)
Buckingham, Paul (University of Alberta)
Cheung, Amy (University of Calgary)
Christie, Aaron (University of Calgary)
Cipra, Barry (Freelance)
Cunningham, Clifton (University of Calgary)
Fodden, Brandon (University of Lethbridge)
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Goswami, Souvik (University of Alberta)
Greenberg, Matthew (University of Calgary)
Guy, Richard (University of Calgary)

Jacobson, Michael (University of Calgary)
Kadiri, Habiba (University of Lethbridge)
Kostiuk, Jordan (University of Alberta)
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McNeilly, David (University of Alberta)
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Musson, Matthew (University of Calgary)
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Chapter 44

PIMS Mathematical and Statistical Graduate Education Roundtable (10w2062)

May 21 - May 23, 2010

Organizer(s): Malcolm Roberts (University of Alberta)

Introduction

The PIMS round-table on math/stat graduate education took place from the 21st to the 23rd of May, 2010. In attendance, by alphabetical order by university and name, were:

- from the University of Alberta: Thomas Hillen (faculty; graduate chair), Cody Holder (grad student; GAME president), Remkes Kooistra (grad student), Jochen Kuttler (faculty), Malcolm Roberts (grad student), and Tara Schuetz (administration);
- from the University of British Columbia: Neil Balmforth (faculty, AIM director), Peter Bell (grad student) David Kohler (grad student), Greg Martin (faculty, grad advisor), David Steinberg (grad student), and Lee Yupitun (administration);
- from the University of Calgary: Ted Bisztriczky (faculty, dept. head), Matthew Musson (grad student), Cristian Rios (faculty), Jedrzej Sniatycki(faculty, acting grad head), and and Colin Weir (grad student);
- from the University of Lethbridge: Wolf Holzmann (faculty) and Hadi Kharaghani (faulty, dept. chair);
- Michael Cavers (grad student) from the University of Regina;
- from the University of Victoria: Chris Bose (faculty), Kseniya Garaschuk (grad student), and Scott Lunney (grad student);
- from the University of Saskatchewan: Christine Soteros (faculty) and Raj Srinivasan (faculty, dept. head);
- and Alexander Dahl (grad student) from the University of Toronto.

The format of the workshop was a series of round-table discussion (though lacking an actual round table) which were led by a variety of people.

Graduate Student Involvement in Decision-Making and Governance

This discussion was led by Remkes Kooistra from the University of Alberta.

The subject of this discussion was the role of graduate students in the operation and decision making processes of a department. This mostly refers to graduate student participation on departmental councils and committees. Remkes began by talking about the written rules and policies that govern graduate student participation. For example, at the University of Alberta, there is university-wide regulation that creates a position for graduate student on department council. However, that policy is vague and relatively unknown, and it doesn't apply to departmental committees, which may not have easily accessible terms of reference. Clear guidelines for student participation are a good starting point, though often less important than culture and precedent.

Better participation might be achieved by clarifying the role of student members, and presented several different models, such as representative, advisory, and supervisory. Another idea for encouraging participation included an honorarium for students to sit on committees. This supports the idea that administration and committee work is a integral part of the academic life towards which many graduate students are working. It was suggested that perhaps committee work could be included in a TA duty, particularly for 3rd and 4th year PhD students.

The discussion then moved away from formal rules to discussing departmental culture: even if the rules are well written and available, departments need to set up a culture to encourage participation. Many aspects of departmental culture were discussed. Transparency is an important aspect of departmental culture. There is a need for confidentiality in many parts of governance, such a financial discussion, discipline, and awards. Departments may benefit from a more open governance in other areas, where students are able to attend meetings, view minutes and budgets, and understand how decisions are made. Openness in these areas can encourage participation from the student population. Transparency is not always consistent: e.g. when a student is recommended for withdrawal at the UofA, there is graduate student representation at the appeal level but not the departmental level. However, there is a risk of conflict-of-interest and confidentiality breaches; one suggestion was that the Departmental Graduate Committee should include a Graduate student from another department to maintain confidentiality.

Another cultural problem with some departments have struggled with is a clash between student and administration. Students need to feel that the department respects their opinions in order to have the confidence to speak up at council or committee meetings. This need for respect goes both ways, and it is important that students avoid a confrontational mentality. A culture of respect is necessary from both sides in order for student participation to be successful.

It is important to recognize the needs of both sides in order to maintain a culture that encourages cooperation. Remkes spoke with students and administrators at the University of Alberta to try to gather this information, and several points were raised at the round-table.

The administration has the following needs from students:

1. Feedback: The department needs students who can act as a conduit from the student body, can speak for the whole, and can inform the department of issues and problems affecting other graduate students.
2. Communication: The department needs students who can share with their peers what the department is planning, and can help educate their fellow students on policy.
3. Culture: Students need to be well-prepared and professional. In particular, students need to respect confidentiality.

Several idea were prominent on the student side:

1. Culture: Students wish to be treated as professionals.
2. Transparency: They want some level of oversight so they can understand departmental decisions.

3. Input: Students need to be able to influence how their department is run.

Research Internships

This discussion was led by Peter Bell from the University of British Columbia.

Industrial internships are available through a number of industries: MITACS IPS (4 month projects) and USRAs, and NSERC internships (12 month projects). Typically, the student must drive the work, including pitching the project to a supervisor and industry, and the funding organizations are often hands-off.

Prospective students who are uncertain about what to do with their degree are good candidates for internships, which can clarify for which jobs a math/stats degree is suitable. Obviously, internships can be an important source of funding, and may help recruit foreign students. Most importantly, there is a huge gap between the mathematics of academeia and those used by industry; internships can help bridge this gap, which could be as straight-forward as implementing an already-established technique.

Internships are difficult to organize:

1. The interaction with industry can restrict what one is able to research; pure science is more difficult to pursue, and the work is often not technically advanced.
2. These internships take real work to organize: the funding org. industry, faculty, and the student all need to be on-board. Some money also comes from the supervisor, which is not always available.
3. The results of the internship may be viewed as trade secrets, so the student and supervisor may not be able to publish the fruits of their labour.
4. The projects are often deadline-oriented, which limits the academic scope of the work. The projects may, however, be seeds for larger MSc/PhD projects.

There is pressure from government and industry that graduate students have skills suitable for industry; there is certainly interest in this area.

Teaching Graduate Students

This discussion was led by Thomas Hillen from the University of Alberta.

Skills students bring

Students enter a graduate program with an important skill set, which can be divided into two general categories (This list was compiled with math students in mind; stats requires somewhat different topic skills):

Soft Skills	Topic Skills
Language (reading and writing)	Math reasoning
Patient problem solving	Proof
Communication skills	Real analysis
Writing skills	Linear algebra
Math talent	Basic algebra
Passion	Computer skills

Determining if an applicant has these necessary skills is not a straightforward process, and there didn't appear to be a consensus on what methods were effective.

The soft skills can be checked by English proficiency exams (of questionable worth), interviews, reference letters, and the personal statement section of the application. Interviews can be very useful, and can be done relatively inexpensively via Skype, but may bias against students for whom English is a second language. Topical skills are estimated from transcripts and reference letters. Self-evaluation can also play an important role: by letting students know what material is expected of them, we can discourage students from applying to degrees beyond their current reach. Additionally, do-at-home entrance exams provide both applicants and institutions with an accurate evaluation while not preventing students from poor countries from applying, albeit at a higher administrative cost for the department.

Evaluation is important in the early stages of the degree. The PIMS universities have the following systems in place:

University	Type of Exam	Time-line (condition)
U of Vic	Qualifying exam	18 months
U of A	Stat entrance exam, core courses	10 days (no fail)
UBC	Entrance exam	2 years (no fail)
U of S	Qualifying exam	12 month
U of T	Comprehensive exam	1 year
U of C	Preliminary exam	1 year

Skills they learn

Teaching graduate students is obviously a complicated task. We provide but an overview in this section.

Each topic has its own particular set of skills. Soft skills are more universal. When students leave their program, they should have developed:

1. Communication: mathematical writing

2. A sense of mathematical taste,

3. Math outside course-work: The student should be able to study math without the direction of a classroom environment,

4. Networking: Conferences, collaboration, corporation, and

5. The ability to learn new fields.

This can be summarized as the “three Cs”: C^3 = competence, criticism, creativity:

Competence	Become an expert in something Responsible for program Ethical standards Be resourceful and ready beyond course material Learn to read papers Know how to get help Learn computer skills, software, latex TA skills Communicating research How to apply for grants/scholarships
Criticism	Self criticism Supervisor is not always correct Challenge ideas Æsthetics of math
Creativity	Direction by supervisor Teach to ask god questions Keep "big picture" in mind Lead by example Build confidence in their (students) own ideas Creative simplification

Some of these skills (e.g. those in the creativity category) may not be directly teachable, and discussion centered ways that we we can influence improvement in these areas.

Skills they need to find jobs

Students should be able to find a job when they leave. In addition to the skills listed above, graduates should be able to deal with complex systems, make connections between research areas, find structures, and generalize. They should have experience with committees, leadership, and teaching. Finally, it is important to know the job market (choose your supervisor and area wisely!) and have the potential to do research.

Recruitment Strategies and Open Houses

This discussion was led by Greg Martin and Lee Yupitun from the university of British Columbia.

How is recruitment important?

Recruitment is an important aspect to every graduate program if they are interested in attracting the best students to apply and to choose their university as the place to continue their graduate education. Collecting feedback from current graduate students is a good way to determine effective recruitment strategies and strengthen the department in general.

Why do students choose a particular university?

Most students who responded to the survey indicated that it was the faculty and areas of research that helped convince them to make their decisions. Other times, the reasons could be just personal, for instance, their spouse was offered admission there as well or it was closer to home. Another advantage is when the students already have friends attending the university and they have heard great things about it. Word of mouth is an excellent recruitment tool! Alumni and postdocs may encourage their students to apply if they had positive experiences at that university. The following key factors could also influence their decisions: financial offer, scholarships available, number of graduate courses offered, standard of living, tuition and university ranking.

Recruitment Strategies

1. Create a poster, postcards, or brochures for faculty or students to bring with them when they travel to conferences.

2. Faculty connections with other universities can help connect and encourage applicants from abroad to apply.

3. Reduce or waive the application fee for students from third world countries so that its more affordable for them to apply.

4. Host an open house for prospective students, especially those who have been offered admission but havent decided where to pursue graduate school.

5. Enhance your graduate website so that its easier to navigate and information is readily available for prospective students, for example, list of graduate course offerings, faculty and research pages.

6. Respond to emails promptly especially from prospective graduate students help them gather information about your program.

Graduate Student Self-Governance

This discussion was led by Colin Weir from the University of Calgary.

Math and stat graduate student organizations are a relatively recent phenomenon in PIMS universities. Their role in the department is often unclear and prone to change, the more so because of the high turn-over rate of graduate students. The following organizations are in place at participating universities:

University	Math-Stat GSA
UofA	GAME
UofC:	GUMS
UBC:	Math Grad Committee
UofR:	Math Actuarial Science Stats (MASS) (undergrad)
UVic:	MASCU (though much is done informally)
SFU:	MSU math student union (grad and undergrad)
ULeth:	Combined grad and undergrad organization
UofS:	TBA: still being organized
UofT:	MGSA

From the discussion, math-stat graduate student organizations (MSGSAs) were created to initiate policy change, coordinate existing events, help organize academic events, and for community outreach. MSGSAs can help the department:

1. as part of the recruitment strategy (e.g. UBC),

2. by providing a point-of-contact between administration and students,

3. by running various programs (e.g. graduate colloquia, graduate-level conferences, and mentoring new students),

4. by providing access to funds for graduate student activities,

5. by acting as a framework for providing graduate student representatives for other university committees, and

6. by highlighting the importance of graduate students in the department.

In addition to the problem of graduate-student turnover, MSGSAs face a variety of challenges. The student body is often not involved in the MSGSA (which is sometimes seen as a clique), increasing the workload for those that do participate and leading to burnout. This can be overcome by having a clear mandate, and advertising what the organization does. Notably, participation by stats grad students is often very minimal - perhaps because stats degrees are often industry-oriented, though the connection is not entirely clear.

Graduate Students as Instructors

This discussion was led by Raj Srinivasan from the University of Saskatchewan.

The natural progression is to first grade written work, then TA, and then lecture courses. Grading and TAing are important sources of funding for graduate students. A typical workload is 12 to 15 hours a week, often including exam grading. Training is often simply a pep talk at the beginning of term and occasional university-wide teaching seminars.

Should graduate students lecture? Lecturing is generally limited to students in the later years of their PhD program (UBC allows master's students to teach as well), often following university regulations. Grad students usually teach first or second year courses, often under the supervision of a mentor and/or with formal training. The results are generally positive. However, there are a variety of issues associated with graduate students lecturing:

1. Monetary:

   (a) Graduate students compete for teaching positions with sessional and post-docs, which may have first right of refusal.

   (b) Funding structures may prevent graduate students from teaching, e.g. if there are different costs for grad students or sessionals lecturing, or if graduate students cannot be paid from the sessional budget.

2. Philosophical:

   (a) First-year classes can be large and difficult to teach; smaller classes are better (but more expensive). Summer courses are a good option.

   (b) Grad school has a heavy workload: post-docs might be a more appropriate time to learn to teach.

   (c) On the other hand, teaching experience is important when applying to academic positions, even post-docs.

   (d) Teaching during grad school helps students decide if teaching is something they would like to pursue later in their career.

Whether students are to TA or lecture, training is important. UVic has a faculty position for graduate-student mentoring, which provides subject-specific training. Other solutions are teaching seminars (there was some discussion as to their effectiveness) and TA accreditation programs, as in UBC.

The consensus reached after this discussion was that graduate students should teach, keeping in mind that this not greviously interfere with their thesis- and course-work.

Inter-University Teaching Collaboration on Hot Topics

Universities in the Netherlands have a unique opportunity: the universities are so closely situated that it is feasible for students to attend classes at different universities each day. This allows special topics to be taught at one place to students from all the universities nearby.

The situation is quite different in western Canada, where commuting between universities isn't an option. However, technology is in-place in many PIMS universities to collaborate over the Internet using virtual-classroom technology and PIMS has already expressed interest in supporting such collaboration. The number-theory group at the UofA and the UofC are already using this for seminars; it is a natural extension to use this for classes as well. The facilities in place are:

Faculties	
U of SK	
U of C	Already used by number theory
U of R	Too small
U of Leth	
SFU	Coast to coast
U of A	Already used by number theory
U of BC	Being built

Thanks to the Western Deans Agreement, it is relatively straightforward to include such courses on a student's transcript. In terms of teaching, it needs to be decided how this will counted in the professor's teaching load, particularly if the class is team-taught by two professors at different universities.

The advantage of inter-university collaboration is that one is able to offer high-level classes which would otherwise not run due to lack of enrollment. Exactly which topics could be taught in what areas remains to be decided. A pilot project has been proposed as an action item (section 44).

Outcomes for Graduate Students

This discussion was led by Jochen Kuttler the University of Alberta and David Kohler from the University of British Columbia.

Where do students go after graduating? UofC, UVic, and UBC all have some data, but outcomes are generally unknown. The AMS collects data on employment; the CMS and PIMS do not, though NSERC has data on those students they funded during grad school. It was decided that we should gather more data on where students go after they graduate (section 44).

Employment in mathematics is heavily dependent on the field, university, and supervisor. Unpopular fields (even if still worthwhile) often won't lead to academic jobs, unless students switch fields and/or are extremely good. There was a generally reported administrative push to increase the size of the graduate program - this may be harmful, if there number of graduates is more than the job market can absorb. Knowing more about the job market for graduates would help us determine the correct course of action. The situations is quite different in stats, where there is a very good, industry-driven job market. PhDs are accordingly rare, which reduces competition for academic positions.

Four important outcomes were discussed:

1. Academic Track. Each professor produces more PhDs than are needed for replacement, and, despite a predicted "huge retirement wave", academic positions remain difficult to get. The post-doc system creates a difficult work environment, particularly for those wishing to start a family. In the last five hiring attempts at the UofA, no PhDs from Canadian universities were hired.

2. Industrial. One though was to orient masters programs towards industry. Noted employers mentioned were Google and NIST.

3. Educational. In contrast to the academic track, colleges and smaller universities hire mainly PhDs from Canadian universities. There is an increased demand for PhDs in math from recently university-accredited institutions.

4. The Love of Mathematics. It is important to mention this as a separate item: even if graduates end up working in a field other than what they studied, attaining a PhD in math or stats can be an end in itself.

Wrap-up and Action Items

The many interesting discussions we had over the course of the workshop will have an effect on our universities only if we act on them when we return. This report is the first step of that. This section also describes action-items we wish to see implemented.

Gather more data on student outcomes

It was noted in section 44 that we have very little data on where graduate students go after they graduate. This action item describes how we would like to rectify this.

For purposes of simplicity, it was decided to collect data on students who were graduated with a PhD in the last 10 to 15 years. They can be reached via their former supervisors (included perhaps in their annual report). The questions that we would like answered are:

1. Where are they now?

2. What job do they have? What path led them there?

3. What is the student's background? (Gender, citizenship, education.)

At the departmental level, we would like to know the immediate outcome for PhD students after they graduate.

David Kohler agreed to make the template for this survey.

Sample Exams for PIMS Universities

In section 44 it was suggested that sample exams be made available to students who are thinking of applying to grad school.

Thomas Hillen agreed to get sample exams and put them on the PIMS webpage so that all PIMS universities can use these in their application process. Thomas also agreed to start a project whose aim is to standardize the expectation for incoming students between PIMS universities.

Creation of a PIMS-level GSA

The idea was put forward during an informal discussion that we create a graduate student organization within PIMS. The mandate for this organization would be:

1. to organize the young researcher's conference in mathematics and statistics,

2. to organize future round-table meetings on graduate education,

3. to help organize shared graduate-level courses,

4. and to represent graduate students to PIMS by having a (non-voting) graduate representative on the PIMS board.

The PIMS GSA was thought to be a fairly flexible organization (perhaps as simple opting-in to a mailing list), and can be run via the PIMS offices in each participating university. Since graduate students are not able to travel extensively, the creation of a regional body was suggested as a more workable alternative to existing national organizations.

David Kohler, Colin Weir, and Cody Holder agreed to act on this item.

Inter-University Courses on Hot Topics

In section 44, we discussed teaching using WestGrid collaboration facilities. These are already in use for number-theory seminars between the UofA and the UofC.

Thomas Hillen agreed to collect ideas for what course to run for the winter term. He will send an email to round-table participants as a proposal. The immediate goal is to find people who are willing participate and start a pilot project to determine the effectiveness of the idea.

Future Round-Table Meetings

Follow-up is important if we want our ideas to have an effect. There was discussion about making the round-table an annual or biannual event. This item is part of the mandate of the PIMS GSA.

Conclusion

I would like to take this opportunity to thank the participants of this workshop for their time, ideas, and willingness to listen - this is particularly important for mathematicians; if you ask n mathematicians for their opinions, you can get up to $\aleph_n$ answers! I would also like to thank Thomas Hillen and Tara Schuetz for their help in organizing this workshop, and BIRS for their on-going support for not only this workshop, but the mathematics community in general. The research station is a unique institution, without which this and many other important workshops would not take place.

The workshop provided time for us to discuss an activity on which we expend a great deal of energy, but rarely have time to think about, and the more philosophical discussions were not included in this report not because they are unimportant. However, this round-table will be a success only if it influences how we run our graduate programs; follow-up is the most important part. I look forward to seeing the participants at future workshops.

Participants

Balmforth, Neil (University of British Columbia)
Bell, Peter (University of British Columbia)
Bisztriczky, Ted (University of Calgary)
Bose, Chris (Mathematics and Statistics, University of Victoria)
Cavers, Michael (University of Regina)
Dahl, Alexander (University of Toronto)
Garaschuk, Kseniya (University of Victoria)
Hillen, Thomas (University of Alberta)
Holder, Cody (University of Alberta)
Holzmann, Wolf (University of Lethbridge)
Kharaghani, Hadi (University of Lethbridge)
Kohler, David (UBC)
Kooistra, Remkes (University of Alberta)
Kuttler, Jochen (University of Alberta)

Lunney, Scott (University of Victoria)
Martin, Greg (University of British Columbia)
Musson, Matthew (University of Calgary)
Rios, Cristian (University of Calgary)
Roberts, Malcolm (University of Alberta)
Schuetz, Tara (University of Alberta)
Sniatycki, Jedrzej (University of Calgary)
Soteros, Christine (University of Saskatchewan)
Srinivasan, Raj (University of Saskatchewan)
Steinberg, David (University of British Columbia)
Weir, Colin (University of Calgary)
Yupitun, Lee (UBC)

Chapter 45

New geometric and numeric tools for the analysis of differential equations (10w2134)

Aug 13 - Aug 15, 2010

Organizer(s): Elizabeth Mansfield (University of Kent) Greg Reid (University of Western Ontario) Andrew Sommese (University of Notre Dame) Jukka Tuomela (University of Joensuu)

Summary

This meeting focused on geometrical approximation techniques and symbolic algorithms for differential equations with a particular focus on symbolic invariant calculus and discrete invariant calculus. A key goal of the meeting was to bring together researchers working at the intersection of the above areas; and highlight open problems in the development of these areas.

Remarkably for a 2 day workshop, the meeting attracted a very large number (32) of participants: 18 from Canada, 9 from the US and 5 from Europe. We had 3 undergraduates attend who gave well received posters. In an email after the meeting one told us that they had decided to continue to graduate research based on their experience. Another 4 in attendance were either PhD students or Postdoctoral fellows.

We mention some highlights of the presentations. Brynjulf Owren's (Trondheim) talk focused on a general framework for geometrical integrators for PDE. Most existing work has focused on ODE. Jonathan Hauenstein's (Field's PDF) presentation gave the first extensions of numerical algebraic geometry, an exciting emerging area, to the computation of non-unique equilibrium solutions for certain reaction diffusion systems. Conventional BVP techniques require initial guesses close to solutions - the new homotopy methods stably find all such solutions. Peter Hydon's (Surrey) talk gave algorithms for the computation of conservation laws for difference equations, essential for applications to numerics. Melvin Leok (UCSD) characterized the exact discrete Hamiltonian which provides an exact correspondence between discrete and continuous Hamiltonian mechanics, yielding a discrete Hamilton-Jacobi theory providing a new approach for discrete integrable systems. Olivier Verdier (PDF, Trondheim) described reduction procedures for arbitrary constrained linear PDE through generalizing a function space approach fulfilling an *inf-sup* condition to the constrained case. His examples included elastodynamics, and some "mixed" formulations of the Poisson problem, together with

subsequent application of Galerkin methods. Greg Reid described new developments in numerical Jet geometry, where jet manifolds of constrained differential systems are efficiently represented using witness points computed using numerical algebraic geometric techniques.

Despite a fairly dense schedule the talks were well attended and energetic discussion generated. A poster session was also well subscribed; as well as a book display. We, the organizers felt that the schedule was too dense, and that a 5 day format would have been more appropriate. Feedback from participants was very positive, especially from an enthusiastic group of undergraduates from Alberta. Strong participation from industry included Elena Shmoylova (Maplesoft) and Charles Wampler (General Motors) who spoke on a numerical local dimension test to compute the mobility of mechanisms.

In conclusion the meeting was very successful, driven partly by the rapid developments, and the enthusiastic response from participants.

Overview and Recent Developments in the Field

Our workshop proposal was prompted by remarkable recent progress in three areas in the geometric analysis of differential equations:

1. Geometrical Approximation Techniques
2. Symbolic Invariant Calculus
3. Discrete Variational Calculus

These topics are united under the umbrella of effective algorithmic algebraic-geometric approaches. Geometry, viewed as the study of group actions and their invariants, pervades all three. The aim of the workshop is to promote interaction between researchers from these areas, and to make progress on the many open problems that lie at their intersections. Computer implementation of methods is an important sub-theme of the workshop.

The basic idea behind these approaches is that geometric objects characterize various properties of differential equations. However, to study these properties in a constructive way we must first formulate the problem in algebraic terms and then try to solve the corresponding algebraic problem. In non-trivial situations this in turn requires the use of intensive symbolic and numeric computation.

Recent Developments and Open Problems

This new approach leads for example to applications of Lie group integrators for numerical schemes that guarantee the solution remains on the manifold of the Lie group. This is vital for geometric integrators such as those used in computer graphics where the animation needs to emulate the correct physics in order to be convincing. This would significantly extend the existing work on geometric integration pioneered by Iserles, Budd, Hairer and others (e.g. see [1]).

The deep connections between symmetries and conservation laws constitute the relationship between symbolic invariant calculus and variational calculus. The importance of variational principles in finite element techniques has prompted the recent development of discrete variational and discrete exterior calculus, and its related homological constructions. Our focus on unification of geometric and numeric methods means that variational calculus and its discrete formulations are of particular interest to us, and another of the three main areas of the workshop. There are several related major advances here. One is the seminal work of Douglas Arnold and his collaborators, in the construction of numerically stable “compatible discretisations” for the finite element method. Finally there are several important recent applications of the discrete variational formulations, such as Leok’s application of such methods to the Schrödinger Equation.

While algebraic methods are powerful and provide an algorithmic foundation for manipulations on the underlying manifolds, in each of the areas and applications above, they are not stable when applied to the approximate data that usually accompany real applications. Thus the other ingredient of our workshop, which addresses this issue, will be the new area of Numerical Algebraic Geometry. In this area solution sets of polynomial systems are represented stably by certain approximate (witness) points, which are efficiently computed by homotopy continuation methods. This topic was pioneered by Sommese, Verschelde and Wampler (with the first book on the subject by Sommese and Wampler [2]. Their work builds on previous work on homotopy methods and the computation of isolated solutions of polynomial systems by Allgower, Georg, Li, Morgan, Shub, Smale and others. Numerical algebraic geometry provides the first stable approximate version of algebraic geometry that deals with positive dimensional solution sets. Previous unsuccessful attempts had been more or less literal translations of exact approaches resulting in seriously unstable computations.

