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Contents

Five-day Workshop Reports

Chapter 1

Free Probability, Extensions, and Applications (08w5076)

Jan 13 - Jan 18, 2008

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Overview of the Field

Free probability theory is a line of research that parallels aspects of classical probability, in a highly noncommutative context where tensor products are replaced by free products, and independent random variables are replaced by free random variables. It grew out from attempts to solve some longstanding problems about von Neumann algebras of free groups. In the almost twenty years since its creation, free probability has become a subject in its own right, with connections to several other parts of mathematics: operator algebras, the theory of random matrices, classical probability and the theory of large deviations, algebraic combinatorics.

Since free probability relates to random matrices, its tools and techniques have a significance for questions about random matrices. Consequently, various communities which use random matrices in their models have started to use notions and results from free probability for their calculations. A prominent example of this kind are the investigations of electrical engineers on multiuser communication systems. Furthermore, there are presently quite a number of attempts to extend the methods and the applicability of free probability in various directions.

The workshop put special emphasis on applications of free probability and the attempts to extend its framework. In the following we will first give a brief general description of some of the main results and directions of free probability. Then we will address the applications of free probability in applied fields and point out some of the directions for extensions of the framework of free probability.

Recent Developments

Some of the fundamental results of free probability

Recently, Haagerup and Schulz [26, 18] achieved a crucial break-through on the famous invariant subspace problem; by relying on free probability techniques and ideas, they showed that every operator in a II_1 factor whose Brown measure is not concentrated in one point has non-trivial invariant subspaces.

Free probability provides new ideas and techniques for investigating random multi-matrix models. Recently, in this direction, Haagerup and Thorbjornsen [19] obtained a sweeping generalization to several matrices for a number of results concerning the largest eigenvalue of a Gaussian random matrix, see also [26].

A celebrated application of free entropy was Voiculescus proof [31] of the fact that the free group von Neumann algebras do not have Cartan subalgebras (thus solving a longstanding problem); many other powerful applications of free entropy to questions on operator algebras are due to Ge, Stefan, Jung, and Shlyakhtenko. Recently, Connes and Shlyakthenko [8] introduced a kind of L^2-Betti number for von Neumann algebras. There exist close relations between this theory and free entropy.

The study of free group factors via free probability techniques has also had an important application to subfactor theory: not every set of data for a subfactor inclusion can be realised in the hyperfinite factor; however, the recent work of Shlyakhtenko, Ueda, and Popa has shown that this is possible using free group factors. Thus the connection of free group factors to free probability and random matrices appears to be also related to a key role of this class of factors within von Neumann algebras.

First elements of a stochastic calculus and a stochastic analysis for free Brownian motion were developed by Kmmerer and Speicher, and by Biane and Speicher [6]. These are expected to be crucial tools for getting a deeper understanding of random multi-matrix models. A groundbreaking result in this direction, on the fluctuations of two non-commuting Gaussian random matrices, is due to Cabanal-Duvillard [7].

In relation with probability, the work of Ben-Arous, Guionnet, and Cabanal- Duvillard ([1, 9]) shows that Voiculescus free entropy is useful in the study of the rate functions of large deviation principles for special random matrices. A significant progress on one of the most intriguing problems in this context (the unification problem for the two approaches to free entropy) was recently achieved by Biane, Capitaine, and Guionnet [4].

Free probability has a significant combinatorial facet. Speicher [27] showed that the transition from classical to free probability consists in replacing all partitions by non-crossing partitions. The combinatorial machinery of free probability was used by Nica and Speicher to obtain new results in free harmonic analysis (see [23]); and by Biane to derive new results on the asymptotics of representations of symmetric groups; it gives rise to new interesting conjectures in that area, in particular in connection with the Kerov polynomials, see [3, 26, 15].

Other important recent directions currently pursued in free probability are free Wasserstein distance and free log Sobolev inequalities, processes with free increments and analytic subordination, properties of cyclic derivatives and automorphisms of the free group factors, duality for coalgebras of free difference quotients and more general ”free analysis” questions.

Applications of free probability in applied fields

Through the quite unexpected relation between free probability theory and random matrices (which was discovered by Voiculescu in [29]), the tools and techniques from free probability theory have a significance for questions about random matrices. The power of those tools from free probability (in particular, the R-transform and S-transform, and the notion of free cumulants) has become more and more apparent in recent years to various communities which use random matrices in their models.

One active line of research in this spirit is the use of the free probability machinery in investigations of electrical engineers for multi-user wireless communication systems. This direction was initiated by Tse; the relevance of free probability for such problems has been pointed out to the engineering community in the survey article of Tulino and Verdu [54]. Whereas simple models have been treated very succesfully, more realistic/complicated models still have to be solved and present new challenges for free probability theory.

Statistics is another field where random matrices (in particular, Wishart matrices and their variants) are of eminent interest and where the interest in free probability techniques has risen during the last years. A present point of contact between statistics and free probability are results on linear statistics or eigenvalue fluctuations, which are closely related to the new concept of second order freeness [10]. Other statistical topics of interest, like the statistics of the largest eigenvalue, are still not within the realm of free probability but could serve as inspiration for further developments.

Another interesting link between applied fields and free probability is provided by the implementation by Edelman and Rao (see [12]) of the tools of free probability on a computer by using symbolic software (building on MATLAB). On one side, this has made available the tools of free probability to a much wider audience and, on the other side, presents the challenge of incorporating new developments into this ’free calculator’.

Random matrices are also used in various models in theoretical physics. An interesting recent contribution to this connection was made by Guionnet and Maurel-Segala [16] who could give rigorous proofs (and connect them with the concept of free entropy) of some expansions for multi-matrix models, which had appeared before on a formal level in the physical literature.

Extensions of free probability

One of the main focus of the workshop was on various extensions of the framework of free probability theory. The motivation for such extensions comes from various sources, both theoretical and applied. We put much effort into having a good balance of people who are confronted with concrete problems and those who might develop the tools for solving them.

We describe below some of the present ideas for extensions of free probability.

Voiculescu introduced from the very beginning a more general version of free probability: operator valued free probability theory, where the scalars are replaced by more general algebras and the role of the underlying state is taken over by a conditional expectation. This extension of free probability has a much wider applicability but still shares many of the features with usual free probability. Some of the basic results of free probability theory were extended right away to the operator valued version [30, 27]. However, the more advanced theory and also the detailed examination of fundamental examples has only started recently, and we expect a surge of new investigations in this direction. Further progress on operator-valued free probability seems to be instrumental both for pure and for applied questions. E.g., on the pure side, recent work of Junge [J1, J2] on realizations of the Hilbertian operator space OH relies on generalizing norm inequalities for sums of free variables to the operator-valued context. Further results in this direction promise a deeper understanding of OH, which is a central object in the theory of operator spaces. On the applied side, operator-valued versions of free probability have turned out to provide new techniques for dealing with more complicated types of random matrices; see, in particular, the results of Shlyakhtenko [25] on Gaussian band matrices. Recently, this was taken up and extended in [24], who considered block matrices which are of relevance in wireless communication MIMO models.

A few years ago, Biane, Goodman, and Nica [5] introduced a type B version of free probability theory. The usual, type A, free probability theory relates to the permutation groups. Replacing those by corresponding type B Coxeter groups leads to type B free probability. There exists a nice combinatorial theory of this version, however, random matrix models for this extension are still missing. Models used in applied problems might provide some inspiration for this.

Whereas free probability deals with operators on Hilbert spaces, corresponding to square random matrices, Benaych-Georges [2] introduced recently a version of free probability which deals with operators between different Hilbert spaces and relates to rectangular random matrices. The latter show up, in particular, in the context of Wishart matrices, and thus rectangular free probability promises to provide the right framework for some applied problems in wireless communication and statistics.

In the random matrix literature there has been a lot of interest in linear statistics or global fluctuations of random matrix eigenvalues (see, e.g, [11]). In order to extend the framework of free probability to be able to deal with such problems, Mingo and Speicher [22] introduced the concept of ’second order freeness’. They developed, with Collins and Sniady [10], an extensive combinatorial theory for this concept and are presently applying, with Edelman and Rao [13], their theory to statistical eigen-inference problems.

Other extensions of the framework which are presently under investigation are, e.g., q-deformations of the free Fock space, free extreme values, or monotone convolution.

Presentation Highlights

Since the workshop brought together researchers from quite different communities there were a couple of survey talks which presented aspects of free probability and random matrix theory from various points of views. Particular emphasis in those talks was given to pointing out open problems and possible future directions.

- Voiculescu gave an introduction to free probability with special emphasis on the recent developments and questions around the coalgebra structure and operator-valued resolvents.
- Bercovici gave a survey covering limit theorems in free probability, and regularity issues for free convolutions. He discussed in particular the prospects of extending these results to operator-valued variables, and to other variants of noncommutative probability theory.
- Verdu gave a survey on the questions in wirleless communications, and the use of free probability theory and random matrix theory in such models. This was complemented by a talk of Tulino who described in more detail specific models.
- Letac showed the use of random matrices in statistics by presenting results on the computation of moments for beta distributions, and applications of such tools.
- Mingo gave an introduction to the calculation of unitary matrix integrals in terms of the so-called Weingarten function, and presented the main results about the asymptotics of the Weingarten function.
- Speicher gave a survey on the questions, ideas, and results behind the notion of higher (in particular, second) order freeness.
- Nowak showed how in physics a quaternion valued extension of free probability theory is used to treat new examples of non-normal random matrix ensembles.
- Silverstein outlined recent work on spectral properties of random matrices, in particular in connection with the ”spiked population model”, with is of relevance in statistics, and in connection with some random matrix models which appear in the modeling of MIMO systems in wireless communications.
- Edelman gave a survey on computational aspects of random matrices and free probability.
- Nica gave an introduction to recent developments on the combinatorial side of free probability theory.

The other talks presented more specific results; but in each case the speaker provided some background and motivation for the considered question.

The other talks can roughly be divided into two groups. The first group consisted of mathematial results about free probability and random matrices:

- Capitaine and Donati-Martin talked about the asymptotics spectrum of deformed Wigner matrices, with particular emphasis on the behaviour of the largest or smallest eigenvalue.
- Dykema presented calculations about the microstates and the free entropy dimension in amalgamated free products over a hyperfinite subalgebra.
- Hiai discussed the notions of free pressure and microstates free entropy from the point of view of hypothesis testing. In particular, he considered a free analogue of Stein’s lemma.
- Kargin defined the notion of Lyapunov exponents for a sequence of free operators and showed how they can be computed using the S-transform. He also discussed the relations with corresponding results on the product of large random matrices.
- Kemp presented results about the resolvent behaviour of a prominent class of non-normal, so-called R-diagaonal, operators.
- Shlyakhtenko discussed the relation between planar algebras, subfactors and random matrices and free probability. In particular, he showed how random matrix constructions of planar algebras can be used to give a new proof of a theorem of Popa on realization of subfactors.
- Anshelevich presented his results on polynomial families (Appell, Sheffer, Meixner) in the context of Boolean probability.
- Collins introduced the notion and presented the analytic and combinatorial aspects of free Bessel laws and explained its connection with quantum groups and random matrices.

The second group treated concrete problems in wireless communications:

- Moustakas discussed the application of diagrammatic methods developed in physics to the calculation of the asymptotic eigenvalue spectrum of specific random matrix models. He also discussed the use of the replica method in such a context.
- Müller considered the problem of minimizing random quadratic forms and explained the relevance of this problem in transmitter processing of wireless communications.
- Ryan presented the use and implementation of free probability methods for an example of channel capacity estimation in MIMO systems.

Open problems and possible future directions

There was also scheduled a special discussion meeting on Thursday afternoon in which open problems and possible future directions of free probability theory were discussed. In the following we list some of the major relevant problems which were pointed out in this discussion meeting and in numerous other discussions between the participants throughout the workshop.

- What is the relevance of free entropy in applied fields. Free entropy is clearly a major notion in free probability (with many technical problems still open), but there was also the feeling that similar to classical entropy it should play a fundamental role in statistics and information theory. In this context, it seems that one also needs a more general notion of relative free entropy.
- The use (and the success) of the replica method in many calculations has no mathematical justification. Can free probability justify the replica method, or at least provide other tools for deriving results which are obtained by the replica method.
- The need for a better understanding of the analytic theory of operator-valued freeness and resolvents is not only mathematical apparent, but there are also many applied quite successful methods (as quaternion extension of free probability, or deterministic equivalents of Girko for random matrix models) which might benefit from such a theory.
- Tulino and Verdu presented calculations on the Gaussian Erasure Channel; some of the results are the same as one would obtain if one assumes freeness between involved operators; however, no freeness is apparent. Does this hint at a new instance of asymptotic freeness in this model or is there something else going on?
- The recent results of Belinschi and Nica revealed a deeper connection between free and boolean convolution. This deserves further clarification.
- Whereas complex random models are the most basic in mathematics and engineering, in statistics one is usually only interested in real random matrices. Whereas for questions about the eigenvalue distribution the distinction between complex and real does not play a role, it becomes significant for finer questions, like the fluctuations of eigenvalues. This asks for an extension of the theory of second order freeness from the complex to the real case.
- Whereas engineers have no problems in applying asymptotic freeness results for unitarily invariant ensembles it has become apparent that they do not have the same confidence in the analogous results for Wigner matrices. The main reason for this is the lack of precise statements on this in the literature. This has to be remedied in the future.

List of Participants

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Donati-Martin, Catherine (Université Paris 6- CNRS)
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Hiai, Fumio (Tohoku University)
Kargin, Vladislav (Courant Institute)
Kemp, Todd (Massachusetts Institute of Technology)
Letac, Gerard (Universite Paul Sabatier)
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Mingo, James A. (Queen's University)
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Chapter 2

Combinatorial Game Theory (08w5075)

Jan 20 - Jan 25, 2008

Organizer(s): Michael Albert (University of Otago), Elwyn Berlekamp (University of California, Berkeley), Ezra Miller (University of Minnesota), Martin Mueller (University of Alberta), Richard Nowakowski (Dalhousie University), David Wolfe (Gustavus Adolphus College)

Overview of the Field

Combinatorial game theory deals principally with two-person games of perfect information and without chance elements. It provides techniques for determining who can win from a game position and how. While ad hoc techniques for such analysis are as old as humanity, the modern theory employs more powerful and general tools such as the notion of a game-theoretic value. From a mathematical standpoint, these techniques can be brought to bear to solve completely a wide variety of games. From the algorithmic perspective (that is, when the efficiency of the analysis is considered), there are efficient methods to analyze certain GO endgames and capture races, and various classes of impartial games. In addition, complexity results abound, and when a game is provably NP-hard, there are heuristic methods that can be employed.

All the above is true for games played under the *Normal* play rules, that is games in which the last player to move wins. The situation for misère play games (last player to move loses) is very different. A few games have been analyzed but even quaternary games (simple extensions of subtraction games) have shown themselves to be very difficult.

The *disjunctive sum* of games G and H, written $G + H$, is the game in which a player can choose to play in G or H but not both. The two players are usually called *Left* and *Right*. Games can be in one of four outcome classes: $\mathcal{L}$, if Left wins regardless of who moves first; $\mathcal{R}$, if Right wins regardless of who moves first; $\mathcal{N}$, if the next player to move wins regardless of whether this is Left or Right; and $\mathcal{P}$, if the next player loses regardless of who moves first. Two games, G and H, are said to be *equal* if the outcome class of $G+X$ is the same as the outcome class of $H+X$, for every game X. This defined equality is clearly an equivalence relation. For both Normal play and misère play rules, there is a set of reductions (obviously different in both cases) that give a unique—*canonical*—representative for each equivalence class. The algorithm for the Normal play canonical form is given in [8, 6] but an algorithm for misère play was not found until 2007 [30], and presented for the first time at this Workshop. In Normal play, these equivalence classes are very large but in misère play these are very small, in many cases of size 1, hinting that misère play will be the more difficult to analyze.

The field is growing and is attracting the interest of many people. There have been major workshops at MSRI in 1994 and 2000, Dagstuhl in 2003, and BIRS in 2005. The MSRI and BIRS Workshops resulted in three books, *Games of No Chance*, *More Games of No Chance*, and *Games of No Chance III*. The last includes twenty research papers, four top-level surveys, and updated versions of *Unsolved Problems* and

Bibliography of Combinatorial Games. The field is new and is growing. The call for a special volume of the Journal of Theoretical Computer Science on results from the Dagstuhl workshop brought 26 submissions. The electronic journal INTEGERS (started in 2000) opened a special games section in 2002 and this has had a steady stream of submissions.

Recent Developments and Open Problems

There have been many important developments in the last few years most of which were announced at the BIRS 2005 meeting. The main objectives of the workshop were to air the new results and to introduce new people and techniques to the area. Specifically:

- **Misère games.** Normal play games (last person to move wins) form a partially ordered commutative group. The corresponding structure for misère games (last person to move loses) is more complicated and is not yet understood. As was reported at the conference by Meghan Allen, *disjunctive sum* is the correct sum as far as category theory is concerned (see [14]), this is not true for misère games and indeed, there is no natural game-playing decomposition that would satisfy a category theorist. At the level of impartial games, Normal play evaluation involves finding elements in the direct sum of (possibly infinitely many) copies of Z_2. These are usually called the Sprague-Grundy or nim values and there is a well understood recursive mechanism for determining them. This is not true for misère play. The approach of "use the Normal play strategy until close to the end of the game" is too naive. A more mathematical version of this idea, called the "Normal-play Kernel Conjecture", has recently appeared and has proved to be false although it still seems to form a reasonable heuristic. One major development is Plambeck's breakthrough in the analysis of impartial misère games (first announced at BIRS 2005). He showed that the solution to an impartial misère game G can be described by its misère quotient, a commutative monoid that encodes the additive structure of G. Aaron Siegel has designed algorithms for computing misère quotients, and together Plambeck and Siegel have begun to develop a structure theory. These monoids are very special. For example, there are between 1,000,000 and 256,000,000 monoids on 8 elements but there is only one that arises from impartial misère impartial games. This class of monoids has not been identified in the literature. A major thrust of this workshop was to invite and interact with algebraists so as to better understand these monoids. Ezra Miller joined the organizing committee for this reason and attracted several algebraists to the meeting.

- GO is a hot topic and its analysis is expanding the theoretical tools as well as the algorithmic tools (Müller[11, 14, 15], Siegel [19]). Nowakowski, Ottaway and Angela Siegel recently (2005) introduced the game of WOODPUSH to allow for an analysis of ko-like situations without requiring the rest of the structure of GO. At the last BIRS meeting, Dr Nakamura presented his results showing that cooling by 2 points was essential to the analysis of races to capture. Nakamura's results bear so many resemblances to the atomic weight theory that there may be deeper connections waiting to be discovered. Elwyn Berlekamp reported on his recently successful efforts to increase the dialog between combinatorial game theorists and professional players of GO, the world's premiere intellectual board game.

  Many GO players are aware of the book, *Mathematical* GO, by Berlekamp and Wolfe [7], which was published in 1994 and subsequently translated into Japanese. This book is widely considered to be the last word on getting the last point. However, most professional GO players believe they can do almost-as-well using their well-honed reading skills instead of mathematics. But subsequently, Berlekamp, Fraser, Spight, and Siegel (see [11, 20, 31]) developed another theory, related to thermography, which allows one to assign numerically precise values to GO positions and to the sizes of moves. These values are often rational fractions, such as $1\frac{5}{12}$. Most professional GO players have superb skills at finding the best local moves, and of finding their approximate values very quickly. But they tend to think only in terms of integers and half-integers, so they might characterize a move of value $1\frac{5}{12}$ as "about $1\frac{1}{2}$". In some situations, the outcome of a close endgame can depend on the very small differences between the values of different moves, and sometimes professional GO players lose a game that could have been won if they knew how to do these calculations precisely.

  Berlekamp has long sought to raise the awareness of these results among professional GO players, and also to get their advice about which directions of further development of this theory might have most relevance to the classical version of the game. To this end, he formed a partnership with the North American GO Foundation to sponsor the first professional COUPON GO Tournament at the Baduk Association in Seoul Korea on November 28-29, 2007. The contestants were six of the world's foremost professional GO players: Sang-Hun Han, Tae-gon Song, Sung-jin Won, Jo-Young Ahn, Naiwei Rui, and Jujo Jiang.

Each of the contestants played a round-robin with 15 contests partitioned into five "duplicate" rounds. Each round consisted of two endgames each, once as Black and then again as White against the same opponent starting from the same initial endgame position. The player who obtained the better score was declared the winner of that contest. All five endgame positions had been chosen from classic games originally played by Go Siegen, the legendary GO player who dominated the game for more than a decade in the middle of the 20th century.

In COUPON GO, in addition to the GO board, there is also a stack of 20 coupons, arranged in descending order with values $10, 9.5, 9, 8.5, 8, \ldots$, down to 0.5. At each turn, the player may either play any legal move on the board OR he may instead elect to take the top coupon. When the game is over, the values of the coupons each player has taken are added to his score.

The tournament drew great interest in Korea. One pair of games was covered in full on national television. All of the contestants expressed interest in participating in a second annual COUPON GO Tournament next year. Several of them suggested that next year the difference between successive cards be reduced to $\frac{1}{4}$ point instead of $\frac{1}{2}$. This is a welcome step in the direction of the case about which we have the most mathematical results. That is the idealized case of an infinitely "thick" stack of coupons, each of which differs from its predecessor by only an infinitesimal amount. Like Carnot cycles in thermodynamics, this idealized case ensures that the temperature must decrease adiabatically, and that leads to theorems which relate COUPON GO with thick stacks to the results which were called "thermography" in Winning Ways [6].

- All-small games: recent partial analyses of CLOBBER[4], CUTTHROAT[23] and DRAGOVER[5] have given impetus to the analysis of all-small-games. In addition, John Conway (2006), in a personal communication to the authors of [5], suggested a new representational theory that could greatly simplify the canonical form representation of all-small games. Again, the underlying algebraic structures pose interesting and challenging questions. Neil McKay reported on some of his thesis work [17]. In the weeks between the conference and the time this report was written, it has already shown itself to be an invaluable tool in the analysis of the Chip-firing games and Cleaning games on graphs [23].

- Complexity issues: This is always an important topic. In particular, a relatively new tool for proving high complexity demonstrated its strength, and a new method of proving polynomiality was presented in the workshop.

Presentation Highlights

There are very few conferences or Workshops in Combinatorial Game Theory. Consequently, all the talks in the Workshop were interesting, had new results and engendered discussion. The complete list of speakers and titles is given first which is then followed by a synopsis of those talks.

Talks

- *Richard Guy - Impartial Games.*

  Synopsis: This invited talk was an overview given] by one of the pioneers in combinatorial game theory. The basic theory and results behind impartial games (games in which both players have the same moves) were discussed. Some items discussed included NIM sums, reversible moves, the Tweedle-Dum Tweedle-Dee strategy, the Sprague-Grundy theory, and Ferguson's Pairing Principle. Also discussed were open problems in subtraction games and octal games. An open problem mentioned was whether the period of a subtraction game $S(s_1, s_2, \cdots, s_n)$ was bounded by some polynomial of degree $\binom{n}{2}$. The talk was run in an interactive manner, with the speaker presenting games and soliciting responses from the willing audience.

- *Thane Plambeck - Algebraic Problems in Impartial misère Games.*

  Synopsis: This invited survey talk set out the present state of play in the theory of misère impartial games. Note that very little of the material has yet made it into the published literature, it is that recent. (Or not depending on your view of the impact of French Cinema on mathematics).

  The speaker opened with an amusing movie clip demonstrating the use of misère games in the French New Wave cinema, *Last Year in Marienbad*. He posed the question of why there isn't a comparable Sprague-Grundy theorem for misère games. He then gave an overview of the theory he developed in conjunction with Aaron Siegel, that of the indistinguishability quotient. An important distinction with Normal play theory is that under this analysis of misère games we consider a game only with respect to other positions in that game rather than with the set of all impartial games. This theory, when applied to games played under the normal play convention, gives the classical representation of an impartial game as a direct sum of copies of $\mathbf{Z_2}$. However, under misère play, the quotient can be a wide variety of monoids. Some examples of working with the monoid for a small game were given. The speaker concluded his presentation by asking whether under this context there is a analogue of the mex function for computing values in the monoid. In subsequent discussion, the hypotheses necessary for the Normal play quotient were discussed, as were strategies in relating winning moves in Normal play to winning moves in misère and vice versa. Also discussed was how to deal more effectively with quotients which have infinite cardinality.

- *Martin Müller - Race to Capture: Analysing Semeai in* GO*.*

  Synopsis: In this talk, the speaker gave an introduction to the theory of semeai, a concept in GO in which two non-live groups attempt to capture one or the other to live. An algorithm was given detailing who, under perfect play, should win the semeai. Details included looking at the eye shape of each group, as well as the number of liberties, the shared liberties between the groups, etc. The speaker concluded by discussing the implementing this algorithm as one often encounters Class 2 semeais, positions with unsettled eyes which are not accounted for in the earlier algorithm.

- *Elwyn Berlekamp - Report on Professional* COUPON GO *Tournament.*

  Synopsis: This invited talk was very important for setting the stage for the Workshop. The COUPON GO tournament was a breakthrough in getting GO professionals to explore the approaches suggested by combinatorial game theory. Berlekamp has worked for over a decade to bring these tools to their attention. Many participants of this Workshop spent most of their 'free' time poring over these records.

  The speaker, an expert in the mathematical analysis of GO, discussed a recent experiment in attempting to bring together professional GO players with combinatorial game theorist. He, along with the American GO Association, and with the help of Professor Chihyung Nam of Meonju University, sponsored a COUPON GO tournament in Seoul, November 28 and 29, 2007. In the tournament, the participants played a variation of GO where on their turn, the players could either play a move continuing a game starting from a preset GO position or take a coupon awarding them a certain number of points. The tournament television and newspaper coverage in Korea, as well as attracting the participation of some of the world's most highly ranked GO players. The speaker hopes to analyse these games using his temperature theory approach to further understand his and the players' end-game positions in GO.

- *Aaron Siegel - The Structure of misère Quotients.*

  Synopsis: This invited talk dovetailed with Plambeck's presentation and delved more deeply into the algebraic aspects and presented algorithms.

  The speaker began by reviewing the idea of the misère quotient. He then proceeded to discuss the abstract idea of a reduced bipartite monoid as well as homomorphisms thereof. The goal of this abstraction is to formalize the notion of a misère quotient in a more formal context. For this goal, several examples were given. Three questions were posed:

1. What is the structure of an misère quotient?
2. How many unique misère quotients are there of order n?
3. When is a reduced bipartite monoid a misère quotient?

To give the flavour of proofs in this theory, the speaker demonstrated that every finite misère quotient has even order. He also gave a strong estimate of the number of unique misère quotients up to order 18. He characterised tame games under the misère quotient framework, as well as noting an extension result for calculating misère quotients. The normal kernel hypothesis—*that optimal misère play is the same as Normal play until 'close' to the end of the game*—was touched upon briefly.

- *Mike Weimerskirch - Another Algorithmic Approach to misère Quotients and an Infinite Quotient on a Finite Heap Alphabet.*

  Synopsis: This was a small counterpoint to the previous talk of Aaron Siegel and helped broaden the discussion by indicating another algorithmic approach. In this talk, the speaker demonstrated a new method for calculating misère quotients. To do so, he analysed the octal game **0.3122** with heap sizes up to and including seven tokens. His method involves determining pre-period and period length of the $\mathcal{N}$ and $\mathcal{P}$ positions of combinations of certain heap sizes. Identifying heap sizes with generators of a monoid gives a candidate misère quotient. This candidate quotient is then reduced to give the true misère quotient. This method seems to be able to analyse infinite misère quotients in a manner not available via Aaron Siegel's *misère Solver*.

- *Teigo Nakamura - Evaluating Territories in* GO.

  Synopsis: Along with the COUPON GO talk, this was a must-see for anyone interested in the Normal play, partizan theory. The successful application of cooling by 2 is amazing and it solves a very hard problem in actually playing GO. The notion that this approach might have something in common with atomic weight theory gave rise to many discussions which carried on after the Workshop.

  The speaker presented his method of determining the values of Semeai games. He began by reviewing the idea of semeais, as well as the terminology introduced previously by Martin Müller. He then discussed his notion of a Liberty Counting Game. In this game, the liberty count is not just an integer, but rather a combinatorial game. A number of positions were analysed using the Liberty Counting Game, including a full board position. In addition, he gave his method for determining the territory score based on who wins the Liberty Counting Games into which a board separates. He noted that there were two important points: To analyse the positions, one must cool the temperature of the game by 2, and one must assign liberties to terminal end nodes. At the conclusion of the talk, Berlekamp noted that much of the speaker's methodology was similar to the idea of atomic weights and suggested that future research to bring the two areas together might prove fruitful.

- *Takenobu Takizawa - On A Width-Two Entrance Rogue Position.*

  Synopsis: The speaker analysed end-game positions where black and white fight over territory. The main focus was on ”width two room positions”, positions where black surrounds an area of no more than seven free positions with two white invaders. As the speaker noted, many of these rogue positions lead to ko's, which complicate the analysis. Four key examples with their analysis of possible versus best moves were fully presented.

- *Aaron Siegel - misère Canonical Forms of Partizan Games.*

  Synopsis: This was a deceptively unassuming talk. As mentioned in the first section of this report, Normal play games form a very nice structure with equivalence classes and a well-defined recursive procedure to identify a unique representative of the equivalence class. It was known that misère game formed equivalence classes but with few elements, comparatively speaking, in each class. There were no known operations that would reduce a game to a unique representative in its class. A paper by Mesdal [19] had come close but 'close only counts in Horseshoes'—the approach did not give a hint of finding a way of reducing a game to a canonical form. Siegel succeeded in a very nice fashion. This approach already is forming the basis of one Ph.D. in partizan misère games.

The speaker began by reviewing the canonical form question for various types of combinatorial games. He noted that three of the four possibilities, impartial Normal play, partizan Normal play, and impartial misère play, have had the question completely answered in the literature. He then proceeded to demonstrate his method of determining a canonical form for partizan misère play games. The proof consisted of an extension of the impartial misère theory combined with ideas taken from the partizan normal theory. One application of such a method is to give upper bounds, or in small cases, determine the number of misère games born by day n. He also noted that the misère quotient can be extended to partizan games using their canonical forms, although much work remains to be done in this area. Questions arising from this talk included whether there are any partizan misère games with playing experience, how to use this method to analyse partizan subtraction games in misère play, and whether the theory is simplified by restricting ourselves to all-small games, which would remove some of the cases required in the proofs of the theorems given.

- *Sam Payne - Discrete Bidding Games.* Joint work with Mike Develin.

  Synopsis: A skilled CHESS player and a skilled POKER player play a game of CHESS and it will surprise no-one that the CHESS expert will win. Give each player 100 chips and each has to bid for the right to make the next move (the higher bidder gives the money to the lower bidder). Now who wins and in how many moves? This was the coffee-time discussion (with practical experiments) that was engendered by this talk.

  This talk discussed the mathematics behind discrete bidding games, games in which players must have closed bids for the right to play in each move. The speaker began by reviewing Richman's theory of continuous bidding [16], games in which players can bid any real value number. The speaker noted that while continuous bidding yields interesting theoretical results, games played with discrete bidding are often more enjoyable. As the theory for discrete bidding games is less developed, the speaker investigated such games. Many of the results for continuous bidding games had comparable results for discrete ones. He applied the theory to games of TIC-TAC-TOE. Finally, he noted that one could develop an ordering and a theory similar to that for combinatorial games, which may yield more results in the future. A question was asked about the relationship between coupon games to discrete bidding games, but it was decided that the similarities are merely superficial.

- *Urban Larsson - Muller Twists and Variants of Wythoff Nim.*

  Synopsis: In this talk, the speaker examined variations of WYTHOFF'S NIM in which moves are restricted. He began by explaining the notion of a Muller twist: before the next player moves, the previous player restricts the options in some predetermined way. The speaker noted that WYTHOFF'S NIM is ideal for Muller twists, as restricted move sets correspond to removing squares from the chessboard. Three types of restrictions were analysed:

  1) disallowing certain moves along the diagonal

  2) disallowing certain rook type moves

  3) disallowing certain moves in any direction.

  He then showed a variety of complexity results in determining $\mathcal{P}$ positions for these different restrictions.

- *Eric Duchéne - Extensions and Restrictions of* WYTHOFF'S *Game preserving Wythoff's sequence as sets of $\mathcal{P}$-positions.* Joint work with A. Fraenkel, R. J. Nowakowski & M. Rigo.

  Synopsis: A focal point for the researchers in impartial games. The use of automata was new and the idea sparked a flurry of activity that culminated in [10].

  Three known characterisations of the $\mathcal{P}$-positions of WYTHOFF'S game were given. The speaker then discussed his morphic characterisation, which uses formal word strings to determine the $\mathcal{P}$-positions. This gives an polynomial time algorithm for determining $\mathcal{P}$-positions of WYTHOFF'S game. Some properties of the outcome class sequence of WYTHOFF'S game were easier to prove under this new analysis. Using automata theory, the speaker has found a direct link between combinatorics on formal words and numeration systems, giving a new exploration area for impartial games. (Note that Howard

Landman in [15] used automata theory to greatly simplify the proof contained in [9].) The speaker then discussed the problem of characterising all extensions and restrictions of WYTHOFF'S game whose $\mathcal{P}$-positions are the same as in WYTHOFF'S game. Three open questions in this field were posed:

1. Does an algebraic characterization of extensions which preserve the $\mathcal{P}$-positions?
2. Are there other games that are neither extensions nor restrictions of Wythoff's game which preserve the $\mathcal{P}$-positions?
3. The same two questions applied to generalized WYTHOFF'S game.

- *Aviezri Fraenkel - Polynomializing apparently hard P-positions using surrogate sequences.* Joint work with Udi Hadad

  Synopsis: This is a new method for providing a polynomial-time strategy for apparently hard games. Normally, approximation methods are sought when a problem is proved NP-hard. In the present approach, this process is reversed: first a close approximation using poly-time surrogate sequences to seemingly hard sequences of P-positions was established. Then the approximation is used to formulate an exact recursive poly-time algorithm for computing the P-positions of the hard looking sequences. In particular, the method establishes polynomiality of a certain variation of WYTHOFF'S game considered by Eric Duchene and Sylvain Gravier, and certain blocking games with a Muller twist considered by Larsson and Hegarty.

- *Tristan Cazenave - Monte-Carlo approximation of temperature.*

  Synopsis: Another must-see talk about GO. T he Monte-Carlo approach has been responsible for the biggest jump in the strengths of computer GO playing programs in recent history.

  The speaker discussed his very successful Monte-Carlo approach to playing GO. In particular, he discussed how Monte-Carlo methods could be used to approximate the temperature of a position. The speaker began by reviewing the history of the Monte-Carlo approach for GO programs. He noted that the latest advances in the Monte-Carlo approach had gone from ten kyu to one kyu for 19x19 boards in merely one year. Using upper bound confidence trees, the speaker gave results pairing different search algorithms against each other on 7x7 boards: Global, Dual, and Threat. Threat is better than dual but twice as slow. Dual is better than Global. The speaker noted that for games too complex to analyze, a Monte-Carlo method might be best to approximate the temperature.

- *Thatsaporn Thanatipanonda* - TOADS-&-FROGS *and* CHESS *Endgames.*

  Synopsis: The speaker began by giving an introduction to the game of TOADS-&-FROGS. He noted that it was an interesting game to analyse because of the wealth of patterns which occur for a variety of positions. The speaker presented a new, recursive method of analysing TOADS-&-FROGS positions, the Finite State Method. This method has parallels to the methods used in solving recurrence relations and differential equations. Using this method, four open conjectures regarding TOADS-&-FROGS positions, were solved:

$$\begin{array}{ll} (a) & T^a..F^b = \{\{a-3|a-b\}|\{*|3-b\}\} \\ (b) & T^a...FF = (a-2)* \\ (c) & T^a...F^3 = a - 7/2 \\ (d) & T^a.^aF^{a-1} = 1 \text{ or } 1*. \end{array}$$

  An open problem on TOADS-&-FROGS was discussed, namely: $TT.^aFF = *$ if $a = 7 + 6n$, 0 else. The speaker concluded by noting that this method may be applicable to analysing CHESS endgames.

- *Paul Ottaway - Some classes of partizan misére games.*

  Synopsis: In this talk, the speaker examined a class of games which, while being partizan, are very close to being impartial. In particular, the speaker defined a class of games which have a consecutive move ban. That is $G^{LL} = G^{RR} = \emptyset$, as well as all the followers of G having the same property. Following the ideas of Siegel and Plambeck, he defined a consecutive move ban quotient, in which only games in the class of consecutive move ban games are considered. The speaker further restricted his class of games by examining left and right handed games, games in which $G^R = \emptyset$ or $G^L = \emptyset$ respectively. In this object, for any game G, we can construct its negative such that $G + (-G) = 0$. Some examples of games with all the properties discussed in the talk were given.

- *Neil McKay - Uptimals.*

  Synopsis: The speaker discussed all-small games, games in which either both players have an option or neither play has an option. An example of such a game is ALL-SMALL PUSH. The speaker used this game to demonstrate many of the concepts discussed in his talk. In particular, the idea of uptimal notion was reviewed. Uptimal notation is a short hand for defining certain games in terms of up and down. The speaker mentioned that, in joint work with *Wolfe and Nowakowski*, that a canonical form theorem for uptimals has been obtained. A comparison between uptimal notation and canonical form was given for a certain example, with the speaker noting that in certain cases, uptimal notation is more concise and easier with which to work than canonical form. An open problem was easily solved by finding canonical forms for different uptimals.

- *Carlos Santos - Nim-Dimension of Konane is Infinite.*

  Synopsis: The concept of Nim-Dimension has been in the air for a long time. Berlekamp (see [1], Guy, Unsolved Problems in Combinatorial Game Theory) first asked for 'the habitat of $*2$'. Santos has expanded that question to $*2^n$.

  In this talk, the speaker discussed the problem of finding arbitrary nimbers in combinatorial games. The first example discussed was the game of KONANE. One constructs arbitrary nimbers through an iterative process of taking a position, enlarging it, rotating it, and appending it to the previous position. In addition to KONANE, the problem of finding arbitrary nimbers in AMAZONS and CHESS was discussed. A construction was given for $*4$ position in AMAZONS, a feat that had eluded others. He concluded by looking at several interesting nimbers that arose from zugzwang positions in CHESS.

- *Bob Hearn - Constraint Logic.*

  Synopsis: Almost all participants knew a few of the results that Hearn presented but it appeared to be the first time that all were presented in a coherent framework.

  The speaker discussed constraint logic, a method for determining the complexity of a variety of games. This method is not restricted to two player games, but also can involve zero player (e.g. game of LIFE), one player (e.g. sliding block puzzles), or team player (bridge with certain restriction) games. Constraint logic is a hybrid of game analysis, Turing machine methodology, and quantified boolean formulae. The method was to translate the moves of a game into a constraint logic graph. Once translated, complexity results were more easily shown on these graphs than on the games from which they were generated. For example, his proof of various block puzzle complexity results was simpler than those previously presented in the literature. He concluded by noting that his method showed possible deep connections between game theory and computation theory.

- *Kevin Saff - Ordinal Multiplication of Games.*

  Synopsis: The games discussed in this talk were a subset of poset games. On her turn, a player removes a node as well as all higher nodes. In particular, he wished to discuss the ordinal sums of poset games. He discussed the notions of mex for ordinal sums, as well as a concept he denoted by lens, which allows one to focus in on a variety of parts of the analysis. The speaker concluded by presenting his generalisation of Byrne's Theorem, a game which has ties to the combinatorial game CHOMP.

Scientific Progress Made

One of the major aims of the Workshop was to have the algebraists and game theorists engaged in conversation. On this alone, the Workshop was a major success.

During the non-scheduled times, the Workshop participants divided into three groups: those interested in misère games; those interested in GO; and those interested in impartial games. Given that there is a non-trivial overlap between these groups, it was difficult for many people to choose.

One of the major aims of the Workshop was to get a dialogue between researchers in algebra and those in misère games. The talks by Plambeck, Siegel, and Weimerskirch set the stage, presenting the approaches and algorithms from the game theory point of view. As mentioned in Section 2, there is as yet no characterization of these monoids. Indeed, given a game, there is nothing known to help decide the size of the monoid or indeed that it will be infinite. These two groups set aside much of the free time and a lively dialogue ensued—amongst others, the fields of topology and category theory were invoked. The groups are planning other meetings to further the fascinating structures that appear as the monoids of impartial heap games. There has yet to be a discussion about the structures that occur as monoids of partizan misère games and, because of this absence, one graduate student has made this her Ph.D. thesis topic.

The group interested in GO met regularly to start the analysis of the Coupon Games on which Berlekamp reported.

The impartial group mainly discussed the some of the variants of WYTHOFF'S NIM —changing the rules as to what a player may take away from the heaps. One interesting aspect was that the talk by Duchene, with its automata approach, sparked an idea that led a group of four to the solution of an actively-worked-on, 4-year-old conjecture from the game of TOPPLING DOMINOES. What is surprising is that the idea was originally applied to an impartial game but was the key to a conjecture in a partizan game.

One aspect of these Game Workshops has been that of designating a tournament game, a game that has not been well-explored, that has not given in easily to analysis and has some tie-in with the Workshop theme. The rules are given out a few days in advance. There was a human and a separate computer tournament[1]. This Workshop the game was misère DOTS AND BOXES, i.e. the player with the fewer number of boxes wins. The misère aspect obviously fitted in well with the misère theme of the Workshop, but as a score game, it is slightly outside the usual purview of combinatorial game theory. It was not clear, and still isn't, how much, if any, of the Normal play analysis carries over. The discussion and tactics that evolved during play seem to indicate that very little carries over. However, there were groups actively working on the problem after the end of the Workshop. The Monte Carlo method that has been so successful recently in computer GO proved to be very unsuccessful when applied to this game. Cazenave noted that in GO, the optimal strategy has many other almost-as-good strategies that differ only in a few moves. In misère DOTS AND BOXES given a winning line, any slight deviation leads to a devastating loss. This might explain why both human and machine required an inordinate amount of time to play the games. One hour was not unusual for a 5×5 array of 25 boxes.

One potentially fruitful area that has yet to be explored is the overlap of the areas of classical and combinatorial game theory. Sam Payne's talk on Richman games gave an impetus. It really intrigued the participants'. There were many chess games played with the new bidding rules for each move. It became clear that, given the participants low level of expertise, the game was determined after only a few rounds but as the expertise grew so did the length of the games.

Outcome of the Meeting

The proceedings of the Workshop will appear as *Games of No Chance IV* and will include not only the talks that were presented but also the papers that originated in or were sparked by the talks. Many new research partnerships were formed at the Workshop and the next few years should be quite productive for the area because of the opportunities afforded by the Workshop.

[1] A previous Workshop had CLOBBER[4] as the tournament game. In the human-side final, the losing move was the phrase'I resign' uttered by the player who had a winning position. On the computer side, there was the strange situation where computer A reported that it could see to the end of the game and it determined that it had won. Its opponent, computer B, couldn't see that far and the human operator asked to play on. Computer A made a move, followed by computer B, at which point computer A said that it could see to the end of the game and it now lost! Off-the-board tactics?

List of Participants

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Chapter 3

Mathematical Advancement in Geophysical Data Assimilation (08w5096)

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Overview of the Field

Mathematical Overview of Data Assimilation

The issue of fusing data into models arises in all scientific areas that enjoy a profusion of data. In the geophysical community, this is referred to as data assimilation (DA) and has the goal of estimating an unknown true state of the atmosphere or ocean. The most routinely performed practice of geophysical DA is numerical weather prediction. The current atmospheric state is estimated 'optimally' by fusing the relevant atmospheric observations over the preceding few hours of a DA cycle into an output computed by a large atmospheric model as a forecast based on a past initial condition. The resulting analysis of the current state is then used as a new initial condition to start a forecast of the next assimilation cycle.

The mathematical problem of fusing data into a model is both fundamental in that it aims at the estimation of an unknown, true state and challenging as it does not naturally afford a clean solution. It has the two equally important elements of observations and computational models. Observations measured by instruments provide direct information of the true state, whether they are taken in situ or by remote sensing. Such observations are heterogeneous, inhomogeneous in space, irregular in time, and subject to differing uncertainty. In contrast, computational models use knowledge of underlying physics and dynamics to provide a complete description of state evolution in time. Models are also far from perfect: due to model error, uncertainty in the initial conditions and computational limitations, model evolution cannot accurately generate the true state. In order to obtain an analyzed state that is more complete and accurate than the raw observations or model simulations by themselves, DA merges observations into the models.

The DA schemes in use have been built on a variety of mathematical theories and techniques originating in such areas as statistics, dynamical systems and numerical analysis. Recent technological advances have elevated both sides of the DA equation to a new level: innovative observing techniques have led to an enormous surge in the amount of available data, and increased knowledge of the underlying system advances geophysical modeling, while ever faster computers have given us the capability of new levels of computational modeling. Accordingly the need to develop more sophisticated yet efficient DA schemes has grown commensurately.

By its very nature, DA is a complex interdisciplinary subject. The development of effective methods of DA must now be viewed as one of the fundamental challenges in scientific prediction. Nevertheless, the part of the mathematical community interested in these issues has been limited until recently. In particular, timely and exciting subjects that badly need input from mathematicians include the potential of ensemble-based methods, the unifying effect of a Bayesian perspective, and the present shift towards probabilistic forecasts. Mathematical theories and computation such as Markov-chain Monte Carlo methods and stochastic computing give promise of significant advancement for DA. We now have a tremendous opportunity to bring the relevant scientific areas together in a focused effort aimed at developing new approaches, understanding the underlying issues and testing the implementation of new schemes.

Background for This Workshop

This intensive workshop was organized to bring together mathematicians, particularly those working in dynamical and stochastic systems, statisticians, and domain scientists who have a vested interest in fusing data with models. The workshop aimed to host a mathematical effort for a genuinely interdisciplinary subject in that the participants will explore and define mathematical investigations necessary to advance DA further beyond the current state-of-the-art.

To lay the groundwork and respond to the growing need for mathematical and statistical techniques, a pilot mathematical program on DA was run collaboratively by the Statistical and Applied Mathematical Sciences Institute (SAMSI) and the Institute of Pure and Applied Mathematics (IPAM) during spring 2005. Communication between the various groups is being established. The area is now ripening for fostering effective collaborative efforts as a community begins to gel around the key questions and mathematicians are brought in to tackle the hard problems. The timing of this workshop is chosen judiciously to collectively maximize the impact of this workshop and keep up the momentum after three years since the pilot program.

Recent Developments and Open Problems

Data assimilation has made significant progresses recently. Progresses may be categorized mainly into two areas. One area concerns the development of mathematical approaches to assimilate data. In the past, two approaches have been considered as the advanced approach. They are the variational approach (either 3D-Var or 4D-Var) and the sequential approach (mainly ensemble Kalman filter for large-dimensional problems). Both approaches basically solve the same problem but make different approximations in order to be computationally feasible for large atmospheric and oceanic problems. A new approach based on the Bayesian estimation has been gaining its popularity because it makes less approximations than the variational and sequential approaches. However, the most severe limitation of the Bayesian approach so far is that it quickly becomes computationally unfeasible to implement as the dimension of the system increases. The other area concerns how to deal with the complex systems like the atmosphere and the oceans, while the currently available models cannot fully represent such systems.

As more mathematicians get involved in data assimilation, we expect that significant progress will be made in the coming years. Some open questions and challenges raised by the participants prior to the workshop included:

1) Can fully Bayesian method be developed and practically implemented? In the case of ensemble methods, the main difficulty seems to be the large dimension of atmospheric and ocean models, which have so far been prohibitive for algorithms such as particle filters;

2) Ensemble estimation, which aims at defining probability distribution, is of a different nature than deterministic estimation, which aims at determining a point estimate. What are the ways for properly evaluating ensemble estimation?

3) Model errors, and different types of observational errors too, are certainly correlated in time. Sequential assimilation cannot be optimal in the presence of time-correlated errors. What are the ways to deal with temporal correlation?;

4) Turbulence is associated with complex interaction between spatial scales. What is the impact of those interactions on assimilation? For instance, is it possible to reconstruct the small scales of the motion from observations of the large scales?

In Section 3 we summarize the progress made during this workshop.

Workshop Presentations

This section presents a short summary of the presentations made during the workshop. The presentations themselves are available online at http://kayo.bol.ucla.edu/birs/.

Atmospheric Data Assimilation

Andrew Lorenc *"Research Issues in Data Assimilation for Operational NWP"*
Operational NWP has improved predictive skill by about a day per decade since the 1970s. Much of this is due to four-dimensional data assimilation methods, which fit the best available numerical forecast model to observations, allowing for the error characteristics of both. Statistically based methods are needed because observations, although plentiful in the satellite era, are incomplete and relatively inaccurate, compared to the information carried forward by a good forecast model from past observations.

Variational methods use Gaussian models to characterise the errors in the forecasts and observations; the cost and complexity of good forecast models means that the true errors are unknowable. Error modelling assumptions are essential, and the Gaussian assumption leads to computationally tractable linear systems. Recently, in order to continue to improve, it has become necessary to allow for the flow dependence of forecast errors. Statistically based four-dimensional variational methods (4D-Var) are used in most of the best synoptic-scale NWP systems, while ensemble methods for characterising errors are increasingly important. Another issue topic is the modelling of the effect of forecast model errors, rather than initial condition errors, on forecast errors. The development of these methods is the subject of much current research.

Gaussian assumptions, with a linearisable forecast model, lead to methods related to the Kalman filter (KF). Although the KF itself is not affordable, its linear equations enable approximations such as 4D-Var and the Ensemble KF which are feasible even for complex NWP models; it is likely that operational NWP will be based on such methods for some time. Nevertheless nonlinear relationships and the related non-Gaussian distributions are important; methods must be adapted to perform well in such cases (sometimes in an ad hoc way). One possible consequence of nonlinearity is that the Kalman filter 'blows up' if there are chaotic features which are so poorly observed that they remain chaotic in the assimilation system. This can happen in the upper stratosphere, and will happen in a global convective-scale model. In the real world, and in realistic nonlinear models, there is a climate attractor. Nonlinear processes damp perturbations (from the climate mean state) which are large compared to the climate variability. In the Kalman filter, and in the linear models used in 4D-Var, this damping needs to be added explicitly. Another consequence of this attractor is the existence of coherent structures such as fronts, inversions and cyclones. Forecasts often have plausibly structures, in the wrong place. This can lead to a significantly non-Gaussian and biased error distributions. Adaptations include the incremental approach and nonlinear initialisation. Much harder to deal with is a model with errors which mean its attractor does not match the atmosphere's.

Increases in computer power mean we can now develop convective-scale NWP systems; a major challenge is to extend the above approaches. Except perhaps in limited regions with good Doppler radar coverage, nonlinear effects will be more important; we need to spin-up realistic convective cells which match available observations. Luckily for our ability to make forecasts, convection is often largely determined by larger-scale and topographic forcings, so multi-scale assimilation methods are needed which preserve large-scales from an optimal global system, while still fitting detailed observations when they exist.

Pierre Gauthier *"Mathematical Problems Associated with Atmospheric Data Assimilation and Weather Prediction"*
The duality principle presented by Courtier (1997) states that the 3D-Var and the Physical-Space Analysis System (PSAS) (or dual form) are just different algorithms to solve the same problem. It was also shown that the two algorithms with their own specific preconditioning can be expected to converge at a similar rate as

their Hessian matrices have the same condition number. A 4D-Var algorithm being merely an extension of 3D-Var, the so-called 4D-PSAS should also be equivalent. In this presentation, results will be presented to establish the equivalence of the two approaches. To tackle the nonlinear problem, an incremental formulation is introduced and the equivalence will be established to stress the role of the outer loop process. Results from El Akkraoui *et al.* (2008) indicate some convergence problems that were encountered with the dual form. Moreover, when cycling an assimilation system, the Hessian from the previous minimization can be used to precondition the next assimilation. This is beneficial but cannot be done as easily in a PSAS system. An approach is proposed that takes advantage of the equivalence between the eigenvectors of the dual and primal problems. The interest of the dual form is motivated by the fact that it permits to compute the observation impact through adjoint sensitivities with respect to observations (Langland, 2004). An intercomparison experiment is being carried out at the moment to assess the robustness of the method when used at different NWP centres. Finally, the weak-constraint 4D-Var can also be formulated in either its primal or dual form, the latter having the advantage of using a control variable with a considerably lower dimension. This avenue is now being examined in the context of a simplified barotropic model.
Joint with Amal El Akkraoui, Simon Pellerin and Samuel Buis.

Oceanic Data Assimilation

Robert N. Miller *"Estimation of Representation Error in Ocean Models"*
Much of the variability in the observed data arises from physical causes that are often neglected in ocean general circulation models (GCMs). Models that are commonly used as components of climate models or coupled to models of ocean ecology are implemented with resolution too coarse to resolve western boundary currents or eddies, so signals present in the observed data resulting from these phenomena cannot be usefully assimilated. That part of the variability contributes to the model-data misfits and must be treated as error. It is therefore referred to as 'representation error', since the physics of the model are inadequate to represent it.

We describe the construction of a static optimal interpolation scheme based on projection of the model-based misfits into the space whose variability can be reliably simulated by a common non-eddy resolving GCM applied to the north Pacific ocean, and use our scheme to assimilate remotely-sensed SST observations. Most of the correction to the model run appears in regions where the model output is reliable. Correction is minimal in the Kuroshio. Our method for calculating the forecast error covariance allows us to explicit estimate of the statistics of the representation error.

We also present an ensemble calculation to show that our error estimates are sufficient to produce ensembles with statistical properties that are similar to the model-data misfits. Similar error estimate could be used to implement an ensemble Kalman filter that would account for representation.

Zhijin Li *"Development of Data Assimilation Schemes in Support of Coastal Ocean Observing Systems"*
The Integrated Ocean Observing System (IOOS) is an emerging national program, whose goal is to develop and sustain a network of integrated coastal and ocean observations. One major component of IOOS is the Regional Coastal Ocean Observing Systems (RCOOSs). For RCOOSs, a real-time data assimilation and forecasting system has been considered as an integrated component. We have developed a three-dimensional data assimilation (3DVAR) scheme in association with the Regional Ocean Modeling System (ROMS) in support of coastal ocean observing systems. The formulation is described, and several challenges are addressed. The major challenges are those related to complexity of topography, uncertainties of atmospheric and fresh water runoff forcing, and observability.
Joint with Yi Chao, James C. McWilliams, Kayo Ide

Keith Thompson *"Predicting Mesoscale Variability of the North Atlantic Using a Simple Physically Motivated Scheme For Assimilating Altimeter and Argo Data"*
A computationally-efficient scheme is described for assimilating sea level measured by altimeters and vertical profiles of temperature and salinity measured by Argo floats. The scheme is based on a transformation of temperature, salinity and sea level into a new set of physically-motivated variables for which it is easier to specify spatial covariance functions. The scheme allows for sequential correction of temperature and salinity biases, and online estimation of time-dependent background error covariance parameters. Two North Atlantic application, both focused on predicting mesoscale variability, are used to assess the effectiveness of the

scheme. In the first application the background field is a monthly temperature and salinity climatology and skill are assessed by how well the scheme can recover Argo profiles that have not been assimilated. In the second application the backgrounds are forecasts made by an eddy permitting model of the North Atlantic. Skill is assessed by the quality of forecasts with lead times of 1 to 60 days. For both applications it is shown that the scheme has useful skill. The benefits of using physical constraints to reduce the computational cost of assimilation is discussed in general, and compared to other cost-reducing approaches such as those used in the SEEK filter.
Joint with Yimin Liu

Variational Method

Mark Buehner *"Towards an Improved Use of Flow-Dependent Background Error Covariances in a Variational Data Assimilation System"*
Since early 2005, Environment Canada has been operationally running both a global four-dimensional variational analysis system (4D-Var) and an ensemble Kalman filter (EnKF). Both systems employ the same atmospheric model though with different spatial resolution. The co-existence of these two operational systems at a numerical weather prediction (NWP) centre provides a unique opportunity. In this talk approaches for incorporating background-error covariances estimated from the EnKF ensembles in the variational assimilation system are discussed. The techniques of spatial and spectral localization are briefly described and demonstrated with a simple one-dimensional problem. Then, the impact of localizing ensemble-based covariances in the variational system are shown. The practical challenge of simultaneously applying localisation in both spectral and spatial domains within a realistic NWP data assimilation system is also presented.

Ricardo Todling *"Catching up to the World: The GMAO 4d-Var and its Adjoint-Based Tools"*
The fifth generation of the Goddard Earth Observing System (GEOS-5) Data Assimilation System (DAS) is a 3d-var system that uses the Grid-point Statistical Interpolation (GSI) system developed in collaboration with NCEP, and a general circulation model developed at Goddard, that includes the finite-volume hydrodynamics of GEOS-4 wrapped in the Earth System Modeling Framework and physical packages tuned to provide a reliable hydrological cycle for the integration of the Modern Era Retrospective-analysis for Research and Applications (MERRA). This MERRA system is essentially complete and the next generation GEOS is under intense development. A prototype next generation system is now complete and has been producing preliminary results. This prototype system replaces the GSI-based Incremental Analysis Update procedure with a GSI-based 4d-var which uses the adjoint of the finite-volume hydrodynamics of GEOS-4 together with a vertical diffusing scheme for simplified physics. As part of this development we have kept the GEOS-5 IAU procedure as an option and have added the capability to experiment with a First Guess at the Appropriate Time (FGAT) procedure, thus allowing for at least three modes of running the data assimilation experiments.

The prototype system is a large extension of GEOS-5 as it also includes various adjoint-based tools, namely, a forecast sensitivity tool, a singular vector tool, and an observation impact tool, that combines the model sensitivity tool with a GSI-based adjoint tool. These features bring the global data assimilation effort at Goddard up to date with technologies used in data assimilation systems at major meteorological centers elsewhere.
Joint with Yannick Trémolet

Nancy Nichols *"Use of Reduced Order Models in incremental Four-Dimensional Variational Data Assimilation"*
Incremental methods used operationally for 4D-variational data assimilation aim to solve a sequence of linear approximations to the full nonlinear problem. These methods consist of inner iteration loops for solving each linear approximation via an adjoint procedure and an outer iteration loop in which the nonlinear analysis is updated and the problem is re-linearized about the current estimate of the analysis. In order to increase the computational efficiency of these methods, low rank approximations to the inner linear systems are used, thereby reducing the work needed in each inner iteration loop. Low resolution models derived from spatial or spectral truncations of the full system commonly provide the reduced rank approximations. Convergence of these procedures depends on how accurately the low order models approximate the full system model.

New techniques for finding reduced rank models based on balanced truncation methods developed for

large scale control system design are presented here with application to the incremental 4D-Var procedure. Reduced models determined by these methods are optimal in the sense of producing the best match to the frequency response of the full system. More of the dynamical information of the full system is therefore retained by these reduced models than by a low resolution system. Results obtained for simple shallow water test cases illustrate the superior performance of these reduced models and show that the same accuracy in the analysis can be obtained more efficiently with a much lower dimensional reduced order approximation than with a low resolution model.
Joint with Amos S. Lawless, Caroline Boess, Angeliza Bunse-Gester

Ensemble-Based Method

Martin Ehrendorfer *"Ensemble-Based Data Assimilation"*
Ensemble-based data assimilation methods related to the fundamental theory of Kalman filtering have been explored in a variety of mostly non-operational data assimilation contexts over the past decade with increasing intensity. While promising properties have been reported, a number of issues that arise in the development and application of ensemble-based data assimilation techniques, such as in the basic form of the ensemble Kalman filter (EnKF), still deserve particular attention.

The necessity of employing an ensemble of small size represents a fundamental issue which in turn leads to several related points that must be carefully considered. Attempts to reduce effectively the sampling error due to small ensembles and at the same time maintaining an ensemble spread that realistically describes error structures has led to the development of variants of the basic form of the EnKF. In this presentation, several of the above-mentioned issues are discussed and illustrated together with a brief review of the methodology that has been developed by varying the basic form of the EnKF.

Zoltan Toth *"Towards an Improved Use of Flow-Dependent Background Issues Related to the Use of Ensembles in Data Assimilation and Targeting"*
The assimilation of observations into numerical models of dynamical systems ideally builds on both dynamical and statistical principles. The presentation focus is on the interface between dynamics and statistics, exploring some aspects from both fields that may either be critical, or could possibly be compromised for achieving a balanced solution, leading to successful data assimilation (DA). Questions and issues explored include: The role of a numerical first guess in traditional and ensemble-based DA; Alternative ways of generating first guess fields for ensemble-based DA; Statistical and dynamical considerations when estimating the background error covariance; How to assimilate data with an imperfect model? Can information from highly non-linear forecasts be used for targeting observations to improve such forecasts? What other issues one must consider for an integrated observing, data assimilation and forecast system for chaotic systems?
Joint with Malaquias Pena, Mozheng Wei, Yucheng Song

Istvan Szunyogh *"Flow Dependence of the Performance of an Ensemble Based Analysis-Forecast System"*
Data assimilation is problem at the intersection of dynamical systems theory and mathematical statistics. In this talk, we focus on the dynamical systems aspects of the problem. In particular, we argue that most techniques of dynamical systems theory, which have already been applied to geophysical fluid dynamical systems, have a solid theoretical foundation only for low-dimensional systems. Since geophysical fluid dynamical systems are inherently high-dimensional, a systematic approach to extend the theoretical machinery to increasingly more complex systems would be highly desirable. In this talk, we outline one potential approach to address this issue: the high-dimensional system is viewed as the collection of local systems; the local state vector is defined by the variables of the original high-dimensional system from a local neighborhood of each physical location; and properties that smoothly vary with the location are computed based on the local state vectors. We illustrate this approach by using it to explain the spatio-temporal variability of the performance of an ensemble-based analysis-forecast system. This system consists of the Local Ensemble Transform Kalman Filter data assimilation scheme and a reduced resolution version of the model component of the Global Forecast System of the National Centers for Environmental Prediction.

Eric Kostelich *"Recent Results of the 4D Local Ensemble Transform Kalman Filter (4D-LETKF)"*
I outline the latest results of the Maryland/ASU implementation of the Local Ensemble Transform Kalman

Filter (LETKF) to the Global Forecast System of the National Centers for Environmental Prediction (NCEP). Measures of forecast accuracy and comparison with with operational NCEP analyses are described. The computational efficiency of our implementation of the LETKF also is assessed, including issues of scaling, load balancing, and data transport.

Hybrid Methods

Fuqing Zhang *"Coupling Ensemble Kalman Filter with Four-Dimensional Variational Data Assimilation"*
This study examines the performance of coupling deterministic four-dimensional variational assimilation (4D-VAR) with an ensemble Kalman filter (EnKF) to produce a superior hybrid approach for data assimilation. The coupled assimilation scheme (E4D-VAR) benefits from using the state-dependent uncertainty provided by EnKF while taking advantage of 4D-VAR in preventing filter divergence. The 4D-VAR analysis produces posterior maximum likelihood solutions through minimization of a cost function about which the ensemble perturbations are transformed, and the resulting ensemble analysis can be propagated forward both for the next assimilation cycle and as a basis for ensemble forecasting. The feasibility and effectiveness of this coupled approach are demonstrated in an idealized model with simulated observations. It is found that the E4D-VAR is capable of outperforming both 4D-VAR and the EnKF under both perfect- and imperfect-model scenarios. The performance of the coupled scheme is also less sensitive to either the ensemble size or the assimilation window length than that for standard EnKF or 4D-VAR implementations.
Joint with Meng Zhang, James A. Hansen

Observations

Gérald Desroziers *"Use of Observations in Data Assimilation Schemes"*
Modern operational data assimilation schemes rely on the use of a large range of types of observations. This is made possible via the implementation of observation operators that allow to go from model space to observation space and that especially permit the direct assimilation of satellite radiances. Because most data assimilation schemes rely on the theory of estimation, they is also a need to diagnose and specify observation error covariances. Some observations, such as satellite data, are known to be biased. In that case, a particular procedure such as variational bias correction has to be implemented. Interestingly, ensembles of perturbed assimilations are classically based on a perturbation of observations. Such ensembles allow to document background error covariances that are a key ingredient in a data assimilation scheme. On another hand, the variances given by such ensembles have most often to be inflated. Such an inflation can be tuned via the comparison of ensemble variances to the variances deduced from statistics of the innovation vector. Other aspects are discussed such as the different ways to measure the impact of observations on analyses and subsequent forecasts.