Objectives

The aim of the workshop is to foster interaction between mathematicians, engineers, and scientists working with algorithmic geometrical methods for differential equations at the intersection of the three areas: geometrical approximation techniques; symbolic invariant calculus; discrete variational and discrete exterior calculus. A key motivation underlying the objectives of the workshop is that problems from applications are now big enough and the inputs have enough numerical error that methods are needed that take full advantage of the geometry with the numerics always in sight. Symbolic tools should be used to the extent they can be, but in the end we need to develop tools that address problems that actually arise.

The expected outcomes include significant progress on creation and development of new algorithmic tools for the geometric analysis of differential equations and their approximations. Specific goals of the workshop include sharing progress made, open problems, and technical set-ups, with a view to developing or applying tools that utilize the best ideas in the three areas. In particular the specialists of each subtopic will learn of the techniques and software being developed in other areas which will help them to tackle overlapping facets of the common problems.

The relevant technical background comes from numerical algebraic geometry, algorithmic algebraic geometry, differential algebra, symbolic invariant calculus, moving frames, and invariantization methods. The growing common realization that nontrivial computational advances in the above sub-areas, requires a combination of geometrical and numerical techniques, has already prompted initial contacts between people working in the above sub-areas. While many conferences and workshops have considered geometric analysis of differential equations, and discrete exterior and variational calculus, none have considered them all with an underlying theme of approximation using numerical algebraic geometry.

The unique combination of themes exposes many new open problems and has a high potential for important breakthroughs. As examples we can cite combining Lie group integrators with numerical applications of moving frames; combining discrete variational methods with discrete exterior calculus in the context of Finite Element Methods; using Numerical Algebraic Geometry to characterize singular orbits of group actions and special solutions of PDE; determining hidden constraints and compatibility conditions using numerical approaches.

Further presentation highlights

Andrew Sommese (Notre Dame) gave an overview of Numerical Algebraic Geometry in his talk with applications on striping for Zebra fish and tumor growth models. Existing techniques only find highly symmetric tumors while the new homotopy techniques search for all solutions. In order to do this one must be able to analyze systems of thousands of nonlinear equations in thousands of variables. This is possible using a new technique called *Regeneration*. The standard numerical software for the solution of BVP for PDE is designed for the case where there are as many equations as unknowns (square systems). Jukka Tuomela presented a new framework for over-determined BVP based on using the compatiblity operator and the compatibility complex associated to the given overdetermined system. This permits the return to square systems and then standard finite elements can again be used, and at the same time the relevant constraints are taken into account. Promising numerical results were obtained for the Stokes problem and a microfluidic system. Tuomela also described open problems related to the algebraic computation of compatibility operators. Elena Celledoni (Norwegian University of Science and Technology) presented a new class of numerical methods for Hamiltonian systems that preserve an input first integral exactly.

Young faculty members Silvana Ilie (Ryerson), JF Williams (SFU) and Theodore Kolokolnikov (Dalhousie) gave well-received talks. In particular Ilie discussed geometric adaptivity that rigorously establishes polynomial cost numerical methods for constrained differential systems and scale-invariant adaptive geometric integrators for PDE with finite time blow up. B.K. Muite from the University of Michigan presented a poster *Numerical Study of the Davey Stewartson System* using geometric integration.

We even had some undergraduates attend the meeting, and contributed posters. One of them emailed us after the meeting to let us know that the positive experience had inspired him to continue to apply to grad school. New PhD student Austin Roche (Maplesoft) presented a poster on an equivalence method for functional decomposition of invariants and the Solution of Abel's equation. PhD student Wenrui Hao (Notre Dame) presented a poster on *A free boundary problem modeling tumor growth* using Numerical Algebraic Geometry. An enthusiastic group of undergraduates Paranai Vasudev, Philippe Gaudreau and Richard Slevinskyz from the University of Alberta presented some excellent posters (see the programme). Carl Wulfman and Yang Zhang (Manitoba) presented well received posters. A lively book display was also given with most of the authors in attendance [3], [2], [4] provided some good background material for the conference.

Participants

Anco, Stephen (Brock University)
Bluman, George (University of British Columbia)
Butz, Edward (University of British Columbia)
Celledoni, Elena (Trondheim Norway)
Gaudreau, Philippe (University of Alberta)
Hao, Wenrui (University of Notre Dame)
Hauenstein, Jonathan (Fields Institute)
Hydon, Peter (University of Surrey)
Ilie, Silvana (Ryerson Canada)
Kolokolnikov, Theodore (Dalhousie University)
Leok, Melvin (University of California, San Diego)
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Mazalov, Vadim (University of Western Ontario)
McCoy, Timothy (University of Notre Dame)
Muite, Benson (University of Michigan)
Owren, Brynjulf (Norwegian Institute of Science and Technology)
Reid, Greg (University of Western Ontario)
Roche, Austin (Maplesoft)
Shmoylova, Elena (Waterloo Maplesoft Inc)
Slevinsky, Richard (University of Alberta Campus Saint-Jean)
Sommese, Andrew (University of Notre Dame)
Tsogtgerel, Gantumur (McGill University)
Tuomela, Jukka (University of Joensuu)

Vasudev, Pranai (University of Alberta)
Verdier, Olivier (Norwegian University of Science and Technology)
Wampler, Charles (General Motors and Notre Dame)
Williams, JF (Simon Fraser University)
Wolf, Thomas (Brock University)
Wulfman, Carl (University of the Pacific)
Zhang, Yang (University of Manitoba)
Zheng, Zhonggang (Northeastern Illinois University)

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Chapter 46

Information processing, rational beliefs and social interaction (10w2133)

Aug 27 - Aug 29, 2010

Organizer(s): Giacomo Bonanno (University of California), James Delgrande (Simon Fraser University), Randy Goebel (University of Alberta), Jerome Lang (Universite Paris-Dauphine) Hans Rott (University of Regensburg)

Overview of the Field

The study of the mathematical aspects of belief formation, information processing and rational belief change is of central importance in a number of different fields, namely artificial intelligence, computer science, game theory, logic, philosophy and psychology. The area of belief change studies how a rational agent may maintain its beliefs about a possibly changing environment after obtaining or perceiving new information about the environment. This new information could include properties of the actual world, occurrences of events, and, in the case of multiple agents, actions performed by other agents, as well as the beliefs, preferences or actions (including communication acts) of other agents. Such agents could be acting and sensing in a dynamic world, coalescing information obtained from various sources, negotiating with other agents, or otherwise augmenting and revising their knowledge.

The most important question in Game Theory is how to rationally form a belief about other players' behavior and how to rationally revise those beliefs in light of observed actions. Traditionally Game Theory has relied mostly on probabilistic models of beliefs, although recent research has focused on qualitative aspects of belief change. A new branch of modal logic, called Dynamic Epistemic Logic, has emerged that investigates the effects of events that involve information being revealed to a group of agents in a variety of ways, such as through a public announcement or a private announcement. In artificial intelligence, the relatively recent emergence of the field of cognitive robotics, which is concerned with endowing artificial agents with cognitive functions that involve reasoning about goals, actions, the states of other agents, collaboration and negotiation, etc., has given impetus to the development of computational operators for belief change and the identification of issues arising from concrete, evolving sets of knowledge. Another, related, new field of research, called Social Software, maintains that mathematical models developed to reason about the knowledge and beliefs of a group of agents can be used to deepen our understanding of social interaction and aid in the design of successful social institutions. Social Software is the formal study of social procedures focusing on three aspects: (1) the logical and algorithmic structure of social procedures (the main contributors to this area are computer scientists), (2) knowledge and information (the main contributors to this area are logicians and philosophers) , and (3) incentiv! es (the main contributors are game theorists and economists). The area of belief change is thus of interest to many research communities. To date, there has been limited interaction among these communities. The purpose of this 2-day workshop was to bring together researchers from these different areas in an attempt to find some common ground and to identify general principles that underly the different approaches.

Recent Developments and Open Problems

The initial research in belief change came from the philosophical community, wherein belief change was generally studied from a normative point of view, providing axiomatic foundations about how rational agents should behave with respect to the information flux. Subsequently, computer scientists, especially in the artificial intelligence and the database communities, have been building on these results and relating them to computational systems. Belief change, as studied by computer scientists, not only pays attention to behavioral properties characterizing evolving databases or knowledge bases, but must also address computational issues such as how to represent beliefs states in a concise way and how to efficiently compute the revision of a belief state. More recently, the economics and game theory community, in particular the emerging field of cognitive economics, has become active in belief change research, adopting a normative point of view, like philosophers, but paying more attention to the ”cognitive plausibility” of the belief change operators.

Belief change is an area that leads to complex formal problems, not least of which is the problem of specifying an agent’s epistemic state. That is, not only must an agent’s beliefs be formally characterized, but so too must (effectively) the agent’s strategy for responding to new information. The dominant approach to belief revision is known as the AGM theory, following the pioneering contribution of Alchourrn, Grdenfors and Makinson (1985). The AGM theory deals with the transition from a belief state to a new belief state in response to a piece of information. Information is treated as veridical and the ”success axiom” is assumed, which requires that information be believed. While belief revision is an active area of research, there are important open problems that remain to be addressed or further explored.

The first open problem concerns the notion of information. Belief revision is about incorporating reliable information into one’s beliefs. What constitutes reliable information? Years ago, perhaps, a photograph could be taken as ”indisputable evidence”. Nowadays, with the advent of sophisticated image-editing software, photographs can be manipulated to misrepresent facts or to create the appearance of an event that did not happen. Videos and voice recordings are, nowadays, equally manipulable. What can one trust as a source of reliable information? The testimony of a witness? A newspaper article? A book? A television news report? A claim by the president of the USA? Many of us rely on the internet for information. Can material found on the internet be trusted as accurate? The theory of belief revision needs to address the issue of belief formation and revision in a world where no information can be fully trusted. Furthermore, in a social context, the ince! ntives to convey wrong information need to be studied and incorporated into a theory of belief revision.

A second open problem is how to deal with sequences of items of information which are in partial or full contradiction with each other. This can happen when the same source, over time, provides contradicting information or when different sources (e.g. different experts) provide conflicting information or different opinions or assessments. To some extent, this issue has been studied in the literature on iterated belief revision, where various principles have been suggested (for example, the principle that the most recent item of information should prevail over earlier ones). However, the proposed principles seem rather *ad hoc* and in need of a firmer foundation.

A third problem concerns the notion of ”minimal” belief change. The AGM theory is often referred to as a theory incorporating the principle that beliefs should be changed in a minimal way, so as to ensure that there is minimal loss of prior beliefs. While this is true when new information is compatible with prior beliefs, in the case where the new information contradicts the earlier beliefs, there is really no constraint imposed by the AGM postulates in terms of preserving as many of the old beliefs as possible. Indeed one way of revising beliefs, which is consistent with the AGM postulates, if to form a new belief set consisting exclusively of the learned information and anything that can be logically deduced from it. More work needs to be done on what minimal belief change entails.

Presentation Highlights

This was a multidisciplinary workshop, covering different fields. Two participants were from economics and game theory (Giacomo Bonanno, University of California Davis, USA and Daniel Eckert, University of Graz, Austria), two from philosophy (Hansa Rott, University of Rotenburg, Germany and Bryan Renne, University of Groningen, The Netherlands), three from computer science and artificial intelligence (James Delgrande, Simon Fraser University, Canada, Ken Satoh, National Institute of Informatics, Japan and Thorsten Schaub, Technical University of Darmstadt, Germany), one from linguistics (Jeffry Pelletier, University of Alberta, Canada) and one from Information Science and Media Studies (Thomas Ågotnes, University of Bergen, Norway). There was also a graduate student in computer science (Mehrdad Oveisi, Simon Fraser University, Canada). The first day of the workshop was devoted to individual presentations. However, the speakers were encouraged to avoid focusing on narrow t! echnical contributions and instead try to highlight approaches and issues that spanned more than one field. Each talk lasted 30 minutes. Giacomo Bonanno talked about using the AGM theory of belief revision developed in computer science and philosophy to gain new insights into game theory, in particular the solutions of dynamic games with imperfect information. Ken Satoh talked about the brand new field of Juris-informatics and the attempts to analyze principles of legal reasoning in terms of non-monotonic logic and counterfactuals. Thomas Ågotnes drew a connection between the methods and tools used to analyze cooperative or coalitional games and the relatively new field of dynamic epistemic logic. James Delgrande and Thirsten Schaub talked about new developments in the theory of belief revision, from both a theoretical and a computational perspective. Hans Rott talked about the connections between rational choice theory and principles of belief revision. Bryan Renne talk! ed about attempts to model communication and exchanges of opin! ions in terms of justifying one's own beliefs. Daniel Eckert drew a connection between model theory and impossibility results in social choice theory. Jeffrey Pelletier talked about experiments aimed at understanding how well people reason from a logical point of view. Mehrdad Oveisi gave an overview of his thesis where he analyzes changes in belief bases. Each talk was followed by a lively discussion. The second and last day was devoted to two round-table discussions which spanned the topics touched upon in the previous day as well as new topics.

Scientific Progress Made

Given the very short length of this workshop (one and a half day) one could not expect to achieve much in terms of scientific progress. However, all the participants agreed that the workshop had been very fruitful, both in terms of exposure to new topics and issues and in terms of highlighting possible new avenues for research.

Outcome of the Meeting

It is expected that one of the outcomes of the meeting will be to stimulate interdisciplinary research. During the several informal discussions that took place during the one and a half day, some of the participants saw the possibility of establishing new connections between their areas of research and talked about possible joint projects. It was also agreed that the workshop had been very beneficial and that a follow-up or similar workshop would be highly desirable. However, it was also agreed that a longer workshop that spanned more than one and a half days would be better. Six out of the ten participants came from very far (five from Europe and one from Japan) and felt that a longer workshop would be needed in order to justify traveling such a long distance.

Participants

Agotnes, Thomas (University of Bergen)
Bonanno, Giacomo (University of California)
Delgrande, James (Simon Fraser University)
Eckert, Daniel (University of Graz)
Oveisi, Mehrdad (Simon Fraser University)
Pelletier, Francis Jeffry (University of Alberta)
Renne, Bryan (University of Groningen)
Rott, Hans (University of Regensburg)
Satoh, Ken (National Institute of Informatics)
Schaub, Torsten (Universitat Potsdam)

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Chapter 47

Hierarchical Bayesian Methods in Ecology (10w2170)

Sep 10 - Sep 12, 2010

Organizer(s): Devin Goodsman (University of Alberta (Ph.D candidate), Christian Robert (Ceremade, Universite Paris-Dauphine), Francois Teste (University of Alberta)

Workshop Context

Ecosystems are dynamic in both space and time, hence involve multiple spatial and temporal scales, and are often heterogeneous in both of those dimensions, leading to spatial and temporal clustering. Accommodating this complexity in the context of scientific (statistical) hypothesis testing necessitates more advanced methods than those available within the classical null hypothesis testing paradigm.

Rather than ignoring ecological complexity, the modern approach in ecology is to incorporate this complexity into more realistic models. This leads to a more holistic portrayal and understanding of ecology. Once such models are constructed, they can be estimated based on the available data (and statistical principles). Environmental scientists can compare models of divergent ecological hypotheses by comparing their fit to data or predictive power. Thus an essential skill for modern ecologists is to be able to translate scientific hypotheses into ecologically relevant numerical constraints on natural processes, prior to more traditional statistical model comparison or model choice.

Ecologists use many types of statistical models to accommodate ecological complexity. These include random effect and multi-level models to incorporate clustering; ordinary and partial differential equations to model time-continuous changes through time and across space; and Markov models in discrete time that describe changes in ecosystems based on their previous state. There are many variations within each of these model types and many further types that are not covered here. Modern ecological models often have both stochastic and deterministic features, thereby accounting for the inevitable effects of measurement error, process error and natural variability on model performance. The Bayesian framework and paradigm [8] easily conforms to both temporal and spatial variability, as well as to both stochasticity and dynamical process models. However, from the ecologist user perspective, it requires a reasonably deep understanding of the tools of probability theory and probabilistic calculus, as well as statistical inference and stochastic approximation techniques.

Therefore, high-level “numerical literacy” has become an increasingly essential asset for modern ecologists. However, calculus, Monte Carlo approximation, and dynamical modelling courses are rarely part of graduate-level ecological training [1]. The resulting deficit in mathematical training leaves ecologists at a disadvantage and requires arduous self-teaching. This workshop was intended to introduce (mostly local) ecologists to advanced numerical and stochastic techniques and to modelling methodology for better accommodating ecological complexity.

Current Ecological Models

The heterogeneity of ecosystems means that they often require spatially explicit models: Moving from one domain to another corresponds to changes in ecosystem parameters and patterns. Incorporating heterogeneity in space and time is difficult using classical statistical methods while more tractable using Bayesian methods. As an illustration, ecologists have used a Bayesian model to reconstruct spatially correlated vegetation composition at a tree level based on fossilized pollen [2]. The complexity involved in reconstructing tree locations from pollen dispersal is evident. Wind impacts where pollen lands relative to the source plant and pollen disperses differently depending on the species.

Dynamical ecological models with unknown model parameters (to be estimated), incorporation of errors due to model inadequacy (termed "process error"), and observation errors are among the most sophisticated stochastic models used by ecologists [3]. These state-space models can be implemented in the frequentist statistical paradigm using the Kalman filter, with the limitation of the Gaussian requirement of this filter, or through Markov Chain Monte Carlo (MCMC) simulation methods in the Bayesian framework, which offers a much wider diversity in the modelling range. Although MCMC algorithms are now standard, their use in complex models remains limited by the current computing power. Due to their flexibility and novelty, Bayesian state space models are beginning to proliferate in the ecological literature despite the high learning cost due to their computational complexity. For instance, ecologists recently used such a model to predict tree growth based on sparse data from tree ring and diameter measurements [4]. State space models are appropriate for such data because they are able to fill in the gaps in the data with estimates, while acknowledging estimate uncertainty thereby enabling a more complete analysis.

Other types of dynamical ecological models involve changes in state variables over continuous time or space. The process models at the core of these dynamical models are often systems of ordinary differential equations. When many state variables are involved, and when there are many interactions in the model, these quickly become high-dimensional. At the current time, Bayesian methods provide the most feasible method of estimating parameters in high-dimensional systems while including stochastic processes to model uncertainty [5]. One example of such high-dimensional system is the ocean biogeochemical cycle involving nitrate, ammonium, dissolved organic nitrogen, phytoplankton, zooplankton and bacteria as state variables [6]. This biogeochemical cycle can be modeled with a system of six ordinary differential equations with parameters estimated using MCMC algorithms that take advantage of the availability of reliable prior knowledge [6]. The predictions of the model were true to observed temporal patterns demonstrating the utility of such methods [6].

Workshop Problems and Mathematical Approaches

Each of the participants brought models and datasets to the two-day workshop with the intention of exploring Bayesian parameter estimation techniques. The models that the participants brought to the workshop could be divided into three classes based on complexity and model type: The simplest models were random effect models which usually accounted for clustered experimental designs. The second class of problems were continuous time dynamical models, which typically had ordinary or partial differential equations modeling their processes. The third and most complex class of models were hidden Markov models which are to be fitted in discrete time. These include unmeasured latent variables, and allow for the estimation of observation and process error.

One ubiquitous model type in the whole of environmental science is the random effect model. Random effect models are a special case of both hierarchical and latent models [7]. One variant of random effect models is the random intercept model. A highlight of the workshop was an interactive and fruitful R programming session to estimate parameters for a random intercept Poisson regression of resin canals, a defensive tree trait, as predicted by two tree characteristics. The data were from lodgepole pine trees sampled in a clustered fashion in sites ranging from Grande Prairie to Sundre, Alberta. A Gibbs sampling algorithm was embedded in a Metropolis Hastings algorithm to build posterior probability densities for the parameters including the random intercepts. Posterior densities were built based on the data and uninformative priors. This elicitated a very strong response from the participants, because it showed how much a local decomposition by conditioning and the corresponding Gibbs sampler simplified the analysis of a globaly complex model.

Therefore, although far from being at the cutting edge of statistical science, this random effect model enabled participants to see Metropolis–Hastings and Gibbs sampling algorithms under a realistic perspective, applied to a hierarchical problem they knew. The simplicity of the model enabled participants to much better understand the underlying computational machinery, which can be difficult to apprehend at the conceptual level. Statistical approaches to the more complex model classes explored during the workshop involved application of the same computational machinery. The following models provided by participants are comparable in sophistication to those described in the Current Ecological Models section above.

Until recently, the dynamical models used by ecologists typically ignored observation uncertainty. However, dynamical models that incorporate observation uncertainty within the uncertainty around parameter estimates are increasingly common in the ecological literature. One such model explored during the workshop described the abundance and movement of planktonic larval lice from a salmon farm in the Broughton Archipelago. The process model was an diffusion-advection-decay equation:

$$\frac{\delta \mathrm{n}}{\delta \mathrm{t}} = D\frac{\delta^2 \mathrm{n}}{\delta x^2} - \gamma \frac{\delta \mathrm{n}}{\delta x} - (\mu_n + \theta_n)\mathrm{n}, \tag{47.1}$$

where n is the density of planktonic larval lice, the diffusion coefficient D represents the combined effect of tides and winds, and random movements of individuals, γ is the advection (flow) of larvae due to currents, and individuals die at a per capita rate of μn and transform to a post-larval life stage at a rate of θn.

The steady state solution of equation (47.1) gives the larval lice density along a 1-D corridor. One can obtain a likelihood function by assuming observed lice counts on fish are Poisson distributed, with an expected value equal to the model prediction. Using prior information for the parameters (D, γ, μ, θ), in combination with the calculated likelihood and the data for n, we can employ a Metropolis–Hastings algorithm to arrive at a posterior density function for each parameter that includes uncertainty due to variability in the data, and the uncertainty of prior information.

A hidden Markov model explored during the workshop differentiated between ice movement and polar bear movement based on data from global positioning collars that recorded bear movement, but did not distinguish between a bear's own movement and movement due to moving sea ice. The mathematical approach we discussed was to use a state-space model which includes two equations: The first was the observation equation which described the relationship between the movement of the ice and the movement recorded by the global positioning collars. The second equation was a process equation that described the movement strategies of polar bears.

Like with the simplest example, the parameters of this complicated model can be estimated using a combination of Gibbs sampling and Metropolis–Hastings algorithms. Gibbs sampling algorithms are especially useful for hierarchical structures such as those within state space models as they capitalize on conditional dependence relationships that result from the hierarchical structure [9]. In other words, they enjoy a local simplification that allows for a mostly straightforward implementation.

Outcome of the Meeting

The intention of this workshop was not to extend the boundaries of statistical science and to achieve new advances in statistical methodology *per se*. Rather, the objective was to enable ecologists, who are not directly involved in statistical research, to understand modern ecological models and to use modern statistical and Monte Carlo techniques in their on-going and future research. In order to accomplish this goal, it was essential that ecologists could freely communicate with statisticians at the forefront of statistical modeling. However, such an exchange requires some investment on the part of ecologists to raise their mathematical fluency and correspondingly a receptive ear from statisticians to understand which were the stumbling blocks towards a better understanding of those methods.

We are aware that many of the workshop participants found the pace of the workshop to be too fast and the material covered to be very challenging. We believe that future workshops dealing with complex ecological models require more than 2 days and more than a single interlocutor/statistical discourse. Two-day workshops—even such as the current running almost round-the-clock over the two days—provide enough time to understand basic applications without delving into mathematical complexity but obvious fall short of providing the “big picture” that would benefit the intended audience. Bearing this self-criticism in mind, we believe that the workshop nonetheless provided participants with the fundamental tools required to explore more complex ecological methods on their own, assuming they are willing to invest the time and effort. As evidence of this, an ecological modeling reading group was initiated at the workshop and continues to the present at the University of Alberta. Like the workshop, the objective of the reading group is to enable ecologists to understand and use sophisticated ecological models in their research. The reading group membership includes nine of the participants from the Hierarchical Bayesian Methods in Ecology workshop.

Participants

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Blanchet, Guillaume (University of Alberta)
Daemi, Maryam (University of Alberta)
Gaertner, Stefanie (University of Alberta)
Goodsman, Devin (University of Alberta (Ph.D candidate))
Hahn, Aria (University of Alberta)
Horn, Hannah (Heidi) (University of Alberta)
Koh, Saewan (University of Alberta)
Lopez, Claudia (University of Alberta)
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Chapter 48

Operator Algebras and Representation Theory: Frames, Wavelets and Fractals (10w2163)

Oct 08 - Oct 10, 2010

Organizer(s): Palle Jorgensen (The University of Iowa), Berndt Brenken (University of Calgary), Gestur Olafsson (Louisiana State University), Sergei Silvestrov (Lund University)

This weekend workshop offered a great opportunity for the participant researchers to further the subject, the ongoing collaborations, and to make headway on a list of problems. It helped us to gain insight into the open questions. The subject is at the cross roads of Operator Theory/Algebras, harmonic analysis, and applied mathematics.

Our workshop has been especially important for the young participants, postdocs and recent Ph.D students. Since many of us have met and collaborated at other conferences, we were able to make headway in the relatively short time. This includes research collaborations, planning, and exchange of ideas. This is vital for research advances, and headway was made with several research papers that had been in the planning stage for some time.

Presentation Highlights

The list of speakers with titles is as follows.