Art Krener *"Eulerian and Lagrangian Observability of Point Vortex Flows"*
We study the observability of one and two point vortex flow from one or two Eulerian or Lagrangian observations. By observability we mean the ability to determine the locations and strengths of the vortices from the time history of the observations. An Eulerian observation is a measurement of the velocity of the flow at a fixed point in the domain of the flow. A Lagrangian observation is the measurement of the position of a particle moving with the fluid. To determine observability we introduce the observability and the strong observability rank conditions and compute them for the various flows and observations. We find that vortex flows with Lagrangian observations tend to be more observable then the same flows with Eulerian observations.

We also simulate extended Kalman filters for the various flows and observations and find that they perform poorly when the observability rank condition or the strong observability rank condition fails to hold.

Richard Ménard *"Model Error as an Unobserved Variable: What Do We Know From Estimation Theory"*
Model error can be accounted as an unknown tendency in the dynamics equation. Since most observation operators relates to state variables as opposed to their tendencies, model error can be accounted as an 'unobserved variable'. Its impact however built up with time. We review several of the known schemes, making the links between variational and Kalman filter and smoother formulations. In a simple model we present some

results and discuss the issue observability of the model error estimation problem. Some ideas about the use of lagged innovations to obtain critical error statistics are also presented. Finally, using an information filter formulation, we note some specific properties arises in the estimation of unobserved variable and speculate that it could be used to distinguish it from observation error.

N. Sri Namachchivaya *"Target Detection in Multi-Sensor and Multi-Scale Environments"*
We describe nonlinear filtering in multi-scale environment, dimensional reduction for noisy nonlinear systems, and reduced order nonlinear filters for physically-motivated problems.

Lagrangian Aspects

Andrew Tangborn *"Assimilation of Vorcore Polar Balloons"*
25 long lived constant volume stratospheric balloons were flown over Antarctica from September 2005 - January 2006. They produced position, pressure and temperature data every several minutes. Wind vectors were derived from the position measurements. We present the results of assimilating Vorcore balloon winds into the GEOS-4 data assimilation system. Improvements to the wind field are found by comparing with an independent data set. The analyzed winds are used to transport ozone fields during the same period in the GMAO ozone assimilation system. Modest improvements to the ozone forecasts are found. We also discuss current plans for assimilation in the GEOS-5 assimilation system and the upcoming Concordiasi balloon campaign.

Kayo Ide *"Lagrangian Data Assimilation: Method and Mathematical Issues"*
The Lagrangian data assimilation (LaDA) is a method for the direct assimilation of Lagrangian observations. Lagrangian instruments in the oceans, such as drifters and floats, are often designed to sample ocean properties while remaining on a two-dimensional surface in the three-dimensional ocean except when descending to or ascending from the desired depth. By augmenting the model state vector with the coordinates of the instruments, the LaDA can assimilate the Lagrangian positions without the need for any commonly used approximations to transform Lagrangian observations into Eulerian (i.e., velocity) observations.

We describe the LaDA method and the observing system design for optimal deployment of Lagrangian instruments. Using the judicious design of the deployment strategy, the LaDA is strikingly efficient in tracking the local coherent structures, such as ocean eddies, as well as estimating the large-scale ocean circulation.
Joint with Guillaume Vernières, Chris Jones

Guillaume Vernières *"Lagrangian Data Assimilation: Application to Gulf of Mexico"*
We demonstrate effectiveness of LaDA in a realistic setting for ocean-eddy tracking in Gulf of Mexico. We evaluate three types of observations for ocean eddy tracking: the measurement of velocities at fixed station, the horizontal position of surface drifters, and the three dimensional position of isopycnal floats. By considering the "volume of influence", we examine how and to what extent the LaDA propagates the information vertically to estimate the three-dimensional ocean structure. We show that as little as one judiciously placed drifter or isopycnal float is needed to recover an eddy being shed by the loop current.
Joint with Kayo Ide, Chris Jones

Bayesian Approaches and Non-Gaussianity

Peter Jan van Leeuwen *"Particle Filtering in Large-Scale Systems: Problems & Potential Solutions"*
Starting from Bayes theorem, it is shown how the Kalman filter and 4D-Var can be derived. Then we concentrate on methods that use a particle representation of the model probability density function (pdf). The Ensemble Kalman Filter (EnKF) is derived, and we shortly touch upon the Ensemble Kalman Smoother. For applications in large-scale problems the number of particles is limited to typically 10-100 because of computational limitations. Given the number of independent unknowns, of the order of 1 million, the ensemble size is way too low. In that case the general formulation does not work, and adjustments have to be made. One of them is to do the analysis locally, i.e., use only observations close to a certain gridpoint to determine the analysis there. This procedure increases the effective ensemble size by a substantial factor, sometimes a factor 1000. While this is still too low, first-order statistics can be determined with reasonable accuracy. A serious

drawback is that the EnKF assumes that the pdf is Gaussian, which can be bad for strongly nonlinear systems. In that case a so-called particle filter can be used in principle, in which the analysis consists of weighting the particles according to their 'distance' to the observations (importance weighting/sampling). Again, the affordable number of particles is too low for most geophysical applications. The localization cannot be applied directly in the particle filter, because it tends to break local geophysical balances, so other solutions have to be found. We discuss several possibilities, such as reduced-space solutions, merging particle filters, marginal pdf's, localization guided by the EnKF etc. Although all these ideas have potential, the final answer is still to be found.

Chris Snyder *"Obstacles to Particle Filtering in High Dimensions"*
Particle filters are ensemble-based assimilation schemes that, unlike the ensemble Kalman filter, employ a fully nonlinear and non-Gaussian analysis step. Evidence is presented that, if the observation log-likelihood has an approximately Gaussian distribution, the ensemble size required for a successful particle filter scales exponentially with the variance of the observation log-likelihood, rather than the state dimension per se. Asymptotic results, following the work of Bengtsson, Bickel and collaborators, are provided for two cases: one in which each prior state component is independent and identically distributed, and one in which both the prior pdf and the observation errors are Gaussian. I also discuss 'effectively low dimensional' situations in which the observation log-likelihood is far from Gaussian despite large state dimension and large numbers of observations.

Mike Dowd *"Sequential Monte Carlo Approaches for Parameter and State Estimation"*
Statistical methodologies for estimating state and parameters for time dependent stochastic dynamic systems are now well established. For nonlinear dynamics and non-Gaussian observations these data assimilation approaches rely on Monte Carlo solutions implemented via particle or ensemble methods. In this talk, I overview new developments in such state estimation methods which rely on resampling/bootstrap and MCMC (or combinations thereof). The associated parameter estimation problem for nonlinear stochastic DE based numerical models is also considered using likelihood and state augmentation approaches. Simple toy models of ocean biogeochemistry using non-Gaussian ecological measurements from a coastal ocean observatory are used for illustration throughout. Challenges for adaptation to data assimilation in large dimension PDE based systems are discussed.

Christopher K.R.T. Jones *"'Bayesian Approach to Lagrangian Data Assimilation"*
Lagrangian data arise from instruments that are carried by the flow in a fluid field. Assimilation of such data into ocean models presents a challenge due to the potential complexity of Lagrangian trajectories in relatively simple flow fields. We adopt a Bayesian perspective on this problem and thereby take account of the fully nonlinear features of the underlying model. In the perfect model scenario, the posterior distribution for the initial state of the system contains all the information that can be extracted from a given realization of observations and the model dynamics. We work in the smoothing context in which the posterior on the initial conditions is determined by future observations. This posterior distribution gives the optimal ensemble to be used in data assimilation. The issue is then sampling this distribution. We develop, implement, and test sampling methods, based on Markov-chain Monte Carlo (MCMC), which are particularly well-suited to the low-dimensional, but highly nonlinear, nature of Lagrangian data. We compare these methods to the well-established ensemble Kalman Filter (EnKF) approach. It is seen that the MCMC based methods correctly sample the desired posterior distribution whereas the EnKF may fail due to infrequent observations or nonlinear structures in the underlying flow.
Joint with Amit Apte, Andrew Stuart

Nonlinearity, Non-Gaussianity, and Multi-Scaleness

Marc Bocquet *"Non-Gaussian Data Assimilation: Application to Inverse Modelling of Atmospheric Tracers"*
On the practical side, the goal of this talk is to demonstrate that data assimilation techniques can be used to identify the source of an accidental release of pollutant into the atmosphere, and forecast (possibly in real-time) the subsequent dispersion plume. On the methodological side, the aim is to show that there are

circumstances when the use of non-Gaussian techniques in data assimilation is profitable.

A first method is based on the principle of maximum entropy on the mean and briefly reviewed. A second approach, which has not been applied in this field yet, is based on an exact Bayesian approach, through a maximum *a posteriori* estimator. The methods share common grounds, and both perform equally well in practice. When specific prior hypotheses on the sources are taken into account such as positivity, or boundedness, both methods lead to purposefully devised cost-functions, thanks to non-linear convex analysis. These cost-functions are not necessarily quadratic because the underlying assumptions are not Gaussian. As a consequence, several mathematical tools developed in data assimilation on the basis of quadratic cost functions in order to establish *a posteriori* analysis, need to be extended to this non-Gaussian framework. Concomitantly, the second-order sensitivity analysis needs to be adapted, as well as the computations of the averaging kernels of the source and the errors obtained in the reconstruction. All of these developments are applied to a real case of tracer dispersion: the European Tracer Experiment (ETEX). Examples are also given on the Chernobyl accident. Comparisons are made between a least squares cost function (similar to 4DVar) approach and a cost function which is not based on Gaussian hypotheses. Besides, the information content of the observations which is used in the reconstruction is computed and studied on the application case.

Alternatively these methods can be interpreted as weakly constrained 4DVar-like approaches with a non-Gaussian formalism for model error. Here, model error would be the pollutant source field, which is very uncertain but still the main forcing of the plume dynamics. Possible generalizations of these methods to non-linear physics are sketched.

Youmin Tang *"Advanced Data Assimilation in Strongly Nonlinear Systems"*
Performance of advanced derivativeless, sigma-point Kalman filter (SPKF) data assimilation schemes in a strongly nonlinear dynamical model is investigated. The SPKF data assimilation scheme is compared against traditional Kalman filters such as extended Kalman filter (EKF) and ensemble Kalman filter (EnKF) schemes. Three particular cases, namely the state, parameter and joint estimation of states and parameters simultaneously, from a set of discontinuous noisy observations were studied.

The celebrated Lorenz model with highly nonlinear condition is used as the test bed for data assimilation experiments. The results of SPKF data assimilation schemes were compared with those of traditional EKF and EnKF where a highly nonlinear chaotic case is studied.

Tomislava Vukicevic *"Analysis of the Impact of Model Nonlinearities, Modeling Errors and Gaussian Prior in Inverse Problem Solving"*
In this study, the relationship between nonlinear model properties and inverse problem solutions is analyzed using a numerical technique based on the inverse problem theory formulated by Mosegaard and Tarantola. According to this theory, the inverse problem and solution are defined via convolution and conjunction of probability density functions that represent stochastic information obtained from the model, observations and prior knowledge in a joint multidimensional space. This theory provides an explicit analysis of the nonlinear model function, together with information about uncertainties in the model, observations, and prior knowledge through construction of the joint probability density, from which marginal solution functions can then be evaluated. The numerical analysis technique derived from the theory computes the component probability density functions in discretized form via a combination of function mapping on a discrete grid in the model and observation phase space, and Monte-Carlo sampling from known parametric distributions.

The efficiency of the numerical analysis technique is demonstrated through its application to two well known simplified models of Atmospheric physics: Damped oscillations and Lorenz' 3-component model of dry cellular convection. The major findings of this study are:

- Use of a non-monotonic forward model in the inverse problem gives rise to the potential for a multi-modal posterior pdf, the realization of which depends on the information content of the observations, and on observation and model uncertainties,
- Cumulative effect of observations, over time, space or both, could render unimodal final posterior pdf even with the non-monotonic forward model,
- A greater number of independent observations are needed to constrain the solution in the case of a non-monotonic nonlinear model than for a monotonic nonlinear or linear forward model for a given number of degrees of freedom in control parameter space,

- A nonlinear monotonic forward model gives rise to a skewed unimodal posterior pdf, implying a well posed maximum likelihood inverse problem,
- The presence of model error greatly increases the possibility of capturing multiple modes in the posterior pdf with the non-monotonic nonlinear model, and
- In the case of a nonlinear forward model, use of a Gaussian approximation for the prior update has a similar effect to an increase in model error, which indicates there is the potential to produce a biased mean central estimate even when observations and model are unbiased.

Milija Zupanski *"Dynamical Approach to Nonlinear Ensemble Data Assimilation"*
We present an overview of ensemble data assimilation methods by focusing on their approach to nonlinearities. This subject is introduced from the dynamical, rather than a typical statistical point of view. As such, most problems in ensemble data assimilation, and in data assimilation in general, are seen as means of producing an optimal state that is in dynamical balance, rather than producing a state that is optimal in a statistical sense. Although in some instances these two approaches may produce the same results, in general they are different. Details of this difference are discussed, and also related to variational data assimilation.

Nonlinearities are of special interest in realistic high-dimensional applications, which implies the need for considering the number of degrees of freedom. The means for increasing the degrees of freedom in ensemble data assimilation are briefly discussed, in particular their impact on dynamical balance.

An algorithm named the Maximum Likelihood Ensemble Filter (MLEF) is presented as a prototype nonlinear ensemble data assimilation method. Some results with the MLEF are shown to illustrate its performance, including the assimilation of real observations with the Weather Research and Forecasting (WRF) model for the hurricane Katrina.

Olivier Pannekoucke *"Background Error Correlation Modeling: Representation of the Local Length-Scale From (small) Ensemble"*
Ensembles of perturbed assimilations and forecasts are now a well known method. They mimic the time evolution of the dispersion of possible states in model space. However this method is costly and only a few assimilations can be computed. The issue of how to extract some robust information from an ensemble is discussed. In a first part, some features about background error correlation functions are reminded. In particular, it is shown how diagnoses of local correlation length-scale can illustrate the geographical variations of correlation functions. A second part of the talk is focused on the representation of geographical variations through the wavelets diagonal assumption. In particular, some interesting properties of this formulation are illustrated: it allows the representation of length-scale variations, and it offers interesting filtering properties. The last part of the talk deals with an alternative way to represent geographical variations of correlation functions via a modelisation based on the diffusion equation.
Joint with Loïk Berre, Gérald Desroziers, Sébastien Massart

Future Perspectives

Olivier Talagrand *"A Few Future Perspectives for Assimilation"*
A number of questions relative to the theory and practice of assimilation are discussed. Particular emphasis is put on ensemble and assimilation validation criteria. Validation requires comparison with unbiased *independent observations* that have not been used in the assimilation. For ensembles, reliability and resolution are key elements. One element that needs to be considered in data assimilation is the presence of observation and model errors that may be correlated in time. Time-correlated errors cannot be taken into account in sequential schemes that discard observations as they are used. 4D-Var and smoother schemes can take into account errors that are correlated in time. Is it possible to develop fully Bayesian algorithms for systems with dimensions encountered in meteorology and oceanography? Would that require totally new algorithmic developments? Finally, the objective evaluation of an assimilation system raises a number of questions to extend notions of information content to the general nonlinear case. Estimation of the first and second order moments of observation errors is needed but current observations may not be sufficient to fully characterize them. Given all those limitations, one could ask instead how to make the best of an assimilation system.

Summary of Scientific Progress

The objective of this workshop was to explore and discuss areas and specific problems in which collaborative efforts with the mathematical community could help to address fundamental and challenging issues in data assimilation. The BIRS workshop brought together practioners of data assimilation with mathematicians and statisticians for a period of time and at a place where the intensive focus and energy could serve to define the way forward. It offered a unique and much needed opportunity to go beyond what we were able to achieve in the previous programs. The outcome of the workshop is expected to lead to significant contributions to geophysical DA through the development of new statistical, dynamical and computational strategies.

During the workshop, several mathematical issues were raised and discussed. Those relate to current problems that need to be investigated to make advances in data assimilation methodology in support of atmospheric and oceanic modeling.

Addressing and accounting for uncertainties

The statistical estimation problem necessitates the characterization, representation and estimation of uncertainties within the assimilation. It would also be important to relax some of the constraints embedded within the current assimilation systems:

1. *Non-gaussianity in probability density function of the state*: linearity and Gaussianity still underlie most assimilation systems. There is evidence that these assumptions are not verified in many cases. However, the extension to the non-Gaussian p.d.f. brings up many difficulties regarding the modeling of the probability distributions and their estimation. From a practical point of view, the question is then to know whether it is at all possible to develop fully Bayesian algorithms for systems with large dimensions such as those encountered in meteorology and oceanography.

2. *Sampling*: ensemble-based methods are using ensembles of finite-size and this raises some questions about the *optimal* sampling of a non-Gaussian pdf in large dimensional spaces while preserving dynamical constraints.

3. *Representation of model errors*: most assimilation methods assume that the forecast error can be explained by errors in the initial conditions. It is important to take into account the fact the model itself contains error. This includes systematic and random error which is correlated in time.

4. *Algorithmic issues*: large scale problems present algorithmic difficulties that must be addressed. This is a concern for minimization algorithms used in variational forms of data assimilation. Optimal sampling of a phase-space of large dimensions is not so obvious particularly when the underlying p.d.f. is unknown. Assimilation algorithms also involve linear algebra problems such as singular value decomposition, generalized inverse, etc. Finally, efficient nonlinear solvers are needed as well in the more general Bayesian formulation.

Mathematical issues in (geo)physical systems

1. *Physical balance vs. localization, large-dimension, high-resolution*: geophysical systems are constrainted by the dynamical laws that govern them. This leads to some *balance constraints* that are approximately imposed. Although large scale constraints like quasi-geostrophy have been imbedded within the formulation of background-error covariances for a long time, dynamical constraints are not so well known for smaller scale dynamics. In ensemble systems, it is often necessary to “localize” and, in this case, how to impose balance constraints remains an open question.

2. *Scale interactions*: the current thinking is that the evolution of the small scales is to a great extent determined from the large scale part of the flow. Although a simple downscaling of the large scales may capture most of the details of the flow, the scale interactions need to be better understood to adequately represent the influence of the small scales on the large scales.

3. *Parameter estimation in very large dimensional systems*: in meteorology, data assimilation focuses mainly on the analysis of the initial conditions. However, in several applications, it would be more important to determine some unknown parameters that define the system. In atmospheric chemistry for instance, sources and sinks of pollutants are far more important than the initial distribution of the chemical species. Parameterizations schemes are used to represent subscale processes which also involve a number of parameters that are often determined by "tuning" the system. Parameter estimation would then seek to estimate such parameters and the associated estimation error.

4. *Observability*: the volume of meteorological observations is fairly large but this is not the case for oceans. Atmospheric chemistry also requires observations of numerous chemical species which are not observed. This puts some limitations on the estimation of the different error sources (e.g., observation, model, background). The volume of observations that is needed depends on the dynamical couplings and constraints of the systems which may reduce the dimensionality of the problem. The volume of available observations then puts some limitations on the estimation of the state of the atmosphere and its variability.

Incorporationg ideas from mathematics

From the summary presented above, some directions emerge in which mathematical ideas could help to address key problems. The evolution of the atmosphere and the oceans is governed by dynamical systems which embeds the balance constraints and processes acting on different spatial and temporal scales. How to tackle the problems associated with multiscale phenomena can then be cast in terms of the theory of dynamical systems. Can the dynamical constraints be used to reduce the dimension of the problem. For example, dynamical systems provided a framework in which the onset of instabilities could be reduced to systems of low dimensions (center manifold theorem).

Data assimilation and ensemble prediction already use concepts of information theory to evaluate the information content of observations. However, this relies on some assumptions that are not respected for nonlinear systems. Any progress made on extending ideas of information theory to nonlinear systems and non-Gaussian p.d.f. could be most useful.

Finally, in presence of model error, current assimilation algorithms are faced with algorithmic problems given the computing load they involve. Variational assimilation relies on iterative algorithms that are not well suited for massively parallel architectures. Would it be possible to design new algorithms. exploring more than one dimension at the time? This could be cast in some hybrid form of variational ensemble data assimilation to move away from purely sequential schemes that is at the heart of ensemble Kalman filtering. This may also give rise to problems that would require nonlinear solvers.

Dissemination of the Outcome of the Workshop

The organizers and participants to this workshop express our sincere appreciation to the Banff International Research Station for hosting and supporting this exciting and fruitful event. The outcome of this workshop will be disseminated as follows:

Two meeting reports are planned to the society bulletin for both the atmospheric/oceanic community and the mathematical community.

1. *Bulletin of the American Meteorological Soceity (BAMS)*: This report targets scientists who are actively involved in data assimilation. This exposes the scientists to the new directions and development in data assimilation made possible by the means of mathematics. P. Gauthier and K. Thompson (organizers of the workshop) lead this report.

2. *Society for Industrial and Applied Mathematics (SIAM) News*: This report targets mathematicians who are not currently working on data assimilation yet but are experts on the related areas of mathematics. This stimulates the mathematicians to contribute to advancement of data assimilation. K. Ide and C.K.R.T. Jones (organizers) lead this report.

A special issue of the collections of papers based on this workshop in one of the leading journals on data assimilation,*Monthly Weather Review (MWR)*, published by the American Meteorological Society. K. Ide (Organizer) and F. Zhang (participant, editor of MWR) are the co-editors of this special issue.

List of Participants

Bocquet, Marc (Université Paris-Est / INRIA)
Buehner, Mark (Environment Canada)
Desroziers, Gerald (Meteo-France)
Dowd, Mike (Dalhousie University)
Ehrendorfer, Martin (University of Reading)
Gauthier, Pierre (Université du Québec à Montréal)
Ide, Kayo (University of California, Los Angeles)
Jones, Chris (University of North Carolina / University of Warwick)
Kostelich, Eric (Arizona State University)
Krener, Arthur (Naval Postgraduate School)
Li, Zhijin (NASA Jet Propulsion Laboratory)
Lorenc, Andrew (Met Office)
Menard, Richard (Meteorological Service of Canada)
Miller, Robert (Oregon State University)
Nichols, Nancy (University of Reading)
Pannekoucke, Olivier (Meteo-France)
Snyder, Chris (National Center for Atmospheric Research)
Sri Namachchivaya, N. (University of Illinois at Urbana-Champaign)
Szunyogh, Istvan (University of Maryland)
Talagrand, Olivier (Laboratoire de Meteorologie Dynamique / Ecole Normale Superieure)
Tang, Youmin (University of Northern British Columbia)
Tangborn, Andrew (NASA Goddard Space Flight Center)
Thompson, Keith (Dalhousie University)
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Toth, Zoltan (National Centers for Environmental Prediction)
van Leeuwen, Peter Jan (Utrecht University)
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Zhang, Fuqing (Texas A & M University)
Zupanski, Milija (Colorado State University)

Chapter 4

Facets of Heteroepitaxy: Theory, Experiment, and Computation (08w5050)

Feb 10 - Feb 15, 2008

Organizer(s): Joanna Mirecki-Millunchick (University of Michigan), Christian Ratsch (University of California, Los Angeles), Peter Smereka (University of Michigan)

Introduction

The word epitaxy comes from the Greek words *taxis* meaning in an ordered manner and *epi* meaning above. For our purposes epitaxial growth is a process in which thin films are grown in a vacuum by deposition onto a crytalline substrate. The deposition is, relatively speaking, slow and the resulting film is also crystalline (well ordered). There are basically two types of epitaxial growth, namely homoepitaxial growth and heteroepitaxial growth. In the former, the deposited material is the same as that of the substrate. In heteroepitaxial growth, atoms of different species are deposited on to a substrate of different type (which also may be composed of a various atomistic species i.e. an alloy). One prototypical system is Germanium deposited on Silicon.

One significant difference between homoepitaxial and heteroepitaxial growth are elastic effects. These arise because the natural bond length of the deposited species often are different from the substrate. The effects on film growth can be dramatic since the system can lower its elastic energy by forming mounds (sometimes called three dimensional islands) while at the same time remaining a coherent solid (i.e. no dislocations form). However, the mound formation will increase the surface energy. Therefore the morphology of the growing film is determined not only by kinetic effects but also by the thermodynamic competition between surface energy and elastic energy (which is a bulk effect). In many systems it turns out that the system can lower its total energy forming these mounds. Therefore, we see that the mounds are self-assembled. Not only are such systems intrinsically interesting but they also are important from a technological perspective. This is because the mound size can be on the order of tens of nanometers. Mounds this small are often called quantum dots. Such quantum dots have interesting optical and electronic properties. For example solid state lasers have been made using such materials.

An ambitious goal would to be to predict the film composition and morphology under a wide variety conditions. A more modest goal would be to a least understand the experiments and suggest new experimental parameters or materials to consider. From a theoretical point of view, either of these goals is an enormous challenge. One fundamental difficult is the vast range of time scales and length scales that must be properly treated in order to have faithful models. For example, if one would like to simulate an epitaxial system with molecular dynamics then the time and length scales are on the order of 10^{-12} sec and 10^{-4} microns (atomistic scale). However, we need to understand the system on the scale of seconds and microns (macroscale). To complicate matters there are processes that occur on this small scale that can have direct consequences on the macroscale. It should be pointed out that much of the current understanding is still driven by experimental results. For example, the notion that one could have self-assembled islands driven by misfit strain was first seen experimentally and was very surprising from a theoretical perspective. The wisdom at the time was that dislocations would provide stain relief.

There are many issues involved in improving our understanding of epitaxial growth from a mathematical point of view. However one can not make progress without working closely with experimentalists. Probably the single most important issue is modeling. There are many different types of models ranging from atomistic which are discrete in nature to coarse-grained models which are typically phrased in terms of partial differential equations. One advantage of atomistic models is that the need to model is considerably reduced. For example, if one is using molecular dynamics all that is required is a model of the intermolecular potential. As one proceeds to coarse-grain the problem more and more information is needed. The advantage is that one achieves not only greater understanding but also a more efficient description. The problem of coarse-graining atomistic problems is incredibly difficult but is central to the issue of modeling and simulation of epitaxial growth. However little progress can be obtained without working closely with experimentalists. The aim of this workshop was to bring together a diverse group: people who focus on computational aspects, experimentalists, and those who develop models.

Meeting Content

Overview Talks

The workshop began with two overview talks.

Overview Talk 1. The first was by Jerry Tersoff who spoke on the basic issues involved in modeling heteroepitaxial growth using continuum models. He outlined the important interplay between elastic energy, surface energy, anisotropic effects, intermixing, and surface segregation. He described situations where the form of the anisotropic surface energy would permit barrierless formation of faceted islands for a rippled surface.

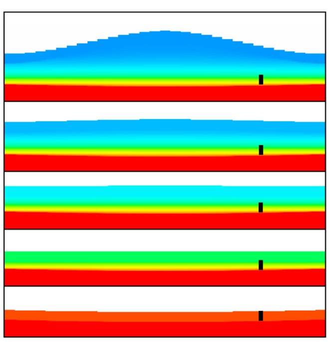

FIG. 1 (color online). Evolution of structure and composition during heteroepitaxy, for nominal $Si_{0.60}Ge_{0.40}$ on Si(001), at deposition rate of 10^4 (arbitrary units). The onset of nonplanar morphology is more abrupt at lower growth rates. Colors indicate composition, from pure Si substrate (bottom) to $Si_{0.62}Ge_{0.38}$ (top). The bottom panel is the initial surface (slightly nonplanar), and subsequent panels are at equal time intervals. The figure shows one unit cell of periodic system; the lateral size is $640w_s$. Surface-layer thickness w_s is indicated by a black rectangle in bottom panel; the vertical scale is greatly expanded to show the small perturbation. The rectangle is repeated in the same position in subsequent panels for reference. Surface steps are a graphical artifact.

Figure 4.1: This figure is from [1] and was discussed in Jerry Tersoff's overview talk.

His talk also discussed his recent work with Y. Tu which showed that segregation could play an important role in the morphology of the growing film. [1, 2, 3] An interesting feature of this work is that the model suggests that wetting layer in Stranski-Krastinov (SK) growth should really be thought of as a transition thickness where the growth rate increases dramatically. In this way, they are claiming that SK growth is really a kinetic effect. This view departs from the conventional wisdom, and sparked a spirited discussion of experimental and theoretical results that both refute and support this hypothesis.

Overview Talk 2. The second overview talk was by Tom Tiedje who presented both experimental results and a model for the epitaxial growth of Gallium Arsenide. [4]. However, the model developed is rele-

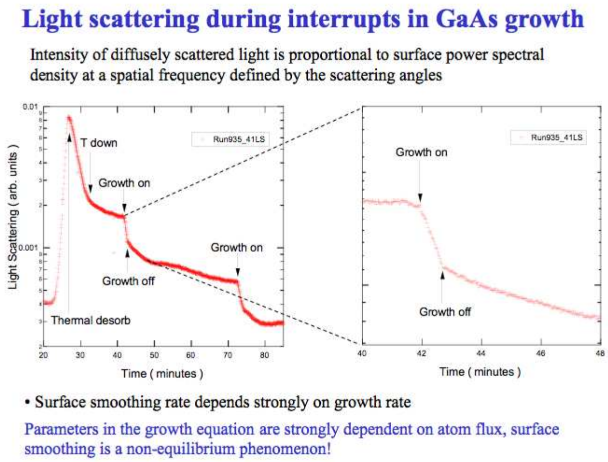

Figure 4.2: Light scattering data for the growth of GaAs homoepitaxial films. In these experiments, the surface continues to evolve even after the growth flux is removed, and has important implications for the development of appropriate models (from Tom Tiedje's talk).

vant to any homoepitaxial system. It was based on a combination of physical intuition and experimental results. Experimental results showed that in the growth regimes considered the film was better modeled by an Edwards-Wilkinson model rather than surface diffusion (Mullins). A nonlinear term, based on physical principles, due Villain was added.

In addition, effects of a step-edge barrier were included by incorporating a current. An interesting feature of the model present was the inclusion of effects of nucleation which allows one to study both island growth and step flow. The model was also in good agreement with kinetic Monte Carlo.

Regular Talks

The remainder of this review provides a summary of the talks in the order they were given.

Jeff Drucker. This talk began by presenting experimental results of the Ostwald ripening of Ge/Si huts and pyramids. [5] These results were based on in situ STM. It was observed that the huts were less stable than the pyramids and the presence of a large dislocated island would alter the ripening of the small islands. Many features of the experiment were modeled by a mean field nucleation theory.

Vivek Shenoy. Work was presented in which composition maps of quantum dots were numerically computed using a continuum model. The model was based on minimizing the total free energy using a finite element method. The results suggested that shallow pyramids do not have extreme composition profiles whereas steeper islands would have high concentrations of Germanium near the top. There was some discussion on the relationship of these energy minimizing solutions as compared to experimental results especially in the of kinetic effects.

Robert Hull. In his talk the speaker presented some novel self assembled nanostructures comprised of pits surrounded by multiple quantum dots, which occur in a very narrow regime of experimental conditions. One feature of these conditions is that the adatoms have limited mobility. It is hoped that such structures will have applications in quantum cellular automata, spin exchange and coherent spin exchange switches. This was joint work with Jennifer Gray (a workshop participant). Relevent material can be foound in Ref. [7].

Ernesto Placidi. Features quantum dot transitions in InAs/GaAs were discussed in this talk. [26] It was experimentally determined that volume of the quantum dots exceeds that of the material deposited from which is was speculated that the extra material must come from intermixing with the substrate, most likely

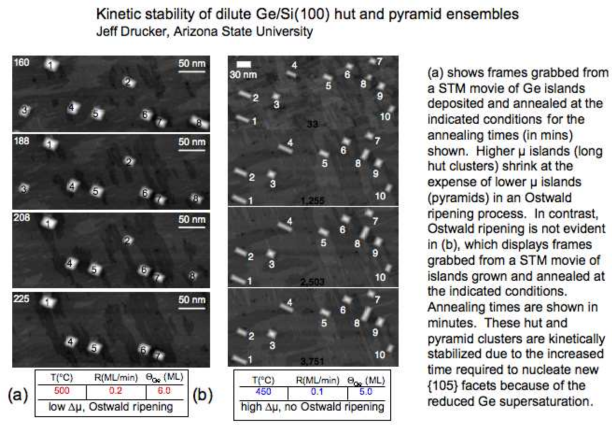

Figure 4.3: A slide from Jeff Druckers talk showing frames of a movie made by a scanning tunneling microscope (STM) that demonstrates the evolution of islands on the surface.

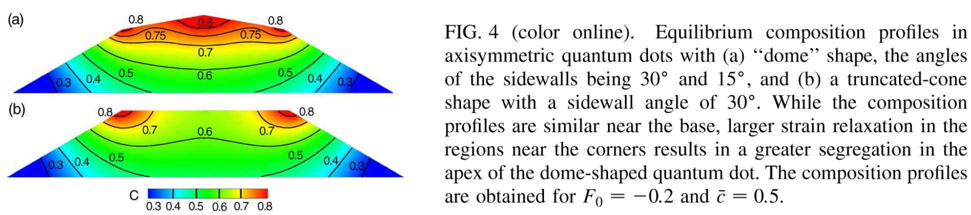

Figure 4.4: This figure is from [6] and was discussed in Vivek Shenoy's talk.

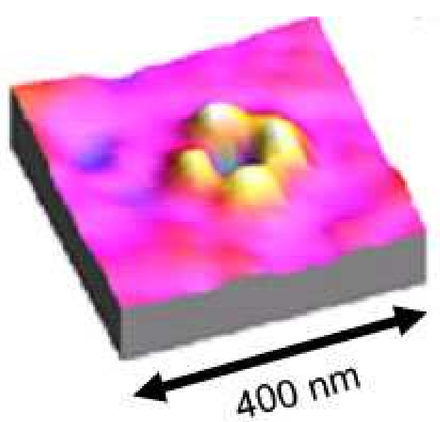

Figure 4.5: An AFM image showing a new class of nanostructure discovered by Gray, Hull, and coworkers, the quantum fortress. It consists of a pit surrounded by discrete islands.

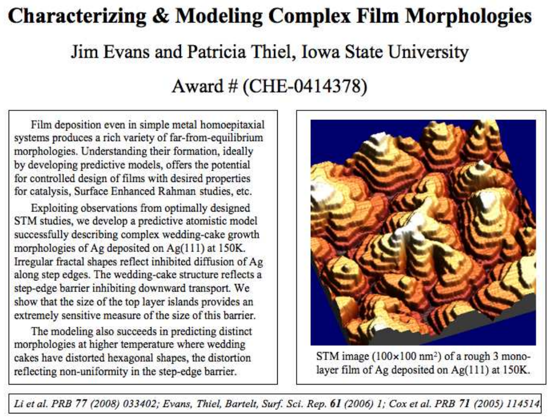

Figure 4.6: A picture showing Silver on Silver epitaxy from the talk by Jim Evans

from adatom detachment from step edges from the surface steps. **Jim Evans.** Evans discussed homoepitaxy

of silver on silver, which gives rise to very interesting film morphology due its large step edge barriers (see Figure 4). He showed how the strength of the step edge barrier can be inferred from the island shape [9]. He also spoke about growth of Silver on Nickel/Aluminum which results in bilayers [10]. Because this system is lattice matched the bilayer are not due to strain, but instead result from the strong anisotopy between the Silver and the Nickel/Aluminium substrate.

Wei Lu. This talk was concerned with self assembly of submonolayer-thick lead films on copper [11]. He presented a continuum model that includes effects of elastic interaction and phase segregation. He showed how the different patterns form depending on the relative strength of various material parameters. He also discussed the effects of prepatterning on the final structure.

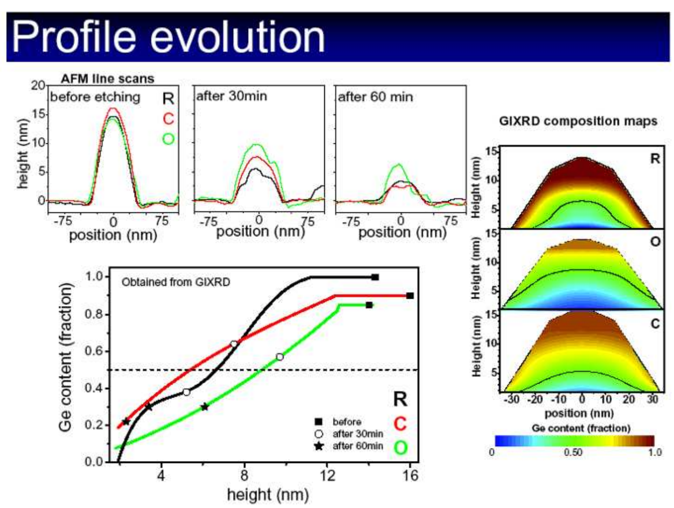

Figure 4.7: The morphological and compositional evolution of SiGe quantum dots, according to Medeiros-Ribeiro.

Gilberto Medeiros-Ribeiro. The thermodynamics of the composition of self-assembled quantum dots was the focus of this talk, which began with a presentation of experimental results showing detailed compositions maps of quantum dots before and after annealing [12]. The results indicated there was a noticeable difference in the compositional maps. This led to considerable discussion as to the mechanism causing the difference since several people argued that bulk diffusion should be quite small in such systems. This experimental result points directly to the need for strong interactions between experimentalists, theorists, and simulators in order to unravel all of the mechanisms of film growth.

Vitaly Shchukin. The topic of this presentation was the importance of nanofaceting and heteroepitaxy in III-V type systems with special emphasis on electronic device manufacturing. [13] He spoke about alloy phase segregation on vicinal surfaces and discussed experimental results that show high index samples give rise to lateral composition modulation.

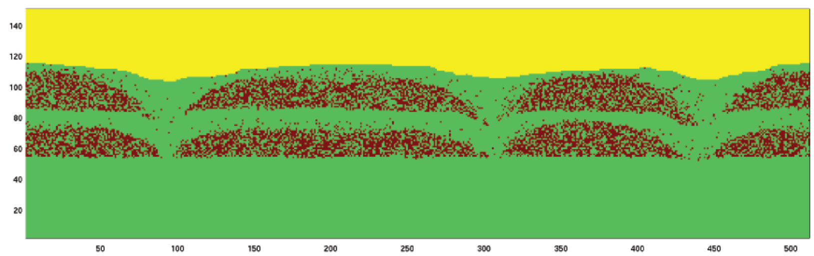

Figure 4.8: Simulation of stacked quantum dots from Arvind Baskaran's presentation

Arvind Baskaran. This talk was concerned with the simulation of heteroepitaxial growth using kinetic Monte Carlo. Much of the talk focused on efficient numerical methods based on the multigrid and the expanding region methods. He also presented results showing that surface segregation can lead to Stranski-Krastinov growth, as has been suggested by Cullis et al[3] and Tu and Tersoff[1]. Arvind's talk was joint work with Tim Schulze, Giovanni Russo, Jason Devita, and Peter Smereka (workshop participants). Two pertinent references for this material are [3] and [4].

Robert Kohn. Professor Kohn spoke on a variational model of faceted film evolution. He described the mathematical framework of gradient descent with respect to the H^{-1} norm [16].. The numerical implementation of such evolution equations was outlined, especially those schemes that are consistent with the gradient descent form of the equations. Finally, Professor Kohn described self similar solutions of this equation and sketched the proof of stability.

Zbig Wasilewski. The effect of defects on the fabrication of a new type of quantum well infrared GaAs/AlGaAs photodetector was discussed in this talk [17, 18]. The source of the defects was not completely understood, but evidence suggested that the defects were not threading dislocations, but maybe the result of contamination. This work shows the importance of challenging commonly held expectations in film growth, and look to other considerations to explain observed phenomena.

Ya Hong Xie. Professor Xie spoke on the dependence of surface roughening on the sign of the strain in Si-Ge systems [19]. They found that the more tensile the Si layer the smoother the resulting film, in contrast to the behavior of compressively stressed films. This result was one of the first of its kind to show that existing models, which assumed symmetry in the role of strain, were incomplete.

Giovanni Russo. Professor Russo outlined an efficient numerical technique for computing displacement fields in elastically strained thin films. The method he described was based on two ideas, the first was an artificial boundary condition which allows one to include the semi-infinite substrate[3]. The second was a multigrid method that can handle complex domains and yet take advantage of the underlying Cartesian structure[4].

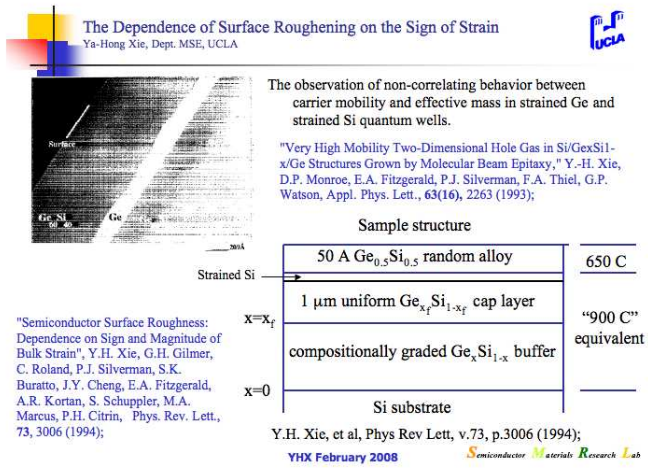

Figure 4.9: A slide from the talk by Ya Hong Xie that shows experimental evidence for a sign dependence on mismatch induced roughening.

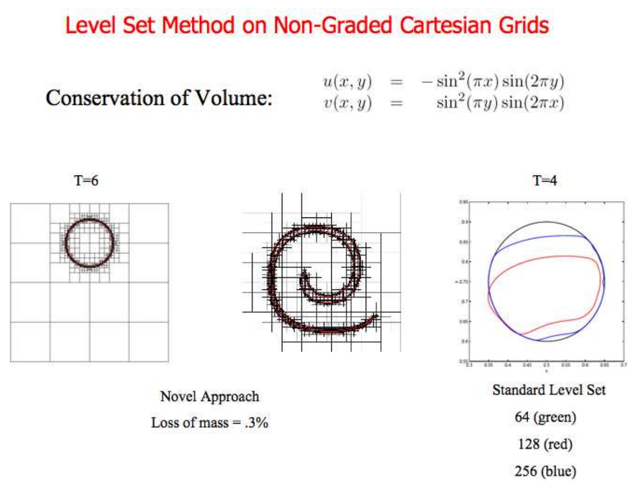

Figure 4.10: A slide from Frederic Gibou's talk showing a nongraded adaptive cartesion grid used for the test problem of simple advection.

Frederic Gibou. A new approach to solving partial differential equations on non-graded Cartesian grids was described by Gibou [20]. Non-graded Cartesian grids are those that allow an arbitrary level of refinement between regions. They have many advantages in terms of construction and computational efficiency. The talk concluded with several applications including crystal growth.

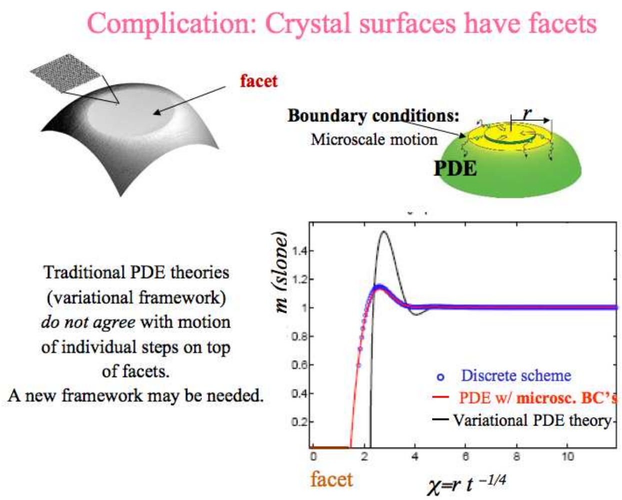

Figure 4.11: A slide from the talk of Dionisios Margetis

Dionisios Margetis. In this talk, Professor Margetis described work in which a continuum model was formulated for step motion in the presence of a facet. The main result is that microscale effects, which enter the PDE solutions via boundary conditions at facets, can affect the surface profiles macroscopically. This consideration aims at enabling predictions for the stability of nanostructures. More details can be found in Ref. [21].

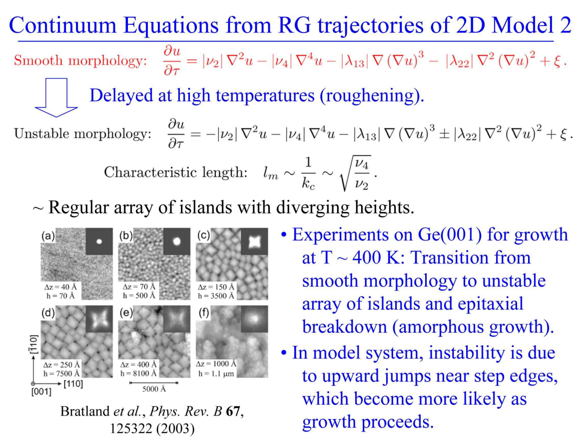

Figure 4.12: A summary slide from the presentation of Christoph Haselwandter

Christoph Haselwandter. This talk was concerned with the development of partial differential equations (PDE) that provide a coarse-grained description of various discrete stochastic processes. [26] Starting with the master equation of a discrete process, he outlined how one could systematically derive a PDE. The asymptotic behavior of the resulting PDE was analyzed using a renormalization group (RG) approach. This results in a set of ordinary differential equations that show the effective behavior as the system evolves.

Kristen Fichthorn. In this talk, Professor Fichthorn described algorithms to improve the computational speed when simulating film growth using atomistic scale methods. A new approach, termed the connector model, was presented that provides a systematic approach of accounting for many body interactions. This framework was used to study hut formation of Al on Al (110) in which two, three and higher particle interactions all have comparable interactions. Also discussed was an approach based on accelerated molecular dynamics that temporally coarse-grained the fast adatom motion resulting in a more efficient algorithm. Pertinent references for this talk include Refs. [22, 23].

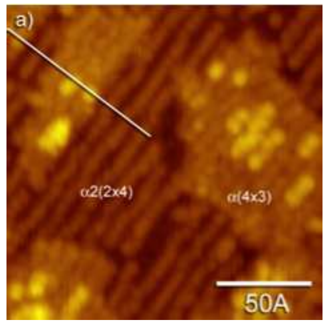

Figure 4.13: A figure from the talk of Jessica Bickel. It shows STM image of surface coexistence of $\alpha2(2\times4)$ and $\alpha(4\times3)$ reconstructions in h ∼1.7ML Sb/GaAs(001).

Jessica Bickel. The role of strain in the surface reconstructions of III-V alloys was discussed in this talk. It was shown that in InGaAs, atomic strain due to the placement of cations induces a surface dimer ordering in the $\alpha2(2\times4)$ reconstruction which is not seen in the InAs and GaAs systems. [25]. She also showed that in the GaAsSb system, lattice relaxation at step edges results in a surface coexistence of two reconstructions with the surface reconstruction coupled to the surface morphology. This was based on joint work with workshop participants Norman Modine and Joanna Mirecki Millunchick.

Axel Voigt and Dong-Hee Yeon. There were two separate talks on the phase field crystal model. In this approach, one starts with classical density functional theory and derives a model that temporally coarse-grained. The resulting phase field model requires finer that atomistic resolution in space but has the advantage of modeling on much longer time scales. As a consequence this formulation can simulate a wide range of phenomena such as elastic and plastic deformation, solidification, and grain growth. The speakers outlined both the basic ideas and the current state-of-the-art. See [11] for more details and background information.

Michael Tringides. Professor Tringides presented results in which High Resolution Electron Diffraction was used to study the growth of Lead on Silicon (111) [27]. The issue was to understand the narrow height distribution of the Lead islands. Depending on growth conditions, islands of heights 5,7, or 9 were observed. The evidence suggests that this is the result of quantum size effects, thus pointing to other mechanisms for self assembly of nanostructures.

Mark Goorsky. An entirely different technique for stacking dissimilar materials was discussed in this presentation. The basic idea was to transfer one layer to another by implanting hydrogen into the semiconductor and anneal to form blisters and induce exfoliation. [28] These blisters grow and ultimately fracture the surface and allow for placing the thin film onto a new handling wafer. While this talk was not strictly concerned with issues in heteroepitaxy, it did bring up issues relevant to defect formation and propagation.

Christian Ratsch and Xiaobin Niu. In this talk a level set formulation for island dynamics was presented. In this approach the island boundaries are iso-contours of a continuous function (the level set function). The strain and adatom fields are found by solving partial differential equations that are coupled to the islands through the level set function. Models for attachment, detachment, and nucleation are incorporated to yield the motion of island boundaries. A particular intriguing feature of this method is the fact the computational

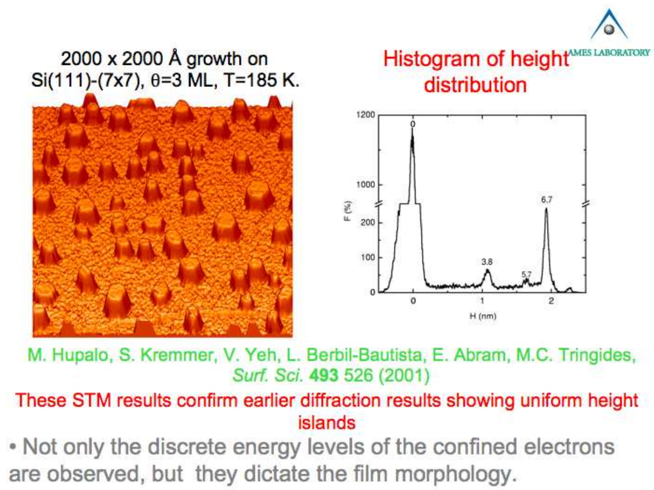

Figure 4.14: A slide from the talk of Michael Tringides that demonstrates quantum size effects in the growth of Lead on Si(111) films.

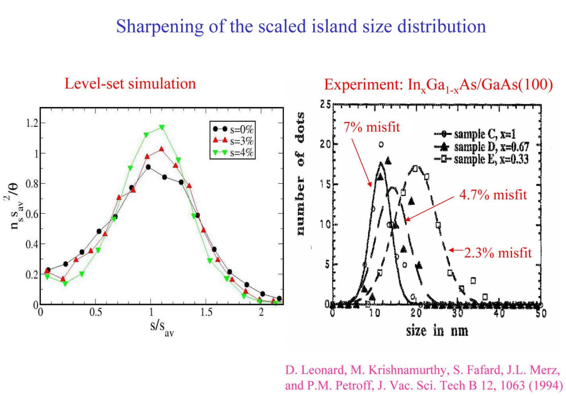

Figure 4.15: A slide from Christian Ratsch's talk

timestep can be chosen orders of magnitude larger than the timestep of typical atomic motion (diffusion). Therefore, it is possible to do the (expensive) calculation of the entire strain field at every computational timestep. Computed island size distribution functions are in good agreement with experiments. Some of the material presented can be found in Ref. [29]. The work presented was joint work with the workshop participants Ya-Hong Xie and Peter Smereka.

Outcome of the Meeting

As mentioned before, we believe that many of the outstanding problems in understanding heteroepitaxial growth can only be solved in tandem, between experimental work and modeling and computations. One immediate challenge that is well known to everyone in the community (and is often very frustrating) is the fact that experimentalists and theorist look at a problem from very different perspectives, and almost "speak a different language". It was therefore one of the main goals of this workshop to help break down this barrier, and help facilitate interactions between theorists and experimentalists. We believe that we succeeded in this respect.

The schedule was of the workshop was organized in a way that theoretical and experimental talks alternated. Most sessions were mixed. We also provided lots of time during and between talks, for many questions, and plenty of discussion. Therefore, we believe (and are supported by the feedback we got) that the environment of this workshop fostered the interactions between theorists and experimentalists. As an example, Bob Kohn (a mathematician) and Tom Tiedje (an experimentalist), who did not know each other prior to the workshop, engaged each other in long discussions during their respective talks, and for long periods of time during some of the "free time". Mike Tringides commented that he enjoyed the extensive discussions he had with Ya-Hong Xie.

Another important outcome of this conference was that some new collaborations have been formed, and that many previous collaborations got strengthened because of this workshop. Some examples of this are the following: Dionisios Margetis (Maryland) established relationships and potential collaborations with Vivek Shenoy (Brown) and Henrique Versieux (Courant, NYU). He also made contact with M. Tringides and his experiments, and expects to develop further communication with him. Moreover, he recently started a collaboration with Matthias Scheffler (FHI Berlin), and this workshop gave him a chance to strengthen this collaboration. Christian Ratsch has recently started a collaboration with Tim Schulze, comparing fast KMC schemes with levelset method. This workshop gave them a chance to deepen this collaboration, and in fact include some new aspects that have been incorporated in their first joint publication. Ratsch is also collaborating with Peter Smereka and Frederic Gibou. These 3 recently submitted a joint proposal. They plan to combine the levelset method (as developed by Ratsch and co-workers) with the efficient strain solver of Smereka and Russo, and with efficient and elegant numerical schemes to accommodate a mixed boundary condition for the diffusion equation, as proposed by Gibou. Meeting at this workshop gave them an opportunity to discuss in more detail their planed joined future work.

We also want to point out that not only the more senior participants of the workshop gave talks, but several talks were made by more junior people. For example, A. Baskaran, J. Bickel, and X. Niu are currently graduate students. C. Haselwandter and D.H. Yeon are a post-docs whereas D. Margetis and F. Gibou are assistant professors. Such exposure is important. As an example, Xioabin Niu got a chance to present some of his Ph.D. work. He is now considered for a postdoctoral position by Kristen Fichthorn, who also attended this workshop. Jessica Bickel, a student of Joanna Mirecki Millunchick, was urged to apply to the Summer School on Surface and Nanoscale Materials to be held in Spain in May 2008 and organized by Matthias Scheffler and Kristen Fichthorn. Bickel is currently a finalist for the Young Research Prize.

List of Participants

Baskaran, Arvind (University of Michigan)
Bickel, Jessica (University of Michigan)
Chen, Hui-Chen (University of Michigan)
Drucker, Jeff (Arizona State University)

Evans, James (Iowa State University)
Fichthorn, Kristen (Pennsylvania State University)
Gibou, Frederic (University of California, Santa Barbara)
Goorsky, Mark (University of California, Los Angeles)
Gray, Jennifer (University of Pittsburgh)
Haselwandter, Christoph (MIT)
Hull, Robert (Univerisity of Virginia)
Kohn, Robert (New York University)
Lu, Wei (University of Michigan)
Margetis, Dionisios (University of Maryland)
Medeiros-Ribeiro, Gilberto (Laboratorio Nacional de Luz Sincrotron)
Mirecki-Millunchick, Joanna (University of Michigan)
Modine, Normand (Sandia National Lab)
Niu, Xiaobin (University of California, Los Angeles)
Placidi, Ernesto (University of Rome Tor Vergata)
Ratsch, Christian (University of California, Los Angeles)
Russo, Giovanni (Universita' di Catania)
Scheffler, Matthias (Fritz Haber Institute)
Schulze, Tim (University of Tennessee)
Shchukin, Vitaly (VI Systems GmbH and Technical Unversity of Berlin)
Shenoy, Vivek (Brown University)
Smereka, Peter (University of Michigan)
Tersoff, Jerry (IBM)
Tiedje, Thomas (University of British Columbia)
Tringides, M.C. (Iowa State University Ames Laboratory)
Versieux, Henrique (New York University)
Voigt, Axel (Techniche Universitat Dresden)
Wasilewski, Zbig (National Research Council of Canada)
Wessels, Bruce (Northwestern University)
Wu, Jia-Hung (University of Michigan)
Xie, Ya-Hong (University of California, Los Angeles)
Yeon, Dong-Hee (University of Michigan)

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Chapter 5

Special Structures in Riemannian Geometry (08w5039)

Feb 17 - Feb 22, 2008

Organizer(s): Gordon Craig (McMaster University/ Bishop's University), Spiro Karigiannis (University of Oxford), Naichung Conan Leung (Chinese University of Hong Kong), Maung Min-Oo (McMaster University), Shing-Tung Yau (Harvard University)

Overview of the Field

Special structures often arise naturally in Riemannian geometry. They are usually given by the existence of globally defined tensors satisfying some (usually elliptic, almost always non-linear) partial differential equations.

One important type of structure is a special curvature condition on the Riemannian metric itself. The most important class of such structures is that of constant Ricci-curvature, or Einstein metrics. Such metrics are often the best candidates for the role of canonical metrics on manifolds, and thus play a very important role in topology. They have also long been a subject of intense interest in theoretical physics, initially in general relativity but more recently in superstring theories as well. Other typical examples in this setting are constant scalar curvature metrics, conformally flat metrics, and others. (The two best survey volumes on Einstein manifolds are [Bes] and [LeW].)

Sometimes a Riemannian manifold admits a globally defined tensor which is parallel with respect to the induced Levi-Civita connection. In this case the Riemannian holonomy reduces. For instance, a manifold admits a parallel almost complex structure if and only if it is a Kahler manifold. Manifolds with special holonomy give examples of Einstein metrics. Calabi-Yau, hyperKahler, G_2, and $Spin(7)$ manifolds are always Ricci-flat, while quaternionic-Kahler manifolds are positive Einstein. The special holonomy condition is a first-order reduction of the second-order Einstein condition. (See [Joy1] for background on Riemannian holonomy.)

Another example of special structures are those isometrically immersed submanifolds which themselves satisfy some non-linear condition on their second fundamental forms, such as minimal submanifolds, CMC (constant mean curvature) submanifolds, or more complicated fully non-linear relations among the eigenvalues of the second fundamental form. The notion of a calibration on a Riemannian manifold fits into this category. The associated calibrated submanifolds are always minimizing, although this is a reduction to a first order equation, similar to the special holonomy condition. ([Joy2] is a good source on calibrated manifolds and their relation to special holonomy.) The interesting calibrations seem to be in one-to-one correspondence with the special holonomies, a relationship which is still not fully understood.

Finally, vector bundles over Riemannian manifolds can admit connections with special properties. An important example is that of Yang-Mills connections, of which anti-self dual connections are a special case.

Many of the most spectacular results in low-dimensional topology and geometry from the last twenty years has have arisen via the study of these gauge theories. Recently, analogues of anti-self dual instantons in the context of G_2 and $Spin(7)$ geometry have been discovered, the Donaldson-Thomas connections. Much work remains to be done in this area.

It is always of interest to find explicit examples of special structures, and usually easier to do so on non-compact manifolds. Often, we can even specify the asymptotic behaviour of such a structure. For the cases of exceptional holonomy, for example, there are several explicit examples of such metrics of cohomogeneity one on non-compact manifolds, due to Bryant, Salamon, and the physicists Gibbons-Page-Pope, and many others([Joy1]). It would be interesting to find explicit examples of higher cohomogeneity. In the case of general Einstein metrics, the work of Graham-Lee and Anderson(see the survey article [And1],) among others, has clarified the structure of Einstein metrics which are asymptotic (in a precise sense) to real hyperbolic space. Biquard has extended some of the existence and uniqueness results to the case of Einstein metrics which are asymptotic to other rank one symmetric spaces([Biq]), but there remain many interesting questions. Explicit constructions of calibrated submanifolds have been found by Harvey-Lawson, Bryant, Joyce, and many others(c.f. [Joy2]). These also tend to have high degrees of symmetry, reducing the complexity of the equations to something which is exactly solvable. The anti-self-dual connections on $\mathbb{R}^4$ were completely classified by Atiyah-Drinfeld-Hitchin-Manin and there has also been more recent work by Hurtubise and others for the cases of $S^k \times \mathbb{R}^{4-k}$.

On compact manifolds, the elliptic, fully non-linear partial differential equations which characterize such special structures are much more difficult to solve. Usually the best we can hope for are non-constructive existence results involving very hard analysis. For instance, Yau's solution of the Calabi conjecture to prove the existence of Ricci-flat Kahler metrics on compact Kahler manifolds with trivial canonical bundle([Yau]). The existence of compact examples of G_2 and $Spin(7)$ manifolds was first shown by Joyce([Joy1]). A general theorem similar to the Calabi-Yau theorem for classifying which 7 or 8 dimensional manifolds admit such Ricci-flat metrics is still missing. In fact, there are not even any obstructions in dimensions greater than 4 to manifolds admitting ordinary Einstein metrics([LeW]).

Manifolds with special holonomy exhibit the phenomenon of mirror symmetry, which is better understood in the hyperKahler and Calabi-Yau cases, but which for the exceptional cases is at present still mysterious. It is also expected (Strominger-Yau-Zaslow, Gukov-Yau-Zaslow) that understanding mirror symmetry will involve studying the moduli spaces of calibrated submanifolds that these manifolds possess, as well as the moduli spaces of ASD connections or their exceptional holonomy analogues. It seems that at least in some cases, these three categories of 'special structures' are all interrelated in some way whose precise formulation is still far from clear.

Another important aspect is the role of spinors and Dirac operators in these settings. Spin geometry seems to be natural for describing many of these structures. For example, the Ricci-flat manifolds that have special holonomy admit parallel spinors, but there also exist classes of Einstein metrics which have a form of 'weak' holonomy, and admit non-trivial Killing spinors. Similarly there exist characterizations of minimal or CMC submanifolds in certain cases using spinors.

Finally, it is important to note that all of these problems involve similar analytic issues. The partial differential equations are all elliptic, often with similar types of non-linearity. Many techniques used for minimal or CMC surfaces, for example, have also been applied to Yamabe metrics, and then to Einstein metrics (such as gluing techniques or understanding of the structure of spaces of conformally compact Einstein metrics; compare for example the gluing constructions in [Kap], [MPU] and [And2].) Differential geometers are finding more and more connections between these research areas all the time. Therefore it is vital to bring together researchers from the individual areas who up to now may not be familiar with the techniques and results from the other areas.

Objectives of the Workshop

Our main goal was to foster new research collaborations by bringing together mathematicians studying special metrics and their special submanifolds with those working in the area of gauge theory to promote cross-fertilization of their different techniques and approaches. Specifically we hoped that many analytic techniques which have been useful in each individual area should prove to be applicable to the other area as well. These research groups have not worked together enough, and through this workshop we hoped to encourage more interaction.

Additionally, most of these special geometric structures play a central role in general relativity and superstring theories. We hoped that by bringing in some physicists, as well as the participation of mathematical physicists, there would be a further opportunities for discussion and collaboration. Theoretical physics has proven time and again to dictate many of the directions of research in differential geometry and global analysis.

It was very important for us that the event be a workshop, and not just a conference. Our hope was that there would be a significant number of collaborations arising from the workshop. To this end, we arranged the schedule so that there would be a fair number of lectures, but also a large amount of open time, with the specific goal of encouraging informal discussions during this time. In the lectures, experts gave talks discussing their recent research, thereby allowing participants working in other fields to get an idea of the state of the given disciplines. Our hope was that these lectures would serve as the launching points for the informal discussions. We also organised a problem session, allowing experts to share the main open problems in their fields with colleagues.

Additionally, we made an effort to invite a significant number of young researchers, both graduate students and recent Ph.D.s, to the meeting in order that they could benefit from contact with more senior scholars.

Overview of meeting

As we hoped, there were a large number of informal discussions, encouraged both by our scheduling large blocks of open time in between talks and by the excellent facilities at BIRS. Of course, it is in the nature of informal discussion that we don't have any records of them.

As for the talks, here are the abstracts, in alphabetical order by speaker surname:

Speaker: **Michael Anderson** (SUNY Stony Brook)
Title: "Spaces of Einstein metrics on bounded domains"

Abstract: There are two natural classes of Einstein metrics on bounded domains. (I) metrics which extend smoothly to the boundary, and (II) complete metrics which conformally extend to the boundary, (conformally compact metrics). We will discuss similarities and differences on the structure of these spaces of Einstein metrics, in particular in regard to the "natural" boundary value problems.