1. Marcin Bownik, Existence of frames with prescribed norms and frame operator
2. Peter Casazza, Kadison-Singer: A few results and a lot of questions
3. Jens Gerlach Christensen, Sampling and representations of Lie groups
4. Dorin Dutkay, Fourier bases on fractal measures
5. Jean Pierre Gabardo, Convolution inequalities and Beurling density of wavelet systems
6. Bin Han, Some results and open problems on nonhomogeneous wavelet systems
7. Deguang Han, Group representation frames: questions and partial results

8. Keri Kornelson, Operators on Bernoulli measures spaces
9. Michael Lamoureux, Generalized frames in seismic imaging
10. Shidong Li, Sparse dual frames and the most compact dual Gabor function
11. Peter Massopust, Exponential B-splines and the partition of unity property
12. Judith Packer , Operators arising from generalized multiresolution analyses
13. Qiyu Sun, Nonlinear Wiener's lemma and numerical implementation

Scientific Progress Made

This weekend workshop has allowed the participants to collaborate and to prepare for future longer workshops with time for in-depth follow-up. While the subject has always been closely related to quantum physics, very recently, other connections to more applied sciences, in particular to engineering, have emerged and stimulated research in mathematics which in turn has led to such interdisciplinary work as: wavelet theory, frame theory, fractals, function spaces related to representations, analysis on loop groups, the geometry of geometric tilings, approximation theory, numerical mathematics, and microlocal analysis; all topics covered in the workshop.

The Kadison-Singer conjecture

Overview of the Field

A main focus was an early problem in operator theory and quantum physics is the Kadison-Singer problem or conjecture on pure states, originating from the work of Paul Dirac: Does every pure state on the algebra of bounded diagonal operators on l^2 have an unique extension to a pure state on the von Neumann algebra of all bounded operators on l^2? In the past few years, it has been shown that this problem in operator theory and physics is equivalent to fundamental unsolved problems in a dozen areas of pure and applied mathematics and engineering. These equivalent problems includes the Paving conjecture, the Feichtinger conjecture in frame theory, and the Bourgain-Tzafriri conjecture in operator theory. This problem also has a strong connection to number theory (frames of exponentials) and to the theory of Toeplitz operators on reproducing kernel Hilbert spaces.

Recent Developments and Open Problems

While the subjects in the workshop are diverse, they were focused on a single conjecture; in turn known to be equivalent to fundamental unsolved problems in a dozen areas of pure and applied mathematics, and even in engineering. In mathematics this includes operator theory, Banach space, harmonic analysis, frame theory, including the theory of fusion frames, and signal/image processing. The first speaker was P. Casazza, who has been a pioneer, and recently, together with co-authors, has made great strides; see e.g., [1]. Renewed interest in these problems has also stimulated new advances in these other diverse areas of mathematics and applications.

Outcome of the Meeting

Frames, and their refinement, fusion frames, like the notion of bases, offer numerical representations of vectors. While the representations are stable, they are typically non-unique, hence their use in applications with intrinsic redundancies: filter bank theory, sigma-delta quantization, image processing, and wireless communications. Other applications to distributed processing and sensor networks in the human brain require clever splitting of large frame systems into sets of (overlapping) smaller systems.

The organizers and the participants have a long history of significant contribution to the field and collaboration, both in research and organization of workshops, special sessions and conferences. This includes a mini-workshop in Oberwolfach, two workshops on the Kadison-Singer problem at the American Institute of Mathematics, a week-long workshop at Banff International Research Station (BIRS, 2006), and several special sessions at AMS meetings.

The organizers.

Participants

Bownik, Marcin (University of Oregon)
Brenken, Berndt (University of Calgary)
Casazza, Peter (University of Missouri)
Christensen, Jens (University of Maryland)
Dutkay, Dorin (University of Central Florida)
Gabardo, Jean Pierre (McMaster University Canada)
Giordano, Thierry (University of Ottawa)
Han, Deguang (University of Central Florida)
Han, Bin (University of Alberta)
Jorgensen, Palle (The University of Iowa)
Kornelson, Keri (University of Oklahoma)
Lamoureux, Michael (University of Calgary)
Li, Shidong (San Francisco State University)
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Chapter 49

Canadian Math Kangaroo Contest Workshop (10w2174)

Nov 26 - Nov 28, 2010

Organizer(s): Rossitza Marinova (Concordia University College of Alberta), Valeria Pandelieva (Statistics Canada), Olga Zaitseva-Ivrii (University of Toronto)

The First Canadian Math Kangaroo Workshop was planned for a long time. The event, generously supported by BIRS and PIMS, became a reality in November 2010. Math Kangaroo city coordinators from the Greater Toronto Area, Ottawa, Montreal, St. John's, Winnipeg, Calgary, and Edmonton as well as volunteers from Edmonton and Calgary attended the workshop. Also, there was one participant from a city intending to organize the contest in the future. Eleven presenters gave talks, two of them undergraduate students.

Overview of the Field

In 2010, the international Math Kangaroo contest involved over 5.5 million students and hundreds of mathematicians from 46 countries internationally. The 2010 Canadian edition of the competition was administered in Ottawa, the Greater Toronto Area, Edmonton, Calgary, Montreal, St. John's, Winnipeg, Sudbury, Langley, and Lunenburg. Almost 1200 students participated in the contest, and hundreds were involved in various training and learning activities prior to the contest day.

The Math Kangaroo outreach programs focus on providing students in the age range of 8 to 18 with the opportunity to experience and explore mathematics. The organization's purpose is to share the joy of mathematics with youth through an annual math competition and short-term and year-long training opportunities. Since joining the International Association in 2006, the Canadian Math Kangaroo is continuously seeking ways to further expand its geographic reach and its high-demand unique programs.

Recent Developments and Open Problems

The Canadian Math Kangaroo program contributes to the science, engineering and education communities through its activities that revolve around the contest but go far beyond its organization.

- Practice sessions and math clubs provide opportunities for school children to explore and expand their math and logical skills in a non-competitive environment; they inspire and promote interest and excellence in math and science. More than 500 students per year receive training.

- Math Kangaroo engages university students; they gain a valuable experience by volunteering in the preparation and delivery of the training, as well as in the supervision and marking on the contest day.
- Canadian Math Kangaroo provides professional development for teachers and educators; workshops at professional conferences enhance their knowledge in the field of challenging mathematics.
- The math outreach educational materials developed through Canadian Math Kangaroo help teachers and parents to reach each student and address individual strengths and learning styles.
- Universities benefit from the students' visits on campus; they organize recruiting and promotion activities, simultaneously with the CMKP activities.
- Canadian Math Kangaroo activities not only promote mathematics; they build confidence and inspire further interest in math and science. Moreover, they build a sense of community and provide enjoyable experience to everyone involved.
- Canadian Math Kangaroo activities are family-oriented. Parents and older siblings volunteer during the training activities, participate in the informal parents' contest, and enhance their own knowledge and appreciation about science through numerous activities such as lectures by university professors on science topics, science presentations, and engineering summer camps, etc.

The Math Kangaroo contest is unique to Canada. Students can participate in it independently of their home school's involvement. It is one of the very few math contests available for Canadian elementary students. While the reputation, the merit, and the quality of inspired learning are at a very high level, the atmosphere on the contest day is unique compared to most of the other contests. Students get the chance to be in real university classrooms; the friendly and welcoming space is enhanced by snacks and small presents; the content is not boring (in fact, the Math Kangaroo is considered a contest-game because of the intended fun element of the problems). Last but not least, the competition allows international comparability of standards, which can be of interest for researchers in the area of math education.

The positive feedback Canadian Math Kangaroo organization receives from parents, students, teachers, and communities proves that its activities are in a high demand. Some of the needs merge with the broader call and need for increasing the overall mathematical, scientific, and technological literacy and skills of young Canadians. However, the most prominent need for the program is to correct the existence of a gap in the math and science outreach programs and activities for elementary students. The Canadian Math Kangaroo team believes in the benefits of exposing young school children to math challenges. This belief is in agreement with the leading educational and cognitive research in the field. Studies confirm that it is extremely important to start challenging these students at a younger age, ”well before students reach the sixth or seventh grade” [1]. Delivering high quality year-long training programs across Canada, and providing students with opportunities to express themselves in competitive events and informal communications, significantly contributes to improving their analytical skills and helps them build confidence, which, in turn, motivates them to advance and to look for new challenges and goals.

Presentation Highlights

The workshop consisted of eleven presentations and several discussions on topics of interest to the organization and the workshop participants.

- **Valeria Pandelieva**, President: Opening remarks; current state of the organization in Canada; International sense and news; general information regarding the 2011 Math Kangaroo contest.

  Valeria Pandelieva started with a brief history of the Canadian Math Kangaroo and its relationship with other similar organizations including the international organization ”Kangaroo without Borders.” The annual meetings of the international association are held every October in one of the member countries. Also, information in regard to the next year contest was provided to the audience.

- **Rossitza Marinova**, Finances: Financial matters, fund-raising information and initiatives.

  Financial challenges the Math Kangaroo organization face were presented and discussed. The financial statements of the organization were reported. The presentation also included fund-raising initiatives recently taken by the Canadian Math Kangaroo. As well, a discussion took place on how to attract funding for local activities that are specific for the individual cities.

  The planned activities and associated budgetary challenges were presented and discussed. These include:

  - Canadian Math Kangaroo Contest;
  - Training activities: math clubs, practice sessions, online interactive training, local summer Math Kangaroo camps, international summer Math Kangaroo camps;
  - Expert support to broader professional educational communities: developing learning materials, professional development opportunities for teachers, research in math competitions and math education;
  - Promotional math and science-related activities for the general public: special sessions for bringing together interactive, hands-on science and engineering experiences.

- **Olga Zaitseva**, Problems Coordinator: Math Kangaroo as the first jump to Mathematics.

  Olga Zaitseva explained the way the contest problems are selected and edited. There are challenges associated with the French version of the problem sets that will have to be solved as soon as possible. Also, the presentation included the importance of organizing long-term training activities such as math clubs. Math clubs run for a long period of time and have a stand-alone curriculum composed of appropriate math enrichment topics. The math clubs are environments in which a greater depth and breath of the training can be achieved. Development of relevant materials for training is work in progress.

- Next, the regional representatives gave 10-15 minutes presentations regarding the competition in their city. These presentations included: *Calgary* (**Mariya Svishchuk**); *Edmonton* (**Rossitza Marinova**); *Montreal* (**Ildiko Pelczer**); *Ottawa* (**Todor Pandeliev**); *Toronto* (**Sophie Chrysostomou**); *St. John's* (**Margo Kondratieva**); *Winnipeg* (**James Currie**).

- **Eddy Essien** presented the Website, in particular users' view and administrator's view; what is in place, what is coming, what will be good to have. The audience suggested better support to regional representatives to be provided through the Website, which include:

  - Bank of forms and templates to be created and made accessible from the administrator portal. New forms and templates to be added by all cities.
  - Bank with shared training materials to be made available.
  - Bylaws and instructions for regional representatives to be posted on the Website.
  - Pages for regional centres to be created and made accessible from the main Website.
  - Other technical details for improvement of the Website.

- Another important presentation followed by a discussion was the club and contest organizational matters given by **Josey Hitesman**. this included how to recruit volunteers, positions, code conduct, and other business/management issues. It was decided that relevant materials will be provided to all participants and made accessible through the administrator portal.

- The last presentation was about the IEEE Teacher In-Service Program (TISP) and the Math Kangaroo delivered by **Mooney Sherman**, the chair of the IEEE Northern Canada Section. Mooney Sherman introduced IEEE and TISP and also discussed some security and confidentiality issues.

Meeting Progress Made

Extensive discussion took place on how to do *marking and calculating the contest results*. Indeed, the Website and its functionality are important for assisting administrators.

It has been noted that there is a need for *more regular communication*; a forum could be used for this purpose. Of course, annual meetings are still needed; however, communications take place throughout the entire year, in particular during the period January - May.

Promoting the contest and its accompanying programs was discussed. It was made clear that the Canadian Math Kangaroo organization prefers to associate with academic institutions rather than organizations aiming to promote their business through the competition. An outcome of this discussion was that some of the participants offered help in attracting new centres through universities.

The Canadian Math Kangaroo outreach programs aim to dispel the myth that mathematics is boring by creating a positive environment with fun events that emphasize the practical nature of mathematics. The IEEE TISP connections could be used for *joint activities of Math Kangaroo coordinators and IEEE volunteers*, example of which was the IEEE TISP Math Kangaroo project in Edmonton.

Ideas for inspiring *award ceremonies* were shared. For example, Edmonton and Calgary invite students to perform during the awards day which makes the day very special to parents, winners, other guests.

Exploring opportunities for *math clubs and summer math programs* would be activities of the local centres, which will be supported by the Canadian Math Kangaroo if funds are available. It is nice to see that lots of city started or plan to start math clubs in near future.

Organizing *workshops for teacher's and teachers candidates* on challenging math content was suggested. These workshops could be delivered during teachers conventions and conferences.

A plan for *development of materials for training* was proposed. Several workshop participants expressed interest in contributing to a series of math club materials that the Canadian Math Kangaroo will develop and publish.

Research into students performance is another aspect of the Math Kangaroo contest. This includes research in the field of math competitions and math education (e.g., conducting studies and presenting results to conferences and peer-reviewed journals). A discussion took place on how results can be used including privacy and confidentiality issues.

Outcome of the Meeting

The workshop is a significant milestone for the Canadian Math Kangaroo Contest organization. Representatives from various cities and provinces had their first meeting to exchange ideas and discuss issues.

The major meeting outcomes include:

- Groups were formed to develop online training program, math clubs and other training materials. Of course, existing materials will be shared among coordinators through the administrator's interface of the website.

- The sets of solutions from past three years (2008-2010) was distributed for editing.

- A small group worked on the selection of problems for the 2011 edition of the contest.

- Decisions were made on issues associated with the Website that will be implemented for the 2011 contest; others changes will be started and completed after the 2011 contest.
- Financial matters were discussed and budgetary specifics for the local centres.
- Holding workshops for teachers workshops on challenging mathematics and the ways to expose young students with diverse learning abilities to it.
- Organizing activities with the purpose to show how mathematics, science, and engineering are related through collaboration with other organizations such as IEEE Canada.
- Math Kangaroo centres are encouraged to organize local summer camps that will run for a week during the summer holidays, and will provide participants with rich instructional and problem solving experience, as well as with opportunities for socializing and communicating with other people of similar interests.

Participants

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Killough, Brady (Mount Royal University)
Kondratieva, Margo (Memorial University of Newfoundland)
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Meneses, Laura (Mount Royal University – Guest)
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Sherman, Mooney (IEEE Northern Canada)
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Focused Research Group Reports

Chapter 50

Hyperbolicity in the symplectic category (10frg147)

Mar 28 - Apr 04, 2010

Organizer(s): Richard Hind (University of Notre Dame), John Bland (University of Toronto), Marianty Ionel (University of Toledo), Min Ru (University of Houston), Jens von Bergmann (University of Calgary)

In this report, we remember our dearest friend and colleague, Pit-Mann Wong. It was his inspiration which lead to the proposal for this workshop and its organization. In the weeks before the workshop, he was diagnosed with a severe form of liver cancer, and was unable to attend the workshop; unfortunately, he has since passed away, on July 3 of this year. We will remember him and miss him.

Overview of the Field

The Kobayashi metric is a key intrinsic quantity associated to complex manifolds, if it is nondegenerate then the manifold is said to be hyperbolic; the study of hyperbolicity is central in much of complex geometry. This workshop aimed to extend notions and theorems regarding hyperbolicity to the (much more general) area of almost-complex and symplectic geometry, thus finding a range of applications to an exciting field of modern mathematics.

Let (M, J) be an almost complex manifold and $\Delta_r, r > 0$, be the disc of radius r, centered at the origin, in the complex plane $\mathbb{C}$. At a point $x \in M$ and a tangent vector $v \in T_xM$, denote by $\mathrm{H}ol(\Delta_r, M)(x, v)$ the space of all J-holomorphic curves from Δ_r into M with the properties that $f(0) = x$ and $f'(0) = v$. The J-Kobayashi pseudo-metric is defined by

$$\kappa_J(x, v) = \inf \frac{1}{r}$$

where the infimum is taken over all $r > 0$ such that $\mathrm{H}ol(\Delta_r, M)(x, v)$ is non-empty. An almost complex manifold (M, J) is said to be *J-Kobayashi hyperbolic* if $\kappa_J(x, v) > 0$ of all $x \in M$ and $v \neq 0$.

A compact almost complex manifold M is said to be J-Brody hyperbolic if there are no non-constant J-holomorphic curves $f : \mathbb{C} \longrightarrow M$. This implies, in particular, there are no rational or elliptic curves in M.

It is easy to see that J-Kobayashi hyperbolic implies J-Brody hyperbolic. The converse is false in general, however it is valid if M is compact;

Lemma 0.1 *For a compact almost complex manifold (M, J), J-Kobayashi hyperbolic is equivalent to J-Brody hyperbolic.*

In the complex case this is a consequence of Brody's reparametrization lemma together with a convergence argument using the fact that M is compact. In the almost complex case the argument is identical since Brody's reparametrization lemma only acts on the domain and the existence of a convergent subsequence follows from Arzela-Ascoli.

Recent Developments and Open Problems

In the literature there are several results concerning J-hyperbolicity. Bangert showed in [Ban98] that T^{2n} equipped with a standard symplectic structure ω is not J-Brody-hyperbolic for any ω-tame almost complex structure J. These results were extended by Biolley in her thesis [Bio04], where she proves the same result for a Stein manifold satisfying an algebraic condition in Floer homology. In all of these cases, the manifolds were shown to be not J-Brody hyperbolic for all tamed almost complex structures J.

On the other hand, Duval showed in [Duv04] that the complement of 5 J-holomorphic lines in $(\mathbb{P}^2, \omega_{FS})$, where J is any ω_{FS}-tame almost complex structure, is Kobayashi-hyperbolic.

Scientific Progress Made

In the results in the literature concerning J-hyperbolicity described above, a symplectic manifold was shown to be either hyperbolic or not hyperbolic for all tamed almost complex structure. We extend these examples by investigating the hyperbolicity of the complement of a divisor in ruled symplectic surfaces.

We review some necessary background on symplectic ruled surfaces. For details we refer the interested reader to [MS98]. Let $\pi : X \to \Sigma$ be a smooth sphere bundle over a compact genus g Riemann surface Σ. Up to diffeomorphism there are exactly two such bundles for each g, the product $X_0 = S^2 \times \Sigma$ and the non-trivial bundle X_1. The trivial bundle X_0 admits sections σ_{2k} of even self-intersection number $2k$ and the non-trivial bundle admits sections σ_{2k+1} of odd self-intersection number $2k+1$. The second homology group $H_2(X;\mathbb{Z})$ is generated by the class of a section and the class of a fiber f, and we have $[\sigma_n] + f = [\sigma_{n+2}] \in H_2(X;\mathbb{Z})$, $[\sigma_n] \cdot f = 1$, $[\sigma_n] \cdot [\sigma_n] = n$ and $f \cdot f = 0$. It is completely understood which cohomology classes can be represented by symplectic forms and any two cohomologous symplectic forms on X are symplectomorphic.

Examples of such bundles are given by taking a holomorphic line bundle $L \to \Sigma$ and setting $X = \mathbb{P}(L \oplus \mathbb{C}) \to \Sigma$.

Let (X, ω) denote a symplectic sphere bundle over a Riemann surface of genus g and let J be an ω-tame almost complex structure on X. Denote the homology class of a fiber by f and let s denote the section with self-intersection 0 or 1, depending on whether X is the trivial or non-trivial bundle, respectively.

Definition 50.0.0.8 *Fix a symplectic ruled surface (X, ω) with tamed almost complex structure J.*

Let m and n be non-negative integers and let L_f be the disjoint union of images of m J-curves in the class f, and define L_σ to be the union of images of n generic smooth J-curve in the class $[\sigma_{k_i}]$ for some integers $k_1, k_2, \ldots k_n$, assuming that such curves exist. Here generic means that every J-curve in the class f intersects L_σ in at least $n-1$ distinct points. Set $L = L_f \cup L_\sigma$. Then set

$$X(m, n) = X \setminus L.$$

Theorem 1 *$X(m, n)$ is J-Kobayashi hyperbolic if either*

- *$n \geq 4$, and one of the following holds*

  1. *$g > 2$ or*

2. *$g = 1$ and $m \geq 1$ or*
3. *$g = 0$ and $m \geq 3$,*

or

- *$n = 3$, X is the trivial bundle and all curves in L_σ represent the class of the trivial section $[\sigma_0]$.*

Theorem 2 *$X(m,n)$ is not J-Kobayashi hyperbolic if either*

- *$n < 4$ (unless $n = 3$, X is the trivial bundle and all curves in L_σ represent the class of the trivial section $[\sigma_0]$), or*
- *$g = 0$ and $m \leq 2$, or*
- *$g = 1$ and X is the trivial bundle and $m = 0$.*

We also have one theorem giving a criterion of the non-hyperbolicity of symplectic manifolds admitting a plurisubharmonic exhaustion.

Theorem 3 *Let (M, J_0) be a symplectic manifold, possibly with boundary. Suppose there exists a J_0-plurisubharmonic exhaustion ψ with uniformly bounded gradient with respect to the metric of the compatible triple $(\omega = d\, d^{\mathbb{C}}\psi, J_0, g_0)$ and so that the curvature is uniformly bounded.*

Then (M, ω, J) is hyperbolic for any uniformly tamed J that is uniformly bounded w.r.t g_0.

Open Questions

The results concerning the hyperbolicity of the complement of a divisor in a ruled surface are incomplete since the case of the non-trivial bundle over T^2 with no section removed is not addressed. Moreover, the theorem only applies where L is the union of distinct curves as described. It would be nice to extend this to the case where L is a general divisor in the class. But this is much harder and very little is known even in the complex category.

Participants

Bland, John (University of Toronto)
Brudnyi, Alex (University of Calgary)
Hind, Richard (University of Notre Dame)
Ru, Min (University of Houston)
von Bergmann, Jens (University of Calgary)

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Chapter 51

Theory of Rotating Machines (10frg138)

May 09 - May 16, 2010

Organizer(s): Peter Lancaster (University of Calgary), Seamus Garvey (University of Nottingham, UK), Ion Zaballa (Euskal Herriko Unibertsitatea)

Introduction

The timing of this focussed research group (FRG) was excellent. Five of the six participants (from Canada, Spain, and the UK) are all involved in a 3-year research programme funded by the UK Engineering and Physical Sciences Research Council (EPSRC) for the three year period, July 1, 2007 to June 30, 2010. Thus, the FRG provided a golden opportunity to reflect on achievements under this aegis, and to consider future activities of a similar kind.

We consider the EPSRC programme to have been highly successful. Bringing together personnel with diverse backgrounds in engineering, mathematics, and computation has been productive, and reveals some exciting vistas for continued collaboration.

The daily programme consisted of a collective working session in the morning, relaxation in the early afternoon, collective and/or private working sessions later in the day.

Overview of the Field

There is a class of mathematical models of linear systems which occurs in a geat variety of physical and engineering problems; namely second order differential systems

$$M\ddot{q}(t) + D\dot{q}(t) + Kq(t) = f(t).$$

Depending on the context, the setting may be in infinite or finite dimensional spaces, and analysis frequently leads to study of time-independent nonlinear eigenvalue problems of the form

$$(\lambda^2 M + \lambda D + K)p = g \tag{51.1}$$

where λ is a real or complex parameter. Again, the context may be either infinite or finite-dimensional vector spaces. In particular, when it comes to computation it is *finite-dimensional* models which must be understood (when M, D, K are almost always square matrices - possibly very large). This is the mathematical environment for this FRG. It is also the environment for a vast body of literature in engineering and applied mathematics. Spectral theory, stability, control and optimization, and the design of algorithms are among the major concerns.

In many problems M, D, K enjoy symmetries. For example, for physical reasons, M is frequently positive definite, and similarly for D and K, but general purpose algorithms cannot assume that this will always be the case. Also, in the analysis of rotating machinery, D, and possibly K, will have a significant skew-symmetric part and, if a mechanical system is free to move in at least one space dimension, M may be singular.

If the model is infinite-dimensional it is necessary that, for the purpose of computation, finite dimensional approximations be made. We do not consider the associated "truncation" errors, but work in the context of the resulting finite-dimensional systems, $\lambda^2 M + \lambda D + K$. Much of the activity in analysis and computation involves the formulation of systems which are isospectral with with $\lambda^2 M + \lambda D + K$, but are of *first* degree in the parameter λ. This is a process known as "linearization". Efficient algorithms for eigenvalues act on the linearized system and will often preserve their characteristic "block" structure - leading to the idea of "structure-preserving transformations" which are also isospectral (i.e. preserving the eigenvalues, their multiplicities and, in the case of real eigenvalues, their "sign characteristic").

In general, there is an insatiable appetite "out there" for faster, more robust algorithms tailored to particular problem areas, and capable of handling larger and larger problem sizes. This provides constant stimulation in the study of algorithms.

Recent Developments and Open Problems

In engineering practice there is great dependency on models in which the three matrix coefficients $M,\ D,\ K$ can be diagonalized simultaneously; and the so-called "modal analysis" works in this context. This has been carefully examined in [7] and expressed in mathematical terms - and provides a useful basis for some of our subsequent investigations.

Research of the group has focussed primarily on the theory and practice of diagonalizing $L(\lambda) = M\lambda^2 + D\lambda + K$ by the application of simple λ-dependent transformations which we call "filters". This can be done without recourse to linearization strategies. Thus, we show that (in general), if systems $L(\lambda) = M\lambda^2 + D\lambda + K$ and $\tilde{L}(\lambda) = \tilde{M}\lambda^2 + \tilde{D}\lambda + \tilde{K}$ are isospectral, then there exist *first degree* polynomials $\tilde{F}(\lambda)$ and $F(\lambda)$ such that

$$\tilde{F}(\lambda)L(\lambda) = \tilde{L}(\lambda)F(\lambda).$$

The "decoupling" then consists in finding filters for which $\tilde{L}(\lambda)$ is *diagonal*. The importance of this is that there are mechanisms admitting physical implementation of such filters using *feedback* mechanisms (familiar in engineering and control theory).

Numerical experiments of S.D.Garvey with S.Jiffri suggest that there are constraints on the spectra of achievable filters which require further analysis. This is in progress and is complemented by the physical construction of model systems (see below). In particular, it has been discovered that filters can be expressed in terms of the "structure preserving transformations" mentioned above, and this is the central idea of [2]. (It has also been found that structure preserving transformations can play a role in perturbation theory [1]).

In the context of linearized systems a thorough analysis has been made of the nature of (suitably defined) structure preserving transformations. Complete parametrizations of such transformations are obtained in [8] in terms of the centralizer of the underlying Jordan structures. This includes systems with or without symmetries in the coefficients M, D, K.

In this context, discussions at the FRG have revealed some gaps in our understanding of canonical "Jordan canonical triples" for real symmetric quadratic systems. This involves some fundamental algebraic ideas and has stimulated refinements in the paper [9] - now near completion.

Presentation Highlights

S. D. Garvey made a presentation concerning the Garvey/Popov/ Lancaster project on the application of a Rayleigh-quotient algorithm to "dilated" quadratic systems. This admits calculation in real arithmetic for real or complex eigenvalues and treats defective eigenvalues seamlessly. This presentation stimulated further polishing of the paper [3].

I. Zaballa presented a careful analysis of a new subspace iteration technique for triangularizing quadratic matrix polynomials.

A. A. Popov described the development of test-rigs nearing completion at the University of Nottingham to be used in collecting sample data to test our theories and algorithms. There are two such experiments in progress. One is made up of electrical circuits with controllable voltage, and the other is a mechanical rotor with controllable bearings.

F. Tisseur made a presentation concerning work of her group on *in situ* "deflation" of quadratic systems (without recourse to linearization). Her collaborations with members of the group (see [4] and [6]) suggest her inclusion in future plans (so providing expertise in computational science).

Scientific Progress Made

As mentioned above, fundamental properties have been found pertaining to Jordan canonical forms - in the context of hermitian and, particularly, real symmetric systems. In the FRG meeting, and at the time of writing, these are still being polished. They give new and important insights into spectral structures. In particular, we obtain fundamental orthogonality properties of eigenvectors providing natural generalizations of classical properties of real symmetric matrices. This points the way to extensions of the Lancaster/Prells studies of orthogonality properties of eigenvector structures (see [5]).

More generally, the FRG provided a golden opportunity for assessing achievements to date and for planning future research directions.

Outcome of the Meeting

This FRG meeting allowed the participants to assess their three years of group-research, to polish and re-evaluate investigations nearing completion and, most important, to look ahead, identify problem areas, and consider future plans. These will include further funding applications in the UK, extending the Canadian participation and, possibly, seeking Canadian funding. It was also agreed that the directions of research would include more specialist expertise in computation.

Participants

Garvey, Seamus (University of Nottingham, UK)
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Popov, Atanas (University of Nottingham)
Prells, Uwe (University of Nottingham)
Tisseur, Francoise (The University of Manchester)
Zaballa, Ion (Euskal Herriko Unibertsitatea)

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Chapter 52

Sparse pseudorandom objects (10frg131)

May 23 - May 30, 2010

Organizer(s): Penny Haxell (University of Waterloo), Vojtech Rodl (Emory University)

Overview

It has been known for a long time that many mathematical objects can be naturally decomposed into a 'pseudorandom', chaotic part and/or a highly organized 'periodic' component. Theorems or heuristics of this type have been used in combinatorics, harmonic analysis, dynamical systems and other parts of mathematics for many years, but a number of results related to such 'structural' theorems emerged only in the last decades. A seminal example of such a structural theorem in discrete mathematics is Szeméredi's Regularity Lemma, which was discovered by Szeméredi in the mid-seventies when he proved his famous result on arithmetic progressions in dense subsets of natural numbers. It states that the set of edges of any dense graph can be 'nearly decomposed' into 'pseudorandom' bipartite graphs. The Regularity Lemma has long been recognised as one of the most powerful tools of modern graph theory.

The aim of the meeting was to follow this structural theme and investigate structural results for sparse combinatorial objects. The meeting brought together a number of experts in the area together with several junior researchers and PhD students.

Presentations and Discussions

Each presenter described recent developments on a particular topic, outlined some of the main related open problems, and led an interactive discussion on these results and problems. The topics addressed were as follows.

Extremal problems for random discrete structures (M. Schacht)

We study thresholds for extremal properties of random discrete structures. We determine the threshold for Szemerédi's theorem on arithmetic progressions in random subsets of the integers and its multidimensional extensions and we determine the threshold for Turán-type problems for random graphs and hypergraphs. In particular, we verify a conjecture of Kohayakawa, Łuczak, and Rödl for Turán-type problems in random graphs. Similar results were obtained by Conlon and Gowers.

Extremal Graph Theory – the Regularity Lemma Revisited (T. Łuczak)

For a graph H and natural numbers k and n let us define the parameter $\nu_\chi^{(k)}(H,n)$ [$\nu_\tau^{(k)}(H,n)$] as the smallest a such that each H-free graph G with n vertices and the minimum degree $\delta(G) \geq an$ can be homomorphically mapped to K_k [some H-free graph F on k vertices]. The behavior of these two parameters has been studied since the early seventies, for instance, the Andrásfai-Erdős-Sós Theorem determines the asymptotic behavior of $\nu_\chi^{(k)}(K_k,n)$ for large n. Here we propose to concentrate on computing the infimum of the sets $\{\nu_\chi^{(k)}(H,n)\}_k$ and $\{\nu_\tau^{(k)}(H,n)\}_k$ rather than finding their complete characterization. Thus, for a graph H, we study the parameters

$$\nu_\chi(H) = \inf_k \liminf_{n\to\infty} \nu_\chi^{(k)}(H,n)\,,$$

as well as

$$\nu_\tau(H) = \inf_k \liminf_{n\to\infty} \nu_\tau^{(k)}(H,n)\,.$$

and survey some recent results, open problems, and methods which fit the above framework.

In particular, using Szemerédi's Regularity Lemma we reprove the result of Thomassen from 2008 who, answering an old question of Erdős and Simonovits, showed that $\nu_\chi(C_{2k+1}) = 0$ for all $k \geq 2$. We also use the Regularity Lemma together with some local resilience argument to show that $\nu_\tau(K_k) = \frac{2k-5}{2k-3}$ for all $k \geq 3$.

This talk is based on joint work with Stéphan Thomassé.

Triangle removal lemma (Y. Person)

The theorem of Szemerédi states that for every $\epsilon > 0$ and every $k \in \mathbf{N}$ there exists $n_0 \in \mathbf{N}$ such that every set $A \subseteq [n]$ with $|A| \geq \epsilon n$, $n \geq n_0$, contains an arithmetic progression of length k. A special case of it is the theorem of Roth for arithmetic progressions of length 3. The best known lower bounds on ϵ in terms of n come from Fourier analytic proofs and the currently best lower bound is due to Bourgain, who showed $\epsilon = \frac{C(\log\log n)^2}{(\log n)^{2/3}}$ is enough. On the other hand, Ruzsa and Szemerédi observed more that 30 years ago that the so-called triangle removal lemma yields another, purely combinatorial, proof of Roth's theorem. This lemma states the following.

Triangle removal lemma. For every $\epsilon > 0$ there exists $\delta > 0$ such that if G is a graph on n vertices with at most δn^3 triangles, then one can remove at most ϵn^2 edges to make G triangle-free.

Until recently, the only known proof of this lemma was via Szemerédi's regularity lemma and therefore the dependency of δ^{-1} on ϵ is a tower of twos polynomial in ϵ^{-1}. Quite recently, Fox gave a new proof of the triangle removal lemma which avoids the use of the regularity lemma and shows that δ can be taken to be a tower of twos of height $200\log\epsilon^{-1}$. Still, the dependency of ϵ and n for Roth's theorem is far from the result of Bourgain mentioned above, but Fox's proof suggests new perspectives and it gives better bounds for testing if a graph is triangle-free or is far from it.

In this talk I will discuss the ideas of Fox and present his proof.

Regular subgraphs (D. Dellamonica)

A paper of Pyber, Rödl and Szemerédi shows: (I) for any k there exists c_k such that any graph with maximum degree Δ and average degree d satisfying $d \geq c_k \log\Delta$ contains a k-regular subgraph. They also show: (II) the existence of graphs with Δ doubly exponential on d which do not contain 3-regular subgraphs. We discuss results and problems related to the following questions.

Question 1: Is $d \geq c_k \log\Delta$ the lowest lower bound possible in (I)?

Question 2: What are the structural properties of graphs which do not contain regular subgraphs? It is possible to show that graphs avoiding regular subgraphs necessarily contain subgraphs which are in some sense similar to the random construction establishing (II). However, in order to transfer properties of the random model used in (II) one would need a finer description of this structure.

Extremal problems for triple systems (D. Mubayi)

1. Regular substructures: Let $f(n)$ denote the maximum number of edges in a linear triple system on n vertices that contains no 2-regular subsystem. Here 2-regular means that every vertex lies in exactly two edges and linear means that every two edges have at most one point in common. About ten years ago, Verstraëte and I (using an idea of Lovász) proved that $n \log n < f(n) < 4n^{5/3}$. It appears that there have been no improvements to either of the above bounds. There are absolutely no results on this problem for k-regular subsystems where $k > 2$.

2. Induced substructures: The induced Turán number $exind(n, F)$ of a k-uniform hypergraph is defined as follows. Let H_1 be a collection of k-element subsets of $[n]$ that are regarded as present and H_2 be a collection of k-element subsets of $\binom{[n]}{k} \setminus H_1$ that are considered as absent. Let $H_3 = \binom{[n]}{k} \setminus (H_1 \cup H_2)$. Suppose also that for every subset of k-subsets M of H_3, the k-graph $H_1 \cup M$ contains no induced copy of F. Then $exind(n, F)$ is the maximum size of H_3 subject to the restrictions above. This parameter is crucial to our understanding of the extremal theory of induced structures.

Let G_i be the (induced) 3-graph with four vertices and i edges. A few months ago I proved that $(1/9)n^2 < exind(n, G_1, G_4) < (1/6 - c)n^2$ for some positive c. I conjecture that the lower bound is tight. This is related to recent results of Razborov and Pikhurko about the usual Turán number of the family G_1, G_4. If the conjecture above is true, then one can attempt to prove a much more challenging conjecture (due to Balogh and me) that characterizes the structure of almost all 3-graphs with vertex set $[n]$ that contain no induced copy of G_1 or G_4. Such questions are related to results of Nagle, Rödl and others on counting hypergraphs with forbidden induced substructures.

Counting induced substructures (B. Nagle)

Let F be a k-graph on f vertices, and let H be k-graph on n vertices. In this talk, we consider the algorithmic problem of computing the number $\#(F, H)$ of (labeled, or unlabeled) induced copies of F in H. (The greedy algorithm can do this in time $O(n^f)$.) In 1986, Nešetřil and Poljak gave an algorithm for graphs for computing $\#(F, H)$ in time $O(n^e)$, where the exponent $e = \omega\lfloor f/3 \rfloor + r$ for remainder $r = f$ (mod 3). In 2005, Yuster studied the problem of computing $\#(F, H)$ for hypergraphs with $k \geq 3$, and conjectured that this quantity may be computed in time $o(n^f)$. In this talk, we present such an algorithm with running time $O(n^f / \log n)$. We formalize the problem that this running time should be reducible to $O(n^{f-\epsilon})$, for an absolute constant $\epsilon > 0$.

We also discuss a few approximation algorithms for estimating $\#(F, H)$. In 1992, Duke, Lefmann and Rödl showed that $\#(F, H)/n^f$ can be determined asympototically in time $O(n^2)$. In 2005, Haxell, Nagle and Rödl showed that $\#(F, H)/n^f$, for 3-graphs, can be determined asymptotically in time $O(n^6)$. Very recently, these results were extended to linear k-uniform hypergraphs by Nagle, Schacht and their graduate students.

Scientific Progress Made

All participants of the meeting worked together on three group projects. A question about what structure of a graph is forced when one knows an upper bound on the number of copies of a fixed tree was proposed by Schacht. The question of finding better bounds on $f(n)$, the maximum number of edges in a linear triple system on n vertices that contains no 2-regular subsystem, was proposed by Mubayi (see 52). The problem of estimating the extremal function $exind(n, G_1, G_4)$ (see 52) was also proposed by Mubayi. Here we describe in detail only the first of these projects, as progress on the others is still ongoing.

Trees force almost regular graphs

Sidorenko's conjecture in extremal graph theory due to Erdős and Simonovits [7] and Sidorenko [5, 6] asserts the following for every bipartite graph F and every $p > 0$. If an n-vertex graph G contains at least $p\binom{n}{2}$ edges, then the number of labeled copies of F in G is at least $(1-o(1))p^{e_F}n^{v_F}$, where $o(1)$ tends to 0 as $n \to \infty$. This conjecture is known to be true for several classes of graphs including forests, even cycles, and complete bipartite graphs [6], Boolean cubes [4] and bipartite graphs F which contain a vertex that is connected to every vertex in the other vertex class [3]. A related and somewhat stronger conjecture was stated by Skokan and Thoma [8]. Those authors asked if every bipartite graph F which contains at least one cycle *forces* a graph G to be *quasi-random* if the number of labeled copies of F in an n-vertex graph G with at least $p\binom{n}{2}$ edges is at most $(1+o(1))p^{e_F}n^{v_F}$. Here a graph G is quasi-random if it satisfies the properties considered in the Chung-Graham-Wilson theorem [2]. Since Sidorenko's conjecture is known to be true for trees and the Chung-Graham-Wilson theorem asserts a matching lower bound for the number of any graph F in a quasi-random graph G, a resolution of the *forcing conjecture* would yield a proof of Sidorenko's conjecture.

We studied a similar question when F is a tree. In view of the forcing conjecture for bipartite graphs F which contain a cycle, one may ask which structure or how much control over a graph G we can force by an upper bound on the number of labeled copies of a given tree T. We say a graph $G = (V, E)$ (more precisely a sequence of graphs $(G_n)_{n\in\mathbf{N}}$) is *nearly p-regular* for some $p > 0$, if

$$\sum_{v\in V} \big|\deg(v) - p|V|\big| = o(|V|^2).$$

It is easy to see for every fixed $\ell \in \mathbf{N}$ that if an n-vertex graph G is nearly p-regular, then for any tree F with ℓ edges the number $N_F(G)$of labeled copies of F in G satisfies

$$N_F(G) = (1 \pm o(1))p^\ell n^{\ell+1}\,.$$

At the workshop we obtained the opposite implication, stating that trees force the property of being nearly regular, i.e., every graph G with $N_F(G)$ being close to the minimal value must be nearly regular. As a consequence we obtain the following characterization of nearly regular graphs.

Theorem. Let $p > 0$ and let $(G_n = (V_n, E_n))_{n\in\mathbf{N}}$ be a sequence of graphs with $|E_n| \geq p\binom{|V_n|}{2}$. The sequence $(G_n)_{n\in\mathbf{N}}$ is nearly p-regular if and only if there exists some tree F with $\ell \geq 2$ edges such that $N_F(G_n) \leq (1+o(1))p^\ell|V_n|^{\ell+1}$.

This theorem follows from a more precise lower bound estimate on $N_F(G)$ in terms of the degrees of G. For that we verify a counting formula for a graph $G = (V, E)$ of the following form

$$\hat{N}_F(G) \geq 2|E|\left(\prod_{v\in V}\deg(v)^{\frac{\deg(v)}{2|E|}}\right)^{\ell-1}, \qquad (52.1)$$

where $\hat{N}_F(G)$ denotes the number of homomorphisms from F to G. Note that for dense graphs G we have

$$N_F(G) \leq \hat{N}_F(G) \leq N_F(G) + o(n^{v_F})\,.$$

It is easy to show that (52.1) is minimized when G is a regular graph and in this case we obtain $N_F(G) \geq (1-o(1))p^\ell|V|^{\ell+1}$. Moreover, one can show that a "matching" upper bound on $N_F(G)$ forces the graph G to be nearly regular.

For the proof of (52.1) we extend the ideas of Alon, Hoory and Linial [1] who obtained the same formula for paths.

Outcomes of the Meeting

We expect several papers to result from the group projects outlined in the previous section. In addition, all the participants derived great benefit from being together in Banff and able to focus on fundamental problems related to spearse pseudo-random objects. We believe the meeting was of particular benefit to the young researchers in the group, and we close with some representative comments from one of the more junior participants.

"My research experience at the BIRS workshop 10frg131, Sparse pseudorandom objects, was extremely positive. This workshop brought together 8 researchers with sharp interests in pseudorandom graph and hypergraph theory for 6 full days of rich discussion and problem-solving. The workshop used an excellent mix of senior and junior researchers. As I consider myself still a junior researcher, I benefited tremendously from time spent with such talented and knowledgable experts, and also appreciated tremendously making collaborative ties with other young researchers whom I didn't previously know. I believe the insights I gained from my mentors, and the relationships I grew with my peers, will assist me invaluably in my career."

Participants

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Person, Yury (Humboldt University)
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Schacht, Mathias (University of Hamburg)

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Chapter 53

The Mathematical Genesis of the Phenomenon called 1/f noise (10frg132)

Jun 06 - Jun 13, 2010

Organizer(s): Priscilla Greenwood (Arizona State University), Lawrence Ward (University of British Columbia)

Overview of the Field

"$1/f$ noise" refers to the phenomenon of the spectral density, $S(f)$, of a signal, having the form

$$S(f) = constant/f^{\alpha},$$

where f is frequency and α is a signal-dependent parameter. In physical situations the phenomenon is often considered to occur on an interval bounded away from both zero and infinity because these endpoints are not observable. Mathematically, however, the behavior of $S(f)$ near these endpoints, particularly as $f \to 0$, is of considerable interest. $1/f^{\alpha}$ signals with $0.5 < \alpha < 1.5$ are found widely in nature, occurring in physics, biology, astrophysics, geophysics, economics, psychology, language and even music [1, 2] (note this overview closely follows parts of [2]). The case of $\alpha = 1$, or "pink noise", is both the canonical case, and the one of most interest; surprisingly, as illustrated in Figure 1, many of the values for α found in nature are very near 1.0. Henceforth the term "$1/f$ noise" will refer only to this case; the value of α will be specified if it is other than 1.0.

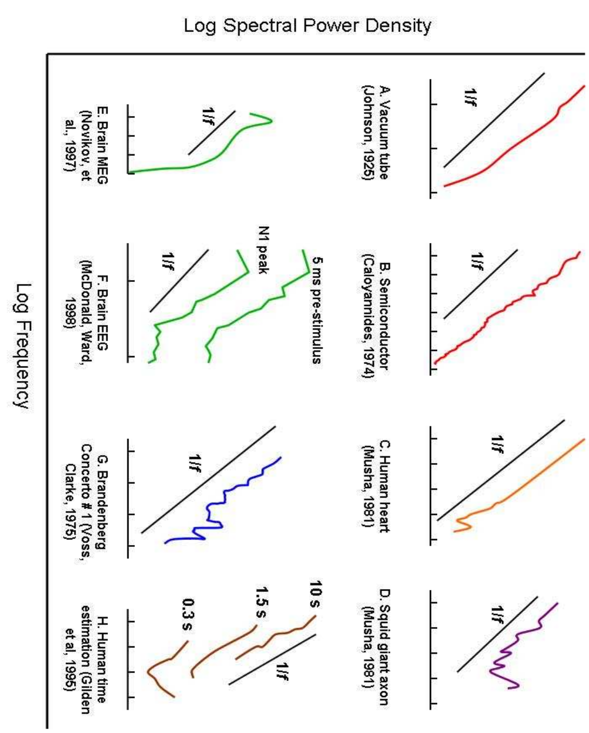
Log Spectral Power Density
Log Frequency
1/f
A. Vacuum tube (Johnson, 1925)
B. Semiconductor (Caloyannides, 1974)
C. Human heart (Musha, 1981)
D. Squid giant axon (Musha, 1981)
E. Brain MEG (Novikov, et al., 1997)
F. Brain EEG (McDonald, Ward, 1998)
N1 peak
5 ms pre-stimulus
G. Brandenberg Concerto # 1 (Voss, Clarke, 1975)
H. Human time estimation (Gilden et al, 1995)
10 s
1.5 s
0.3 s

Figure 1. Some examples of roughly $1/f$ power spectra from various empirical domains. Reprinted from [2].

$1/f$ noise is an intermediate between white noise ($\alpha = 0$) with no correlation in time and a random walk (Brownian motion, $\alpha = 2$) with no correlation between increments. Brownian motion is the integral of white noise; integration of a signal increases α by 2 whereas differentiation decreases it by 2. Therefore, $1/f$ noise cannot be obtained by integration or differentiation of such convenient signals. Moreover, there are no simple, even linear stochastic differential equations generating signals with $1/f$ noise. The widespread occurrence of signals exhibiting such behavior suggests that a generic mathematical explanation might exist. Except for some uninformative formal mathematical descriptions like "fractional Brownian motion" (half-integral of a white noise signal), however, no generally recognized physical explanation of $1/f$ noise has been proposed. Thus, the ubiquity of $1/f$ noise is one of the oldest puzzles of contemporary physics and of science in general.

$1/f$ noise was discovered in 1925 by Johnson [3] in data from an experiment designed to study shot noise in vacuum tubes. Schottky [4] attempted to describe Johnson's pink noise mathematically by assuming that an exponential relaxation,

$$N(t) = N_0 e^{-\lambda t}, t \geq 0,$$

of a current pulse was caused by release of electrons from the cathode of the vacuum tube. For a train of such pulses at an average rate n the power spectrum is the "Lorentzian" form

$$S(f) = \frac{N_0^2 n}{\lambda^2 + f^2},$$

which is nearly constant near $f = 0$ and nearly proportional to $1/f^2$ for large f, with a narrow transition region where the power spectrum resembles that of the pink noise found by Johnson. Bernamont [5] later pointed out that only a superposition of such processes with a variety of relaxation rates, λ, would yield $1/f$ noise for a reasonable range of frequencies. He showed that if λ is uniformly distributed between λ_1 and λ_2, the power spectral density is

$$S(f) = \begin{cases} N_0^2 n & \text{if } 0 \ll f \ll \lambda_1 \ll \lambda_2 \\ \frac{N_0^2 n \pi}{2f(\lambda_2 - \lambda_1)} & \text{if } \lambda_1 \ll f \ll \lambda_2 \\ N_0^2 n \cdot \frac{1}{f^2} & \text{if } 0 \ll \lambda_1 \ll \lambda_2 \ll f. \end{cases}$$

In other words $S(f)$ is proportional to $1/f$ for $\lambda_1 \ll f \ll \lambda_2$. This form, derived from a superposition of Lorentzians, describes the power spectrum in many, but not all, models that have been proposed since Bernamont's.

Another interesting approach to modeling $1/f^\alpha$ noise is related to Granger's [6] classic model in which a long-memory process is produced by the superposition of a number of autoregressive short-memory processes. Erland and Greenwood [7] considered a collection of (discrete-time) AR(1) processes with different parameters, θ_m:

$$X_t^m = \theta_m X_{t-1}^m + \sigma \epsilon_t,$$

where the ϵ_t are i.i.d. Gaussian variables, with mean 0 and standard deviation σ, and $0 < \theta_m < 1$. The autocorrelation function of each X_t^m decays exponentially in time with rate θ_m. The spectral density of each time series X_t^m is the Lorentzian-like function

$$S_m(f) = \frac{\sigma^2}{(1-\theta_m)^2 + 2\theta_m(1 - cosf)} \approx \begin{cases} \sigma^2/(1-\theta_m)^2 & \text{if } 0 \ll f \ll 1 - \theta_m \\ \sigma^2/\theta_m f^2 & \text{if } 1 - \theta_m \ll f \leq 1. \end{cases}$$

Let $Y_t = \frac{1}{m} \sum_{i-1}^{m} X_t^i$, and let the coefficients, θ_m, be distributed as $(1-\theta)^{1-\alpha}$ for $\theta_{min} < \theta < \theta_{max}$. Then the power spectral density of Y_t for large m, is approximately

$$S(f) \propto \begin{cases} 1 & \text{if } 0 \ll f \ll 1 - \theta_{max} \\ 1/f^\alpha & \text{if } 1 - \theta_{max} \ll f \ll 1 \\ 1/f^2 & \text{if } 1 - \theta_{min} \ll f \ll 1. \end{cases}$$

If the θ are uniformly distributed ($\alpha = 1$), then we get a good approximation of $1/f$ noise simply by averaging the individual series. This corresponds to the classical result that the power spectrum of a uniform mixture of exponentially decaying autocorrelation functions has a $1/f$ form. Even the sum of as few as three AR(1) processes with widely distributed coefficients (e.g., 0.1, 0.5, 0.9) gives a reasonable approximation to a $1/f$ power spectrum [1].

Unfortunately such a superposition of Lorentzians is not found in many long-memory models that are concerned with the behavior of $S(f)$ as $f \to 0$. Most long-memory models are driven by a heavy-tailed probability distribution (one in which the tails are not exponentially bounded). In other words, a time series with long memory is one whose autocorrelations decay so slowly with lag that they are not summable, indicating a persistence of dependence of current values on previous values a very long distance in the past of the series. As just demonstrated above, however, a sum of AR(1) processes whose parameters are distributed within a certain range can display a form similar to many of the more physical models [7]. It is possible, therefore, that a similar relationship between other long-memory processes and processes that produce $1/f^{\alpha}$ noise within a specified range can be found.