Speaker: **Adrian Butscher** (Stanford University)
Title: "Gluing Constructions for Constant Mean Curvature Surfaces"

Abstract: I will review the now classical Kapouleas gluing construction for CMC surfaces in Euclidean space and present some results and work in progress concerning the extensions of this theory to general ambient manifolds. An important feature which emerges is that the ambient Riemannian curvature seems to play a significant role in the existence of such surfaces; and exploiting this, it seems possible to construct examples of CMC surfaces having properties very different from their Euclidean analogues.

Speaker: **Benoit Charbonneau** (Duke University)
Title: "Existence of periodic instantons"

Abstract: Yang–Mills instantons on $S^1 \times \mathbb{R}^3$ (often called calorons) are in correspondence, via the Nahm transform, to solutions to Nahm's equations on the circle. In joint work with Jacques Hurtubise, we completed Nye and Singer's proof of this Nahm transform correspondence.

We also proved that the solutions on the circle are in correspondence, by a twistor transform, to certain classes of vector bundles on an associated twistor space. Those correspondence allow us to compute the moduli space of these objects, settling some very natural existence questions.

Speaker: **Andrew Dancer** (Jesus College, University of Oxford)
Title: "Symplectic versus hyperKähler geometry"

Abstract: We look at symplectic constructions such as cutting and implosion and investigate their analogues in hyperKähler geometry.

Speaker: **Robin Graham** (University of Washington)
Title: "The ambient metric beyond the obstruction in even dimensions"

Abstract: The ambient metric construction in conformal geometry will be reviewed, and also the equivalent formal construction of asymptotically hyperbolic Poincaré-Einstein metrics. A modification of the construction in even dimensions will be described which results in a family of smooth infinite order generalized ambient and Poincaré metrics. The generalized ambient metrics can be used to extend conformal invariant theory to all orders in even dimensions. This is joint work with Kengo Hirachi.

Speaker: **Marco Gualtieri** (Massachusetts Institute of Technology)
Title: "Constructions of generalized Kähler structures"

Abstract: I will describe a construction of generalized Kähler structures on holomorphic Poisson manifolds, which uses the concept of a holomorphic Poisson module. I will also describe some properties of the resulting generalized Kähler metric, which is a Riemannian metric admitting two different Hermitian complex structures.

Speaker: **Sergei Gukov** (University of California, Santa Barbara)
Title: "Deformations of Hyper-Kähler Metrics and Affine Hecke Algebras"

Abstract: I will explain how studying deformations of hyper-Kähler metrics on complex coadjoint orbits can provide a simple geometric explanation of certain deep results in representation theory, including categorification of the affine Hecke algebra. This talk is based on a joint work with Edward Witten.

Speaker: **Mark Haskins** (Imperial College London)
Title: "Gluing constructions of special Lagrangians"

Abstract: We describe joint work with Nicos Kapouleas that constructs infinitely many special Lagrangian cones whose link is an orientable surface of genus 4 or of any odd genus. These are the first special Lagrangian cones with links that are surfaces of genus greater than one. We use a geometric PDE 'gluing' method. Time permitting, we will sketch higher dimensional generalisations of these gluing constructions.

Speaker: **Marianty Ionel** (University of Toledo)
Title: "Austere submanifolds of dimension 4"

Abstract: An austere submanifold has the property that its second fundamental form in any normal direction has its eigenvalues symmetrically arranged around zero. The class of austere submanifolds was first introduced by Harvey and Lawson in 1982. The main motivation was their result showing that the conormal bundle of an austere submanifold in $\mathbb{R}^n$ is a special Lagrangian submanifold of $\mathbb{R}^{2n}$. The austere submanifolds of dimension 3 in Euclidean space were classified by R. Bryant. In this talk I will present some results towards a classification of austere submanifolds of dimension 4 in Euclidean space. Depending on the type of the second fundamental form, we get both non-existence results as well as new examples of austere submanifolds. This is joint work with Thomas Ivey.

Speaker: **Jim Isenberg** (University of Oregon)
Title: "Constructing solutions of the Einstein constraint equations"

Abstract: The first step in finding a spacetime solution to the Einstein gravitational field equations via the inital value formulation is to construct initial data which satisfy the Einstein constraint equations. There are three ways of carrying out this construction which have been found to be useful: the conformal and conformal thin sandwich methods, the gluing techniques, and the quasi-spherical approaches. We describe each of these, we discuss their advantages and disadvantages, we outline some of their recent successful applications, and we present some of the outstanding questions remaining to be solved from each of these perspectives.

Speaker: **John Loftin** (Rutgers University Newark)
Title: "Affine Hermitian-Einstein Metrics"

Abstract: A special affine manifold is a manifold with an atlas whose gluing maps are all constant affine maps in $\mathbb{R}^n$ preserving the standard volume form. The tangent bundle to a special affine manifold has the structure of a complex manifold with holomorphic volume form. We develop a theory of stable bundles and affine Hermitian-Einstein metrics for flat vector bundles over a special affine manifold. The proof involves adapting the proof of Uhlenbeck-Yau on the existence of Hermitian-Einstein metrics on Kähler manifolds, and the extension of this theorem by Li-Yau to the non-Kähler complex case of Gauduchon metrics. Our definition of stability involves only flat vector subbundles (and not singular subsheaves), and so is simpler than the complex case in some places.

Speaker: **Dan Pollack** (University of Washington)
Title: "Singular Yamabe metrics and Space-times with Positive Cosmological Constant"

Abstract: The Delaunay (aka Fowler) metrics form the asymptotic models for isolated singularities of conformally flat metrics of constant positive scalar curvature metrics. The Kottler-Schwarzschild-de Sitter space-times form the model family for black hole solutions of the Einstein field equations with a positive cosmological constant. We will show why the former coincides with the time-symmetric initial data sets for that latter. We will then demonstrate how to construct large families of initial data sets for the vacuum Einstein equations with positive cosmological constant which contain exactly Delaunay ends; these are non-trivial initial data sets whose ends coincide with those for the Kottler-Schwarzschild-de Sitter metrics. From the purely Riemannian geometric point of view, this produces complete, constant positive scalar curvature metrics with exact Delaunay ends which are not globally Delaunay. The construction provided applies to more general situations where the asymptotic geometry may have non-spherical cross-sections consisting of Einstein metrics with positive scalar curvature. This is joint work with Piotr Chrusciel.

Speaker: **Martin Reiris** (Massachusetts Institute of Technology)
Title: "The Einstein flow and the Yamabe invariant of three-manifolds"

Abstract: We will explain how the long time evolution of the Einstein flow is related with the Yamabe invariant of three-manifolds. We will set the main conjectures and elaborate on partial results. The discussion will be based on the importance of volume in General Relativity.

Speaker: **Andrew Swann** (University of Southern Denmark)
Title: "Intrinsic Torsion and Curvature"

Abstract: For a Riemannian G-structure a large part of the Riemannian curvature is determined by the intrinsic torsion. Representation theoretic techniques lead to a number of constraints and relations and in many situations much can be gleaned from the exterior algebra. This talk will discuss recent work in this area, including particular results for almost Hermitian and almost quaternion-Hermitian structures.

Speaker: **Christina Tønnesen-Friedman** (Union College)
Title: "Hamiltonian 2-forms in Kähler geometry"

Abstract: Hamiltonian 2-forms, introduced in [1], induce isometric Hamiltonian torus actions and underpin many explicit constructions in Kähler geometry. This talk will take off as a survey and discussion of the techniques developed in [1] and [2]. Some of these techniques have already been applied in subsequent works with my co-authors, but we believe that there are still exciting avenues to take – in particular in the case of higher order Hamiltonian 2-forms and, in general, higher order toric bundles.

[1] "Hamiltonian 2-forms in Kähler geometry, I General Theory"; V. Apostolov, D.M.J. Calderbank, and P. Gauduchon; *J. Diff. Geom.*, **73** (2006), 359–412.

[2] "Hamiltonian 2-forms in Kähler geometry, II Global Classifications"; V. Apostolov, D.M.J. Calderbank, P. Gauduchon , and C. Tønnesen-Friedman; *J. Diff. Geom.*, **68** (2004), 277–345.

Speaker: **Guofang Wei** (University of California at Santa Barbara)
Title: "Comparison Geometry for the Smooth Metric Measure Spaces"

Abstract: For a smooth metric measure space $(M, g, e^{-f}dvol_g)$ the Bakry-Emery Ricci tensor is a natural generalization of the classical Ricci tensor. It occurs naturally in the study of diffusion processes, Ricci flow, the Sobolev inequality, warped products, and conformal geometry. We prove mean curvature and volume comparison results when the ∞-Bakry-Emery Ricci tensor is bounded from below and f is bounded or $\partial_r f$ is bounded from below, generalizing the classical ones (i.e. when f is constant.) This leads to extensions of many theorems for Ricci curvature bounded below to the Bakry-Emery Ricci tensor. In particular, we give extensions of all of the major comparison theorems when f is bounded. Simple examples show the bound on f is necessary for these results. This is a joint work with W. Wylie.

Here is a list of the problems suggested during the open problem sessions:

First Problem: Conan Leung asked the following question related to G_2-manifolds: Let L be a special Lagrangian submanifold of $\mathbb{C}^3$, or more generally of some Calabi-Yau 3-fold X. Does there exist a G_2-manifold M^7 such that there exists a map $\pi : M^7 \longrightarrow \mathbb{C}^3$ with the property that $\pi^{-1}(x) = S^1$ if x is a point not lying on L, and $\pi^{-1}(x)$ is a point if $x \in L$. The motivation for this problem is that given a Calabi-Yau 3-fold X, closed string theories predict a duality between $X^6 \times \mathbb{R}^{3,1}$ and $X \times S^1 \times \mathbb{R}^{3,1}$, and $X^3 \times S^1$ admits a canonical G_2-structure. In the case of an open string theory, the string boundary in the Calabi-Yau manifold X would lie in a special Lagrangian submanifold L, which explains the above condition on π.

Second Problem: Benoit Charbonneau presented a conjecture of Jardim. Consider an anti-self dual(ASD) connection A on a $SU(n)$-bundle E over $\mathbb{R}^2 \times T^2$. Jardim has conjectured that if F_A, the curvature of A, is in L^2, then F_A must be $O(r^{-2})$ or perhaps even $o(r^{-2})$.

The motivation for this arises from the Nahm transform

$$\mathcal{N} : \mathcal{M}_{ASD/QD}\left(\mathbb{R}^2 \times T^2\right) \longrightarrow \mathcal{M}_{SHP}\left(T^2\right),$$

where $\mathcal{M}_{ASD/QD}\left(\mathbb{R}^2 \times T^2\right)$ is the space of ASD connections with quadratic curvature decay on $\mathbb{R}^2 \times T^2$, and $\mathcal{M}_{SHP}\left(T^2\right)$ is the space of singular Hitchin pairs on T^2. It turns out that if you start off with A with non-trivial limit at infinity and satisfying $F_A = O(r^{-1-\epsilon})$ for small ϵ, then $\mathcal{N}(A)$ exists, and $\mathcal{N}^{-1}(\mathcal{N}(A))$ has quadratic decay. Moreover, being L^2 is the usual condition on curvature for the domain of the Nahm transform on $\mathbb{R}^4$ and other spaces.

Third Problem: Spiro Karigiannis suggested the following problem: let M be a compact spin manifold, and let $\not{D}$ be its associated Dirac operator. Do there exist natural flows $\frac{\partial s}{\partial t} = \not{D}s$? This is a spinor analogue of the heat flow on forms. This question is motivated by the fact that such a flow exists on manifolds with special holonomy, with $\not{D}$ being replaced by another first-order operator which is similar to a Dirac operator. Since this operator is first-order, there is no maximum principle available to understand this flow. Studying the above flow on spin manifolds could allow a better understanding of these more complicated flows on manifolds with special holonomy. Here is an example of one of these flows. It gives an impression of how complicated they are, and of how they resemble Dirac operators. Consider $\mathbb{R}^7$ with its standard G_2 structure, and let φ be the associated parallel three-form. Let $\psi = *\varphi$. Then an oriented three-dimensional submanifold $L \subset \mathbb{R}^7$ is associative iff the restriction of φ to L is the volume form of L. This is in turn equivalent (up to a change of orientation) to the vanishing of χ on L, where $\chi \in \Lambda^3(T^*) \otimes T$ is given by $\chi^i_{klm} = g^{ij}\psi_{jklm}$. Now consider an embedded 3-dimensional submanifold $f : U \longrightarrow \mathbb{R}^7$ where $U \subset \mathbb{R}^3$. Then we obtain the flow

$$\frac{\partial f}{\partial t} = \chi\left(\frac{\partial f}{\partial u_1}, \frac{\partial f}{\partial u_2}, \frac{\partial f}{\partial u_3}\right).$$

(Note that $\chi|_{T(f(U))}$ is a normal vector field to the submanifold.) In the special case where $L^3 = \Sigma^2 \times \mathbb{R} \subset \mathbb{C}^3 \times \mathbb{R}$, the L^3 is associative iff $\Sigma^2 \subset \mathbb{C}^3$ is a complex curve. Then we can simplify the embedding above to $h : V \longrightarrow \mathbb{C}^3$, where $V \subset R^2$, and the corresponding flow also reduces to

$$\frac{\partial h}{\partial t} = \Omega\left(\frac{\partial h}{\partial u_1}, \frac{\partial h}{\partial u_2}\right),$$

where $\Omega = dz^1 \wedge dz^2 \wedge dz^3$ is the canonical holomorphic volume form on $\mathbb{C}^3$. If we write out $h(u_1, u_2) = (z^1(u_1, u_2), z^2(u_1, u_2), z^3(u_1, u_2))$, then in coordinates the flow looks like:

$$\frac{\partial z^k}{\partial t} = (\text{Cauchy Riemann Eq}) \cdot (\text{Other first-order terms}).$$

Fourth Problem: The next question was proposed by Dan Pollack. Consider complete metrics of the form

$$g = u^{\frac{4}{n-2}}(t, \theta)(dt^2 + d\theta^2)$$

on $\mathbb{R} \times S^{n-1}$ with constant scalar curvature $R(g) = n(n-1)$. It follows from the work of Gidas, Ni and Nirenberg, that all solutions are independent of θ and that $u = u(t)$ must satisfy an explicit ODE. This ODE has a one-parameter family of positive periodic solutions which corresponds to the set of ”Delaunay metrics”. Now, say that we replace S^{n-1} in the warped product above by some other Einstein manifold M^{n-1} with scalar curvature $R(g) = (n-1)(n-2)$, and we look once again the periodic solutions to the associated ODE. They are of course the same. What can we say about the possibly more general set of complete metrics with $R(g) = n(n-1)$ which are conformal to this product metric? For example, what is the dimension of the space of solutions? In the case of Delaunay metrics, as the parameter ϵ tends to 0, the metric degenerates to the incomplete metric on the sphere minus two antipodal points. In the case of more general M, the degenerations may be more complicated due to the topology.

One of the reasons for studying Delaunay metrics is that the ends of the complete constant scalar curvature metrics constructed by Schoen, Mazzeo and Pacard, and Mazzeo, Pollack and Uhlenbeck on $S^n - \{p_1, ..., p_n\}$ are asymptotically Delaunay. Moreover this behavior must hold in general about any isolated non-removable singular point (at least in the conformally flat case, or in low dimensions). It would be very interesting to know whether there are manifolds with constant positive scalar curvature whose ends are (asymptotically or exactly) generalized Delaunay, in the above sense, but are not diffeomorphic to the product manifold. The construction of such an example would probably involve a gluing argument.

Fifth Problem: The session ended with a conjecture from Robin Graham: suppose $I(g)$ is a scalar conformal invariant of weight $-n$ on an n-dimensional manifold, with n even. Further suppose that $I(g)$ can be written as a linear combination of contractions of covariant derivatives of the Ricci tensor. Then $I(g) \equiv 0$.

The background for this conjecture is the following: let $I(g)$ be a scalar Riemannian invariant which is a linear combination of contractions of covariant derivatives of the curvature tensor. If for every conformal rescaling $\hat{g} = \Omega^2 g$, we have

$$I(\hat{g}) = \Omega^w I(g),$$

then we say that I is a conformal invariant of weight w. For example, W, the Weyl tensor, is a pointwise conformal invariant, so its norm squared $\|W\|^2$ is a conformal invariant of weight -4. If $w = -n$, then

$$\int_M I(g)\, dV$$

is a global conformal invariant, since the scaling of the volume form under a conformal transformation is cancelled out by that of $I(g)$.

Outcome of the Meeting

As we mentioned above, there were many informal discussions, in particular a great deal of exchanges between experts in different fields. Although it is too early to say exactly what collaborations will arise from this workshop, we are confident that the meeting allowed a significant cross-fertilization between fields, and in particular allowed several of the younger participants to advance their research programme thanks to the advice of more senior scholars.

All of the participants were very enthusiastic about BIRS: the natural setting, the infrastructure and the warmth, hospitality and professionalism of the staff were all very much appreciated.

List of Participants

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Chapter 6

Quantum Chaos: Routes to RMT Statistics and Beyond (08w5091)

Feb 24 - Feb 29, 2008

Organizer(s): Gregory Berkolaiko (Texas Agricultural and Mechanical University), Uzy Smilansky (Weizmann Institute of Science, Israel), Robert Whitney (Institut Laue-Langevin, Grenoble)

Summary

The objective of this workshop was to bring together applied mathematicians and theoretical physicists in order to address the following question: *what happens to chaos theory when it meets quantum mechanics?* We worked to understand why the statistical properties of quantum systems whose classical analogues are chaotic are often well-described by random matrix theory (RMT). We then looked beyond RMT, to systems which are now known to have non-RMT properties.

These issues are at the centre of the field known as *quantum chaos*, and large steps have recently been taken towards addressing them in theoretical physics. This in turn is leading to a burst of activity in applied mathematics, both in terms of trying to put the physicists' theories on a mathematically rigorous footing, and in terms of addressing a whole family of interesting combinatorial problems that arise naturally in the context of those theories. Thus the objective of the workshop was to review the state of this rapidly changing field and to stimulate future progress.

Overview of quantum chaos

Chaos theory and Newton's laws. Chaos theory has revolutionized our view of how complexity emerges from very simple rules. Simple rules can generate fractals, such as the Mandelbrot set, which are sets that have detailed and complex structure at whatever scale one looks at them. One aspect of the fractals' complexity is their non-integer dimension.

A marble rolling around in a bath-tub obeys Newton's laws of motion ($F = ma$, etc). It has been shown that these simple rules can cause the marble to follow a chaotic path. Chaotic paths are exponentially sensitive to the initial position and velocity of the marble. Suppose we record the path followed by a marble in the bath with a given initial position and velocity. We can then take the marble and try to make it repeat the same path. If we get the initial position and velocity *exactly* the same as before, then the marble will follow the same path. However tiny differences in the initial position or velocity will result in the marble diverging *exponentially* from the original path. This exponential sensitivity to initial conditions (which we never known exactly) makes specific predictions impossible. It means, that even the smallest of variations in the initial data makes the outcome random. Thus much of chaos theory is dedicated to predicting the probabilities of an event occurring; much like weather forecasts which say there will be a 10% probability of rain next Tuesday (the weather is a good example of a chaotic system).

Whether the paths of a marble in a bath tub are chaotic or not depends on the shape of the bath. For example, in a circular bath-tub, the motion is regular. However, for many other simple shapes, the paths turn out to be chaotic. In fact, the chaoticity is *generic* in the sense that small perturbations to the shape of a chaotic domain do not make paths regular, while arbitrarily small perturbations to a regular domain can make the paths chaotic. We stress that when talking about "chaotic domain" we do not mean that the shape of the domain is irregular. Rather, "chaotic" refers to the properties of the resulting motion.

Fractals can also arise in the context of marble's motion in a bath-tub. A simple example is the following. Imagine having two plug-holes; one at each end of the bath. We mark a line in the bottom of the bath, place the marble somewhere on that line and flick it in a certain direction. The marble will roll around in the bath and eventually fall into one of the plug-holes. Suppose you plot a graph, putting the initial position on the line on one axis and the direction the marble was flicked on the other axis. We then color *red* all points on the graph for which the marble ends up falling in one plug-hole, and color *blue* all points for which the marble falls into the other plug-hole. The plot we end up with will be a fractal, it will have structure on all scales. The large scales are for initial conditions which correspond to the marble falling quickly into a plug-hole. The small scale structures are for initial conditions which correspond to the marble rolling around for a long time without falling into a plug-hole.

Wave-particle duality. Quantum mechanics is the theory of wave-particle duality; it tells us that all objects actually move as waves. The wave spreads out and goes to many places at once. If part of that wave crosses another part (perhaps after reflecting off something) then the two parts of the wave interfere (like light interferes in the well-known Young's double-slit experiment). The probability to find the particle in the places where destructive interference (cancellations) occurs is then greatly reduced compared to the places of no interference and espesially places where two waves enhance each other. Waves can also go around and through small obstacles because they rarely have a well-defined position or energy. The position-momentum uncertainty principle means waves can diffract around obstacles, while the energy-time uncertainty principle means they can tunnel through obstacles.

Remarkably, waves often look like particles if one looks at them on a scale much greater than their wavelength. Visible light (a wave with a wavelength of a few hundred nanometres) reflects off a surface in the same way as a marble would bounce off that surface (i.e. the angle of reflection equals the angle of incidence). This is why Newton's laws work well for relatively heavy objects, whose wavelength is too tiny to ever be observed. Even a marble is heavy enough so that when moving with a velocity of just a few mm per second, it has a wavelength of about 10^{-37}m, which is much too small to be ever observed. However it does not work for lightweight (or massless) objects such as electrons, photons, etc, whose wavelength is often observable. Photons have wavelengths from hundreds of metres (radiowaves) to a few hundred nanometres (visible light) and smaller (x-rays, gamma-rays, etc); electrons in semiconductors can have wavelengths of a few tens of nanometres. Quantum mechanics tells us that we will clearly see all of the wave properties (interference, tunneling, etc) of any object, if we are able to zoom in to the scale of that object's de Broglie wavelength.

Chaos theory meeting quantum mechanics. Suppose the marble in the bath-tub is replaced by an electron or photon in a bath-shaped container. What happens when we start studying the behavior of the particle at the scale of its wavelength? At this scale the particles move much like ripples do (imagine filling the bath-tub with water and making small ripples on the surface with your finger). So one *cannot* use Newton's laws of motion to predict the particle's behavior.

The first thing one notices is that the ripples are smooth at scales much smaller than their wavelength. This means that in quantum mechanics there are no fractals. One can have a plot that looks like a fractal at large scales, but once zoomed in to less than a wavelength the plot becomes smooth and featureless. The next thing one notices is that the structure at the scale of a wavelength is very complicated and unlike that predicted by applying chaos theory to Newton's laws. The central topic of our workshop was the study of this complicated structure at the scale of a wavelength. We are particularly interested in the statistical properties of these complicated structures (much like the example of the weather forecast we gave above).

Level-statistics in quantum chaos. In Newtonian mechanics steady-states, when the system is at rest, and periodic motion are of particular importance. In quantum mechanics, the concept of periodicity gives rise to the discrete energy levels (*eigenvalues*) of a quantum system. Indeed the name "quantum mechanics" itself is coming from the observation that atoms absorb and emit energy (typically light) in discrete portions, "quanta", and, therefore, only certain values of energy are allowed. The set of allowed energies is called the *spectrum* of a system. The *eigenfunctions* (the steady-states of the quantum system) describe the quantum system when it is in a state with a particular (allowed) energy. A quantum system is fully specified by its spectrum and the set of all eigenfunctions. Thus the *quantum chaos* can be broadly described as a study of generic properties of the eigenvalues and eigenfunctions of a quantum system which, in the limit of short wavelength, exhibits many features associated with chaotic motion.

One of the central themes of quantum chaos research has been to explain the so-called Bohigas-Giannoni-Schmit conjecture [8], made in 1984. The conjecture (based on numerical simulations of simple quantum chaotic systems) was that the statistical distribution of energy-levels in simple chaotic systems is the same as that of a suitably defined random matrix. Random matrix theory (RMT) was developed in the 1960s and has been well-studied and well-used since then; it is used to find the statistical properties of the eigenvalues of matrices whose elements are randomly distributed. The question is why a wave in a chaotically-shaped container should follow random matrix predictions.

In 1971, Gutzwiller [11] had pointed out that the Green's function of a wave in a chaotically-shaped container could be neatly expressed in terms of the stationary-phase points of a Feynman path integral. These stationary-phase points correspond to periodic classical orbits, and so the Green function's phase is given by the action of the periodic orbit. Berry ([6], 1985) then pointed out that some information about the statistical distribution of energy-levels could be obtained by considering only the diagonal terms in a double sum over such periodic orbits, and then assuming ergodicity of the classical orbits. The result of this procedure coincided with the RMT prediction for correlations between distantly spaced energy-levels (i.e. correlations between level n and level $(n+m)$ when $n, m \gg 1$), but not otherwise. Berry argued that for nearby levels (such as nearest neighbors) one could not neglect off-diagonal terms in the double sum. However despite a lot of effort, almost no progress was made in dealing with these off-diagonal terms for the next 15 years.

In 2002, Sieber and Richter [22, 21] managed to perform the first semiclassical calculation of a likely candidate for the next-order term (in an expansion in powers of the inverse distance between the distantly spaced levels). They considered the contributions from pairs of periodic orbits that consisted of two loops and that would nearly cross themselves in the phase space. If viewed from afar, the two orbits would look identical. However, they would traverse one of the loops in the same direction and the other in the opposite directions. Sieber and Richter showed that the contribution of such orbits coincided with the next term in the expansion of the RMT prediction. After this crucial step had been achieved, many researchers worked on extending these ideas to include higher orders in the expansion. Pairs of orbits constructed out of growning numbers of joined loops were considered. Finally, Müller, Heusler, Braun, Haake and Altland [17, 18] generalized the procedure to arbitrary numbers of loops, and managed to reproduce RMT to all orders in the expansion. This required the solution of a difficult problem in combinatorics since the number of ways one could connect loops to form a pair of orbits grows rapidly with the number of loops. Resummation tricks were then used to address statistics beyond the regime of convergence of the expansion, again finding RMT results. Thus in 2007 [19] they showed that this semiclassical procedure explained the Bohigas-Giannoni-Schmit conjecture.

One of the central themes of this workshop was to understand this result. It is important to appreciate that, while reproducing the conjectured result, the method is not mathematically rigorous yet. First, as for any term-by-term expansion, convergence question must be addressed. Gutzwiller trace formula is convergent only in a weak sense, so changing the order of terms can lead to differing results. A related question is whether all pairs of orbits have been accounted for (the answer is negative) and whether it is possible to extend the scheme to account for the missing terms (this question is largely open). Finally, as mentioned by N.H. Abel,[1] resummation techniques should be treated with utmost care. Answering the above questions would enable one to clearly define the regimes of validity of the method, and thereby find systems which do not have behavior which coincides with RMT.

An alternative approach to the question of eigenvalue statistics has been the super-symmetry method. In this context, it was initially use to deal with difficult averaging procedures in diordered systems. More recently it has been of great help in dealing with averages over random matrices and averages over energy in

[1] who wrote, rather strongly, that "the divergent series are the invention of the devil, and it is a shame to base on them any demonstration whatsoever".

quantum graphs. In super-symmetry one makes two copies of the system, describing one with usual (commuting) variables and the other with Grassman (anti-commuting) variables. Averaging in the "doubled-system" is much easier than averaging in each one individually (due to cancellation of a "difficult" denominator). However one is then forced to work with commuting and anti-commuting variables at the same time. Much progress [18] has been achieved by comparing supersymmetric expansions with periodic-orbit ones.

Quantum ergodicity and scarring. As has been mentioned above, the quantum eigenfunctions at the scales smaller than the wavelength look smooth a featureless. Zooming out to the scales comparable to the wavelength one will see complicated structure of the eigenstate. What happens when you zoom out even more? In most cases you will see a picture which is almost uniformly gray.

Coming back to the marble analogy, imagine that the marble is covered in ink and is leaving a trace on the bath-tub. If it is left to roll around for a long time (with no loss of energy due friction), it will cover the accessible areas of the bath-tub with ink. If we smudge the ink a little bit, the lines will disappear and the bath-tub will be painted with ink in a smooth way. Some areas will be darker than the others, indicating that the marble is more likely to be found there at any given time.

It is quite remarkable that if we compute the high energy eigenfunctions of the (quantized) bath-tub, and smudge the intensities of the eigenfunctions a little bit, the result will look remarkably like the classical ink picture described above. This is actually a mathematical result known as Quantum Ergodicity Theorem. It is easy to understand: when marble is quantized, it is still following pretty much the same probability laws as the Newtonian marble.

However, some exceptions to the above picture have been observed by Heller [13]. Every now and then we will come across an eigenfunction which is not uniformly gray but which has a few lines of darkness standing out of the sea of light-gray. These few lines are much like the traces of the marble ball, but a one which is going on a periodic trajectory, repeatedly painting with ink the same path. Such special eigenstates were called *scars*, since they are assumed to be traces of classical periodic orbits in the quantized picture. There are many interesting questions associated with scars, for example, whether scarred eigenstates happen infinitely often, or do they stop when the energy gets higher. To put it more bluntly, do the scars really exist? Are there any systems where there are no scars (this is called Quantum Unique Ergodicity)? Can the intensity of the scar can be arbitrarily high, compared with the intensity of the background light gray?

Recently many of these questions have been resolved mathematically, at least in toy model settings (see *Quantum Maps* section below). The workshop provided a forum for mathematicians to explain the powerful new tools involved in answering these questions and for physicists to propose more difficult questions to tackle next.

Quantum chaos in open systems. Particles can escape from an open quantum system (similarly to the marble rolling around in the bath-tub and falling into a plug-hole). Quantum mechanically such systems are not described by eigenfunctions. Instead one must think in terms of the scattering matrix. If a particle is injected with given initial conditions, the scattering matrix tells us how it will escape the system.

For many years it was thought that such systems were also well-described by random-matrix theory. However it has now become clear that as one makes the wavelength smaller, the behavior changes. Many interference effects become exponentially suppressed and as a result the scattering from such a system becomes increasingly classical. The parameter which controls this cross-over from RMT behavior to "almost classical" behavior is the Ehrenfest time. Crucially the "almost classical" behavior is *universal*, by which we mean that it is not sensitive to the details of the system that one studies (unlike other previously observed deviations from RMT).

A second theme of the workshop was to discuss these results, and try to understand the "almost classical" behavior. In particular we asked which properties would be "classical" and which would not. It is hoped that a better understanding of this non-RMT behavior could lead to the discovery of other universal but non-RMT behaviors.

More rigorous approaches to quantum chaos

Mathematically rigorous progress on the questions of quantum chaos has been hampered by the difficulty of the questions themselves. While a lot is known about lower-lying eignevalues, quantum chaos focuses more on the small but generic variations of the high-lying eigenvalues from the well-known Weyl asymptotics. The prime tool with which one can study high eigenvalues is the trace formula, but it is only weakly convergent, involves an exponentially growing number of periodic orbits and only approximate for most systems. Due to these difficulties, two toy models have arisen: quantum maps and quantum graph.

Quantum Maps. Exactly as classical maps supply minimal models of chaotic dynamics with only one degree of freedom, quantum maps provide the simplest models for quantal manifestation of classical chaos and for the quantum-classical correspondence in this context. Simplified trace formulae help analyze the divergencies occuring in the standard trace formulae. One can probe the long time versus the short wave-length limits of the time propagators. Numerical computation is also much facilitated by the fact that, the quantum evolution is realized as the iteration of a $N \times N$ unitary matrix with N being inversely proportional to the Planck's constant. Thus the short wave-length limit corresponds to the large sizes of the propagator matrix.

The procedures associating a unitary operator to a discrete map were initially developed in [7, 12, 2]. Among the quantized maps are the Arnold "cat" maps (linear maps of the torus) and the baker's map both of which has been favourite quantized models for the mathematical studies of quantum chaos. Among notable recent successes were explanation of the violation of the Bohigas-Giannoni-Schmit conjecture on cat maps by the presense of quantum symmetries without classical analogue (Hecke symmetries) [14], quantum unique ergodicity of the Hecke eigenstates [16], construction of scarred eigenstates of weight $1/2$ [9] and use of enthropy bounds to prove impossibility of strong scars [1]. The workshop gave an opportunity to learn more about these recent breakthroughs and discuss open problems (for example, whether generic perturbation of a cat map is quantum uniquely ergodic) and possible approaches to their solution.