Recent Developments and Open Problems

The search term "$1/f$ noise" retrieves over 37,000 records from Google Scholar and over 149,000 from Google. The *Scholarpedia* article [2] has received over 45,000 hits since it was published in 2007. Thus there is evidence of vast interest in the phenomenon. Publications appear at a fairly steady rate proposing new models for $1/f^{\alpha}$ noise. Similarly work continues on long-memory models. The search term "long memory process" retrieves nearly 2,400 records from Google Scholar and 129,000 from Google, testifying in part to the importance of long memory in economics. Two lines of recent work on $1/f^{\alpha}$ noise models were particularly important to our focus group. These were the work of Bronislovas Kaulakys and colleagues on point process models and stochastic differential equation (SDE) models (e.g., [8]), and the work of Sveinung Erland and Priscilla Greenwood on Markov chain models (e.g., [7]). These models describe very large classes of situations in which $1/f^{\alpha}$ noise appears, and take us some way toward a more general understanding of the phenomenon. Similarly important was a set of four classes of long memory models [9], comprising renewal counting processes, on/off models, infinite source Poisson models, and renewal reward processes, described for us by Vladas Pipiras. Combined with the aggregation of autoregressive processes that was proved by Granger to result in $1/f^{\alpha}$ noise [6], these general classes of models comprised our playing field. Our major open problem was how to reconcile these approaches, many of which on the surface seemed mutually incompatible. We began the week concerned with finding an underlying mechanism or mathematical description that would encompass all of these models.

Presentation Highlights

Each of the participants presented a description of their work relevant to $1/f^{\alpha}$ noise and also additional problems and frameworks to guide our joint work. Some presentation highlights were as follows: introduction and overview, including some conjectures about model convergence, by Lawrence Ward, the four major long-memory models in a group as well as a more rigorous definition of $1/f^{\alpha}$ noise by Vladas Pipiras, a Markov chain framework for many models and the demonstration of its compatibility with the SDE framework by Sveinung Erland, a large group of models involving point processes and SDEs by Bronislovas Kaulakys, a discussion of time series with and without local stationarity and the problems that the latter create by Wolfgang Polonik, the train model as a prototype of a physical model of $1/f^{\alpha}$ noise by Joern Davidsen, statistical procedures for estimating the exponent α by Changryong Baek, and and a survey of known results for roughness and extrema in $1/f^{\alpha}$ noise by Nicholas Moloney. These presentations occupied the first two days of the workshop, as considerable work was accomplished toward setting our goals and clarifying our vocabulary and conceptual structures during each one.

Scientific Progress Made

The major progress we made was in identifying rigorous procedures to translate between several major classes of models and in defining the approaches to finding translations between the remaining classes. We discovered that translations that preserve the power spectrum already exist between Markov process and stochastic differential equation models and possibly also between point process and continuous process models. It is also possible that we can demonstrate that fractional Gaussian noise is the limit of both dependence-driven and heavy-tailed-driven models, as conjectured at the beginning of the workshop, and that a translation exists between heavy-tailed-driven models and point process or Markov chain models. If so we would have a complete mapping of all of the model types onto each other. This would make the problem of finding an underlying process more tractable, and also focus efforts in that direction, rather than on further proliferating more limited models.

Outcome of the Meeting

There were two important outcomes of this meeting. First, the participants were from a variety of different fields and they all learned a great deal from each other. In particular the importance of including models of long memory processes in the discussion of the origins of $1/f^{\alpha}$ noise was made clear to those of us who had previously discounted these models because they involved physically impossible situations close to $f = 0$. Moreover, the utility of moving away from the origin in the spectrum in modeling signals was made evident to those of us interested in long memory. Second, we realized that rather than searching for a single underlying theory for all $1/f^{\alpha}$ phenomena, it would be more productive at present to study whether it is possible to translate between all of the various model classes. If so, then the existence of an underlying theory seems more credible, although not guaranteed. We thus produced the outline of a paper to be entitled "$1/f^{\alpha}$ Noise: Data. Models, Translations," which we intend to complete over the next year.

Participants

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Chapter 54

Discrete Probability (10frg155)

Jun 13 - Jun 27, 2010

Organizer(s): Omer Angel (University of British Columbia) Alexander Holroyd (Microsoft Research)

Summary

This is a report on activities and results of the focused research group meeting held at BIRS on 2010-06-13 to 26. The participants were Omer Angel, Ander Holroyd, Gady Kozma, James Martin, Jim Propp (first week), Dan Romik, Johan Wastlund, David Wilson (second week), and Peter Winkler.

Tho format of the meeting was as follows. Each morning, one or two of the participants would discuss a few open problems in the broad area of discrete probability. These led to an open discussion, which continued in the afternoons, either at the BIRS facilities or occasionally during excursions. While the problems were broadly spread, some unexpected connections were discovered. The problems discussed ranged from very specific questions to more vague ideas and suggested attacks on other problems.

In the second week, the problem exposition component was reduced, and most of the time was spent pursuing the some promising approaches to solving the problems. However, some questions also arose later in the meeting, as a result of discussions.

Over all, the meeting was very successful, over 30 problems were posed and discussed. Several were solved completely, and significant progress was made on others. A number of papers are being currently being written as a direct result of the meeting (two are already complete), and much current research is still being done. A number of questions are of a very fundamental nature, and the resulting work is likely to pave the way to additional research in the future.

Diadic tilings

A direct outcome of the workshop [**?**]:

A dyadic tile of order n is any rectangle obtained from the unit square by n successive bisections by horizontal or vertical cuts. Let each dyadic tile of order n be available with probability p, independently of the others. We prove that for p sufficiently close to 1, there exists a set of pairwise disjoint available tiles whose union is the unit square, with probability tending to 1 as $n \to \infty$, as conjectured by Joel Spencer in 1999. In particular we prove that if $p = 7/8$, such a tiling exists with probability at least $1 - (3/4)^n$. The proof involves a surprisingly delicate counting argument for sets of unavailable tiles that prevent tiling. This problem is also related to bootstrap percolation on lamplighter groups.

Avoidance coupling

Another direct outcome [**?**]:

Two independent random walks on a graph are sure to collide at some time. However, if the random walks are not independent, it is sometimes possible to arrange them so that they never collide. As an application, one may envisage some anti-virus software moving from port to port in a computer system to check for incursions. It is natural to have such a program implement a random walk on the ports so as not to be predictable. If another program (possibly with a different purpose) also does a random walk on the ports, it may be desirable or even essential to prevent the programs from examining the same port at the same time.

We show that on the complete graph on n vertices, with or without loops, there is a Markovian coupling keeping apart $\Omega(n/\log n)$ random walks, taking turns to move.

Tokens on a graph

A problem that gave rise to the avoidance question above: Several tokens are located on a graph. At each step an adversary selects which one to move, while trying to avoid collisions asfor as long as possible. Is it possible to find the optimal strategy and worst locations for the tokens? In particular, does the worst configuration ever include more than 3 tokens?

This question is related to a number of problems on scheduling of random walks [**?**, **?**, **?**].

Random fault trees

Consider binary tree of depth n, and place randomly an and-gate or an or-gate at each node, independently at random. If the inputs at the leaves of the tree are random, $\{0,1\}$ variables, so is the resulting value at the root. What is the distribution of the value at the root if we condition on the gates? Each of the 2^n input bits has probability 2^{-n} of influencing the output, but how sensitive is the output to changing some of the gates? What it other gates are also included?

The dark waiting room

A queueing system evolves according to the following rules. Several people are in a waiting room. Additional people arrive at some rate. At each round, each person can request service. If a unique request is received, it is filled and the person leaves. If more than one request is made, nothing happens.

There are many questions regarding this system. Is there a strategy such that every person is eventually served? If person requests service with probability $1/n$ where n is the number of people in the room then the number of people is recurrent as long as the rate of arrival is at most e^{-1}. However, if the number of people is not known, the problem is open.

A number of variations are also interesting: What if people are told how many requests were made at each round? What is the fastest strategy if there are n people in the room with no new arrivals?

Coupling TASEPs

Is there a coupling of two exclusion processes started from two different initial conditions, so that they are at the same state for all large times? In particular, does the so called standard coupling work? This question cames from recent advances related to these processes [**?**], and a positive answer would have some implications.

Allocations

The following problem has vexed researchers for a number of years. Given a Poisson point process in $\mathbb{R}^2$, an allocation is a rule to associate to each point of the process a set of area 1 in a translation invariant manner, so that the sets are a partition of the plane. A number of allocation rules had been known [**?**, **?**], but it was not known how to allocate bounded, connected sets. We have found ways to construct such allocations. One of our constructions has the unusual properties that the sets of the partition even have disjoint closures.

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Chapter 55

Cortical Spreading Depression and Related Phenomena (10frg116)

Aug 01 - Aug 08, 2010

Organizer(s): Huaxiong Huang (York University), Robert Miura (New Jersey Institute of Technology)

Introduction

The brain is a complex organ composed largely of neurons, glial cells, and blood vessels. There exists an enormous experimental and theoretical literature on the mechanisms involved in the functioning of the brain, but we still do not have a good understanding of how it works. The brain maintains a homeostatic state with relatively small ion concentration changes. The major ions are sodium, potassium, and chloride with a lower concentration of calcium ions, which plays an important role in many phenomena.

Cortical spreading depression (CSD for short) was discovered over 65 years ago by A.A.P. Leão, a Brazilian physiologist doing his doctoral research on epilepsy at Harvard University [9]. Cortical spreading depression, which occurs in the cortex of different brain structures in various experimental animals, is characterized by depression of cellular electrical activity and pathological shifts in ion concentrations, e.g., extracellular potassium concentration can reach values as high as 50 mM, and is manifest as slow nonlinear chemical waves, with speeds on the order of mm/min. CSD is associated with migraine with aura, see [5], where a scintillation in the visual field propagates, then disappears, and is followed by a sustained headache. This connection with migraine with aura strongly motivates our research on understanding CSD mechanisms.

A number of mechanisms have been hypothesized to be important for CSD wave instigation and propagation. These mechanisms involve ion diffusion, membrane ionic currents, osmotic effects, spatial buffering, neurotransmitter substances, gap junctions, metabolic pumps, synaptic connections, and the vascular system. Many of these are discussed in Miura et al. [11]. In spite of knowing many of the basic mechanisms involved in CSD, we still do not understand the relative importance of these mechanisms and details of how they conspire to produce the observed wave phenomena. To date, CSD remains an enigma, and further theoretical investigations are needed to develop a comprehensive picture of the diverse mechanisms involved in producing CSD.

In this FRG, we brought together a group of applied mathematicians involved in biological modelling, mathematical analysis, and scientific computing of fundamental problems in neuroscience (Huang, Miura, Mori, Tao, Wilson, Wylie) and mechanical engineers involved in physiological modeling and fluid dynamics experiments (Sugiyama, Takagi) to address fundamental issues related to CSD. The main objectives of the FRG were to discuss recent issues arising in the context of understanding CSD, which included: 1) the propagation of dilation and constriction waves along blood vessels as a result of electrical and blood pressure waves, 2) the effects of the vascular system on the propagation of CSD waves, 3) the effects of electrodiffusion and chemical diffusion of ions, and in particular the boundary-layer effects along a cell membrane due to unequal charge distributions when embedded in an ionic fluid, and 4) the putative connection between a CSD wave in the visual cortex and the aura in the visual field that precedes migraine.

Blood vessels account for a significant portion of the brain volume. Dilation and constriction of blood vessels during the propagation of CSD waves are important and relevant phenomena affecting the supply of oxygen to the tissue. The exact mechanisms for these are not well understood, and we investigated some of these during the FRG.

To better understand the actual mechanisms involved in CSD (and develop some clues into how the brain is organized to perform its normal functions), it is necessary to start from basic principles and build models based on fundamental biochemical and biophysical principles. Below, we describe some of the problems that we studied during the FRG.

Modelling the Dilation and Constriction of a Blood Vessel

In order to understand the mechanism of blood vessel dilation and constriction, and to gain useful insights into the biochemical and biophysical processes involved in CSD and in normal physiological conditions, we began to explore the role played by the ion concentrations and their relations to the blood perfusion rate, under normal and CSD conditions. It has been shown in the literature that blood vessel radius is correlated with blood pressure as well as the shear stress experienced by the vessel, which are affected by the concentrations of the ions such as calcium [3]. CSD provides an interesting case to test the coupling of neuronal and blood prefusion models.

A variety of hypotheses for the observed vasodilation were developed and examined. For example, it is possible that during CSD, in an effort to restore the depolarized cell membrane potential, it is the increased energy demand (as measured for example by ATP) which leads to the increased blood flow. However, such an hypothesis does not explain the constriction of the vessel. Takano et al. [15] review evidence that hyperpolarisation is key to spreading vasodilation, and examine various hypotheses for mechanisms underlying this spreading hyperpolarisation.

Flow induced: Wall shear-stress releases NO which dilates vessels. However, we identified other experimental studies which indicated that it is possible to disable NO synthesis and still observe vasodilatation.

Perivascular nerves: These may be important in vasoconstriction but not in vasodilatation, since one can use TTX to abolish vasoconstriction but not vasodilatation.

Endothelial Ca^{2+}: Ca^{2+} and IP_3 can pass across gap junctions to adjacent cells. But while Ca^{2+} is observed to rise locally with hyperpolarisation, it has yet to measurably reach a distance of 0.5 mm from the initial application of ACh when hyperpolarisation had travelled to at least 2 mm.

Based broadly on the above, the hypothesis that we spent the most time discussing in this FRG was the possibility of a calcium wave generating the “signal” to cause the blood vessel to dilate or constrict upstream and downstream of the CSD location. A model which we have discussed for investigating this hypothesis involved two compartments: a smooth muscle cell compartment (SMC or MC) and an endothelial cell compartment (EC), following some of the ideas in Kapela et al. [7].

The EC is hypothesised to be the main location for the calcium wave. However, maintaining such a wave requires a positive feedback loop. One possibility for such a loop involves the IP_3 receptors (IP_3R).

It is possible that as the membrane depolarizes, the inwardly-rectifying potassium channel opens (further depolarizing the membrane), leading to an increase in extracellular calcium which opens the potassium-calcium channels, creating positive feedback to the membrane depolarization.

Effects of the Vascular System on CSD

The metabolic demand associated with repolarizing cell membranes and re-establishing resting ion concentrations in the wake of the CSD wave requires an increased supply of oxygen-carrying blood from the cerebral arterial network. Recalling that the CSD wave propagates with speeds on the order of mm/min, the question of local arterial responses is dealt with in line with the work in §55. However, on lateral cortical lengthscales on the order of millimeters or centimeters, we must probe the response of a larger branching network of cerebral arterioles. In fact, we must do this if we wish to consider the communicated effects of CSD at deeper levels within the brain.

In general, this linking of neurons and blood vessels is known as *neurovascular coupling*, and as seen in §55, involves a multitude of pathways connecting blood flow to neuronal activity, and vice versa. Here, we are also interested in how the topology and geometry of the cortical architecture and the cerebral arteriolar network are interrelated. A major challenge in creating an accurate mathematical model of these interdigitating trees is that experimental techniques to determine their topology and geometry are usually mutually exclusive.

Nevertheless, during this FRG, we were able to discuss linking existing models of the arteriolar network, such as that presented in [4], with models of CSD instigation and propagation [6], and the work discussed in §55. In particular, the model in [4], building on [3], features a physiologically-realistic cerebral arterial tree that is able to autoregulate in response to changes in metabolism in the surrounding tissue, such as those caused by the passing of a CSD wave. Our discussion focused on (a) updating the autoregulation model in line with the detailed local study and considerations of §55, and (b) linking a detailed arterial tree model with the compartmental model of CSD instigation and propagation of [6]. As we take this work forward, we expect to also build upon the model developed in [1]. There, we can construct a more detailed coupled model, consisting of both neuronal and vascular components, and carry out numerical simulations on the model.

Electrodiffusion and CSD

Since there are large fluctuations in ionic concentrations in CSD, we discussed the merits of using an electrodiffusion model instead of the more conventional chemical diffusion approach in treating ion concentration dynamics in CSD [14]. One interesting complication that arises in such an effort is the treatment of membrane boundary conditions. The basic equations that govern electrodiffusion in the dilute regime are the Poisson-Nernst-Planck equations, but the smallness of the Debye length makes it attractive to take the electroneutral limit [12, 13]. In this singular perturbation limit, however, a boundary layer of electrical charges forms at the membrane interfaces. The presence of such boundary layers lead to capacitive (or cable) effects, the inclusion of which may be particularly important in studying the initiation of CSD. We worked to clarify the mathematical and physical structure of this boundary layer by revisiting the formal asymptotic computations performed in [13].

Another question we tackled was the validity of using the diffusion approximation in place of ionic electrodiffusion in certain contexts. We were able to show, through formal asymptotic computations, that this is indeed possible when the concentration of the ion of interest has a considerably lower concentration than the other co-ions in the electrolyte solution. This justifies the use of simple diffusion to track calcium concentration inside the cell, which has a 10^4-fold lower concentration than the major co-ions (sodium, potassium, chloride) in the cell. This is an important observation given the widespread use of simple diffusion in modeling intracellular calcium dynamics, a major area of cell biology [8].

Mapping of CSD in the Visual Cortex to the Visual Field

Our study is concerned with a visual experience that accompanies some of the migraine headaches associated with CSD. Among the patients who have migraine headaches, 20% of them have so-called migraine with aura [5]. In these patients, the onset of a migraine is preceded with visual auras. These visual patterns often take the form of expanding arcs in the visual field and can last up to half an hour. It has been conjectured that CSD waves in the occipital lobe in these patients may be responsible for these auras. That is, these visual auras in the visual field do not correspond to exogenous visual stimulus, but are instead perceptions directly related to the neuronal activity patterns of CSD waves in one or more areas of the visual pathway.

During our FRG, we examined how a CSD wave in the primary visual cortex (V1) would appear in the visual field. V1 is the first part of the visual pathway in the neocortex and is thought to be responsible for the processing of simple geometric features in the visual scene (for instance, local orientation, spatial frequency, and other features that presumably would aid in the detection of lines, edges, and contours). The coordinate transformation mapping the locations in the visual field to locations in V1 is well known [2]. We use this retinotopic-V1 map to examine how various wave fronts (modeled as moving lines) in V1 could correspond to objects in the visual field. The conjecture that visual auras could be perceptions of CSD waves in V1 is corroborated, as certain wave fronts that propagate correspond to arcs expanding away from the fovea in the visual field, and thus may be perceived as such.

How spatio-temporal neuronal activity in V1 could be perceived is a much more general problem and is of great interest to the visual neuroscience community. The forward problem of how a visual stimulus is coded as neuronal activity in V1 is well studied (especially for simple geometric patterns, see, for example, [10] and references therein), but the inverse problem of determining which visual stimulus could lead to a given spatio-temporal pattern of neuronal activity is not well understood. During our week at BIRS, we examined a few toy models of small neuronal networks to gain intuition for this problem. For a first problem, we examined a network of two neurons driven by independent inputs. So a natural question is: by observing the two neurons in the network, can we determine the inputs that each neuron is receiving.

We used the so-called linear integrate-and-fire point neuron to model each neuron. Each action potential is modeled as decaying exponentials in the synaptic conductances of individual neurons. This is one of the simplest models that could take a generalized input and produce detailed spike times (i.e., timing of action potentials). Within the framework of this highly idealized model, and assuming that we know the strength of coupling between these neurons, we showed that given the detailed neuronal spiking times, we may be able to reconstruct the input into each neuron that is responsible for the activity. We plan to extend this approach to larger networks of networks with more generalized inputs which may contain correlations in the visual scene and to cases where we have partial information (e.g., all of the couplings between the neurons may not be known) or only have statistical information (e.g., statistics of the neuronal activity, instead of detailed spike timings of each neuron).

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Research in Teams Reports

Chapter 56

Convergence of loop-erased random walk to SLE(2) in the natural parametrization (10rit143)

Jan 17 - Jan 24, 2010

Organizer(s): Robert Masson (University of British Columbia), Tom Alberts (University of Toronto), Michael Kozdron (University of Regina)

Overview of the Field

The area of our research project is probability and statistical mechanics. More specifically, we study the loop-erased random walk (LERW) – a prominent discrete model in statistical mechanics – and its continuous scaling limit, Schramm-Loewner evolution (SLE) with parameter 2. The LERW was invented by Greg Lawler [3] in order to study the self-avoiding walk (SAW). While that approach did not turn out to be fruitful for analyzing the SAW, the LERW is extensively studied today, most notably for its intimate connection to the uniform spanning tree through Wilson's algorithm.

SLE was invented by Oded Schramm [7] as a candidate for the scaling limit of LERW. Under the assumptions of conformal invariance of the scaling limit (which was conjectured to be true for the LERW) and a "domain Markov property" (which is easy to show for the LERW), Schramm proved that the only possible scaling limit was SLE with parameter κ: a random curve satisfying the Loewner equation with a Brownian motion of variance κ as its driving function. In his original paper, Schramm determined that if LERW had a conformally invariant scaling limit, one would have to have $\kappa = 2$. Then, in a later paper [4], Lawler, Schramm and Werner verified that LERW does indeed converge to SLE(2). In addition, many other prominent models from statistical physics such as the uniform spanning tree, the self-avoiding walk, the Ising model at criticality, the Gaussian free field, and critical percolation contain discrete curves that scale or are conjectured to scale to SLE(κ) for various values of κ. Establishing that SLE is the scaling limit of these models rigorously confirms many of the predictions that had previously been made using conformal field theory.

Goal of the Research Project

In the paper [4], Lawler, Schramm and Werner proved the weak convergence of LERW to SLE(2) with respect to the supremum norm on curves modulo reparametrization. The goal of our project is to prove weak convergence in the stronger topology that takes into account the parametrization of the LERW. Namely, if we let X^n be the LERW from the origin to the unit circle on the lattice $(1/n)\mathbb{Z}^2$ and M_n be the number of steps of X^n, then one expects that $Y_n(t) = X^n(\mathbf{E}[M_n]t)$ should converge weakly (as n tends to infinity) in the supremum norm to a suitably parametrized version of SLE(2). Although other models have been shown to scale to SLE, none of them have been proved to converge as parametrized curves.

Recent Developments

There are two recent developments that make this problem appear tractable. The first is the identification of what the suitable parametrization for the SLE(2) curve should be. In the original definition of SLE by Schramm, the SLE curves were parametrized so that their capacity (a measure of how big the curves look in the unit disc when viewed from the origin) grew linearly. This was the best way to analyze the curves by way of the Loewner equation but is not natural when one considers the SLE curves as scaling limits of discrete models. Indeed, Beffara showed that the Hausdorff dimension of SLE(κ) is $d = 1 + \kappa/8$ almost surely ($\kappa \leq 8$). This suggests that for a discrete model to converge to SLE(κ) as a parametrized curve, the parametrization on the SLE(κ) curve should be such that scaling the curve by a factor of r in space is equivalent to scaling by a factor of r^d in time. This "natural parametrization" of SLE has recently been shown to exist by Lawler and Sheffield [5]. It is SLE(2) in this parametrization that one expects the LERW Y_n defined above to scale to. Note that $d = 5/4$ for SLE(2), and the fact that $\mathbf{E}[M_n]$ grows like $n^{5/4}$ was established by Kenyon.

The second result that will be useful for this problem is a tail bound on M_n. Recent work by Barlow and Masson [1] gives both upper and lower exponential tail bounds on M_n. As we describe below, this allows us to establish a tightness result that gives subsequential weak limits of LERW in the topology induced by the supremum norm.

Scientific Progress Made

The natural parametrization for SLE(2) defined by Lawler and Sheffield [5] is more easily described in terms of a random Borel measure μ on $\mathbb{D}$. The measure μ is supported on the SLE(2) curve and in essence gives the amount of time that the curve (in the natural parametrization) spends in each subset of $\mathbb{D}$. By the conformal invariance and the domain Markov property of SLE(2) one expects that it should satisfy the following.

1. μ is measurable with respect to the trace of the SLE(2) curve.
2. μ is almost surely supported on the trace of the SLE(2) curve.
3. $\mathbf{E}[d\mu(z)] = G(z)\,dz$ where $G(z)$ is the "Green's function" for SLE(2) in $\mathbb{D}$.
4. Given any parametrization for SLE(2), $\mu(\cdot \cap \gamma[0,t])$ is $\gamma[0,t]$ measurable.
5. $\mathbf{E}[d\mu(z)|\gamma[0,t]] = |g_t'(z)|^{3/4} G(g_t(z))$ for $z \in \mathbb{D} \setminus \gamma[0,t]$, where g_t is the unique conformal map from $\mathbb{D} \setminus \gamma[0,t]$ to $\mathbb{D}$ such that $g_t(0) = 0$ and $g_t'(0) > 0$.

The exponent $3/4$ arises from the fact that the dimension of SLE(2) is $5/4$.

Lawler and Sheffield [5] proved that a measure satisfying these properties exists. Moreover, this measure is unique. Given μ and an SLE(2) curve $\gamma(t)$ in any parametrization, one sets $\Theta(t) = \mu(\gamma[0,t])$, and then defines SLE(2) in the natural parametrization by

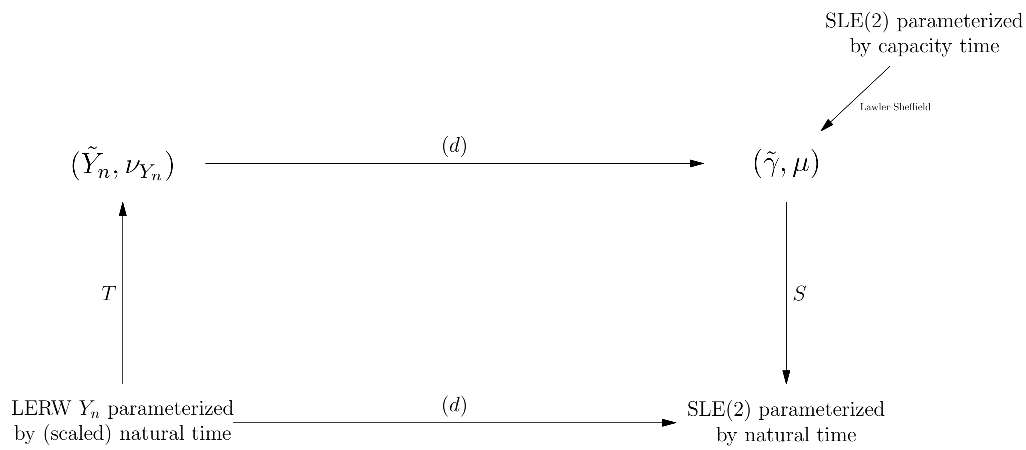
$$\gamma^*(t) = \gamma(\Theta^{-1}(t)). \tag{$*$}$$

Hence, the key step in constructing the natural parametrization is the construction of the natural measure μ.