Quantum graphs. The introduction of quantum graphs as models for quantum chaos in 1997 [15] made it possible to study a broad range of quantum chaotic phenomena in a mathematically rigorous setting. Among the advantages of graphs is the exact trace formula and ease of numerical computations. Furthermore, while quantized maps often have non-universal statistics (successfully explained by the presence of symmetries), the graphs with rationally independent edge lengths typically follow the random matrix predictions.

Among other things, the use of quantum graphs as models have been successful in explaining the cancellation of the off-diagonal contributions in the presence of the magnetic field [5], construction of strong scars [20], application of super-symmetric methods to BGS conjecture without a disorder averaging [10], exploration [4] of the potential mathematical problems with the Müller et al enumeration scheme [17] and studies of the nodal domain count [3]. More recently, a framework for connecting the trace formula on quantum graphs with the similar results on discrete graphs (Ihara zeta function) was proposed in [23]. During workshop we had an opportunity to interact with the specialists in the study of Ihara zeta function as well as hear an update on its connection to the study of quantum graphs.

Conclusions

The workshops was successfull not only in letting researchers report on their latest progress, but also in bringing together people of differing traditions (mathematicians vs physicists). The underlying motive for many discussions during the workshop was to highlight the assumptions made in physical derivations and discuss prospects for their mathematical justifications. The workshop also provided a forum for the young researchers to introduce themselves to the quantum chaos community.

Participants contributions

- Michael Aizenman (Princeton, USA)
  On dynamical localization in the linear and non-linear setup

  Preprint– arXiv:0809.3436
  We consider the spectral and dynamical properties of quantum systems of n particles on the lattice Z^d, of arbitrary dimension, with a Hamiltonian which in addition to the kinetic term includes a random potential with iid values at the lattice sites and a finite-range interaction. Two basic parameters of the model are the strength of the disorder and the strength of the interparticle interaction. It is established here that for all n there are regimes of high disorder, and/or weak enough interactions, for which the

system exhibits spectral and dynamical localization. The localization is expressed through bounds on the transition amplitudes, which are uniform in time and decay exponentially in the Hausdorff distance in the configuration space. The results are derived through the analysis of fractional moments of the n-particle Green function, and related bounds on the eigenfunction correlators.

- Ram Band (Weizmann, Israel)
  Spectral quantum graphs and beyond: a construction method

  Preprint– arXiv:0711.3416
  The purpose of the present manuscript is to collect known results and present some new ones relating to nodal domains on graphs, with special emphasize on nodal counts. Several methods for counting nodal domains will be presented, and their relevance as a tool in spectral analysis will be discussed.

- Harold Baranger (Duke, USA)
  Interactions in Quantum Dots: Does the RMT/Random-Wave Model Work?

  Preprint– arXiv:0707.1620
  We obtain analytic formulae for the spacing between conductance peaks in the Coulomb blockade regime, based on the universal Hamiltonian model of quantum dots. New random matrix theory results are developed in order to treat correlations between two and three consecutive spacings in the energy level spectrum. These are generalizations of the Wigner surmise for the probability distribution of single level spacing. The analytic formulae are shown to be in good agreement with numerical evaluation.

- Gregory Berkolaiko (Texas A&M University, USA)
  Form-factor expansion: some forgotten orbits

  Preprint– arXiv:nlin/0604025
  The form factor of a quantum graph is a function measuring correlations within the spectrum of the graph. It can be expressed as a double sum over the periodic orbits on the graph. We propose a scheme which allows one to evaluate the periodic orbit sum for a special family of graphs and thus to recover the expression for the form factor predicted by the Random Matrix Theory. The scheme, although producing the expected answer, undercounts orbits of a certain structure, raising doubts about an analogous summation recently proposed for quantum billiards.

- Eugene Bolomolny (Paris-Sud, France)
  Spectral statistics of a pseudo-integrable map: the general case

- Oriol Bohigas (Paris-Sud, France)
  Some extreme value statistics problems in RMT

  Preprint– arXiv:0808.2434
  In random matrix theory (RMT), the Tracy-Widom (TW) distribution describes the behavior of the largest eigenvalue. We consider here two models in which TW undergoes transformations. In the first one disorder is introduced in the Gaussian ensembles by superimposing an external source of randomness. A competition between TW and a normal (Gaussian) distribution results, depending on the spreading of the disorder. The second model consists in removing at random a fraction of (correlated) eigenvalues of a random matrix. The usual formalism of Fredholm determinants extends naturally. A continuous transition from TW to the Weilbull distribution, characteristc of extreme values of an uncorrelated sequence, is obtained.

- Jens Bolte (Royal Holloway, UK)
  Semiclassical theory of mesoscopic transport with spin-orbit interactions

  Preprint– arXiv:0704.2702
  We investigate the influence of spin-orbit interaction on ballistic transport through chaotic cavities by using semiclassical methods. Our approach is based on the Landauer formalism and the Fisher-Lee relations, appropriately generalized to spin-orbit interaction, and a semiclassical representation of Green functions. We calculate conductance coefficients by exploiting ergodicity and mixing of suitably combined classical spin-orbit dynamics, and making use of the Sieber-Richter method and its most

recent extensions. That way we obtain weak anti-localization and confirm previous results obtained in the symplectic ensemble of Random Matrix Theory.

- Petr Braun (Essen, Germany)
  Transport through chaotic cavities: RMT reproduced from semiclassics

  Preprint– arXiv:cond-mat/0610560
  We describe a semiclassical method to calculate universal transport properties of chaotic cavities. While the energy-averaged conductance turns out governed by pairs of entrance-to-exit trajectories, the conductance variance, shot noise and other related quantities require trajectory quadruplets; simple diagrammatic rules allow to find the contributions of these pairs and quadruplets. Both pure symmetry classes and the crossover due to an external magnetic field are considered.

- Piet Brouwer (Cornell, USA)
  Anderson localization from classical trajectories

  Preprint– arXiv:0802.0976
  We show that Anderson localization in quasi-one dimensional conductors with ballistic electron dynamics, such as an array of ballistic chaotic cavities connected via ballistic contacts, can be understood in terms of classical electron trajectories only. At large length scales, an exponential proliferation of trajectories of nearly identical classical action generates an abundance of interference terms, which eventually leads to a suppression of transport coefficients. We quantitatively describe this mechanism in two different ways: the explicit description of transition probabilities in terms of interfering trajectories, and an hierarchical integration over fluctuations in the classical phase space of the array cavities.

- John Chalker (Oxford, UK)
  Network models for the quantum Hall effect and its generalisations

  Preprint– arXiv:cond-mat/0201080
  We consider network models for localisation problems belonging to symmetry class C. This symmetry class arises in a description of the dynamics of quasiparticles for disordered spin-singlet superconductors which have a Bogoliubov - de Gennes Hamiltonian that is invariant under spin rotations but not under time-reversal. Our models include but also generalise the one studied previously in the context of the spin quantum Hall effect. For these systems we express the disorder-averaged conductance and density of states in terms of sums over certain classical random walks, which are self-avoiding and have attractive interactions. A transition between localised and extended phases of the quantum system maps in this way to a similar transition for the classical walks. In the case of the spin quantum Hall effect, the classical walks are the hulls of percolation clusters, and our approach provides an alternative derivation of a mapping first established by Gruzberg, Read and Ludwig, ! Phys. Rev. Lett. 82, 4254 (1999).

- Doron Cohen (Ben-Gurion, Israel)
  The conductance of small mesoscopic disordered rings: resistor network analysis of novel sparse and textured matrices

  Preprint– arXiv:0712.0439
  The calculation of the conductance of disordered rings requires a theory that goes beyond the Kubo-Drude formulation. Assuming ”mesoscopic” circumstances the analysis of the electro-driven transitions show similarities with a percolation problem in energy space. We argue that the texture and the sparsity of the perturbation matrix dictate the value of the conductance, and study its dependence on the disorder strength, ranging from the ballistic to the Anderson localization regime. An improved sparse random matrix model is introduced to captures the essential ingredients of the problem, and leads to a generalized variable range hopping picture.

- Sven Gnutzman (Nottingham, UK)
  Quantum Graphs: From Periodic Orbits to Phase Disorder

  Preprint– arXiv:nlin/0508009
  We investigate the spectral properties of chaotic quantum graphs. We demonstrate that the ‘energy’–

average over the spectrum of individual graphs can be traded for the functional average over a supersymmetric non–linear σ–model action. This proves that spectral correlations of individual quantum graphs behave according to the predictions of Wigner–Dyson random matrix theory. We explore the stability of the universal random matrix behavior with regard to perturbations, and discuss the crossover between different types of symmetries.

- Fritz Haake (Essen, Germany)
  Generating function for level correlations in chaotic systems, semiclassical evaluation
  Preprint– arXiv:nlin/0610053
  We present a semiclassical explanation of the so-called Bohigas-Giannoni-Schmit conjecture which asserts universality of spectral fluctuations in chaotic dynamics. We work with a generating function whose semiclassical limit is determined by quadruplets of sets of periodic orbits. The asymptotic expansions of both the non-oscillatory and the oscillatory part of the universal spectral correlator are obtained. Borel summation of the series reproduces the exact correlator of random-matrix theory.

- Jon Harrison (Baylor, USA)
  The effect of spin in the spectral statistics of quantum graphs
  Preprint– arXiv:0712.0869
  The article surveys quantization schemes for metric graphs with spin. Typically quantum graphs are defined with the Laplace or Schrodinger operator which describe particles whose intrinsic angular momentum (spin) is zero. However, in many applications, for example modeling an electron (which has spin-1/2) on a network of thin wires, it is necessary to consider operators which allow spin-orbit interaction. The article presents a review of quantization schemes for graphs with three such Hamiltonian operators, the Dirac, Pauli and Rashba Hamiltonians. Comparing results for the trace formula, spectral statistics and spin-orbit localization on quantum graphs with spin Hamiltonians.

- Philippe Jacquod (Arizona, USA)
  Quantum chaos in mesoscopic superconductivity
  Preprint– arXiv:0712.2252
  We investigate the conductance through and the spectrum of ballistic chaotic quantum dots attached to two s-wave superconductors, as a function of the phase difference ϕ between the two order parameters. A combination of analytical techniques – random matrix theory, Nazarov's circuit theory and the trajectory-based semiclassical theory – allows us to explore the quantum-to-classical crossover in detail. When the superconductors are not phase-biased, $\phi = 0$, we recover known results that the spectrum of the quantum dot exhibits an excitation gap, while the conductance across two normal leads carrying $N_{\rm N}$ channels and connected to the dot via tunnel contacts of transparency $\Gamma_{\rm N}$ is $\propto \Gamma_{\rm N}^2 N_{\rm N}$. In contrast, when $\phi = \pi$, the excitation gap closes and the conductance becomes $G \propto \Gamma_{\rm N} N_{\rm N}$ in the universal regime. For $\Gamma_{\rm N} \ll 1$, we observe an order-of-magnitude enhancement of the conduct! ance towards $G \propto N_{\rm N}$ in the short-wavelength limit. We relate this enhancement to resonant tunneling through a macroscopic number of levels close to the Fermi energy. Our predictions are corroborated by numerical simulations.

- Dubi Kelmer (IAS Princeton, USA)
  Scarring on invariant manifolds for quantum maps on the torus
  Preprint– arXiv:0801.2493
  We previously introduced a family of symplectic maps of the torus whose quantization exhibits scarring on invariant co-isotropic submanifolds. The purpose of this note is to show that in contrast to other examples, where failure of Quantum Unique Ergodicity is attributed to high multiplicities in the spectrum, for these examples the spectrum is (generically) simple.

- Massimo Macucci (Pisa, Italy)
  Shot Noise Suppression in Single and Multiple Chaotic Cavities: the Role of Diffraction, Disorder and Symmetries
  Preprint– arXiv:0802.4329
  We report the results of an analysis, based on a simple quantum-mechanical model, of shot noise

suppression in a structure containing cascaded tunneling barriers. Our results exhibit a behavior that is in sharp contrast with existing semiclassical models predicting a limit of 1/3 for the Fano factor as the number of barriers is increased. The origin of this discrepancy is investigated and attributed to the presence of localization on the length scale of the mean free path, as a consequence of 1-dimensional disorder, while no localization appears in common semiclassical models. The results of the quantum model seem to be compatible with the experimentally observed behavior.

- Sebastian Müller (Cambridge, UK)
  Constructing a sigma model from semiclassics

  Preprint– arXiv:nlin/0610053
  We present a semiclassical explanation of the so-called Bohigas-Giannoni-Schmit conjecture which asserts universality of spectral fluctuations in chaotic dynamics. We work with a generating function whose semiclassical limit is determined by quadruplets of sets of periodic orbits. The asymptotic expansions of both the non-oscillatory and the oscillatory part of the universal spectral correlator are obtained. Borel summation of the series reproduces the exact correlator of random-matrix theory.

- Taro Nagao (Nagoya, Japan)
  Parametric Spectral Correlation with Spin 1/2

  Preprint– arXiv:0707.2276
  The spectral correlation of a chaotic system with spin 1/2 is universally described by the GSE (Gaussian Symplectic Ensemble) of random matrices in the semiclassical limit. In semiclassical theory, the spectral form factor is expressed in terms of the periodic orbits and the spin state is simulated by the uniform distribution on a sphere. In this paper, instead of the uniform distribution, we introduce Brownian motion on a sphere to yield the parametric motion of the energy levels. As a result, the small time expansion of the form factor is obtained and found to be in agreement with the prediction of parametric random matrices in the transition within the GSE universality class. Moreover, by starting the Brownian motion from a point distribution on the sphere, we gradually increase the effect of the spin and calculate the form factor describing the transition from the GOE (Gaussian Orthogonal Ensemble) class to the GSE class.

- Shinsuke Nishigaki (Shimane, Japan)
  Critical level statistics and QCD phase transition

- Stephane Nonnenmacher (Saclay, France)
  Quantum symbolic dynamics

  Preprint– arXiv:0805.4137
  The subject area referred to as ”wave chaos”, ”quantum chaos” or ”quantum chaology” has been investigated mostly by the theoretical physics community in the last 30 years. The questions it raises have more recently also attracted the attention of mathematicians and mathematical physicists, due to connections with number theory, graph theory, Riemannian, hyperbolic or complex geometry, classical dynamical systems, probability etc. After giving a rough account on ”what is quantum chaos?”, I intend to list some pending questions, some of them having been raised a long time ago, some others more recent.

- Marcel Novaes (Bristol, UK)
  Counting statistics of quantum chaotic cavities from classical action correlations

  Preprint– arXiv:cond-mat/0703803
  We present a trajectory-based semiclassical calculation of the full counting statistics of quantum transport through chaotic cavities, in the regime of many open channels. Our method to obtain the mth moment of the density of transmission eigenvalues requires two correlated sets of m classical trajectories, therefore generalizing previous works on conductance and shot noise. The semiclassical results agree, for all values of m, with the corresponding predictions from random matrix theory.

- Cyril Petitjean (Regensburg, Germany)
  Dephasing in quantum chaotic transport (a semiclassical approach)

Preprint– arXiv:0710.5137

We investigate the effect of dephasing/decoherence on quantum transport through open chaotic ballistic conductors in the semiclassical limit of small Fermi wavelength to system size ratio, $\lambda_F/L << 1$. We use the trajectory-based semiclassical theory to study a two-terminal chaotic dot with decoherence originating from: (i) an external closed quantum chaotic environment, (ii) a classical source of noise, (iii) a voltage probe, i.e. an additional current-conserving terminal. We focus on the pure dephasing regime, where the coupling to the external source of dephasing is so weak that it does not induce energy relaxation. In addition to the universal algebraic suppression of weak localization, we find an exponential suppression of weak-localization $\propto \exp[-\tilde{\tau}/\tau_\phi]$, with the dephasing rate τ_ϕ^{-1}. The parameter $\tilde{\tau}$ depends strongly on the source of dephasing. For a voltage probe, $\tilde{\tau}$ is of order the Ehrenfest time $\propto \ln[L/\lambda_F]$. In contrast, for a chaotic environment or a classical source of noise, it has the correlation length ξ of the coupling/noise potential replacing the Fermi wavelength λ_F. We explicitly show that the Fano factor for shot noise is unaffected by decoherence. We connect these results to earlier works on dephasing due to electron-electron interactions, and numerically confirm our findings.

- Saar Rahav (Maryland, USA)
  The classical limit of quantum transport

  Preprint– arXiv:0705.2337

  Quantum corrections to transport through a chaotic ballistic cavity are known to be universal. The universality not only applies to the magnitude of quantum corrections, but also to their dependence on external parameters, such as the Fermi energy or an applied magnetic field. Here we consider such parameter dependence of quantum transport in a ballistic chaotic cavity in the semiclassical limit obtained by sending Planck's constant to zero without changing the classical dynamics of the open cavity. In this limit quantum corrections are shown to have a universal parametric dependence which is not described by random matrix theory.

- Stefan Rotter (Yale, USA)
  Diffractive paths for weak localization in quantum billiards

  Preprint– arXiv:0709.3210

  We study the weak localization effect in quantum transport through a clean ballistic cavity with regular classical dynamics. We address the question which paths account for the suppression of conductance through a system where disorder and chaos are absent. By exploiting both quantum and semiclassical methods, we unambiguously identify paths that are diffractively backscattered into the cavity (when approaching the lead mouths from the cavity interior) to play a key role. Diffractive scattering couples transmitted and reflected paths and is thus essential to reproduce the weak-localization peak in reflection and the corresponding anti-peak in transmission. A comparison of semiclassical calculations featuring these diffractive paths yields good agreement with full quantum calculations and experimental data. Our theory provides system-specific predictions for the quantum regime of few open lead modes and can be expected to be relevant also for mixed as well as chaotic sys! tems.

- Henning Schomerus (Lancaster, UK)
  Staggered level repulsion for lead-symmetric transport

  Preprint– arXiv:0708.0690

  Quantum systems with discrete symmetries can usually be desymmetrized, but this strategy fails when considering transport in open systems with a symmetry that maps different openings onto each other. We investigate the joint probability density of transmission eigenvalues for such systems in random-matrix theory. In the orthogonal symmetry class we show that the eigenvalue statistics manifests level repulsion between only every second transmission eigenvalue. This finds its natural statistical interpretation as a staggeredsuperposition of two eigenvalue sequences. For a large number of channels, the statistics for a system with a lead-transposing symmetry approaches that of a superposition of two uncorrelated sets of eigenvalues as in systems with a lead-preserving symmetry (which can be desymmetrized). These predictions are confirmed by numerical computations of the transmission-eigenvalue spacing distribution for quantum billiards and for the open kicked rotator.

- Martin Sieber (Bristol, UK)
  Periodic orbit encounters: a mechanism for trajectory correlations

  Preprint– arXiv:0711.4537

  The Wigner time delay of a classically chaotic quantum system can be expressed semiclassically either in terms of pairs of scattering trajectories that enter and leave the system or in terms of the periodic orbits trapped inside the system. We show how these two pictures are related on the semiclassical level. We start from the semiclassical formula with the scattering trajectories and derive from it all terms in the periodic orbit formula for the time delay. The main ingredient in this calculation is a new type of correlation between scattering trajectories which is due to trajectories that approach the trapped periodic orbits closely. The equivalence between the two pictures is also demonstrated by considering correlation functions of the time delay. A corresponding calculation for the conductance gives no periodic orbit contributions in leading order.

- Harold Stark (UC San Diego, USA)
  Poles of Zeta Functions of Graphs and their Covers

- Audrey Terras (UC San Diego, USA)
  What is the Riemann Hypothesis for Zeta Functions of Irregular Graphs?

- Steven Tomsovic (Washington State, USA)
  Extreme statistics of random and quantum chaotic states

  Preprint– arXiv:0708.0176

  An exact analytical description of extreme intensity statistics in complex random states is derived. These states have the statistical properties of the Gaussian and Circular Unitary Ensemble eigenstates of random matrix theory. Although the components are correlated by the normalization constraint, it is still possible to derive compact formulae for all values of the dimensionality N. The maximum intensity result slowly approaches the Gumbel distribution even though the variables are bounded, whereas the minimum intensity result rapidly approaches the Weibull distribution. Since random matrix theory is conjectured to be applicable to chaotic quantum systems, we calculate the extreme eigenfunction statistics for the standard map with parameters at which its classical map is fully chaotic. The statistical behaviors are consistent with the finite-N formulae.

- Denis Ullmo (Paris-Sud, France)
  Residual Coulomb interaction fluctuations in chaotic systems: the boundary, random plane waves, and semiclassical theory.

  Preprint– arXiv:0712.1154

  Experimental progresses in the miniaturisation of electronic devices have made routinely available in the laboratory small electronic systems, on the micron or sub-micron scale, which at low temperature are sufficiently well isolated from their environment to be considered as fully coherent. Some of their most important properties are dominated by the interaction between electrons. Understanding their behaviour therefore requires a description of the interplay between interference effects and interactions. The goal of this review is to address this relatively broad issue, and more specifically to address it from the perspective of the quantum chaos community. I will therefore present some of the concepts developed in the field of quantum chaos which have some application to study many-body effects in mesoscopic and nanoscopic systems. Their implementation is illustrated on a few examples of experimental relevance such as persistent currents, mesoscopic fluctuations of Kondo properties or Coulomb blockade. I will furthermore try to bring out, from the various physical illustrations, some of the specific advantages on more general grounds of the quantum chaos based approach.

- Jiri Vanicek (EPFL, Switzerland)
  Dephasing representation of quantum fidelity

  Preprint– arXiv:quant-ph/0506142

  General semiclassical expression for quantum fidelity (Loschmidt echo) of arbitrary pure and mixed states is derived. It expresses fidelity as an interference sum of dephasing trajectories weighed by the Wigner function of the initial state, and does not require that the initial state be localized in position or momentum. This general dephasing representation is special in that, counterintuitively, all of fidelity decay is due to dephasing and none due to the decay of classical overlaps. Surprising accuracy of the approximation is justified by invoking the shadowing theorem: twice–both for physical perturbations and for numerical errors. It is shown how the general expression reduces to the special forms for position and momentum states and for wave packets localized in position or momentum. The superiority of the general over the specialized forms is explained and supported by numerical tests for wave packets, non-local pure states, and for simple and random mixed states. ! The tests are done in non-universal regimes in mixed phase space where detailed features of fidelity are important. Although semiclassically motivated, present approach is valid for abstract systems with a finite Hilbert basis provided that the discrete Wigner transform is used. This makes the method applicable, via a phase space approach, e. g., to problems of quantum computation.

- Daniel Waltner (Regensburg, Germany)
  Semiclassical approach to quantum decay of open chaotic systems

  Preprint– arXiv:0805.3585

  We address the decay in open chaotic quantum systems and calculate semiclassical corrections to the classical exponential decay. We confirm random matrix predictions and, going beyond, calculate Ehrenfest time effects. To support our results we perform extensive numerical simulations. Within our approach we show that certain (previously unnoticed) pairs of interfering, correlated classical trajectories are of vital importance. They also provide the dynamical mechanism for related phenomena such as photo-ionization and -dissociation, for which we compute cross section correlations. Moreover, these orbits allow us to establish a semiclassical version of the continuity equation.

- Simone Warzel (Princeton, USA)
  On the joint distribution of energy levels for random Schroedinger operators

  Preprint– arXiv:0804.4231

  We consider operators with random potentials on graphs, such as the lattice version of the random Schroedinger operator. The main result is a general bound on the probabilities of simultaneous occurrence of eigenvalues in specified distinct intervals, with the corresponding eigenfunctions being separately localized within prescribed regions. The bound generalizes the Wegner estimate on the density of states. The analysis proceeds through a new multiparameter spectral averaging principle.

- Robert Whitney (Institut Laue-Langevin, Grenoble, France)
  Introduction - Ehrenfest time in scattering problems

  Preprint– arXiv:cond-mat/0512662

  Abstract: We investigate transport properties of quantized chaotic systems in the short wavelength limit. We focus on non-coherent quantities such as the Drude conductance, its sample-to-sample fluctuations, shot-noise and the transmission spectrum, as well as coherent effects such as weak localization. We show how these properties are influenced by the emergence of the Ehrenfest time scale τ_{E}. Expressed in an optimal phase-space basis, the scattering matrix acquires a block-diagonal form as τ_{E} increases, reflecting the splitting of the system into two cavities in parallel, a classical deterministic cavity (with all transmission eigenvalues either 0 or 1) and a quantum mechanical stochastic cavity. This results in the suppression of the Fano factor for shot-noise and the deviation of sample-to-sample conductance fluctuations from their universal value. We further present a semiclassical theory for weak localization which captures non-ergodic phase! -space structures and preserves the unitarity of the theory. Contrarily to our previous claim [Phys. Rev. Lett. 94, 116801 (2005)], we find that the leading off-diagonal contribution to the conductance leads to the exponential suppression of the coherent backscattering peak and of weak localization at finite τ_{E}. This latter finding is substantiated by numerical magnetoconductance calculations.

- Brian Winn (Loughborough, UK)
  Quantum graphs where back-scattering is prohibited

  Preprint– arXiv:0708.0839

  We describe a new class of scattering matrices for quantum graphs in which back-scattering is prohibited. We discuss some properties of quantum graphs with these scattering matrices and explain the advantages and interest in their study. We also provide two methods to build the vertex scattering matrices needed for their construction.

- Martin Zirnbauer (Köln, Germany)
  On the Hubbard-Stratonovich transformation for interacting bosons
  Preprint– arXiv:0801.4960
  We revisit a long standing issue in the theory of disordered electron systems and their effective description by a non-linear sigma model: the hyperbolic Hubbard-Stratonovich (HS) transformation in the bosonic sector. For time-reversal invariant systems without spin this sector is known to have a non-compact orthogonal symmetry O(p,q). There exists an old proposal by Pruisken and Schaefer how to do the HS transformation in an O(p,q) invariant way. Giving a precise formulation of this proposal, we show that the HS integral is a sign-alternating sum of integrals over disjoint domains.

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Chapter 7

Quantum affine Lie algebras, extended affine Lie algebras, and applications (08w5015)

Mar 02 - Mar 07, 2008

Organizer(s): Yun Gao (York University), Naihuan Jing (North Carolina State University), Michael Lau (University of Windsor), Kailash Misra (North Carolina State University)

Introduction

Affine Lie algebras appear in many contexts of mathematics and mathematical physics. They have a Kac-Moody presentation in terms of the Serre relations, as well as a loop presentation in terms of maps from the punctured plane to a finite-dimensional simple Lie algebra. Both of these points of view have proved enormously profitable since their introduction 40 years ago, with applications to numerous areas, including Lie theory, number theory, modular forms, Hopf algebras, algebraic groups, combinatorics, knot invariants, quantum field theory, integrable systems, and statistical mechanics.

More recent work has concentrated on generalizations of affine Lie algebras, especially those involving q-deformations of affine structures and multivariable analogues of affine Lie algebras. Two of the most important such generalizations are quantum affine algebras and extended affine Lie algebras.

Quantum affine algebras are defined via a q-deformation of the Serre relations in the Kac-Moody presentation of affine Lie algebras. They combine the power of the $\mathcal{R}$-matrix of the braided tensor category of representations of a (finite) quantum group with a quantum version of the Knizhnik-Zamolodchikov connection on the bundle of conformal blocks in 2-dimensional WZW conformal field theory.

Extended affine Lie algebras are a multivariable generalization of the loop presentation of affine Lie algebras. They have appeared in the context of toroidal symmetries of higher dimensional quantum field theories, as well as in the solution of integrable hierarchies of soliton equations. Recent work by Allison, Berman, Faulkner, Pianzola, and Neher has given a new perspective on the structure theory of extended affine Lie algebras. The representation theory of extended affine Lie algebras is not yet well understood, but it is expected that a better understanding of these algebras will lead to many applications, as has already been the case in affine and quantum affine theory.

The BIRS meeting brought together 38 of the leading experts in the areas of quantum affine algebras and extended affine Lie algebras. There were 19 invited talks of 45-60 minutes duration, as well as informal presentations and collaborations in smaller groups in the evenings. Some of these interactions occurred spontaneously as a result of questions asked during the invited lectures; others were the result of new and existing projects. The abstracts of the formal lectures appear below, along with some selected comments from participants.

Abstracts of Talks

Speaker: Bruce Allison (University of Victoria)

Title: Construction of graded algebras as loop algebras.

Abstract: I will discuss a general construction of graded algebras as loop algebras, and describe necessary and sufficient conditions for a graded algebra to be obtained in this way. An application of this theory is the construction of centreless cores of extended affine Lie algebras as multiloop algebras. The talk will be based on joint work with S. Berman, A. Pianzola and J. Faulkner.

Speaker: Bojko Bakalov (North Carolina State University)

Title: Non-linear Lie conformal algebras with three generators

Abstract: The notion of a Lie conformal algebra encodes the commutators of quantum fields in a vertex algebra. Starting from a Lie conformal algebra one can construct a vertex algebra such that the commutators of generating fields are linear combinations of the same fields and their derivatives. The notion of a non-linear Lie conformal algebra captures the general case when the commutators of generating fields involve not only linear combinations but (normally-ordered) products. We classify certain non-linear Lie conformal algebras with three generators, which can be viewed as deformations of the affine Lie algebra $\widehat{sl(2)}$. We construct free-field realizations of our algebras extending the Wakimoto realization of $\widehat{sl(2)}$ at the critical level -2, and we compute their Zhu algebras. This is joint work with Alberto De Sole.

Speaker: Georgia Benkart (University of Wisconsin-Madison)

Title: What is a Whittaker Module Anyway?

Abstract: In 1978 Kostant introduced a class of modules for complex semisimple Lie algebras, which he called Whittaker modules because of their connections with Whittaker equations in number theory. Since then, Whittaker modules have been appeared in a variety of different settings. This talk will present a survey of this subject. It will include some of our recent joint work with M. Ondrus and will explain how Whittaker modules can be used to construct simple modules for affine Lie algebras.

Speaker: Vyjayanthi Chari (University of California-Riverside)

Title: Representations of quantum and classical affine algebras.

Abstract: We discuss some recent work which relates the representation theory of quantum affine algebras to classical affine algebras. In particular, we give a definition of Kirillov–Reshetikhin modules associated to non–rectangular weights and give a character formula for these modules.

Speaker: Xueqing Chen (University of Wisconsin-Whitewater)

Title: Root vectors and canonical basis of quantum affine algebra of type $A_2^{(2)}$: Ringel–Hall Algebra Approach

Abstract: An integral PBW basis and a canonical basis of the quantum affine algebra of type $A_2^{(2)}$ recently have been constructed by Akasaka. According to the canonical isomorphism between the positive part of the quantum affine algebra of type $A_2^{(2)}$ and the generic composition algebra of the tame algebra with underlying diagram $\bullet \xrightarrow{(1,4)} \bullet$, we provide an alternative route to obtain all root vectors and the integral PBW basis for the later algebra by using Ringel-Hall algebra approach.

Speaker: Chongying Dong (University of California-Santa Cruz)

Title: Rational vertex operator algebras are finitely generated.

Abstract: We will present a recent result on the generators of vertex operator algebras. The main result is that any vertex operator algebra with finite dimensional Zhu's algebra is finitely generated. In particular, any rational vertex operator algebra is finitely generated. We will also discuss some other related results on generators of vertex operator algebras.

Speaker: Jun Morita (University of Tsukuba)

Title: Words, Tilings and Combinatorics

Abstract: We introduce some combinatorics for words and tilings arising from the associated algebraic structures. Such combinatorics can characterize the patterns of words and the local indistinguishability of tilings. Then we will produce certain new combinatorial invariants using functions and positive real numbers. It might be helpful to give good applications to other related areas. We will try to examine several interesting strings.

Speaker: Eugene Mukhin (Indiana University-Purdue University Indianapolis)

Title: Gaudin model and Schubert Calculus.