With this in mind, we show that convergence of the natural measure for LERW to the natural measure for SLE(2) implies the convergence of the associated curves in their naturally parametrized form. Given the LERW Y_n, its natural measure is defined to be

$$\nu_{Y_n}(A) = \int_0^\infty \mathbf{1}\{Y_n(t) \in A\}\, dt. \tag{$**$}$$

Our goal is to prove that ν_{Y_n} converges weakly to μ with respect to the Prokhorov topology on measures. As summarized in the diagram below, this fact plus Lawler, Schramm and Werner's result that the LERW converges weakly to SLE(2) modulo reparametrization implies the same convergence but in the natural parametrization.



Here $\widetilde{Y}_n$ and $\widetilde{\gamma}$ are the equivalence classes of the LERW and SLE(2) curves modulo reparametrization. The mapping T takes the parametrized LERWs Y_n into the pair consisting of the equivalence class and the occupation measure ($**$), while S maps equivalence classes of curves and occupation measures into parametrized curves via ($*$). The map S is continuous at almost all pairs $(\widetilde{Y}, \mu)$, and therefore weak convergence on the top level of the diagram implies weak convergence on the bottom level.

Convergence on the top level follows the usual argument: we show that the pair $(\widetilde{Y}_n, \nu_{Y_n})$ is tight, and that any subsequential weak limit must have the law of $(\widetilde{\gamma}, \mu)$. Tightness of the $\widetilde{Y}_n$ follows from [4], while tightness of ν_{Y_n} is a consequence of the estimate

$$\mathbb{P}\left(\alpha^{-1} \leq \frac{M_n}{\mathbf{E}[M_n]} \leq \alpha\right) \geq 1 - Ce^{-c\alpha^{1/2}}$$

that is due to Barlow and Masson [1].

It remains to show that any subsequential weak limit of $(\widetilde{Y}_n, \nu_{Y_n})$ satisfies the properties 1 through 5 that uniquely define μ. Of these, property 2 is the most straightforward to verify; it follows readily from the fact that ν_{Y_n} is supported on $\widetilde{Y}_n$. Properties 1 and 4 are nontrivial and do not follow from general facts about weak convergence. Some extra information is required and at this point we are not entirely sure what that is.

Properties 3 and 5 can be established once the following conjectures are proved.

Conjecture 4.1. *For all $z \in \mathbb{D}$ and $\epsilon > 0$ sufficiently small,*

$$\mathbf{E}\left[\nu_{Y_n}(B(z,\epsilon)) \middle| Y_n \cap B(z,\epsilon) \neq \emptyset\right] = \frac{\mathbf{E}\left[M_{\epsilon n}\right]}{\mathbf{E}\left[M_n\right]} + o(1)$$

as $n \to \infty$.

This implies property 3 by the following argument.

$$\begin{aligned}\mathbf{E}\left[\mu(B(z,\epsilon))\right] &= \lim_{n\to\infty} \mathbf{E}\left[\nu_{Y_n}(B(z,\epsilon))\right] \\ &= \lim_{n\to\infty}\left[\frac{\mathbf{E}\left[M_{\epsilon n}\right]}{\mathbf{E}\left[M_n\right]} + o(1)\right]\mathbb{P}\left(Y_n \cap B(z,\epsilon) \neq \emptyset\right) \\ &= \epsilon^{5/4}\mathbb{P}\left(\gamma \cap B(z,\epsilon) \neq \emptyset\right) \\ &\sim \epsilon^2 G(z).\end{aligned}$$

The second to last line follows from [4] while the last line is the definition of $G(z)$.

Conjecture 4.2. *Suppose that* D *and* D' *are simply connected domains in* $\mathbb{C}$ *containing* 0 *and* $F : D \to D'$ *is a conformal transformation such that* $F(0) = 0$*. Then for any* $z \in D \cap \mathbb{Z}^2/n$*,*

$$\mathbb{P}\left(F(z) \in X^n_{D'}\right) \sim |F'(z)|^{-3/4}\mathbb{P}\left(z \in X^n_D\right)$$

as $n \to \infty$*, where* X^n_D *is the LERW in the domain* $D \cap \mathbb{Z}^2/n$*.*

This implies property 5 by the following argument. First observe that

$$\int_0^\infty \mathbf{1}\left\{Y_n(s) \in A\right\}\, ds = \int_A \delta_{Y_n(s)}(z),$$

so that by an application of Fubini's Theorem

$$\int_0^\infty \mathbb{P}\left(Y_n(s) \in A\right)\, ds = \int_A \mathbb{P}\left(z \in Y_n[0,\infty]\right)\, dz.$$

Consequently for $A \subset \mathbb{D} \setminus Y_n[0,t]$,

$$\begin{aligned}\mathbf{E}\left[\nu_{Y_n}(A) \,|\, Y_n[0,t]\right] &= \int_0^\infty \mathbb{P}\left(Y_n(s) \in A \,|\, Y_n[0,t]\right)\, ds \\ &= \int_A \mathbb{P}\left(z \in Y_n[t,\infty) \,|\, Y_n[0,t]\right)\, dz \\ &= \int_A \mathbb{P}\left(z \in Y^n_{\mathbb{D}\setminus Y_n[0,t]}\right)\, dz \\ &\sim \int_A |(g^n_t)'(z)|^{3/4}\mathbb{P}\left(g^n_t(z) \in Y^n_{\mathbb{D}}\right)\, dz.\end{aligned}$$

The last line is an application of Conjecture 4.2, via the map $g^n_t : \mathbb{D} \setminus Y_n[0,t] \to \mathbb{D}$ that has $g^n_t(0) = 0$ and positive derivative at zero. Since this holds for all $A \subset \mathbb{D} \setminus Y_n[0,t]$, we have

$$\mathbf{E}\left[d\nu_{Y_n}(z) \,|\, Y_n[0,t]\right] \sim |(g^n_t)'(z)|^{3/4}\mathbb{P}\left(g^n_t(z) \in Y^n_{\mathbb{D}}\right)\, dz$$

as $n \to \infty$. One then uses some form of convergence of ν_{Y_n} to μ to show that the left side converges to $\mathbf{E}\left[d\mu(z) \,|\, \gamma[0,t]\right]$ as $n \to \infty$, and some other form of convergence of LERW to SLE(2) to show that the right side converges to $|g'_t(z)|^{3/4}G(g_t(z))\, dz$.

Outcome of the Meeting

We are currently working on proving these conjectures and intend to produce a manuscript as soon as they have been established.

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Chapter 57

Theory of Functions of Noncommuting Variables and Its Applications (10rit141)

Feb 21 - Feb 28, 2010

Organizer(s): Victor Vinnikov (Ben Gurion University of the Negev), Dmitry Kaliuzhnyi-Verbovetskyi (Drexel University)

Overview of the Project

Polynomials, rational functions, and formal power series in (free) noncommuting variables were considered in a variety of settings. While usually viewed as formal algebraic objects, they also appeared often as functions by substituting tuples of matrices or operators for the variables. Our point of view is that a function of noncommuting variables is a function defined on tuples of matrices of all sizes that satisfies certain compatibility conditions as we vary the size of matrices: it respects direct sums and simultaneous similarities, or equivalently, simultaneous intertwinings. This leads naturally to a noncommutative difference-differential calculus. The objective of our research is to develop a comprehensive theory of noncommutative functions and their difference-differential calculus in both algebraic and analytic setting. We expect this theory to have a wide range of applications from noncommutative spectral theory (compare Taylor [8, 9]) and free probability (compare Voiculsecu [10, 11]) to analysis of linear matrix inequalities (LMIs) in optimization and control (compare Helton [1], Helton–McCullough–Vinnikov [2], Helton–McCullough–Putinar–Vinnikov [3]).

Preliminary discussion: noncommutative polynomials and noncommutative formal power series

The simplest function of several commuting variables is doubtless a polynomial function that arises by evaluating a polynomial on tuples of (say) complex numbers. Let us consider instead the ring $\mathbb{C}\langle x_1, \ldots, x_d\rangle$ of noncommutative polynomials (the free associative algebra) over $\mathbb{C}$; $x_1, \ldots, x_d$ are noncommuting indeterminates, and $f \in \mathbb{C}\langle x_1, \ldots, x_d\rangle$ is of the form

$$f = \sum_{w \in \mathbb{F}_d} f_w x^w, \tag{57.1}$$

where $\mathbb{F}_d$ denotes the free semigroup on d generators, $f_w \in \mathbb{C}$, x^w are noncommutative monomials in $x_1, \ldots, x_d$, and the sum is finite. Notice that f can be evaluated in an obvious way on d-tuples of complex matrices of all sizes: for $X = (X_1, \ldots, X_d) \in (\mathbb{C}^{n\times n})^d$,

$$f(X) = \sum_{w\in\mathbb{F}_d} f_w X^w. \tag{57.2}$$

We can also consider the ring $\mathbb{C}\langle\langle x_1, \ldots, x_d\rangle\rangle$ of noncommutative formal power series (the completion of the free associative algebra) over $\mathbb{C}$; $f \in \mathbb{C}\langle\langle x_1, \ldots, x_d\rangle\rangle$ is of the same form as in (57.1), except that the sum is in general infinite. There are two ways to evaluate f on d-tuples of complex matrices:

- Assume that $X = (X_1, \ldots, X_d) \in (\mathbb{C}^{n\times n})^d$ is a jointly nilpotent d-tuple, meaning that $X^w = 0$ for all $w \in \mathbb{F}_d$ with $|w| = k$ for some k, where $|w|$ denotes the length of the word w; equivalently X is jointly similar to a d-tuple of strictly upper-triangular matrices. Then we can define $f(X)$ as in (57.2), since the sum is actually finite.

- Assume that f has a positive noncommutative multi-radius of convergence, i.e., there exists a d-tuple $\rho = (\rho_1, \ldots, \rho_d)$ of strictly positive numbers such that

$$\limsup_{k\to\infty} \sqrt[k]{\sum_{|w|=k} |f_w|\rho^w} \leq 1.$$

  Then we can define $f(X)$ as in (57.2), where the infinite series converges absolutely and uniformly on any noncommutative polydisc

$$\coprod_{n=1}^{\infty} \left\{X \in \left(\mathbb{C}^{n\times n}\right)^d : \|X_j\| < r_j,\ j = 1, \ldots, d\right\}$$

  of mutiradius $r = (r_1, \ldots, r_d)$ with $r_j < \rho_j$, $j = 1, \ldots, d$.

We notice that in all these cases the evaluation of f on d-tuples of matrices possesses two key properties.

- f respects direct sums: $f(X \oplus Y) = f(X) \oplus f(Y)$, where

$$X \oplus Y = (X_1, \ldots, X_d) \oplus (Y_1, \ldots, Y_d) = (X_1 \oplus Y_1, \ldots, X_d \oplus Y_d) = \left(\begin{bmatrix} X_1 & 0 \\ 0 & Y_1 \end{bmatrix}, \ldots, \begin{bmatrix} X_d & 0 \\ 0 & Y_d \end{bmatrix}\right)$$

  (we assume here that X, Y are such that $f(X)$, $f(Y)$ are both defined).

- f respects simultaneous similarities: $f(TXT^{-1}) = Tf(X)T^{-1}$, where

$$TXT^{-1} = T(X_1, \ldots, X_d)T^{-1} = (TX_1T^{-1}, \ldots, TX_dT^{-1})$$

  (we assume here that X and T are such that $f(X)$ and $f(TXT^{-1})$ are both defined).

Overview of some definitions and results

Both for the sake of potential applications and for the sake of developing the theory in its natural generality, it turns out that the proper setting for the theory of noncommutative functions is that of matrices of all sizes over a given vector space (or a given module). In the special case when the vector space is $\mathbb{C}^d$, $n \times n$ matrices over $\mathbb{C}^d$ can be identified with d-tuples of $n \times n$ matrices over $\mathbb{C}$, and we recover noncommutative functions of d variables, key examples of which appeared in the previous section.

Let $\mathcal{V}$ be a vector space over $\mathbb{C}$ (for the algebraic part of the theory, we can consider more generally a module over any commutative ring with unit). We call

$$\mathcal{V}_{\text{nc}} = \coprod_{n=1}^{\infty} \mathcal{V}^{n\times n}$$

the noncommutative space over $\mathcal{V}$. A subset $\Omega \subseteq \mathcal{V}_{\text{nc}}$ is called a noncommutative set if it is closed under direct sums, i.e., we have

$$X \oplus Y = \begin{bmatrix} X & 0 \\ 0 & Y \end{bmatrix} \in \Omega_{n+m}$$

for all $X \in \Omega_n$, $Y \in \Omega_m$ and all $n, m \in \mathbb{N}$, where we denote $\Omega_n = \Omega \cap \mathcal{V}^{n\times n}$. Noncommutative sets are the only reasonable domains for noncommutative functions, but additional conditions on the domain are needed for the development of the noncommutative difference-differential calculus. Essentially we need the domain to be closed under formation of upper-triangular block matrices with an arbitrary upper corner block, but this is too much (e.g., this is false for noncommutative polydiscs and balls). The proper notion turns out to be as follows: a noncommutative set $\Omega \subseteq \mathcal{V}_{\text{nc}}$ is called upper admissible if for all $X \in \Omega_n$, $Y \in \Omega_m$ and all $Z \in \mathcal{V}^{n\times m}$, there exists $\lambda \in \mathbb{C}$, $\lambda \neq 0$, such that

$$\begin{bmatrix} X & \lambda Z \\ 0 & Y \end{bmatrix} \in \Omega_{n+m}.$$

Our primary examples of upper admissible noncommutative sets are as follows:

- The set $\Omega = \operatorname{Nilp} \mathcal{V}$ of nilpotent matrices over $\mathcal{V}$. Here $X \in \mathcal{V}^{n\times n}$ is called nilpotent if $X^k = 0$ for some k, where we view X as a matrix over the tensor algebra

$$\mathbf{T}(\mathcal{V}) = \bigoplus_{j=0}^{\infty} \mathcal{V}^{\otimes j}$$

  of $\mathcal{V}$; equivalently, there exists $T \in \mathrm{GL}_n(\mathbb{C})$ such that TXT^{-1} is strictly upper triangular.

- Assume that $\mathcal{V}$ is a Banach space and that Ω is open in the sense that $\Omega_n \subseteq \mathcal{V}^{n\times n}$ is open for all n; then Ω is upper admissible.

A special case of the second item — that is crucial for analytic results that are uniform in the size of matrices — is when $\mathcal{V}$ is an operator space This means that there is a sequence of norms $\|\cdot\|_n$ on $\mathcal{V}^{n\times n}$ such that

$$\|X \oplus Y\|_{n+m} = \max\{\|X\|_n, \|Y\|_m\} \quad \text{for all } X \in \mathcal{V}^{n\times n},\ Y \in \mathcal{V}^{m\times m}, \tag{57.3}$$

and

$$\|TXS\|_n \leq \|T\|\|X\|_n\|S\| \quad \text{for all } X \in \mathcal{V}^{n\times n},\ T, S \in \mathbb{C}^{n\times n}. \tag{57.4}$$

An important example of an open noncommutative set is then a noncommutative ball

$$\Omega = \coprod_{n=1}^{\infty} \left\{X \in \mathcal{V}^{n\times n} \colon \|X\|_n < \rho\right\}.$$

(For the general theory of operator spaces, see, e.g., Paulsen [6] or Pisier [7].)

Let $\mathcal{V}$ and $\mathcal{W}$ be vector spaces over $\mathbb{C}$, and let $\Omega \subseteq \mathcal{V}_{\text{nc}}$ be a noncommutative set. A function $f\colon \Omega \to \mathcal{W}_{\text{nc}}$ with $f(\Omega_n) \subseteq \mathcal{W}^{n\times n}$ is called a noncommutative function if:

- f respects direct sums: $f(X \oplus Y) = f(X) \oplus f(Y)$ for all $X \in \Omega_n$, $Y \in \Omega_m$.

- f respects similarities: $f(TXT^{-1}) = Tf(X)T^{-1}$ for all $X \in \Omega_n$ and $T \in \mathrm{GL}_n(\mathbb{C})$ such that $TXT^{-1} \in \Omega_n$.

It turns out that these two conditions are equivalent to a single one: f respects intertwinings, namely if $XS = SY$ then $f(X)S = Sf(Y)$, where $X \in \Omega_n$, $Y \in \Omega_m$, and $S \in \mathbb{C}^{n\times m}$. This condition originates in the pioneering work of Taylor [8].

One can construct noncommutative functions generalizing the formal power series construction discussed in Section 57 to a coordinate free framework. Assume that we are given a sequence $f_k\colon \mathcal{V}^{\otimes k} \to \mathcal{W}$ of linear mappings. Then

$$f(X) = \sum_{k=0}^{\infty} f_k(X^k), \tag{57.5}$$

where the matrix power X^k is taken in the tensor algebra $\mathbf{T}(\mathcal{V})$ and f_k is extended entrywise to a linear mapping from matrices over $\mathcal{V}^{\otimes k}$ to matrices over $\mathcal{W}$, defines a noncommutative function provided we can make sense of the (generally speaking) infinite sum on the right hand side. This can be done in two ways:

- If X is nilpotent then the sum in (57.5) is actually finite; hence (57.5) always defines a noncommutative function on $\mathrm{Nilp}(\mathcal{V})$.
- If $\mathcal{V}$ and $\mathcal{W}$ are operator spaces, and we have a growth estimate

$$\limsup_{k\to\infty} \sqrt[k]{\|f_k\|_{\text{cb}}} \le \frac{1}{\rho}$$

  (where $\|\cdot\|_{\text{cb}}$ denotes the completely bounded norm), then the series in (57.5) converges absolutely and uniformly on any noncommutative ball of radius $r < \rho$; hence in this case (57.5) defines a noncommutive function on the noncommutative ball of radius ρ.

One of the main results of the noncommutative difference-differential calculus is the infinite series expansion, called the Taylor–Taylor expansion[1], that provides a converse to the above construction. It is given by

$$f(X) = \sum_{k=0}^{\infty} \Delta_R^k f(\underbrace{0,\dots,0}_{k+1})(X^k). \tag{57.6}$$

Here the multilinear forms $\Delta_R^k f(\underbrace{0,\dots,0}_{k+1})\colon \mathcal{V}^k \longrightarrow \mathcal{W}$ are the values at $(0,\dots,0)$ of the kth order noncommutative difference-differential operators applied to f. They can be calculated directly by evaluating f on block upper trangular matrices:

$$f\left(\begin{bmatrix} 0 & Z_1 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & 0 & Z_k \\ 0 & \cdots & \cdots & 0 & 0 \end{bmatrix}\right)$$
$$= \begin{bmatrix} f(0) & \Delta_R f(0,0)(Z_1) & \cdots & \cdots & \Delta_R^k f(0,\dots,0)(Z_1,\dots,Z_k) \\ 0 & f(0) & \ddots & & \Delta_R^{k-1} f(0,\dots,0)(Z_2,\dots,Z_k) \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & f(0) & \Delta_R f(0,0)(Z_k) \\ 0 & \cdots & \cdots & 0 & f(0) \end{bmatrix}.$$

The exact meaning of (57.6) is one of the two:

- If f is a noncommutative function on $\mathrm{Nilp}(\mathcal{V})$, then the expansion holds for all $X \in \mathrm{Nilp}(\mathcal{V})$.

[1]In honour of Brook Taylor and of Joseph L. Taylor.

- If f is a bounded noncommutative function whose domain contains an open noncommutative ball of radius ρ and that is bounded there, then the expansion holds on this ball with the series converging absolutely and uniformly on every noncommutative ball of a strictly smaller radius.

This is merely the simplest of the various convergent Taylor–Taylor series. The expansion can be around any point in $\mathcal{V}_{\rm nc}$ rather than about 0, providing for the possibility of analytic continuation. In the case $\mathcal{V} = \mathbb{C}^d$ one can obtain stronger results relating to the absolute convergence of the series (57.2) over the free semigroup, rather than grouping the terms together to obtain a series of homogeneous polynomials as in (57.6). One can also relax the assumptions of local uniform boundedness over all matrix sizes (with respect to an operator space norm); if a noncommutative function f is locally bounded (or even just locally bounded on slices) in every matrix size, it is still true that its Taylor–Taylor series is locally uniformly convergent in every matrix size (of course the convergence is no longer uniform across matrix sizes). Thus a very weak regularity assumption on a noncommutative function implies already a very strong regularity result.

Progress during the Banff RIT meeting

We are currently working on completing the foundations of the theory of noncommutative functions and their difference-differential calculus, including the preparation of the manuscript [5]. During our week at Banff we made a considerable progress, especially with regard to the detailed proof of the convergence theorem for the Taylor–Taylor series in the non-uniform case, including some facets having to do with the classical theory of analytic functions in several and in infinitely many variables (see, e.g., Hille–Phillips [4] for the later).

Participants

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Chapter 58

Local-global principles for etale cohomology (10rit149)

Mar 07 - Mar 14, 2010

Organizer(s): David Harbater (University of Pennsylvania), Julia Hartmann (RWTH Aachen University), Daniel Krashen (University of Georgia)

Overview

Local-global principles have long been an important part of number theory, beginning with the Hasse principle for quadratic forms over number fields F. This classical form of the principle, which asserts that a quadratic form is isotropic over F if and only if it is isotropic over each completion, holds as well for one-variable function fields over finite fields, and thus for all global fields. Other versions of the local-global principle apply to rational points on varieties, and to elements of cohomology groups (or sets). Such a principle relates an object over a field F to the objects it induces over the completions of F at its discrete valuations.

In [3], we obtained results about quadratic forms and about Brauer groups over higher dimensional fields, such as function fields over the p-adics. These results were proven with the use of a new type of local-global principle for this higher dimensional situation, concerning homogeneous spaces for rational connected linear algebraic groups. That principle was obtained using the technique of patching over fields, a method developed in [2] that was an outgrowth of patching methods that had relied on formal or rigid geometry. In that approach, the completions being considered are not at discrete valuations, but rather correspond to "patches" on the curve.

Using [3], Colliot-Thélène, Parimala and Suresh proved analogous local-global principles in terms of completions with respect to discrete valuations, in the case of quadric hypersurfaces (for application to quadratic forms) and for certain cases in which the homogeneous space is a torsor [1]. The validity of such a local-global principle in general remains open, but [1] motivated work of the three of us on local-global principles for torsors. In particular, we recently showed that local-global principles in terms of patches hold for torsors even for disconnected rational groups provided that the reduction graph of the given curve is a tree.

Since torsors are classified by the first étale cohomology group, this raises the question of whether local-global principles can be shown for higher étale cohomology groups, provided that the linear algebraic group is abelian (so that H^i is defined for $i > 1$). This is the subject of our project at BIRS.

Goals

Given a field F and a linear algebraic group G over F, by a local-global principle for étale cohomology we will mean an assertion that the natural map

$$H^i(F, G) \to \prod_{\xi \in \Xi} H^i(F_\xi, G)$$

has trivial kernel, where $\{F_\xi \,|\, \xi \in \Xi\}$ is a collection of fields containing F that are obtained using completions. Here we assume that G is abelian if $i > 1$; while if $i = 1$, this is a local-global principle for torsors. If F is a global field, the natural collection of overfields is the set of completions of F at discrete valuations. For function fields F over a higher dimensional base K (e.g. $K = \mathbb{Q}_p$), it appears that this set of completions will in general be insufficient, though in special cases it may suffice (as shown in [1] for $i = 1$, in the context of quadratic forms, as mentioned above). Instead, in the case that K is a complete discretely valued field, we consider another choice of Ξ, viz. a set obtained by patches, as in [2] and [3] (also see below).

The desired principle would apply not only to p-adic fields, but more generally to complete discretely valued fields, in particular including n-local fields, paralleling results on homogeneous spaces in [3]. Applications of the desired principle could include local-global principles for structures classified by invariants in higher étale cohomology groups, e.g. for octonion and Albert algebras.

Scientific progress at BIRS

We worked to prove a local-global principle for étale cohomology in the case of commutative linear algebraic groups G over function fields F of curves over complete discretely valued fields K. Since we were relying on results in [3], we assumed that the group G is rational, in the sense that each connected component is a birational to some $\mathbb{A}^n_K$. This is not a very restrictive hypothesis.

As in [3], our local-global principle is framed in terms of patches. That is, we consider a regular projective model $\widehat{X}$ of F over the ring of integers of K, say with closed fiber X, and we take a non-empty set MCP of closed points of X that includes every point at which two components of X meet. For each $P \in$ MCP, we take F_P to be the fraction field of the complete local ring of $\widehat{X}$ at P. For each component U of the complement of MCP in X, we take F_U to be the fraction field of the completion of the subring ring of F consisting of rational functions on $\widehat{X}$ that are regular on U; and we let MCU be the set of such components U. For each branch $\wp$ of X at a point $P \in$ MCP along a component $U \in$ MCU, we also consider the fraction field $F_\wp$ of the complete local ring at $\wp$; and we let MCB be the set of branches. (See [3] for more details about this set-up.)

In this framework, we prove in particular a local-global principle for the n-th cohomology of the group $\mu_\ell^{\otimes n-1}$. Namely, we show that for each $n > 1$, the map

$$H^n_{\text{ét}}(F, \mu_\ell^{\otimes n-1}) \to \prod_{\xi \in \mathrm{MC}P \cup \mathrm{MC}U} H^n_{\text{ét}}(F_\wp, \mu_\ell^{\otimes n-1})$$

is injective. There are also similar results for other tensor powers.

In order to show this, we first prove a long exact Mayer-Vietoris sequence for étale cohomology, relating $H^i(F,G)$, $\prod_{\xi\in\Xi} H^i(F_\xi,G)$ and $\prod_{\wp\in \mathrm{MC}P} H^i(F_\wp,G)$. In fact, we show this holds when G is an arbitrary commutative rational linear algebraic group. The proof uses a new "auxiliary" Grothendieck topology, which we call the *patching-étale topology* and which combines the étale topology with the topology defined by patches. The argument also draws on results from [2].

The above local-global principle is then deduced from the Mayer-Vietoris sequence, together with the Bloch-Kato theorem recently proved by Voevodsky, Rost and Weibel (e.g. cf. [4]). Note here that $n \geq 2$.

In particular, there is a counterexample to the local-global principle for torsors (i.e., for H^1), with $G = \mathbb{Z}/2\mathbb{Z}$ and F the function field of a Tate curve (see [1] or [3]). As noted above, this can occur because the group is disconnected and the reduction graph is not simply connected. But the above construction gives another explanation for this failure of the local-global principle for H^1 in such an example. Namely, the cokernel of the map on the H^0 level is non-trivial, as can be seen from a combinatorial description in terms of the incidence geometry of the components of the closed fiber of a semistable model.

Particiapnts

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Chapter 59

H-holomorphic maps in symplectic manifolds (10rit146)

Apr 11 - Apr 11, 2010

Organizer(s): Jens von Bergmann (University of Calgary), Richard Hind (University of Notre Dame), Ely Kerman (University of Illinois at Urbana-Champaign), Olguta Buse (Indiana University-Purdue University Indianapolis)

Overview of the Field

Symplectic manifolds are the natural domains of the modern mathematical formulation of classical mechanics, and they play a prominent role in many areas of mathematics. Since the introduction of the theory J–holomorphic curves by Gromov in [5], a tremendous amount of progress has been made in the study of these manifolds and the maps which preserve their symplectic structures. This progress has been particularly dramatic in the case of symplectic manifolds of dimension 4. For example, for $S^2 \times S^2$, the symplectic forms are classified (see [5], [14]), their symplectomorphism groups are well understood (see [5], [3]), and their Lagrangian spheres are all known to be symplectically equivalent (see [6]). Ruled symplectic 4–manifolds have also been completely classified (see [11]).

The proofs of these results all have the same starting point; the existence of foliations by J–holomorphic spheres for all tamed almost complex structures. There have been several attempts to establish the existence of such foliations in more general settings. It was recently shown in [7] that such existence statements do not hold for foliations by J–holomorphic spheres of manifolds of dimension greater than 4. For index reasons, one can also not expect to find foliations by J–holomorphic curves of higher genus. To overcome this latter limitation, in the setting of symplectizations of a contact 3–manifolds, H. Hofer proposed in [8] to replace the standard J–holomorphic map equation with a parameterized version where the parameter takes values in the space of harmonic 1–forms on the domain. More precisely, they introduce the notion of an $\mathcal{H}$–holomorphic map which is a map u from a Riemann surface (Σ, j) to the symplectization $(\mathbb{R} \times Z, J)$ of a contact manifold Z such that $\bar{\partial}_J u$ takes values in $\mathcal{H}^{0,1} = \mathcal{H}^{0,1}(u^*\underline{\mathbb{C}})$, the space of harmonic $(0,1)$–forms on Σ with values in the trivial bundle $u^*(\underline{\mathbb{C}})$, where $\underline{\mathbb{C}} \subset T(\mathbb{R} \times Z)$ is the trivial complex vector bundle generated by the $\mathbb{R}$–factor.

For $\mathcal{H}$–holomorphic maps many new analytic difficulties arise. For example, local intersections of such maps need not be positive, and the space of these maps is in general not compact (see [15]). Despite these difficulties, $\mathcal{H}$–holomorphic maps have been used to obtain foliations of contact 3–manifolds. In particular, in both [1] and [16], it is shown that every contact structure on a 3–manifold admits a contact form and an almost complex structure which support an open book decomposition whose pages are embedded $\mathcal{H}$–holomorphic maps.

The use of parameterized versions of the J–holomorphic map equation is not new. For example, they were used to find non–trivial elements in symplectomorphism groups by O. Buse in [4]. As well, the parameter space introduced in [10] was recently used to compute the Gromov-Witten invariants of Kähler surfaces in [12].

Scientific Progress Made

We investigated a generalization of the J–holomorphic map equation for maps into symplectic 4–manifolds. One of our goals is to use these maps to obtain foliations by higher genus surfaces that can be used to generalize some of the classification results obtained for ruled symplectic surfaces. The generalized equations we intend to study are defined in analogy with the $\mathcal{H}$–holomorphic map equation for contact 3–manifolds from [2], as follows.

For a hermitian line bundle (L, ω, J) over a genus g Riemann surface (Σ, j), let $\mathcal{H}^{0,1} = \mathcal{H}^{0,1}(L)$ denote the space of harmonic $(0,1)$–forms with values in L, i.e. sections ξ of $\Lambda^{0,1}T^*\Sigma \otimes L$ satisfying $d^\nabla \xi = 0$, where ∇ denotes the induced hermitian connection on L. Suppose that (X, ω) is a symplectic manifold with almost complex structure J. Let $L \subset TX$ be a J–complex line subbundle. A map $u : \Sigma \to X$ is called $\mathcal{H}$–holomorphic (w.r.t. L) if

$$\bar{\partial}_J u \in \mathcal{H}^{0,1}(u^*L) \subset \Gamma(\Lambda^{0,1}T^*\Sigma \otimes u^*TX)$$

Hence, the $\mathcal{H}$–holomorphic map equation for symplectic manifolds is a parameterized version of the J–holomorphic map equation with parameter space given by the finite dimensional vector space $\mathcal{H}^{0,1}$ of twisted harmonic $(0,1)$–forms.

To better understand this definition let (X^4, ω) be a symplectic surface bundle, i.e. X is a fiber bundle $\pi : X \to V$ with connected symplectic fibers of genus g and a symplectic base (V, ω_V) of real dimension 2. Let $F = \ker(d\pi) \subset TX$ be denote the vertical subbundle and let $L = F^\omega$ be its symplectic complement. Fix an almost complex structure J so that the splitting $TX = L \oplus F$ is J–invariant.

In this situation X is foliated by J–holomorphic curves in the class of the fiber. Unfortunately the linearized operator for J–holomorphic maps is not surjective. Indeed, the kernel of the linearized operator is 2–dimensional, but the index of this problem is $2(1 - g)$.

On the other hand, each J–holomorphic map u is also $\mathcal{H}$–holomorphic. The bundle u^*L is trivial so $\mathcal{H}^{0,1}(u^*L)$ has dimension $2g$ by Riemann–Roch and u has index $2(1-g)+2g = 2$. Moreover, the linearized operator for $\mathcal{H}$–holomorphic maps is surjective.

During the workshop we investigated the behavior of $\mathcal{H}$-holomorphic maps for more general choices of almost complex structure J and line bundle L. Unlike in the contact manifold case that was studied before, in the current setting the bundle L is not geometrically trivial. This introduces many analytical difficulties that make some of the arguments significantly harder, and render other results false.

Unlike in the contact manifold case we were not able to prove automatic regularity, i.e. surjectivity of the linearized problem, for $\mathcal{H}$-holomorphic maps, however, for generic compatible almost complex structure J all $\mathcal{H}$-holomorphic maps are regular. Moreover, for any fixed compatible almost complex structure J and generic choice of complex line bundle L, all $\mathcal{H}$-holomorphic maps transverse to L are regular.

Another important step when foliating contact manifolds by $\mathcal{H}$-holomorphic maps is that algebraic invariants guarantee that families of maps that start out transverse to L remain transverse to L. We have found counterexamples to show that this is not true any more in our setting.

In order to foliate the image manifold one needs to show that the linearized operator is superregular, that is that its kernel contains a pair of pointwise linearly independent sections that are transverse to the map. In our setting it is the curvature of L that complicates the situation compared the case in contact geometry, and we were not able to prove superregularity of the operator in our setting.

The main difficulty in generalize the results from contact geometry to our setting is given by the curvature of L. In the cases that we are interested in we always assume that L is topologically trivial, so L always admits a flat connection by choosing a complex trivialization. If we assume that we have a canonical choice of flat connection we can significantly improve on the previous theorem.

Examples of cases where such curvature assumptions hold are symplectic mapping tori (see [9]).

Participants

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Chapter 60

Boundary problems for the second order elliptic equations with rough coefficients (10rit135)

Apr 18 - Apr 25, 2010

Organizer(s): Svitlana Mayboroda (Purdue University), Steven Hofmann (University of Missouri-Columbia), Carlos Kenig (University of Chicago), Jill Pipher (Brown University)

Overview of the Field and the Framework

The main focus of the meeting was on boundary value problems for general differential operators $L = -\mathrm{div}\, A\nabla$. Here A is an elliptic matrix with variable coefficients, given by complex-valued bounded and measurable functions. Such operators arise naturally in many problems of pure mathematics as well as in numerous applications. In particular, they describe a wide array of physical phenomena in rough, anisotropic media. Thus, one of the central questions is: *what kind of medium yields solvable boundary problems*, or, mathematically, *what are the sharp conditions on the matrix A responsible for the solvability of problem $-\mathrm{div}\, A\nabla u = 0$ in a given domain $\Omega \subset \mathbb{R}^n$, $u|_{\partial\Omega} = f$, with boundary data, for instance, in $L^p(\partial\Omega)$*. Despite tremendous advances in the elliptic theory over the past half a century, this question remains largely open.

Recent Developments and Open Problems

For purposes of this discussion let us concentrate on the case $\Omega = \mathbb{R}^n_+ = \{(x,t) : x \in \mathbb{R}^{n-1},\, t \in (0,\infty)\}$.

It has been known for a long time that some restrictions on the matrix A are necessary to ensure solvability, and more precisely, certain smoothness in the transversal direction t is needed [4]. This observation naturally leads to two threshold problems.

Problem 1. *Establish solvability of boundary problems for a t-independent matrix A.*

Problem 2. *Investigate the perturbation: which restrictions on $A - A_0$ would allow one to pass from solvability results for A_0 to those for the matrix A.*

The first results towards Problems 1 and 2 date back to the early 80's. However, both of them are still far from being fully understood.

There are three basic types of boundary value problems: the Dirichlet problem with the prescribed trace on the boundary (stated in Section 1), the Neumann problem with the given flow through the boundary, i.e., normal derivative, and the regularity problem when the tangential derivative is known. In each case, most of the results available pertain to *real and symmetric* coefficients. In this context, the solvability for the Dirichlet problem with t-independent matrix A is due to D. Jerison and C. Kenig [10], and for the Neumann and the regularity problems due to C. Kenig and J. Pipher [11], [12]. Aside from these achievements, only a few results exist, addressing real non-symmetric matrices *in dimension two* [7], [13].

In the direction of Problem 2, a few approaches emerged. The situation when A and A_0 are *real and symmetric* and the discrepancy $A - A_0$ has bounded Carleson norm has been treated in [5], [6], [11], [12]. For *complex* matrices analogous perturbation result was established by S. Hofmann and S. Mayboroda [9] and independently in [2] under additional assumptions that A_0 is t-independent and the Carleson norm of $A - A_0$ is small. It is important to observe that while the Carleson condition is, in some sense, sharp [6], it necessarily requires that A and A_0 coincide on the boundary. Thus, one has to investigate independently a complementary problem: *find the optimal conditions on $A - A_0$, with $A \not\equiv A_0$ on the boundary, such that the solvability for A could be deduced from solvability for A_0*. In this context, it has been only known that the smallness of the L^∞ norm of $A - A_0$ is sufficient [1].

It has long been recognized that any further progress would require introduction of some decisively new methods. A big advantage of real symmetric matrices is availability of the Rellich identity. The latter allows one to compare the tangential and normal derivatives of the solution on the boundary, and has proved to be one of the leading tools in the analysis of boundary value problems. In particular, it was extensively used in the aforementioned works. Unfortunately, there is no analogue of the Rellich identity even for real non-symmetric matrices. Moreover, complex coefficients offer a whole new set of challenges: the positivity of the solutions, comparison principle, and thus, harmonic measure techniques essentially fail. At the same time, a few available methods of the analysis of elliptic operators with non-smooth *complex* coefficients, largely emerging from [3], are still extremely limited and await to be fully developed.

Scientific Progress Made

The meeting has brought significant advancement in the direction of Problems 1 and 2. Already in the first few days we have established the solvability of the boundary problems under the assumption that the matrix A is t-independent and close to identity in BMO. More precisely, we have showed the following.

Theorem 1. *Let $L = -\mathrm{div}\, A\nabla$ be an elliptic operator in $\mathbb{R}^{n+1}_+$ with complex bounded measurable coefficients independent of the transversal direction t. Then there exists $\varepsilon > 0$ such that the boundary value problems for L are well-posed in L^2 whenever $\|A - I\|_{BMO} < \varepsilon$.*

Note that, *in the case when $A_0 = I$*, Theorem 1 is strictly stronger than all previously available results for complex t-independent matrices. Indeed, the space BMO is strictly larger than L^∞ and, thus, in this context, the perturbation in the L^∞ norm discussed in Section 2 immediately follows from Theorem 1.

At the same time, our result opens several new directions of research. For instance, one would like to know what are the optimal restrictions on A_0. Specifically, it is desirable to have an analogue of Theorem 1 with any "good" A_0 in place of I, i.e., such that $L_0 = -\mathrm{div}\, A_0\nabla$ yields well-posed boundary problems.

Furthermore, during the meeting the participants have actively pursued Problem 1. The main theorems in [7] include sufficient conditions on absolute continuity of the elliptic measure (and thus, the solvability of the Dirichlet problem) for real non-symmetric matrices. The most general results were not, however, stated in terms of the conditions on the matrix A, but rather invoking some a priori estimates on the square function and non-tangential maximal function of solutions. At the time, these estimates could be originally verified only in the two-dimensional case. It seems though that the infusion of new methods from [3], [1], [9] could pave a way to a full higher-dimensional result. At the meeting we have built a possible strategy to attack this problem, and currently we are actively working on its major aspects.

Outcome of the Meeting

The meeting has been successful and productive at many levels. Based on the progress outlined above we are now preparing a manuscript of the paper. Moreover, an intensive exchange of the ideas, continuous collaboration and brainstorming allowed us to single out possible strategies for some outstanding problems in the field. In this connection, an opportunity to meet together at BIRS for a full week of an uninterrupted focused research has been invaluable. Now that the foundation for future work is laid, the participants will continue working at their home institutions, and hopefully, many more results are on the way.

Participants

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Chapter 61

Alexandrov Geometry (10rit151)

May 02 - May 09, 2010

Organizer(s): Stephanie Alexander (University of Illinois at Urbana-Champaign), Vitali Kapovitch (University of Toronto), Anton Petrunin (PennState University)

Overview of the Project

The purpose of our research stay was to work on our book "Alexandrov Geometry". Our book is supposed to be a comprehensive text and reference work on the fields of curvature bounded below and curvature bounded above. Although these two fields developed quite independently, they have many similar guiding intuitions and technical tools. Our approach is novel in its attention to the interrelatedness of the two fields, and its emphasis on the way each illuminates the other.

In addition to all the basic material in both fields, the book includes all the important advanced material on spaces of curvature bounded below. This material is unavailable in any book, and not all of it is in the literature. For spaces of curvature bounded above, we are emphasizing topics and proofs inspired by considering the two contexts simultaneously.

Progress Made

At present, our draft is about 250 pages. The final version will be at least twice that. Most of the current draft material is in the attached version of the book.

We were working on the book for more than half a year without face-to-face contact. (Before that we met for a week in October 2008 and S. Alexander and A. Petrunin met in July 2009). During this time, a number of issues accumulated. We were able to get through the complete list of them and make very substantial progress in just one week at Banff.

Many of our discussions during the research stay concerned proofs and advanced topics to be included. Some proofs became more transparent, and new and surprising dualities between the two bodies of material came to light. These findings improve the book's coherence and elegance. More specifically, we mostly worked on Chapter 6 (Definitions of curvature bounded from below) and Chapter 7 (Definitions of curvature bounded above). Chapter 6 is now mostly complete and we feel it's sufficiently ready to be made available to public. Therefore, after coming back from Banff we posted this chapter on the web. It can be accessed here http://www.math.toronto.edu/vtk/the-defs-CBB.pdf , here http://www.math.uiuc.edu/sba/the-defs-CBB.pdf or here http://www.math.psu.edu/petrunin/papers/alexandrov-geometry/

Chapter 7 is now also mostly complete and hopefully we'll soon be able to make it available to public as well.

The visit to BIRS had other unexpected benefits:

- Consistency: The fields of curvature bounded below and curvature bounded above can favor different formulations, and a balance must be negotiated.
- Notation: Our approach requires new notations aimed at transparency and economy. Finally settling on optimal notation to mediate between the reader and the material is challenging.
- Technical: Our figure-preparation and file-sharing arrangements were improved.
- Lastly: We had many interesting conversations with other BIRS visitors at mealtimes and while they were not usually directly related to our main project they were nevertheless quite stimulating.

  Overall we had an extremely productive visit which was absolutely perfect for the kind of project we are involved in.

Participants

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Kapovitch, Vitali (University of Toronto)
Petrunin, Anton (PennState University)

Chapter 62

Borel measurable functionals on measure algebras (10rit156)

Jul 04 - Jul 11, 2010

Organizer(s): Harold Garth Dales (University of Leeds), Anthony To-Ming Lau (University of Alberta)

Overview of the Field

Let A be a Banach algebra. Then there are two natural products, here denoted by $\Box$ and $\Diamond$, on the second dual A'' of A; they are the *Arens products*. For definitions and discussions of these products, see [3, 4, 5, 6], for example. We briefly recall the definitions. As usual, A' and A'' are Banach A-bimodules. For $\lambda \in A'$ and $\Phi \in A''$, define $\lambda \cdot \Phi \in A$ and $\Phi \cdot \lambda \in A'$ by

$$\langle a, \lambda \cdot \Phi \rangle = \langle \Phi, a \cdot \lambda \rangle , \quad \langle a, \Phi \cdot \lambda \rangle = \langle \Phi, \lambda \cdot a \rangle \quad (a \in A) .$$

For $\Phi, \Psi \in A''$, define

$$\langle \Phi \Box \Psi, \lambda \rangle = \langle \Phi, \Psi \cdot \lambda \rangle \ (\lambda \in A') ,$$

and similarly for $\Diamond$. Thus $(A'', \Box)$ and $(A'', \Diamond)$ are Banach algebras each containing A as a closed subalgebra. The Banach algebra A is *Arens regular* if $\Box$ and $\Diamond$ coincide on A'', and A is *strongly Arens irregular* if $\Box$ and $\Diamond$ coincide only on A. A subspace X of A' is *left-introverted* if $\Phi \cdot \lambda \in X$ whenever $\Phi \in A''$ and $\lambda \in X$.

There has been a great deal of study of the two algebras $(A'', \Box)$ and $(A'', \Diamond)$, especially in the case where A is the group algebra $(L^1(G), \star)$ or the measure algebra $(M(G), \star)$ of a locally compact group G. For example, it has been known for a long time that $L^1(G)$ is strongly Arens irregular for each locally compact group G. On the other hand, each C^*-algebra is Arens regular.

Recently, the three participants have studied [5] the second dual of a semigroup algebra; here S is a semigroup, and our Banach algebra is $A = (\ell^1(S), \star)$. We see that the second dual A'' can be identified with the space $M(\beta S)$ of complex-valued, regular Borel measures on βS, the Stone–Čech compactification of S. In fact, $(\beta S, \Box)$ is itself a subsemigroup of $(M(\beta S), \Box)$. See [13] for background on $(\beta S, \Box)$.

Let G be a locally compact group. The algebra $M(G)$ has been much studied. This algebra is the multiplier algebra of the group algebra $L^1(G)$. Even in the case where G is the circle group $\mathbb{T}$, the Banach algebra $M(G)$ is very complicated; its character space is 'much larger' than the dual group $\mathbb{Z}$ of $\mathbb{T}$ [10].

Starting at a BIRS 'Research in Teams' in September, 2006, the three participants have been studying the algebras $(M(G)'', \Box)$ and $(L^1(G)'', \Box)$. Our work continued at other meetings, some at BIRS, and in 2007 and 2008 we established a number of other results that are contained in [6].

The first part of our memoir [6] studied the second dual space of $C_0(\Omega)$, where Ω is a locally compact space. This second dual is identified with $C(\widetilde{\Omega})$ for a certain hyper-Stonean space $\widetilde{\Omega}$; in particular, $\widetilde{\Omega}$ is compact and extremely disconnected. The space $C(\widetilde{\Omega})$ contains as a proper closed C^*-subalgebra the space $\kappa(B^b(\Omega))$, which is an isometric copy of $B^b(\Omega)$, the space of *bounded Borel* functions on Ω. The *Dixmier space*, $D(\Omega)$, of Ω is the quotient of $B^b(\Omega)$ by the ideal of functions that vanish on sets of measure 0. These latter spaces, and their relation to $C(\widetilde{\Omega})$, are themes of our work.

We then turned to the algebras $(M(G)'', \Box)$ and $(L^1(G)'', \Box)$ when G is a locally compact group. For example, [6] contains many results on the semigroup structure of $\widetilde{G}$, which is the natural analogue of βS in the non-discrete case. Indeed it is shown in [6, Chapter 8] that $(\widetilde{G}, \Box)$ is semigroup if and only if G is discrete, and in [6, Chapter 7] that the algebra $(M(\widetilde{G}), \Box)$ determines the locally compact group G.

Finally we mention some strong results [7, 8, 9] of M. Daws, who proved using techniques from the theory of Hopf–von Neumann algebras that the space $W := WAP(M(G))$ of weakly almost periodic functionals on the measure algebra $M(G)$ of a locally compact group G is a commutative C^*-algebra, so resolving a long-standing open question, and also that the character space Φ_W of W is a compact, semi-topological semigroup under the natural product associated with the Arens product on W'. This latter result shows that Φ_W is entirely analogous in the non-discrete case to the well-known weakly almost periodic compactification of a group. The corresponding results about the Fourier algebra $A(G)$ and the Fourier–Stieljes algebra $B(G)$ are apparently open. s

The plan for the present research week had three aspects: s

(1) Let $B^b(\Omega)$ be the C^*-algebra of bounded, Borel functions on a locally compact space Ω, as above, viewing the elements of this space as continuous linear functionals on the measure space $M(\Omega)$. The character spaces of $B^b(\Omega)$ and $D(\Omega)$ are denoted by Φ_b and Φ_D, respectively. The space Φ_b is a topological quotient of $\widetilde{\Omega}$ and is totally disconnected, but it is not a Stonean space; the latter space is a Stonean space. We would like to calculate the cardinalities of key subsets of these spaces; this would be analogous to work in [6]. We also wish to know for which locally compact spaces Ω the space Φ_D is hyper-Stonean.

(2) Let G be a locally compact group. The maximal introverted translation-invariant subspace X of $B^b(G)$ is well-defined, and then $(X', \Box)$ is a Banach algebra. In this case, X is a closed subspace of $B^b(G)$. It is not clear whether X is always a C^*-subalgebra of $B^b(G)$; if so, the character space Φ_X of X is a compact right-topological semigroup analogous to a Stone–Čech compactification. We planned to investigate the linear space X and the compact space Φ_X in various cases. We question whether W and $\kappa(B^b(G))$ are introverted subspaces of $C(\widetilde{G})$.

(3) We planned to investigate which functions on $\widetilde{G}$ belong to the above-mentioned space W. For example, we do not know whether or not the characteristic function of the character space Φ of $L^\infty(G)$ belongs to W. This question is related to questions about the products $\varphi \Box \psi$ for $\varphi, \psi \in \widetilde{G}$ that were studied in [6]; these questions seem to have independent interest, and are related to problems about the products of singular measures on G. We also wished to determine the topological structure of the character space Φ_W.

Recent Developments and Open Problems

We cite two recent results.s

1) A dramatic recent result of Losert, Neufang, Pachl, and Steprans [15] establishes that $M(G)$ is strongly Arens irregular for each locally compact group G.s

2) An impressive calculation of Budak, Işik, and Pym [2] discusses how many points are required to 'determine the topological centre' of the Banach algebras $L^1(G)$ for all locally compact groups and $\ell^1(S)$ for various semigroups S. These results are related to those in [5].

Presentation Highlights

Since this was a workshop for three people assembled for ‘Research in teams’, there were no formal presentations.

Scientific Progress Made

We made progress in three related areas.s
1) The following question was not specifically mentioned in the proposal, but seems to be a key preliminary to our work. *Let X be a compact space such that $C(X)$ is isometrically isomorphic to the second dual space of a Banach space. Is it necessarily true that there is a locally compact space Ω such that $X = \widetilde{\Omega}$?*

In Banff, we established the following result. Here D represents the collection of extreme points of the unit ball of $N(X)$, the space of normal measures on X. As in [6], D can be identified with the set of isolated points of X.

Let X be a compact space such that $C(X)$ is isometrically isomorphic to the second dual space of a separable Banach space. Then either D is countable and $C(X)$ is isometrically isomorphic to $C(\beta\mathbb{N}) = c_0''$, or D has cardinality $\mathfrak{c}$ and $C(X)$ is isometrically isomorphic to $(C[0,1])''$.