Abstract: We show that the representation of the Bethe algebra in a subspace of singular vectors of a given weight in a tensor product of irreducible finite-dimensional gl(N) modules is isomorphic to the coregular representation of the algebra of functions on a suitable intersection of the Schubert varieties. That implies several long standing conjectures: 1) the spectrum of the gl(N) Gaudin model is simple for all real parameters of the model; 2) the intersection of Schubert varieties associated to a normal rational curve and real parameters is transversal; 3) eigenvectors of the Bethe algebra (Bethe vectors) are in one-to-one correspondence with monodromy-free Fuchsian differential operators with specified singular points and exponents.

Speaker: Toshiki Nakashima (Sophia University)

Title: Affine Tropical R and Prehomogeneous Geometric Crystals.

Abstract: We shall define prehomogeneous geometric crystals (PGC) and discuss the properties of isomorphisms between PGC's. We present the sufficient condition for the prehomogeneity of a positive GC, which is given by the connectedness of the crystal ultra-discretized from the positive GC. We shall construct the tropical R-morphisms on some affine PGC's whose ultra-discretizations are limit of perfect crystals and see the properties of the affine tropical R-morphisms.

Speaker: Karl-Hermann Neeb (Darmstadt-Technichal University)

Title: Generalizing toroidal algebras and classifying twists.

Abstract: If M is a smooth manifold and L a simple complex Lie algebra, then the current algebra $C^\infty(M, L)$ is a well-studied object and it is known that its central extensions are parametrized by the space $\Omega^1(M, \mathbb{C})/dC^\infty(M, \mathbb{C})$ which is infinite-dimensional for $\dim M > 1$. Taking covariance with respect to the Lie algebra $\mathcal{V}(M)$ of smooth vector fields on M into account, one is lead to the semidirect product $C^\infty(M, L) \rtimes \mathcal{V}(M)$ and abelian(in general non-central) extension of this Lie algebra. Their classification requires the calculation of cohomology spaces of $\mathcal{V}(M)$ for the action on the quotients $\Omega^p(M, \mathbb{C})/d\Omega^{p-1}(M, \mathbb{C})$. In this talk we report on several aspects of this problem, classification results obtained in joint work with Y. Billig and generalizations to Lie algebras of infinitesimal automorphisms of non-trivial principal bundles.

Speaker: Erhard Neher (University of Ottawa)

Title: Generalizations of extended affine Lie algebras and Lie tori .

Abstract: One of the drawbacks of EALAs is that their definition is somewhat long and technical. Several generalizations of EALAs have been suggested, but the systems of axioms did not get (much) easier. In this talk I will present a new class of Lie algebras, called INV-algebras, which are defined by a simple set of axioms. The class of INV-algebras includes all the previously studied algebras. Every INV-algebra has a centreless core, which turns out to be a so-called ipd-algebra (a generalization of a Lie torus). Conversely, every ipd-algebra arises as the centreless core of an INV-algebra.

Speaker: Arturo Pianzola (University of Alberta)

Title: Descent constructions in infinite dimensional Lie theory.

Abstract: E. Neher has shown that Extended Affine Lie Algebras (EALA) can be ”build up” from Lie tori. This is done, roughly speaking, by taking central extensions of Lie tori and adding suitable ”degree” derivations. On the other hand Lie tori can also be constructed by Galois descent. I will review how (and why) this descent construction takes place, and explain how the descent formalism can be extended to handle the full EALA construction.

Speaker: Alistair Savage (University of Ottawa)

Title: Crystals, Quiver Varieties and Coboundary Categories for Kac-Moody Algebras.

Abstract: Henriques and Kamnitzer have defined a commutor for the category of crystals of a finite dimensional complex reductive Lie algebra, giving it the structure of a coboundary category. Kamnitzer and Tingley then gave an alternative definition of the crystal commutor, using Kashiwara's involution on Verma crystals, that generalizes to the setting of symmetrizable Kac-Moody algebras. In this talk, we will discuss a geometric interpretation of the crystal commutor using quiver varieties. Equipped with this interpretation we show that the commutor endows the category of crystals of a symmetrizable Kac-Moody algebra with the structure of a coboundary category, answering in the affirmative a question of Kamnitzer and Tingley.

Speaker: Anne Schilling (University of California-Davis) and Masato Okado (Osaka University)

Title: Existence of Kirillov-Reshetikhin crystals for nonexceptional types.

Abstract: Using the methods of Kang et al. and recent results on the characters of Kirillov-Reshetikhin modules by Nakajima and Hernandez, the existence of Kirillov-Reshetikhin crystals $B^{r,s}$ is established for all nonexceptional affine types. We also prove that the crystals $B^{r,s}$ of type $B_n^{(1)}$, $D_n^{(1)}$, and $A_{2n-1}^{(2)}$ are isomorphic to recently constructed combinatorial crystals for r not a spin node.

Speaker: Shaobin Tan (Xiamen University)

Title: Twisted Loop Algebras and TKK algebras.

Abstract: Let $\mathcal{A}$ be a commutative associative algebra over the complex field $\mathbb{C}$, and $so(n \geq 3, \mathbb{C})$ be the special orthogonal Lie algebra. We define a Lie algebra $\mathcal{G}_n = \mathcal{G}(E_1, \ldots, E_n) := so(n, \mathbb{C}) \otimes \mathcal{A}$ with a twisted Lie bracket for any fixed elements $E_i \in \mathcal{A}$. When the associative algebra $\mathcal{A}$ is the Laurent polynomial algebra $\mathbb{C}[t_1^{\pm 1}, \ldots, t_\nu^{\pm 1}]$, and $\mathcal{G}_n$ is perfect then $\mathcal{G}_n$ is a $\frac{1}{2}\mathbb{Z}$-graded Lie algebra. We prove that the Lie algebra $\mathcal{G}(t_1, \ldots, t_\nu, 1)$ is isomorphic to a subalgebra of a TKK algebra which gives an A_1 type extended affine Lie algebra. We study the universal central extension $\hat{\mathcal{G}}_n$ and the derivation Lie algebra Der($\mathcal{G}_n$) of $\mathcal{G}_n$. In particular, the Lie algebras for the case $n = 3$ are classified. The finite dimensional representations for the Lie algebras $\mathcal{G}_n$ are classified. We also study the vertex representations for this Lie algebras.

Speaker: Éric Vasserot (Université de Cergy-Pontoise)

Title: Double affine Hecke algebras and affine Lie algebras.

Abstract : We'll review the category O for rational double affine Hecke algebras and will give some recent results on finite dimensional representations and relations with conformal blocks of affine Lie algebras.

Speaker: Rajeev Walia (University of California-Riverside)

Title: Tensor factorization and spin construction for Kac-Moody algebras

Abstract: In this talk I will discuss the "Factorization phenomenon" which occurs when a representation of a Lie algebra is restricted to a subalgebra, and the result factors into a tensor product of smaller representations of the subalgebra. This phenomenon will be analyzed for symmetrizable Kac-Moody algebras (including finite-dimensional, semi-simple Lie algebras). I will present a few factorization results for a general embedding of a symmetrizable Kac-Moody algebra into another and provide an algebraic explanation for such a phenomenon using Spin construction. I will also give some applications of these results for semisimple finite dimensional Lie algebras. I will extend the notion of Spin functor from finite-dimensional to symmetrizable Kac-Moody algebras, which requires a very delicate treatment. I will introduce a certain category of orthogonal g-representations for which, surprisingly, the Spin functor gives a g-representation in Bernstein-Gelfand-Gelfand category O. Also, for an integrable representation Spin produces an integrable representation. I will give the formula for the character of Spin representation for the above category and work out the factorization results for an embedding of a finite dimensional semi-simple Lie algebra into its untwisted affine Lie algebra. Finally, I will discuss classification of those representations for which Spin is irreducible.

Speaker: Yoji Yoshii (Akita National College of Technology)

Title: Locally affine root systems and locally affine Lie algebras.

Abstract: There is a correspondence between locally finite irreducible root systems (as a natural generalization of classical finite irreducible root systems) and locally finite split simple Lie algebras (as a natural generalization of finite-dimensional split simple Lie algebras described by Neeb and Stumme). Also, there is a correspondence between affine root systems (in the sense of Macdonald) and affine Kac-Moody Lie algebras (or loop algebras). I will talk about a natural generalization of these two correspondences. Namely, I will discuss about a correspondence between "locally affine root systems" and "locally affine Lie algebras" (or "locally loop algebras").

Speaker: Kaiming Zhao (Wilfrid Laurier University)

Title: Highest weight modules over pre-exp-polynomial Lie algebras.

Abstract: In my talk, I will introduce pre-exp-polynomial Lie algebras which look like Z-graded local Lie algebras. This class of Lie algebras include some exp-polynomial Lie algebras, for example, loop algebras, Virasoro-like algebras, and some quantum torus Lie algebras. I will show you the relationship of the conditions for non-graded and graded irreducible highest weight modules with the same highest weight having all finite dimensional weight spaces, and the relationship of irreducibility of non-graded and graded highest weight Verma modules with the same highest weight.

Selected Comments from Participants

"[My research areas are] Lie algebras, groups and applications to material science and bio science. [This conference helped me] to know top level research reports to make international research communications to create new research projects. [I would also like to add:] excellent hospitality." [Jun Morita, University of Tsukuba, Japan]

"My research interest lies in the representation theory of Lie algebras and quantum groups. This also includes the theory of vertex algebras and conformal field theory.

I have benefited quite a bit from hearing about what other people are doing for current research. Conferences/workshops such as this BIRS session, give me new ideas on how to proceed on projects that I have been thinking about for a while and many of the main speakers kindly formulated conjectures and problems that they are interested in - this allows other participants to consider joining in the search for their solution or resolution. This workshop also allowed me to work on a joint project with two other the participants and this discussion has been very fruitful.

Due to my busy schedule (or perhaps it is lazyness) I forgot about the deadline for submitting abstracts and I had planned on giving a talk on some of my own work. Next time, if there is a next time, I will be sure to submit the abstract early enough to the organizers for consideration.

The Banff International Research Station provides a wonderful and well organized environment to conduct research and interact with other mathematicians. The facilities which includes a swimming pool and weight room, is icing on the cake. If I had properly read the web site for BIRS I would have known this and a swim suit and gym clothes would have found their way into my luggage. The food in the dining room is top notch and the staff always seem to be happy and friendly.

Thanks for bringing me here." [Ben Cox, College of Charleston, U.S.A.]

"(1) My recent research interests fit very well with the topics of the meeting, as I am interested in Lie tori, extended affine Lie algebras and their generalizations, combinatorial aspects of representations, crystal bases, Hecke algebras, and many other topics discussed in the talks.

(2) The conference program had a nice diversity of topics. Yet participants had sufficiently many common interests that fostered interactions and a lot of communication. I have had mathematical discussions with over

half of the participants. My understanding of such subjects as Kirillov-Reshetikhin modules, coboundary monoidal categories, multiloop algebras, quiver varieties, and several other topics has been greatly expanded by the lectures.

(3) Thanks, Yun, Naihuan, Michael, and Kailash, you have done an excellent job." [Georgia Benkart, University of Wisconsin-Madison, U.S.A.]

"My research interests range from algebraic combinatorics, representation theory to mathematical physics. I have been interested in combinatorial properties of quantum algebras. Quantum algebras have their roots in two dimensional solvable lattice models in statistical mechanics. Kashiwara showed that at zero temperature the quantum algebras exhibit beautiful combinatorial properties. Mathematically these are formulated in the crystal base theory. Recently I have also been interested in aspects of affine Schubert calculus.

* I was able to present a talk on my joint work with Masato Okado on the existence of Kirillov-Reshetikhin crystals and combinatorial models for them. * I was able to collaborate with Masato Okado on new work in progress. * I very much benefited from the talks, in particular the talk by Georgia Benkart on Whittaker modules, Vyjayanthi Chari on conjectural generalizations of Kirillov-Reshetikhin modules to nonrectangular cases, Alistair Savage on Crystals, quiver varieties and coboundary categories for Kac-Moody algebras, Toshiki Nakashima on geometric crystals, and Eugene Mukhin on the Gaudin model and Schubert calculus. * I had the opportunity to talk in person with many people to explain my ideas and listen to theirs.

Additional comments:

BIRS is really located in a unique place! I enjoyed my hike up to Sulphur mountain very much, which also gave me the opportunity to talk in an informal fashion with Eugene Mukhin about his research." [Anne Schilling, University of California, Davis, U.S.A.]

"[My current research interests are]

* Representations of infinite dimensional Lie algebras * Geometric representation theory * Quivers and quiver varieties * Quantum groups and crystal bases

This workshop was very helpful for me in that it gave me the opportunity to meet with other researchers in the field and discuss the connections between our research programs.

The workshop was well-organized and the accomodations, meeting rooms, etc. were excellent." [Alistair Savage, University of Ottawa]

"My research is in the fields of algebra and combinatorics, and my area of expertise is the representation theory of Hecke algebras. Hecke algebras arise naturally in many areas of mathematics and physics, such as quantum groups, quantum field theory, statistical mechanics, and knot theory. I study their irreducible representations (a.k.a. simple modules), which are the most basic objects whose symmetries are encoded in this algebra.

This workshop gave me the opportunity to keep up with the state-of- the-art within my field. Many leading experts were here, talking about their most recent progress and groundbreaking results. One such example is the existence of crystal bases for Kirillov- Reshetikhin modules, and the precise combinatorial structure of their related crystal graphs. Professors Okado and Schilling presented their recent breakthroughs on this topic. They also stated which related problems remain open, which is also important communication that one often relies on workshops such as these to learn.

There were also researchers here in areas just outside (but tangent to) my own area. I had the chance to learn more about these areas from the world experts.

There was also a mixture of junior and senior researchers. I benefitted a lot from the expertise of the senior researchers. I also really enjoyed meeting and interacting with the more junior participants–it was great to hear what projects the graduate students were working on and see how inspired they were by the workshop.

The talks were outstanding. There was also time made during the day for breaks to have discussions with colleagues, and there were many rooms available for such exchanges. The setting here is really amazing, and BIRS does its best to make us very comfortable. There are also good computing, technical, and library resources." [Monica Vazirani, University of California, Davis, U.S.A.]

"My research interests are Lie theory and algebraic geometry.

From this workshop I've learned a lot of new progress in the research of Lie theory. It also gave me a good view of the representation theory of Lie algebras. I also get to know a lot of people in this area and have chance to discuss math with them.

It is an excellent workshop. I enjoy it very much." [Jie Sun, University of Alberta]

"My research interests are Lie algebras and nonassociative algebras. I learned lots of new information, especially about loop algebras, affine Lie algebras and extended affine Lie algebras in this workshop. Also, I am happy to having reported about my results for locally affine Lie algebras in front of experts." [Yoji Yoshii, Akita National College of Technology, Japan]

"My research interests are graded Lie algebras including extended affine Lie algebras, extragraded exp-polynomial algebras, quantum torus algebras, Cartan type Lie algebras, Kac-Moody algebras, and their representations.

This workshop is very successful and very useful to my future research. During the workshop I exchanged research information, research ideas, discussed mathematics with many participants which might lead to some future collaborations. From the talks, I knew new results peoples are doing or have done. I met a lot friends and enhanced my friendship with many participants.

Everything at Banff is excellent, facility, equipment, hotel, administrative service and food." [Kaiming Zhao, Wilfrid Laurier University]

"It was a wonderful meeting. My thanks to the organizers! I benefited tremendously from the meeting and in particular from the informal discussions with the participants. For example, one of the speakers on Monday afternoon discussed a problem that I had solved a year ago, but that I did not publish because I did not think that there would be enough interest. I then gave an impromptu talk on Tuesday night presenting my solution. This in turn stirred up more discussions and on Wednesday afternoon we worked together on generalizing and simplifying part of my solution." [Erhard Neher, University of Ottawa]

"My research interests include Representation Theiry of finite and infinite-dimensional Lie algebras, in particular Kac-Moody algebras, Extended affine Lie algebras, vertex algebras, quantum affine Lie algebras. The workshop was very important and useful for my research. The talks provided new insights in some areas of my interests. As a result of the interaction with other participants I have started 3 new joint projects related to the representations of infinite-dimensional Lie algebras.

The workshop had an excellent organization. Many thanks to the organizers for that. Also many thanks to BIRS for providing excellent working conditions. I found my stay at BIRS extremely fruitful and I hope to come back again." [Vyacheslav Futorny, University of Sao Paulo, Brazil]

"My interests are in infinite dimensional Lie algebras and connections to non-associative algebras. In particular, I study extended affine Lie algebras.

This was one of the best workshops that I have ever attended. Not only were the lectures very interesting, but there was also a great deal of informal discussion during the breaks between lectures and in the evening. As a result of the workshop, I improved my awareness of recent work of others in my field, and I left with several ideas for future research directions." [Bruce Allison, University of Victoria]

"I'm interested in representation theory of quantum groups, crystal bases, geometric crystals.

In this workshop, I knew that there are many new objects, e.g., algebras, representations and their constructions. I'm inspired by those things to consider relations with my interests.

Thank the organizers for inviting me to such a nice workshop. I hope to be in Banff again." [Toshiki Nakashima, Sophia University, Japan]

"[My research interests are:] (Root) graded Lie algebras, presentations by gen and rel'n, graded central extensions, homolgical algebra, quantum groups, representation theory (graded).

It was great to meet the experts in the field and listen to their talks. I really have to point out that the presentation were excellent, it is rare that everybody makes such an effort to be clear and yet bring across some work in progress. Seeing what other people in related areas work on and more more importantly, what kind of methods they apply, was of great benefit for me as Graduate student.

Some of the speakers I have seen on quite a regular basis and I am always excited to get an "up-date" on their work. It is interesting to observe the evolution of a result.

One other good thing was that although all the speakers were experts, they never forgot to point out the red thread that ran through all of the conference.

If I had to choose one word to characterize the conference, it would be coherency." [Angelika Welte, University of Ottawa]

"[My research interests are:] Structure and representations of infinite-dimensional Lie groups and Lie algebras. More specifically I am interested in geometric aspects, such as Lie algebras arising naturally in the context of smooth manifolds and fiber bundles thereon.

I learned a lot from the talks at the workshop. I think that the overall quality of exposition was very high, which made "learning by listening" possible. A fascinating point of Lie theory are that it combines so many perspectives on its structures: structure theoretic (algebraic), such as in Neher's talk, algebraic geometric, as in Pianzola's talk and the smooth geometric perspective which I was talking about.

I had a variety of informal discussions, mostly with Arturo and Erhard, on central extensions of "forms" of Lie algebras and I think that we now got some idea how to address a quite general description of the these extensions which should work in all three perspectives mentioned above." [Karl-Hermann Neeb, University of Darmstadt, Germany]

"The meeting dealt with my main research interest which is EALA theory as well as other topics associated with infinite dimensional Lie theory like quantum theory, crystal base, and representation theory.

This conference was beneficial since I could learn of many recent developments from both the talks as well as through conversations with those present. Such contact helps to foster research as well as to give some direction to various studies.

I know of several cases during the conference where two or three mathematicians had conversations which lead to new results. This was very stimulating to them and beneficial to the area.

This type of personal contact is very important." [Stephen Berman , University of Saskatchewan]

"[My research areas are:] Quantum affine Lie algebras, Crystal bases, Application to integrable systems

I could learn many interesting topics in quantum affine Lie algebras from lectures and also from discussions after that. I could understand roughly recent trends and problems in extended affine Lie algebras. I could also exchange ideas with my collaborators abroad.

Although quantum and extended affine Lie algebras are a bit different subjects, I think it is good for people from these subjects to get together and discuss. I hope this trial become a seed for future development of these two subjects." [Masato Okado, Osaka University, Japan]

"My main subject of research is Representation Theory, in particular the representation theory of Double Affine Hecke algebras. These algebras have been introduced about 20 years ago by Cherednik to solve some conjecture of MacDonald. It is expected that they should play some role in representation theory of p-adic groups, but this is still unclear...despite of some strange coincidences. In any case, they are closely related to many other topics in representation theory such as Kac-Moody algebras, Hall algebras, Springer theory. So this conference, which gathered a large spectrum of mathematicians in Lie theory was very approriate." [Éric Vasserot, Université de Cergy-Pontoise, France]

"[My current research interests are:] representations of infinite-dimensional Lie algebras, including extended affine Lie algebras. Vertex operator algebras.

During the workshop, Slava Futorny and myself obtained a character formula for irreducible representations of a Lie algebra of vector fields on n-dimensional torus.

Thank you for organizing this interesting and stimulating conference." [Yuly Billig, Carleton University]

"I am interested in representation theory, quantum groups, Hecke algebras and Springer fibers. In this moment I am particularly concerned with the representation theory of double affine Hecke algebras and their degenerations as the rational Cherednik algebras.The double affine Hecke algebras have been introduced by Cherednik 15 years ago in order to solve a conjecture of Macdonald on the constant term of some polynomials associated to Weyl groups. Actually they appears in different fields of mathemathics such as quantum groups, harmonic analysis, the study of hypergeometric functions, mathematical physics... Conjecturally they are linked to the representation theory in positive characteristic of affine Lie algebras or p-adic groups as the affine Hecke algebras takes a role in the modular representation theory of Lie algebras or reductive groups over a finite field. I really enjoy the Banff conference where there was people from different areas of Lie theory." [Michaela Varagnolo, Université de Cergy-Pontoise, France]

"My research interests include the representation theory of affine Kac-Moody algebras, in particular the finite-dimensional and integrable representations of loop algebras.

My time spent at the workshop here at BIRS was beneficial for several reasons. I was exposed to many current research topics from around the world. This allows me to connect different areas of research and to search for new ways in which my own work may be related or extended. This first-hand exposure to so many different points of view is inspiring and essential to my development as a young mathematician. On a more personal level, it is very satisfying to spend so much time together with this group of people who are all united by their passion for these pursuits. The atmosphere created at BIRS is one which encourages us all to share our stories in mathematics and in life, and I come away from this workshop reminded that I do not struggle alone, but that I belong to a community." [Prasad Senesi, University of Ottawa]

"I found the workshop extremely productive. I thought most of the talks were well prepared and quite interesting. Even though we are all supposed to be familiar with what is going on in our area, in practice this is not the case. There is simply too much stuff going on. The workshop gave me a very good perspective of how the area is developing.

Just as important for me as the lectures was my interaction with other people in small groups. I found this to be highly beneficial. One question that was raised during this small discussions for sure will lead to an interesting paper. There is also the distinct possibility of collaborating with other people in at least two other projects.

I want to thank you and the rest of the committee for a job well done. It was a great meeting." [Arturo Pianzola, University of Alberta]

Conclusion

The main goal of the BIRS workshop was to bring together experts in the areas of quantum affine algebras and extended affine Lie algebras. The AMS has agreed to publish a conference proceedings for the BIRS meeting in the *Contemporary Mathematics* series. Although many conferences have been held in areas related to these two topics, no previous conference had specifically addressed the interaction between the two groups. We hope that this conference and the resulting conference proceedings will be useful for future work in these areas. There remains great potential for cross-fertilization of ideas and methods, and it is expected that future progress in both quantum affine algebras, extended affine algebras, and their applications will benefit from further dialogue.

List of Participants

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Chen, Xueqing (University of Wisconsin-Whitewater)
Christodoloupoulou, Konstantina (University of Windsor)
Cox, Ben (College of Charleston)

Dong, Chongying (University of California)
Futorny, Vyacheslav (University of Sao Paulo)
Gao, Yun (York University)
Jing, Naihuan (North Carolina State University)
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Misra, Kailash (North Carolina State University)
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Senesi, Prasad (University of Ottawa)
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Chapter 8

New Topological Contexts for Galois Theory and Algebraic Geometry (08w5014)

Mar 09 - Mar 14, 2008

Organizer(s): Andrew Baker (University of Glasgow/University of Oslo), Birgit Richter (University of Hamburg)

Overview of the Field

There were two main themes present in the workshop. One is probably best described by the term *arithmetic of structured ring spectra* and the other might be called *arithmetically defined cohomology theories*.

Cohomology theories are classical subjects in topology and of stable homotopy theory. Different cohomology theories detect different aspects of topological spaces. Particularly nice cohomology theories are the ones that carry a multiplicative structure, for example singular cohomology with coefficients in a ring has cup products, cobordism theories have products related to cartesian products of manifiolds, and K-theories have products related to tensor producs of vector bundles. Such structures make it possible to use algebraic methods in order to investigate generalized cohomology groups of spaces. Cohomology theories can be represented by spectra. These are the objects of study in the stable homotopy category. Multiplicative structures on a cohomology theory give rise to so-called homotopy ring structures on the associated spectrum.

Since the middle of the 90's several symmetric monoidal categories of spectra were developed that model the stable homotopy category, for instance symmetric spectra [10] and S-modules [8]. From now on we will call such strict versions of homotopy ring spectra *structured ring spectra* or just *ring spectra*.

In good cases it is possible to improve homotopy ring structures on spectra to actual monoid structures in these strict models; sometimes this is done using classical approaches [13], but there are other means such as direct constructions, obstruction theories or the application of functors to ring spectra that have ring spectra as an outcome.

With these strict models the analogy to classical algebra is a sound one that can be exploited: it is possible to study the algebraic features of ring spectra such as Galois and Hopf-Galois theory of structured ring spectra as defined by Rognes, and to investigate arithmetic properties by studying algebraic K-theory of ring spectra.

Classical rings give rise to Eilenberg-MacLane spectra, the representing objects of singular cohomology, and this process embeds classical algebra and arithmetic into the world of ring spectra. However, homotopy theory provides a much richer variety of *rings* than algebra: the initial ring spectrum is the sphere spectrum and for instance there are many Galois extensions sitting between the sphere spectrum and the field with p elements for a prime p.

In order to understand algebraic K-theory of ring spectra it is often useful to investigate topological Hochschild homology [7] or topological cyclic homology of ring spectra. These homology theories are topological analogues of Hochschild and cyclic homology for algebras. For commutative ring spectra topological André-Quillen homology [4] is an important homology theory. Determining algebraic K-theory is usually a demanding task, but substantial progress has been made with respect to concrete calculations [3, AY, 1] and with respect to statements about structural properties (see for instance [6, 16]).

The construction of some important examples of structured ring spectra is inspired by arithmetic and algebraic geometric ideas, and relies on machinery from derived algebraic geometry newly developed by Lurie, Toën and Vessozi [11, 17, 18]. Most prominently, Hopkins' spectrum of topological modular forms, TMF [9], and Behrens-Lawson's topological automorphic forms, TAF [5].

Following the foundational developments during the last decade, the subject area seems to be moving into a period in which applications in homotopy theory as well as algebraic geometry and other fields can be seen.

The workshop and talks

The BIRS workshop on **New Topological Contexts for Galois Theory and Algebraic Geometry** took place at a crucial moment in the development of the subject. With many of the leading experts on various aspects of the subject attending the conference, the participants and in particular younger researchers had an excellent opportunity to communicate and exchange their ideas.

The programme was organised around a series of invited talks prepared by small groups of participants or indivduals, and these were intended to provide to give the audience an up-to-date perspective in these (often specialised) topics. The rest of the talks were selected from those offered by participants.

The invited talks included two on Hopf Galois theory [14], three on ∞-categories, one on topological André-Quillen cohomology [4], two on algebraic K-theory for S-algebras, two on topological logarithmic structures, as well as talks on étale K-theory, topological automorphic forms, Hopf Galois extensions in monoidal model categories, realisability of Landweber exact theories, and ended with a timely survey/historical talk by May on E_∞ ring spaces and spectra. The other talks covered a range of topics all well-related to the subject of the workshop.

A poster board was available during the workshop, and a number of posters appeared, with a session during which their authors were available to discuss them.

The last morning consisted of a problem session in which individuals proposed problems and gave short background talks.

The following talks were given at the workshop. We list the speakers in alphabetical order; the abstracts were written by the speakers.

Speakers: **Clark Barwick & David Gepner** (Universities of Oslo, Sheffield)
Title: ∞-*categories and applications, I & II*
Abstracts:
I Infinity Categories and Applications – Models for the ∞-category of ∞-categories.
∞-categories provide an excellent foundation for abstract homotopy theory, offering several advantages over the more traditional approach via Quillen model categories. After discussing some of their merits, we turn to definitions and models for higher categories and specifically $(\infty, 1)$-categories, including simplicial categories, Segal categories, complete Segal spaces, and quasicategories. Finally, we focus on quasicategories, which are in some sense the smallest and most streamlined of the known models.

II Post-Prandial Infinity-Categories – Third Half.
In this talk, I describe the relationship between model categories and infinity-categories. By the coherent nerve construction discussed in part I, one can convert any model category into an infinity category. But when one performs infinity categorical constructions on coherent nerves of model categories, how does one understand the result? The answer comes in the form of the Strictification Theorems, which give models for infinity-categories constructed by homotopy limits and internal homs. Further, there are multi-infinity-category versions of this result as well, which allow for the strictification of weak algebras over weak operads. By combining these results with the theory of operator categories, one can prove a number of interesting

results, including the assertion that the space of E_n structures on the infinity-category of left modules over an E_1 ring spectrum A is canonically equivalent to the space of E_{n+1} structures on A itself.

Speakers: **Christian Ausoni & Christian Schlichtkrull** (Universities of Bonn, Bergen)
Title: *Algebraic K-theory and traces for structured ring spectra, I and II*

The aim of this series of lectures is to give an overview of the trace invariants associated to the algebraic K-theory $K(A)$ of a connective structured ring spectrum A. We begin with the definition of $K(A)$ based on matrices, and we explain how it is related to Waldhausen's A-theory of spaces by means of spherical group-rings. We then review the Bökstedt trace map to topological Hochschild homology, and its refinement given by the cyclotomic trace to topological cyclic homology. We also present some general results, like the theorems on relative K-theory of Dundas and McCarthy. In the second part of this lecture, we turn to more specific examples of computations of $K(A)$, first with rational coefficients, and then with finite coefficients. Finally, we mention an extension of the Lichtenbaum-Quillen conjectures to this context, due to John Rognes.

Speaker: **Maria Basterra** (University of New Hampshire Durham)
Title: *Topological André-Quillen cohomology and related topics*

In his seminal work *Homotopical Algebra*, Quillen defined cohomology in a general model category in terms of the derived functors of *abelianization*. In this talk I will give an overview of my work with Mike Mandell investigating Quillen cohomology in the category of commutative S-algebras. We present several perspectives and some of the results obtained from the different points of view.

Speaker: **Andrew Blumberg** (Stanford University)
Title: *Localization for THH and TC of schemes*

Abstract: In this talk I will give a construction of the topological Hochschild homology and topological cyclic homology of a scheme in terms of the 'spectral derived category' of the scheme. I will discuss the application of this construction to show that there is a localization sequence associated to the inclusion of an open subscheme, naturally connected via the cyclotomic trace to the localization sequence of Thomason-Trobaugh in K-theory. This is joint work with Michael Mandell.

Speaker: **Ethan Devinatz** (University of Washington)
Title: *Towards the finiteness of the homotopy groups of the $K(n)$-local sphere*

Abstract: I will replace the notion of finiteness by a related notion of 'essentially finite rank' which is relevant for certain homotopy or homology groups of finite $K(n-2)$-acyclic spectra which are annihilated by p. Using the Devinatz-Hopkins continuous homotopy fixed point spectra, I will outline a program for proving that, if X is such a spectrum, then the homotopy groups of its $K(n)$-localization are of essentially finite rank, and I will indicate what progress I have made. One consequence of my work is the result that if z is an element of the p-Sylow subgroup of S_n and is non-torsion in the quotient of this group by its center, then the only units in $(E_n)_*$ fixed by z are the units in the Witt vectors.

Speaker: **Paul Goerss** (Northwestern University)
Title: *Realizing families of Landweber exact homology theories*

Abstract: In this overview, I would like to revisit and explore the following realization problem: given a continuous family of Landweber exact homology theories, when can it be lifted to a diagram of commutative ring spectra? This is not always possible, but work of Hopkins, Miller, Lurie, Behrens, and Lawson has given us a number of important examples where realization is possible, and I would like to meditate some on these in order to see what makes them work. Because of the relative simplicity and because it is easy to make explicit the role of p-divisible groups, I will emphasize the example of elliptic homology theories (i.e., topological modular forms) and the Hopkins-Miller realization result.