However, after our stay in Banff, we discovered that this result is already contained in an old paper of H. Elton Lacey [14], with a different proof in [12]; we are grateful to F. Dashiell and T. Schlumprecht for a discussion of the literature. It seems that our proof is quite elementary, and avoids the appeal to some deep results in Banach space theory that Lacey makes. It is not clear whether our proof is sufficiently different from existing proofs to justify publication.

The question in the case when the space $C(X) = E''$ for a space E that is not separable remains open.

The analogous question in the isomorphic theory of Banach spaces was resolved in a similar way by Stegall [17]; for related work, see [11].s
2) Let G be a locally compact group. We asked whether or not the space $B^b(G)$ is left-introverted for each locally compact group G. We proved that this is not the case, at least when the group G is infinite and metrizable. The easy proof uses a strong, old result of Rudin from [16]. We do not yet know the answer in the case where G is not metrizable.s
3) Again, let G be a locally compact group. We considered the space W of weakly almost periodic functionals on $M(G)$. We proved that W can be identified with the space of functions $F \in C(\widetilde{G})$ such that $F(\varphi \,\square\, \psi) = F(\varphi \diamond \psi)$ for all $\varphi, \psi \in \widetilde{G}$, a result also contained in the work of Daws; our proof of this result uses a theorem of Bourgain and Talagrand [1]. Using this result, we can easily see that $\kappa(B^b(G)) \cap W$ is a C^*-subalgebra of $C(\widetilde{G})$, a result that follows from Daws’ work, give examples of various elements that belong to the space W, but not to $\kappa(B^b(G))$, and can show that W is ‘large’ in some sense; we hope to make this statement more precise.

Outcome of the Meeting

The three participants are continuing to work on the mentioned problems, and expect our work to lead to a publication in due course. In particular, we shall meet again in Leeds in December 2010 to attempt to make further progress

Lau will attend a conference on *Harmonic analysis* at the Chern Institute of Mathematics, Nankai University, Tianjin, China in June, 2011,

Dales, Lau, and Strauss will attend the *20th International Conference on Banach algebras in Waterloo, Canada*, 3-10 August, 2011, and will have discussions on their work there.

A proposal has been made to the *Fields Institute* in Toronto for a Thematic Program on *Banach algebras and harmonic analysis* in the second half of 2013; each of the three participants is an organiser or co-organiser of this programme. In particular, this proposal suggests a workshop on *Topological centres*; this topic is closely related to our present work. It is expected that many questions related to our work, and related matters, will be discussed during this semester.

Participants

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Chapter 63

Analytic index theory (10rit136)

Jul 25 - Aug 1, 2010

Organizer(s): Adam Rennie (Australian National University), John Phillips (University of Victoria)

Overview of the Field

The local index formula in noncommutative geometry, initially proved by Alain Connes and Henri Moscovici in 1995, [9], is an analytic formula for the index of Fredholm operators that can be shown to imply the Atiyah-Singer local index formula for Dirac type operators (as shown by Raphael Ponge, [13]) but is more general in that it provides a computable formula for noncommutative index problems. The formula is cohomological in the sense that it is seen to be connected to Connes (b, B) complex in cyclic theory.

The connection to the classical case is that for a compact manifold M, cyclic cohomology of $C^\infty(M)$ is just the de Rham homology of M with complex coefficients. In the noncommutative case the hope is that the cyclic theory, with its long exact sequences, can add computational and conceptual tools to the computation of index pairing problems.

However the original formulation requires working with the standard trace on the algebra of bounded operators on Hilbert space whereas long ago Alain Connes and Joachim Cuntz, [8], showed that any study of cyclic cohomology leads very naturally to traces on semifinite von Neumann algebras not just on the bounded operators on Hilbert space. In [4] and [1] examples of situations where noncommutative geometry methods may be used to compute a semifinite index formula were found.

Subsequently, inspired by a new proof of the local index formula by Higson, [11], the participants in this workshop discovered a new version of the local index formula that is proved in the context of unital semifinite spectral triples under weaker hypotheses than the original theorem [5, 6, 7]. It was proposed that this current workshop would investigate whether the theory had reached a sufficiently stable state so that writing a monograph on the topic would be of use to researchers interested in the problem.

Recent Developments and Open Problems

In the course of preparing for the workshop the relevance of a new viewpoint involving nonunital spectral triples (in the sense of [2]) became apparent. Nonunital spectral triples are relevant to the index theory of Dirac type operators on noncompact manifolds, and particularly to the study of pseudo-Riemannian manifolds which is a topic of considerable interest to physicists.

The notion of nonunital spectral triple has proved rather difficult to properly formulate, and efforts in this direction have actually required rather substantial advances in the theory of operator ideals in von Neumann algebras.

In current work, [3], a very general approach to the problem of proving the local index formula in semifinite noncommutative geometry for nonunital algebras is being explored. It relies on the proof of the index formula in [7], *all* other approaches being impossible *on quite fundamental grounds*.

In finding the minimal conditions and methods needed to push this proof through, this project helped constrain the possibilities for the definition of a nonunital spectral triple.

Scientific Progress Made

The main discussion point for the meeting was whether there were examples of nonunital spectral triples satisfying the tentative definition implied by the approach of [3]. Given that this latter paper was far from being in a final state there was considerable fluidity in the formulation and much interplay between putative examples and the formulation of general theory.

The key examples which should be covered by any useful index theory for nonunital spectral triples are:
- the generalisation of the Atiyah-Singer index formula to noncompact manifolds, as studied in [10],
- the L^2-index theorem for noncompact manifolds, previously unstudied,
- the Phillips-Raeburn theorem for actions of $\mathbb{R}$ on arbitrary C^*-algebras with unbounded trace.

A good understanding of all three problems was reached, and how they all fit into the one context provided by nonunital spectral triples.

One key unifying feature which we wish to point out is the discovery of a single analytic framework dealing with summability and smoothness of spectral triples. The summability and smoothness conditions are the main ingredients in the local index formula, and finding a single framework to discuss these two, seemingly disparate, features was a major conceptual breakthrough.

Less pleasingly, it was realised that *all* papers on the local index formula contain a hidden continuity assumption, which is nontrivial. It is known how to prove this continuity in the case of classical manifolds, though it requires the sophisticated machinary of complex powers of pseudodifferential operators. Higson presents a generalisation and simplification of this method in [11], and shows that it gives the required continuity for more exotic examples arising from manifolds. This continuity question is difficult to address in general, and a case by case approach is still required to check that it is satisfied.

Outcome of the Meeting

A consensus was reached on the correct definition of smooth finitely summable semifinite spectral triple. This was tested by extensive calculations undertaken both at BIRS and in the subsequent week spent by some of the participants at the University of Victoria. Three conjectures were made. The first was in the context of complete Riemannian manifolds M where a formula of Gromov-Lawson type [10] was proposed for Dirac type operators on vector bundles over M. The second was on a smooth version of the nonunital index formula of Phillips-Raeburn [12] for generalised Toeplitz operators. The third was on the extension of the L^2-index theorem to noncompact manifolds. In addition the text of [3] was re-worked to take into account the nature of these two conjectures.

The main outcome of the meeting is expected to be an extended account of the nonunital theory in a rather lengthy text that will greatly extend the current preliminary form of [3]. It is likely the Phillips-Raeburn theorem will be dealt with in a separate text.

Participants

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Chapter 64

Subordination Problems Related to Free Probability (10rit159)

Aug 15 - Aug 22, 2010

Organizer(s): Michael Anshelevich (Texas A&M University) Serban Belinschi (Department of Mathematics and Statistics, University of Saskatchewan) Maxime Fevrier (Universite Paul Sabatier, Institut de Mathematiques de Toulouse) Alexandru Nica (University of Waterloo)

Overview of the field

Our research project is in the area of noncommutative probability. Noncommutative probability emerged in the early '80s as a very powerful tool for the study of finite operator algebras. The fundamental idea is to view a pair (A, τ), where A is a unital algebra over the complex numbers (usually endowed with a suitable norm topology), and τ is a linear, unit preserving, functional on A, as a noncommutative probability space, in which the role of integration is taken by τ, while A plays the role of a function algebra over a probability space from the commutative case. There are several notions of independence specific only to the noncommutative setup. From an operator algebraic perspective, one can think of a noncommutative independence as a rule on how to extend τ from a family of independent subalgebras to the algebra they generate together. Our project is mainly related to the *free independence.* Free independence was introduced by Voiculescu [10] in the eighties with the intention of studying in a probabilistic framework the free group factors $L(\mathbb{F}_n)$ generated by the left regular representation of the free group with n generators $\mathbb{F}_n$. Since then, free probability became a powerful tool in several other areas of mathematics beyond operator algebras, especially in random matrix theory (the paper [11] initiated this direction of investigation, which since then has known a spectacular growth).

The subordination property (in the sense of Littlewood) for free convolutions, which forms the main subject of our research project, has been first noted in [12] by Voiculescu for free additive convolution: it has been shown in this paper (under an easily removable genericity condition) that the Cauchy-Stieltjes transform

$$G_{\mu_X \boxplus \mu_Y}(z) = \int_{\mathbb{R}} \frac{1}{z-t}\, d(\mu_X \boxplus \mu_Y)(t) \quad \Im z > 0$$

of the free additive convolution $\mu_X \boxplus \mu_Y$ of the probability distributions μ_X and μ_Y of the selfadjoint random variables X and Y is subordinated to G_{μ_X}. That is, there exists an analytic self-map of the complex upper half-plane ω so that $G_{\mu_X \boxplus \mu_Y}(z) = G_{\mu_X}(\omega(z))$, $\Im z > 0$. Biane [3] extended this result to a statement about conditional expectations: given two selfadjoint random variables X, Y which are free from each other, there exists a unique analytic self-map of the upper half-plane ω so that:

(1) $\lim_{y\to+\infty}\omega(iy)/iy = 1$, and

(2) $E_X((z-X-Y)^{-1}) = (\omega(z)-X)^{-1}$, where E_X denotes the conditional expectation from the unital algebra generated by X and Y onto the unital algebra generated by X.

(As E_X is trace-preserving, this is indeed a generalization of Voiculescu's result.) This analytic subordination result, and a similar one for free multiplicative convolution, has been used by many authors (Belinschi, Benaych-Georges, Bercovici, Biane, Chistyakov, Götze, Guionnet, Lenczewski, Nica, Voiculescu, Wang, Williams etc) to study free entropy for single random variables, to prove regularity results and arithmetic properties for free convolutions, as well as existence results and connections with other convolutions from noncommutative probability theory.

Another major step in the understanding of the role of subordination in free probability was made by Voiculescu in [14]. Paralleling on the one hand the construction of free products with amalgamation and on the other classical conditional expectations, Voiculescu defined *freeness with amalgamation* over a unital $*$-subalgebra B. In this context, he showed that if X and Y are free with amalgamation over B, then there exists a unique analytic self-map $\omega : B^+ \to B^+$ so that

$$E_{B\langle X\rangle}((b-X-Y)^{-1}) = (\omega(b)-X)^{-1}, \quad b\in B^+,$$

where B^+ denotes the set of elements of B with strictly positive imaginary part, and $E_{B\langle X\rangle}$ is the conditional expectation from $B\langle X, Y\rangle$ (the $*$-algebra generated by B, X and Y) onto $B\langle X\rangle$. (The result is expressed in terms of fully matricial sets and functions, and the proof is based on the observation that certain conditional expectations involved are co-algebra morphisms; however, we will not go into those details here.) Thus, the analytic subordination plays an important role in operator-valued non-commutative probability.

An aspect of considerable interest in the probabilistic approach to operator algebras is the study of joint distributions of k-tuples of selfadjoint random variables. Unlike in classical probability, however, the distribution of $(a_1,\ldots,a_k)$ with respect to τ needs not be a probability measure, as the variables $a_1,\ldots,a_k$ need not commute with each other. Thus, we define the distribution of $(a_1,\ldots,a_k)$ as simply the values that τ takes on all monomials in $a_1,\ldots,a_k$ (we call this sequence the *moment sequence* of $(a_1,\ldots,a_k)$.) As for the case when $k=1$, it is convenient to place the moment sequence in a formal power series in non-commuting variables $z_1,\ldots,z_k$:

$$M_{(a_1,\ldots,a_k)}(z_1,\ldots,z_k) = \sum_{n=1}^{\infty}\sum_{i_1,\ldots,i_n=1}^{k}\tau(a_{i_1}\cdots a_{i_n})z_{i_1}\cdots z_{i_n}.$$

If μ is the distribution of $(a_1,\ldots,a_k)$, then $M_{(a_1,\ldots,a_k)}$ is sometimes denoted by M_μ. By starting from M_μ one defines two other important series, the R-transform R_μ and the η-series η_μ. These series linearize the operation $\boxplus$ of free additive convolution and respectively the operation of Boolean convolution $\uplus$, which is the counterpart of $\boxplus$ in Boolean probability theory.

For the study of sums and products of free k-tuples of random variables, the main tool has been the combinatorial aparatus of free cumulants developed by Nica and Speicher [9]. This tool is based on formal power series in non-commuting variables (as above), and as of this moment no explicit subordination result is known in this context, despite the recent progress realized by Nica in defining a subordination distribution [7].

Operator valued free probability and the study of distributions of k-tuples of free random variables are intimately connected, at least in principle, in the sense that one can rephrase problems from the second in terms of the first. However, despite this fact being known for more than a decade, a precise correspondence of the tools and methods involved is still missing.

Some recent developments

Results related to subordination have appeared recently in literature in significant numbers. We would like to mention some of them which are relevant to our project.

(1) Generalizing Lenczewski's work [6], where an operator model for the so-called subordination distribution was proposed, Nica [7] has constructed a subordination distribution for k-tuples of selfadjoint random variables, and showed that they satisfy the same arithmetic properties with respect to non-commutative convolutions as in the case when $k = 1$.

(2) Recent work of Capitaine, Donati-Martin, Féral and Février [4] uses the subordination property in the investigation of the eigenvalues of spiked perturbations of Wigner matrices.

(3) Using Voiculescu's machinery of fully matricial sets and functions, Belinschi, Popa and Vinnikov [1] have recently proved several limit theorems for operator-valued selfadjoint random variables and given a description of the Boolean-to-free Bercovici-Pata bijection in the operator-valued context.

(4) In [5], Curran extends the free difference quotient coalgebra approach to analytic subordination to the case of a free compression in free probability. Free compressions with a projection have been shown to correspond in terms of distributions to free convolution powers by Nica and Speicher [8]. The subordination property for scalar-valued random variables has been proved by Belinschi and Bercovici.

Scientific progress made

The first two days of the meeting were dedicated to presentations made by the four participants concerning their fields of specialization (Anshelevich on operatorial realizations for distributions, Belinschi on the analytic approach to Voiculescu's theory of fully matricial maps and sets, Février on the use and interpretation of the subordination property in random matrix theory, and Nica on combinatorial aspects of both scalar and operator valued distributions of k-tuples of random variables). For the rest, we have approached several problems, and we can report definite progress on issues.

First, following the realization of subordination distributions for k-tuples by Nica [7], it was a natural question to ask whether this distribution indeed deserves its name: does it satisfy a subordination relation? The following theorem of Anshelevich and Nica answer this question in the affirmative:

Theorem 4 *Let $X_1, \ldots, X_k$ and $Y_1, \ldots, Y_k$ be selfadjoint random variables in a non-commutative probability space $(\mathcal{A}, \tau)$. Assume that $\mathcal{B} \subset \mathcal{A}$ is a unital subalgebra so that $X_i \in \mathcal{B}$ and Y_i are free from $\mathcal{B}$ for all $1 \leq i \leq k$. Let $z_1, \ldots, z_k$ be non-commuting indeterminates, and denote by μ the joint distribution of $(X_1, \ldots, X_k)$ and by ν the joint distribution of $(Y_1, \ldots, Y_k)$ Then*

$$\mathbb{E}_{\mathcal{B}}\left[\left(\mathbf{1} - \sum_{i=1}^{k}(X_i + Y_i)z_i\right)^{-1}\right] = \left((\mathbf{1} - \eta^{\nu,\mu}(z_1, \ldots, z_k)) - \sum_{i=1}^{k} X_i z_i\right)^{-1}.$$

Here $\mathbb{E}_{\mathcal{B}}$ denotes the conditional expectation onto $\mathcal{B}$ and $\eta^{\nu,\mu}(z_1, \ldots, z_k))$ denotes the eta-series *of the subordination distribution of ν with respect to μ (as in [7]).*

The second aspect concerns aspects of free additive convolution and free Brownian motions for operator-valued free probability. As in classical probability, the centered free central limits (the semicircular, or Wigner, distributions) are known [10] to be indexed by their variances $t \in (0, +\infty)$. Moreover, if γ_t is the centered semicircular distribution with variance t, then $\gamma_t \boxplus \gamma_s = \gamma_{t+s}$, so that convolution powers $\{\gamma_t = \gamma_1^{\boxplus t} \colon t > 0\}$ form a convolution semigroup. Voiculescu [13] proved a free central limit theorem for operator-valued distributions, and found the operator-valued semicircular distributions to be naturally indexed by the semigroup of *completely positive* linear maps $\eta\colon B \to B$, so that $\gamma_\eta \boxplus \gamma_{\eta'} = \gamma_{\eta+\eta'}$ (as above, B denotes the algebra of scalars). This fact motivates a natural question (explicitely asked by Hari Bercovici), namely under what conditions one can define convolution powers $\mu^{\boxplus\eta}$ for operator-valued distributions μ and completely positive maps η?

Nica and Speicher found in [8] that any probability measure μ on the real line belongs to a partial free convolution semigroup $\{\mu^{\boxplus t}\colon t \geq 1\}$. This result, together with the connections of such semigroups to free Brownian motions found in [2], motivated our search for the main result of our recent preprint "Convolution powers in the operator-valued framework" (arxiv:1107.2894v1). We denote by $\Sigma(B)$ the set of B-valued positive conditional expectations from the algebra $B\langle\mathcal{X}\rangle$ freely generated by B and the selfadjoint symbol $\mathcal{X}$ onto B. Then,

Theorem 5 *If $\mu \in \Sigma(B)$, then the following inclusion holds:*

$$\{\mu^{\boxplus\eta} | \eta\colon B \to B \textit{ compeletely positive so that } \eta - 1 \textit{ is completely positive}\} \subset \Sigma(B).$$

The set on the left side of the above inclusion is indeed a partial semigroup: $\mu^{\boxplus\eta} \boxplus \mu^{\boxplus\eta'} = \mu^{\boxplus\eta+\eta'}$. If μ is $\boxplus$-infinitely divisible, $\mu^{\boxplus\eta} \in \Sigma(B)$ for any completely positive η. In addition, we obtain among others a correspondence between these partial semigroups and free Brownian motions paralleling the one obtained in [2] for scalar-valued distributions, a subordination formula for operator-valued Cauchy-Stieltjes transforms associated to $\mu^{\boxplus\eta}$ and show that the Cauchy-Stieltjes transform of a free Brownian motion started at a B-valued distribution μ satisfies a B-valued version of the inviscid Burgers equation (the free analogue of the heat equation, as shown in [10]).

Outcome of the meeting

The meeting gave us the opportunity to make significant progress in several areas related to the role of subordination in non-commutative probability. At least one paper will be written as a result of our work together during the RIT meeting in Banff.

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Chapter 65

Research in photonics: modeling, analysis, and optimization (10rit160)

Sep 12 - Sep 19, 2010

Organizer(s): Fadil Santosa (University of Minnesota), David Dobson (University of Utah), Stephen Shipman (Louisiana State University), Michael Weinstein (Columbia University)

Overview of the Field

The focus of this research team is to study mathematical problems arising in photonics. Photonics is the science of manipulating light, including its generation, transmission, and processing. The phenomena in photonics are modeled by Maxwell's equations. Specifically, we are interested in the behavior of the solutions of Maxwell's equations in microstructured materials, where the microstructure is modeled by changes in material property.

One problem we considered has to do with efficient localization of light. The fundamental issue in this problem is a mathematical topic of resonances of wave equations. We are particularly interested in developing novel computational methods that directly approximate the resonances associated with the optical device.

Another problem of interest is the propagation of light in a micro-structured plasmonic material. These are made by creating periodic cells consisting of metallic and dielectric components. The mathematical issue that arises involves characterizing the dispersion relation associated with waves propagating in the structure.

Recent Developments and Open Problems

In the case of the resonance problem, the team has recently discovered numerical evidence for the dependence of the resonances in a 1-D Schroedinger equation on the width of the potential walls. One goal of the team is to develop a full mathematical understanding of the resonances and to devise an efficient general numerical method for solving for resonances that are based on theory.

Raman and Fan [1] performed calculations of dispersion curves of a 2-D plasmonic band-gap structure using a direct finite difference time-domain method. Their calculation revealed so-called plasmonic modes which concentrate energy in the neighborhood of the metal-dielectric interfaces. We set out to develop a mathematical understanding of this phenomenon as well as a theory for wave propagation in periodic structures with metallic components.

Scientific Progress Made

The team made some progress on a number of problems during the visit. The wonderful care-free atmosphere of BIRS contributed to the success of our visit.

(1) **Behavior of resonances in a 1-D Schroedinger equation** We were able to make progress on understanding why when a true potential well is truncated at some distance L, the resonances are close to the bound states of the Schroedinger equation. Moreover, we began to investigate numerically the properties of the resonances for frequencies with large real parts. We were able to obtain asymptotics of these resonances.

(2) **Dispersion curves of plasmonic band-gap structure** We spent some time discussing plasmonic phenomena in wave propagation through media with metals. We formulated a simple model problem from which we hope to gain fuller understanding. We plan to continue working on this problem.

Outcome of the Research in Team

Two projects resulted from the visit to BIRS. The first project has already yielded a manuscript about the behavior of resonances in a 1-D Schroedinger equation [2]. Several other questions are being investigated including the extension of the said result to the case of acoustic wave and Maxwell's equations and problems in multiple dimension.

The second project is an investigation of the dispersion curves of a layered plasmonic band-gap structure, and this is on going. Numerical results obtained during the visit are providing clues to the unusual behavior of waves in such structures.

We are also contemplating writing a joint proposal in this topic.

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Chapter 66

Derived Category Methods in Commutative Algebra II (10rit158)

Oct 31 - Nov 07, 2010

Organizer(s): Henrik Holm (University of Copenhagen), Lars Christensen (Texas Tech University), Hans-Bjorn Foxby (University of Copenhagen)

This workshop was the organizers' second meeting at BIRS to work on their book *Derived Category Methods in Commutative Algebra* which will be published by Springer-Verlag. Unfortunately, illness hindered Foxby's participation in the workshop.

Background

In our report on the first "Derived Category Methods in Commutative Algebra" workshop (2008) we wrote:

"Derived category methods have proved to be very successful in ring theory, in particular in commutative algebra. Evidence is provided by [1, 8, 4, 5, 6, 7, 11, 12, 15, 16, 19, 20, 23, 24, 27], to list some work of considerable importance.

Surprisingly, there is no accessible introduction or reference to the applications of derived category methods in commutative algebra, or in general ring theory for that matter. To be an effective practitioner of these methods, one must be well-versed in a series of research articles and lecture notes, including unpublished ones: [10, 14, 17, 16, 22, 25, 28, 13, 3, 2, 9, 18, 29]. To get an overview of their applications in commutative algebra, the list grows further. The purpose of the BIRS workshop was to make progress on a book manuscript—authored by L.W. Christensen, H.-B. Foxby, and H. Holm—that will remedy this deficiency.

As implied in the discussion above, the book has no direct competition. Many books cover applications of classical homological algebra in (commutative) ring theory, but only a few books address derived category methods and their applications in this field: In *Homological Algebra* [9] by Cartan and Eilenberg, resolutions of complexes and derived functors are briefly discussed in the final chapter; no applications are given. In Weibel's *An introduction to homological algebra* [30], derived categories are introduced in the final chapter; a few applications to ring theory are included as exercises. Derived categories are also covered in *Methods of Homological Algebra* [21] by Gelfand and Manin, but applications to ring theory are not. A very thorough construction of derived categories is given in *Categories and Sheaves* [26] by Kashiwara and Schapira. However, the aim of [26] is sheaf theory, so beyond the construction of derived categories, there is barely any overlap with this book. Finally, Christensen's *Gorenstein Dimensions* [10] has an appendix on derived category methods. It provides a rudimentary and incomplete survey of technical results without proofs. The fact that it has, nevertheless, become a frequently cited reference betrays a significant gap in the existing literature."

Goals and results

The purpose of the workshop was for the authors to finalize the central chapters of their book "Derived Category Methods in Commutative Algebra". As the authors live on different continents, and in different time zones, the extended face-to-face interaction afforded by the workshop was extremely important for resolving scientific as well as editorial questions. It is a great pleasure to thank BIRS for providing this opportunity.

The workshop served three main purposes:

(A) To coalesce the material contributed by each author since their previous meeting

(B) To finalize the construction of index, glossary and other structural elements of the book

(C) To distribute exercises between the sections in the book

Ad (A). Since the authors last met in May 2010, they had rewritten the central chapters on "Modules and Homomorphisms", "Complexes and Morphisms, "Derived Functors", and "A Brief for Commutative Ring Theorists." In the course of the workshop, the authors discussed this material, and decided on the final contents.

Ad (B). Principles for indexing were decided on and implemented and guidelines for the List of Symbols and the Glossary were "tested".

Ad (C). As the manuscript is shaping up to be a genuine graduate textbook, it was decided to add a significant number of exercises. The process of choosing exercises was started this summer and contined at BIRS.

By the end of the workshop, the authors distributed new tasks and revised the time table for completion of the book. The book will be completed within the next year, and it will be published by Springer-Verlag. Finally, the latest version of the manuscript and a revised schedule were sent to Springer-Verlag.

Participants

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Holm, Henrik (University of Copenhagen)

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