Speaker: **Kathryn Hess** (EPF Lausanne)
Title: *Hopf-Galois extensions in monoidal model categories*

Abstract: Rognes introduced the notion of a Hopf-Galois extension of structured ring spectra, of which the unit map from the sphere spectrum to MU is an important example. In this talk I will outline a theory of homotopic Hopf-Galois extensions in a monoidal category with compatible model category structure that generalizes the case of structured ring spectra. I will give examples of homotopic Hopf-Galois extensions in other categories. This is joint work with Cédric Bujard.

Speaker: **Mark Hovey** (Wesleyan University)
Title: *Semisimple ring spectra*

Abstract: In this talk, we present a definition and partial classification of semisimple ring spectra. This can be looked at as part of the general program of extending ring theory to structured ring spectra. It is also very closely related to the following purely algebraic question: for which graded rings R can the category of projective R-modules be triangulated, where the suspension is the shift? This is joint work with Keir Lockridge.

Speaker: **Rick Jardine** (University of Western Ontario)
Title: *Étale K-theory: a modern view*

Abstract: This lecture shows how to construct the étale K-theory of a scheme S and investigate its properties, with modern tools. There is a rather simply defined version of the K-theory presheaf of spectra K on the big site for S that is constructed with Waldhausen's techniques from big site vector bundles, and which is a presheaf of symmetric spectra. Let n be a number which is relatively prime to the residue characteristics of S: then the mod n étale K-theory presheaf of spectra is constructed from the presheaf of spectra K by taking a stably fibrant model FK/n for the presheaf K/n with respect to the etale topology. I shall display descent spectral sequences for mod n étale K-theory, including a spectral sequence of Galois descent type for the mod n étale K-theory of S which starts with Galois cohomology of the Grothendieck fundamental group of S, with coefficients in étale K-groups. We shall also discuss some standard comparisons with other flavours of K-theory.

Speaker: **Tyler Lawson** (University of Minnesota)
Title: *Topological Automorphic Forms*

Abstract: In this talk, I will discuss joint work with Mark Behrens on families of Landweber exact homology theories arising from moduli of higher-dimensional abelian varieties with extra structure. I will explain how these moduli give rise to p-divisible groups and a result of Jacob Lurie that allows realization of them. In particular, I will discuss the case of abelian surfaces with complex multiplication and how these can be related to the case of elliptic homology theories.

Speaker: **Peter May** (University of Chicago)
Title: *E_∞ ring spaces and E_∞ ring spectra*

Abstract: E_∞ ring spectra were defined in 1972, but the term has since acquired several alternative meanings. The same is true of several other terms. The new formulations and constructions are not always known to be equivalent to the old ones and even when they are, the notion of 'equivalence' needs discussion: Quillen equivalent categories can be quite seriously inequivalent. Part of the confusion stems from a gap in the modern resurgence of interest in E_∞ structures. E_∞ ring spaces were also defined in 1972 and and have never been redefined. They were central to the early applications and they tie in to modern applications. We give an informal open ended discussion of the relationships between the original notions and various new ones, explaining what is and what is not known.

Speaker: **Susan Montgomery** (University of Southern California)
Title: *Hopf Galois theory: I & II*

Abstract: The first talk will consist of definitions, examples, and a few basic results about Hopf Galois extensions. In the second lecture, I will try to discuss topics raised by the audience at the first talk.

Speaker: **John Rognes** (University of Oslo)
Title: *Topological logarithmic structures, I and II*

Abstract: A logarithmic structure on a commutative S-algebra B is a suitable map $M \to \Omega^\infty B$ of E_∞ spaces (with zero). It specifies a topological algebro-geometric object, intermediate between $\mathrm{Spec}(B)$ and $\mathrm{Spec}(B[M^{-1}])$. We report on work in progress on how to define logarithmic versions of TAQ and THH. In the case $B = HA$, where A is the valuation ring of a p-adic number field K and M is freely generated by the uniformizer, this agrees with the relative $THH(A|K)$ of Hesselholt and Madsen. In the case $B = ku$, the hope is that this framework provides a setting where the 'fraction field' of complex K-theory makes sense.

Speaker: **Steffen Sagave** (University of Oslo)
Title: *DG-algebras and derived A_∞-algebras*

Abstract: Let A be a differential graded algebra over a commutative ring k. We show that the homology of A admits a k-projective resolution E coming with a family of higher multiplications. This E is an instance of a 'minimal derived A_∞-algebra'. The main result is that minimal derived A_∞-algebras provide an alternative description of quasi-isomorphism types of dgas.

Mathematical outcomes

The Workshop provided a timely event at which a large number of the mathematicians interested in these topics were able to interact. In particular the following conclusions can be drawn from teh activities of the Workshop.

It is clear that the rapidly developing technical subject area of ∞-categories will have a major impact in the near future, with work of Lurie [12], Barwick, Gepner, Töen and Vezzosi being central.

The continuing development of Galois theoretic ideas within the framework structured ring spectra and also more general monoidal model categories, leads to the need to make greater use of existing algebraic Galois theoretic machinery.

Algebraic K-theory, with its links to Hochschild and cyclic homology will continue to provide a major stimulus, with versions for structured ring specra currently being the subject of a great deal of computational and conceptual activity. Topological logarithmic structures and suitable (co)homology theories are being developed and these provide further enrichment of the subject and interactions with existing algebraic and number theoretic areas.

The development of topological modular forms and the more recent topological automorphic forms, particularly as examples of the applicability of Lurie's methods in derived algebraic geometry, point to increasingly rich sources of interaction with algebraic geometry and interesting new objects to study in algebraic topology. One motivation for the latter is its connections (both established and speculative) with the dominant chromatic viewpoint on stable homotopy.

Outcome of the Meeting

The workshop ran at almost 100% capacity (we had a few very late withdrawals and managed to fill all but one place because of the great demand to attend). The programme was a mixture of invited talks and short sequences of talks, as well as talks chosen from those offered by participants.

It was notable that a great number of the speakers were young mathematicians and the standard of presentations was high. We have had many positive comments about the workshop from participants since it occurred. The facilities at BIRS provide a marvellous environment for a research meeting.

There will be a proceedings volume of the conference and we have encouraged all of the invited speakers to produce written versions of their talks. These papers should provide an up-to-date introduction and survey of the topics of the workshop and fill an existing gap in the literature. We have been promised a substantial number of articles which we expect to amount to more than 300 pages.

List of Participants

Ando, Matthew (University of Illinois)
Angeltveit, Vigleik (University of Chicago)

Ausoni, Christian (University of Bonn)
Baker, Andrew (University of Glasgow/University of Oslo)
Barwick, Clark (Institute for Advanced Study)
Basterra, Maria (University of New Hampshire, Durham)
Bauer, Kristine (University of Calgary)
Blumberg, Andrew (Stanford University)
Brun, Morten (University of Bergen)
Bruner, Robert (Wayne State University)
Chebolu, Sunil (University of Western Ontario)
Devinatz, Ethan (University of Washington)
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Richter, Birgit (University of Hamburg)
Rognes, John (University of Oslo)
Roitzheim, Constanze (University of Sheffield)
Roth, Fridolin (University of Hamburg)
Sagave, Steffen (University of Oslo)
Schlichtkrull, Christian (University of Bergen)
Shipley, Brooke (University of Illinois, Chicago)
Strickland, Neil (University of Sheffield)
Whitehouse, Sarah (University of Sheffield)

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Chapter 9

Recent Progress on the Moduli Space of Curves (08w5086)

Mar 16 - Mar 21, 2008

Organizer(s): Aaron Bertram (University of Utah), Jim Bryan (University of British Columbia), Renzo Cavalieri (University of Michigan)

Overview of the Field

Mumford's 1983 paper [1] initiated the systematic study of the intersection theory of the moduli space of curves, in particular emphasizing the importance of tautological classes - Chow classes naturally arising from the intrinsic geometry of curves. Subsequently, Carel Faber explored the properties of the graded intersection ring generated by such classes - the so-called tautological ring of the moduli of curves [4]. About ten years later, based on a substantial amount of numerical data and the Witten conjectures (proved by Kontsevich), Faber conjectured that the tautological ring of curves in each $g \geq 2$ "*behaves like the algebraic cohomology ring of a nonsingular projective variety of dimension* $g-2$." Moreover, he conjectured surprising combinatorial formulas for the "intersection numbers" that have been shown ([5])to follow from a very deep result (the proof of the Virasoro conjecture) of Givental ([**?**]). The drawback of such a high-powered and indirect proof is that it doesn't shed much light on the fundamental geometric reasons for such formulas.

In the last few years, new ideas and techniques have been developed that offer some promising new lines of attack on Faber's conjectures. These include the following:

- *Relative stable maps and localization.* The Hurwitz spaces of branched covers of the Riemann sphere admit different compactifications by spaces of "relative stable maps", depending upon how one treats the collisions of branch points. The Hurwitz spaces have long been useful tools for studying the moduli spaces of curves, but somewhat surprisingly, recent applications of the Atiyah-Bott localization theorem to all compactifications at once have led to some important new insights. One of the most powerful of these is the Theorem "Star" of Graber-Vakil characterizing the support of tautological classes of codimension $> g$ [6].

- *Axiomatic Gromov-Witten theory.* Givental's approach to Gromov-Witten theory in higher genus, regarding the spaces of axiomatic Gromov-Witten theories as a sort of homogeneous space for a "quantized" loop group, led Y.P. Lee to make a series of intriguing conjectures on relations in the tautological rings. In principle, these conjectures ought to reduce the computation of all relations to linear algebra, but in practice the computations are prohibitively complicated. Nevertheless, this point of view has resulted in a systematic rediscovery of many subtle relations, as well as several new ones [3] and [2] .

Recent Developments

In the last two years, the above circle of ideas have led to significant progress in the field. Some examples include:

- Lee's invariance conjectures constituted the backbone for the proof of *Witten's r-spin conjecture* by Faber, Shadrin and Zvonkine([7]).
- Work of Vakil with Goulden and Jackson has led to a new proof of the λ_g conjecture and of the intersection number part of Faber's conjecture for the moduli spaces of curves with rational tails, in the case of a top intersection number given by a small number of factors ([8], [9]).
- Only days before the workshop Liu and Xu posted yet another interesting proof for Faber's intersection number conjecture([10]).
- The analysis from the previous works led Goulden, Jackson and Vakil ([11]) to observe remarkable structure for double Hurwitz numbers: they are piecewise polynomial. Shadrin, Shapiro and Vainshtein ([12]) have described walls and wall crossing formulas in genus 0, and recent work of Cavalieri, Johnson and Markwig ([13]) seems to have identified a very promising combinatorial framework to study the positive genus case.
- The study of Gromov-Witten theory for orbifolds has been extremely lively and exciting. We won't try to list specific works here for fear of being unfair and incomplete. On the one hand, orbifold Gromov-Witten theory can be shown to create yet another bridge between teh moduli space of curves and Hurwitz theory, and hence towards a combinatoruialization of questions about tautological classes. On the other hand, Givental machinery has been successfully adapted to the orbifold setting, providing an extremely powerful computational framework. Perhaps one of the most exciting open questions in the fiels is *Ruan's* (et al. by now) Crepant Resolution Conjecture, predicting a nontrivial equivalence of the orbifold Growov Witten theory of an orbifold with the ordinary Gromov-Witten of a crepant resolution.
- Recent work of Telemann([14]) is using a classification of families of semi-simple field theories to prove a conjecture of Givental, stating that higher genus Gromov-Witten theory can be recovered from the genus 0 case by a process of quantization.

Description of the Scientific Activity

The workshop "Recent progress in the moduli space of curves" counted forty three participants, with particular emphasis on encouraging interaction between estabilished researchers and young mathematicians: participants included fourteen graduate students and eight postdocs, from a variety of institutions all around the world.

The scheduled activities in this workshop consisted of:

- a three hour mini-course given by Y.P. Lee presenting recent work of Teleman([14]). This is a very technical work, and Lee provided an "as soft as possible" introduction to the circle of ideas used by Teleman.
- a three plus two hour mini-course coordinated between Ravi Vakil and Ian Goulden. Vakil gave an overview of the Faber conjectures and presented their history, particularly focusing on the geometric approaches using Gromov-Witten theory. Goulden presented a key combinatorial tool used in these arguments, explaining how and why a lot of the families of intersection numbers arising in this theory are organized by the KP integrable hierarchy.
- five half hour talks by advanced graduate students: Johnson, Pagani, Penev, Todorov and Wise.
- an open ended discussion session on open problems.
- nine one hour long research talks: the speakers were Bryan, Cadman, Edidin, Faber, Farkas, Kimura, Shapiro, Tseng, Yang.

Discussion and Questions Emerged

One afternoon of the conference was devoted to an open ended discussion session. The participants were encouraged to sumbit their questions and ideas. Aaron Bertram led the discussion and acted as a moderator. The discussion was very lively, and several participants participated very actively. Several questions, ranging from basic to very advanced, emerged. This was indeed a crucial moment in the workshop. We wish to emphasize this by reporting here some of the questions and conclusions.

Sam Payne "spayne@stanford.edu" Here's a situation I find intriguing: the moduli space of stable n-pointed rational curves embeds naturally in a toric variety – the toric variety associated to the space of phylogenetic trees with n leaves. For small n, one can show that this toric variety has some exceptionally nice cohomological properties (e.g. the section ring of any ample line bundle is Koszul). Keel and Tevelev have shown similar properties for the kappa embedding of M_0, n. My question in two parts is then:

1. Does the toric variety associated to the space of phylogenetic trees with n leaves have Koszul homoegeneous coordinate rings for every n?

2. Can the Keel-Tevelev Theorem on the kappa embedding be deduced from the geometry of its embedding in the toric variety associated to the space of phylogenetic trees, and can such results be extended to other projective embeddings of M_0, n?

Angela Gibney "agibney@math.upenn.edu" There are some very basic questions about the birational geometry of $\overline{M}_{g,n}$ which by now are kind of old-ish, but that we shouldn't forget are still open.

One of the fundamental objects of study in Mori theory is the closed cone of curves. By understanding the cone of curves of a projective variety X, one could essentially describe what maps there are from X to any other projective variety. Carel Faber is responsible for identifying a natural collection of curves on $\overline{M}_{g,n}$ which he observed, for low g and $n = 0$, actually spanned the extremal rays of the Mori cone of curves. These curves are 1-dimensional boundary strata – they are numerically equivalent to the closures of the loci of points in $\overline{M}_{g,n}$ having $3g - 4 + n$ nodes. Faber's conjecture for the Mori cone is known in a number of intermediate cases between $n = 0$ and $g \leq 24$ to $g = 0$, and $n \leq 7$. Faber's conjecture would be true on $\overline{M}_{g,n}$ if it were true on $\overline{M}_{0,g+n}$, and so of course, knowing what happens in the genus zero case is very important.

In the genus zero case, Faber's conjecture on the cone of curves is equivalent to Fulton's conjecture for cycles. Fulton questioned whether the cycle structure on $\overline{M}_{0,n}$ is analogous to the cycle structure on a normal toric variety X_Δ, where Δ is the fan of cones. On X_Δ, every effective k-cycle would be equivalent to an effective combination of torus invariant cycles of dimension k. Fulton likened the boundary stratification of $\overline{M}_{0,n}$ to the fan of cones of a toric variety and wondered whether an effective cycle of dimension k on $\overline{M}_{0,n}$ might be numerically equivalent to an effective combination of k-dimensional boundary strata. This is actually true for 0-cycles since $\overline{M}_{0,n}$ is rational. Keel and others have shown it is false for cycles of dimension $k \geq 2$. The one remaining open case is for $k = 1$. Fulton's question is whether or not every effective curve is numerically equivalent to an effective combination of boundary curves. In other words, his question asks whether the extremal rays of the Mori cone are spanned by the curves that Faber predicts.

One can rephrase these questions to describe the cone of nef divisors on $\overline{M}_{g,n}$. As Farkas said in his talk, this is the cone spanned by divisors that nonnegatively intersect all curves. So Faber's conjecture can be rephrased as predicting that the cone of nef divisors $Nef(\overline{M}_{g,n})$ is equal to what people call the F-cone of divisors $F(\overline{M}_{g,n})$ which is spanned by those divisors that nonnegatively intersect the boundary curves. In other words, the F-cone is an upper bound for the Nef cone. Faber's conjecture is that the two are equal. Recently, Maclagan and Gibney have proved that the F-cone on $\overline{M}_{0,n}$ is actually the pull back of a cone of divisors on a toric variety X_Δ that contains $\overline{M}_{0,n}$. Gibney and Maclagan also define a lower bound $L(\overline{M}_{0,n})$ of the Nef-cone of $\overline{M}_{0,n}$ by pulling back another cone of divisors from the toric variety X_Δ. In other words, there is a chain of cones

$$L(\overline{M}_{0,n}) \subset Nef(\overline{M}_{0,n}) \subset F(\overline{M}_{0,n}),$$

and we know that for $n \leq 6$ all cones are the same. So a natural question is whether these cones can be distinguished from one another, and whether one can work on the ambient toric variety rather than on the moduli space itself. It also begs the question of whether there is an embedding of $\overline{M}_{g,n}$ in a toric variety in such a way as to explain the F-cone on those spaces for $g > 0$.

Andrew Morrison "andrewmo@math.ubc.ca" I was wondering if the bernoulli numbers that come up in the Hodge intergrals have any geometric meaning, do they count something good? My geuss is that they are just the residues of the Todd class used somewhere...

Someone also said at one point that Poincare' duality is not know for the case of $\overline{M}_{g,n}$ bar. I suppose I am a bit unfamilliar with the basics of its cohomology.

David Steinberg "dsteinbe@math.ubc.ca" Quotients in one form or another are ubiquitous in geometry, they form a basic tool for creating new spaces out of old ones. Of particular interest is a quotient of a space by a group action; here the quotient space is the often the set of orbits of the action. In algebraic geometry, however, one gets into trouble using this definition. The GIT quotient is NOT the collection of orbits, but it is what the quotient "should" be in algebraic geometry. Since GIT quotients are fundamental to the construction of the moduli space of curves, I would be interested to know more about them, in particular: why does the set of orbits fail to be a good quotient in the algebraic category, what is a GIT quotient, and why is the GIT quotient the right quotient.

In the simplest case, the MNOP conjecture states that the GW invariants of a Calabi-Yau 3-fold are related to its Donaldson-Thomas invariants; in particular, a change of variables of the DT (reduced) partition function yields the GW partition function. It has been stressed that this equality after change of variables does not hold for a fixed homology class, that one must work with all the invariants at once in order to obtain the above relation. An explanation of why this is the case would be very interesting.

Dave Anderson "dandersn@umich.edu" I've got a few questions, mainly related to symmetric functions. I'm not sure this is the desired format, but there's a *little* mathematical content at least...

Are the symmetric functions $P_{g,n}(alpha)$ occuring in the ELSV formulas Schur-positive? Or are they positive with respect to other bases (elementary, homogeneous, Q, etc)? If not, do the expansions have any predictable signs or combinatorial meaning? Symmetric functions that come up in geometry often have some such positivity, so it would be nice to know about this. (E.g., polynomials that integrate positively when evaluated at Chern classes of ample vector bundles are Schur-positive.)

Are the "y-augmented" Schur functions Goulden introduced related to factorial Schur functions (aka multi-Schur functions, shifted Schur functions, double Schur functions, ...)? (Okounkov and Olshanski studied them under the name "shifted Schur functions"; also, they represent equivariant Schubert classes in Grassmannians.) They can't be the same exactly, but possibly one gets the factorial Schurs after a substitution in the y's, or summing Goulden's functions appropriately.

What are the betti numbers of the tautological ring – do they have a combinatorial description? What is the dual Hopf algebra of the stable cohomology of M_g? Is there some basis nicer than monomials in psi- or kappa-classes with respect to the Hopf algebra structure? (Motivating these questions: Is there a meaningful rough analogy between the stable tautological ring and the ring of symmetric functions?)

Michael Shapiro "mchapiro@gmail.com" 1. Generalize the description of walls of polynomiality chambers and wall crossing formula for double Hurwitz numbers from genusC 0 to positive genus.

(During the meeting Paul Johnson and Renzo Cavalieri suggested a method to approach the problem using tropical geometry that sounds very promising).

2. Is there any " r-ELSV formula"C for the moduli space of r- spin structures (Zvonkine'sC program)?

Gavril Farkas "farkas@mathematik.hu-berlin.de" A couple of questions on the algebraic-geometry side of M_g:

1) What is really κ_1? We do not known a single explicit example of a very ample divisor class on the coarse moduli space of curves. Write down an explicit ample class on M_g, that is, describe its zero section as a geometric locus in M_g.

2) Find a lower bound on the slopes of effective divisors on M_g. Show that such a bound is independent of g.

3) What is the genus of the smallest curve passing through a general point in M_g. One should expect this genus to be at least $\log(g)$ (assymptotically).

Jonathan Wise "jonathan@math.brown.edu" What can you say about Hurwitz numbers allowing specified branching at an arbitrary collection of branch points? What do orbifold techniques tell you? Does it make life easier or harder to put a stack structure at infinity instead of using relative stable maps?

To what extent can you study FTFTs in purely algebraic terms (i.e., without parameterizing boundary circles)? What are the sources of semisimple FTFTs? Are there any that do not come from Gromov–Witten theory?

Yuan-Pin LEE "yplee@math.utah.edu" Are there other applications of the powerful facts in topology of moduli of curves, like Harer stability and Madsen–Wiess' theorem, to GW theory, besides Teleman's result?

Conversely, are there any implications of Teleman's result to topology on moduli of curves?

(As discussed during the lecture, Teleman's result implies the semisimple GW classes in $\bar{M}_{g,n}$ are tautological.)

Barbara Fantechi "fantechi@ias.edu" Can one give an algebraic definition of the morphism $M_{g,1} \to M_{g+1,1}$ (up to homotopy)?

More precisely, consider the DM stack Y parametrizing morphisms from $\overline{M}_{g,1}$ to $\overline{M}_{g+1,1}$. The gluing morphism $\overline{M}_{g,1} \times \overline{M}_{1,2} \to V_{g+1,1}$ defines a morphism (indeed a closed embedding) $\overline{M}_{1,2} \to Y$. Let X be the connected component of Y containing the image of $\bar{M}_{1,2}$, and let U be the intersection of X with the open substack parametrizing maps which map $M_{g,1}$ to $M_{g+1,1}$. The question above should be answered positively if U is nonempty and connected.

Gueorgui T Todorov "todorov@math.utah.edu" I would like to hear about people's opinion on the behavior of GW invariants under a general birational modification of the target space.

Arend Bayer "bayer@math.utah.edu" In a recent preprint, Constantin Teleman proved a theorem reconstructing higher-genus Gromov-Witten invariants from finitely many genus-zero invariants in the case of semisimple small quantum multiplication. The proof uses various topological results and methods. It would be interesting to try to understand to what extent these methods can be formulated in a completely algebraic geometric setting.

Hsian-Hua Tseng "tseng@math.wisc.edu" Connectedness of moduli spaces of twisted stable maps.

To the best of my knowledge (possibly due to my lack of knowledge), I don't seem to know answers to the following questions.

Part A: Let G be a finite group, and let $\overline{M}_{g,n}(BG)$ be the stack of n-pointed genus g twisted stable maps to BG. We know that it is not connected.

(1) I'd like to know whether the components parametrizing maps with fixed stack structures at marked points are connected. This may be easy or outright false.

(2) More generally, describe the connected components of $\overline{M}_{g,n}(BG)$.

Part B: We can ask the same questions for the stack of twisted stable maps to some nice stacks, say weighted projective stacks.

Melissa Liu "ccliu@math.northwestern.edu" Questions for Jim Bryan: You mentioned that you have been studying orbifold Donaldson-Thomas theory.

(1) Do you have a statement of the crepant resolution conjecture in the Donaldson-Thomas theory (relating the orbifold DT theory of the orbifold to the DT theory of its crepant resolution)?

(2) Do you have a statement of the orbifoldGW/orbifoldDT correspondence?

(3) If the answer to (2) is yes, can one proves it for toric orbifolds of dimension 3?

Questions for Yunfeng Jiang and Hsian-Hua Tseng:

You have stated the Virasoro constraints for orbifolds. Do you know that Virasoro conjecture hold for BG? (Paul Johnson seemed to say so in his talk today ...) If yes, can you modify Givental's proof of the Virasoro conjecture for toric Fano manifolds to obtain a proof of the Virasoro conjecture for toric Fano orbifolds?

Paul Johnosn "pdjohnso@umich.edu" Some questions that I've come up with/thought about while I was here: there are the ones mentioned in the talk. The moduli space $M_{g,\gamma_1,\ldots,\gamma_n}(BG)$ has an obvious forgetful map to $M_{g,n}$, forgetting the principal G bundle, and we have a pretty good understanding of how this interacts with the tautological class. But we also have various maps to $M_{g'}$ that remember just the total space of the principal G bundle, or do a change-fiber construction to replace the $G-$torsor fibers of the fiber with some other G space. The push-forward of tautological classes via these maps seems rather open. The simplest cases are just the images themselves: is the closure of the space of curves with isotropy group G tautological? Or how about the closure of the space of degree d ramified covers, where the monodromy does not generate all of S_d, but just some subgroup?

(Carl Faber comments): there is an example (by Gaber-Pandharipande arXiv:math/0104057) of an algebraic locus in $\mathcal{M}_{2,22}$ that is not tautological. The locus that is degree two covers of curves in $\mathcal{M}_{1,12}$ simply ramified over the last two points.

Constructions of non tautological classes on moduli spaces of curves Authors: T. Graber, R. Pandharipande

Stacky ELSV is known for $\mathbb{Z}_r$ and it can be deduced for an abelian group. 10 **Question:** What about for a general G?

Given a representation $\rho : G \to \mathbb{C}$ is there a formula of the following type.

$$\int_{\mathcal{M}_{g,n}} \frac{\lambda_g^\rho - t\lambda_{g-1}^\rho + \cdots}{(1-\mu_1\psi_1)\cdots(1-\mu_n\psi_n)} = \text{characteristic theoretic formula.}$$

Balazs Szendroi "szendroi@maths.ox.ac.uk" I have come here to find out more about orbifold GW and its possible relations to orbifold DT, algebraic structures on cohomology of moduli space of curves, cohomology theory interpretation of the virtual class, and have been intrigued by wall crossing behaviour of double Hurwitz numbers.

I haven't any explicit problem in mind that would interest the others; as you know I have been intrigued by $[C^3/Z_3]$ for a while.

Charles Cadman "cadman@math.ubc.ca" I think it would be interesting to extend the ELSV formula in some way to higher genus targets. This could provide more interesting relations between Hodge integrals. The original ELSV formula, as well as the extensions of it, use ramified covers of P^1 to compute the relations. Since the target is P^1, it is possible to use localization to quickly obtain the formula. If the target is a higher genus curve, then localization would not work (at least not in any obvious way) and so one would need a different approach. It might be a matter of finding the right compactification of the space of smooth ramified covers, and using some kind of virtual excess intersection method to transform the degree of the branch map into an integral over something which lies in the boundary. I should note that the original ELSV approach used a non-standard compactification of the space of ramified covers of P^1, together with some delicate analysis of the boundary.

Greg Smith "ggsmith@mast.queensu.ca" Can one prove Faber's conjectural presentation of the tautological ring of $\mathcal{M}_g$? Is there a conjectural presentation of the tautological rings if $\mathcal{M}_{g,n}^{\mathrm{rt}}$, $\mathcal{M}_{g,n}^{\mathrm{ct}}$, or $\overline{\mathcal{M}}_{g,n}$?

For $\mathcal{M}_{g,n}(BG)$ or $\overline{\mathcal{M}}_{g,n}(BG)$ describe the connected components. For a fixed conjugacy class, how is this ramified. (Look at Hurwitz papers by Mike Freed et. al)

Is there an analog of Faber's conjecture for $\mathcal{M}_{g,n}(BG)$? How would one even define tautological classes in this case?

Note: Mumford's conjecture for $\mathcal{M}_{g,n}(BG)$ has recently been proved by Ralph Cohen and Soren Galatius.

Renzo Cavalieri "crenzo@umich.edu" Note that λ_g is the evaluation class for curves of compact type and $\lambda_g\lambda_{g-1}$ is the evaluation class for curves with rational tails. A similar statement seems possible for λ_i or $\lambda_g\lambda_i$ for varying i. Note that λ_i "kills" all curves whose dual graph has more than $g-i$ loops; similarly $\lambda_g\lambda_i$ "kills" all curves whose dual graphs have more than $g-i$ vertices of positive genus. One would hope that a Faber-type statement be made for these loci, but perfect pairing fails already in genus 4 with the class $\lambda_4\lambda_2$, as well as with the class λ_3. One may try to recover Renzo's dream with classes other than λ_i or $\lambda_g\lambda_i$: for example, look at the homogeneous pieces of the polynomial $c(\mathbb{E})c(\mathbb{E})$.

Carel's suggestion for a little sisters: The class $\lambda_g\lambda_{g-1}\lambda_{g-2}$ is the class of a fixed curve C in $\mathcal{M}_g$, and it yields a Fulton-MacPherson space $C[n]$ in $\mathcal{M}_{g,n}$. What is the tautological ring of this space? One possible definition is to look at the subalgebra of $A^*(C[n])$ generated by diagonals (no κ classes!).

Another little sister: Look at the n-fold fiber product of C_g over M_g, denoted $(C_g^n)_{\mathcal{M}_g}$.

Conclusions

As organizers, we feel very satisfied with the outcome of the workshop. Our goal of "massaging" the usual structure of a research conference in order to increase the level of participation among participants seems to have been achieved. The mini-courses provided some solid reference points for all participants to focus on. The graduate student talks provided an excellent opportunity of interaction. In particular, during one if the graduate students talks, Carel Faber and Gabi Farkas identified a flaw in the student's thesis problem planned strategy. After the talk, Faber and Farkas discussed the issue at length with the student, and were able to suggest other more promising strategies to go about the same problem. It's needless to point out how valuable such an experience has been for the student. Having a good number of standard research talks helped avoiding "over-focusing", and gave the workshop a significant breadth. Several speakers, such as Cadman and Tseng, chose to give a survey talk on their research rather than focusing on a specific result. This turned out to be extremely pleasant and useful for many of the participants.

Several new collaborations were activated thanks to this workshop. Charles Cadman activated collaborations with Greg Smith and YP Lee, Tyler Jarvis with Dan Edidin; Paul Johnson and Renzo Cavalieri have much to discuss with Misha Shapiro.

We are pretty confident in saying that all participants were very satisfied with this workshop. Of course we organizers like to claim part of the credit for this, but it's no doubt that the amazing work enviroment provided by the Banff Center, and the efficient organization of BIRS were instrumental to such a success of this activity. We would also like to acknowledge the Clay mathematical institute, which provided us with a $10000 grant to subsidize travel expenses for graduate students.

Testimonials

Paul Johnson This conference has been by far the favorite I've attended. I've found that I've been doing a lot more math and, for lack of a better work, schmoozing, between talks. Maybe I'm just further along and starting to understand things and know people and have results, but I also think being here at Banff as a part of it: I'm used to everyone coming to a conference knowing who they wanted to talk to, and rushing off immediately when they have spare time to talk. Having all the meals together at the same place, and all staying at the same place and sharing the common space have made interacting a lot easier. A part of this could just be that I'm one of the people rushing off to talk to people now, but if that's the case it's wonderful that they're all in the same place to talk to.

Misha Shapiro I want to join Paul's email that it is really great conference!

Joro Todorov Thank you so much for a very enjoyable conference and also for the opportunity to give a talk.

Yunfeng Jiang It is my second time to attend conferences in Banff. The working and studying environment here is amazing and I really made some progress on my research.

The workshop is on the hot subject "Moduli of curves" in algebraic geometry in modern mathematics. It not only covers the Gromov-Witten side of the moduli of curves on the talks and discussions, on which I am working, but also contains the birational geometry of the moduli of curves, which is another important subject in algebraic geometry. I have learnt a lot from the talks.

At last, I think that it would be more fascinating if there were some talks on Donaldson-Thomas theory and Pandharipande-Thomas theory, which these theories also encode the enumerative geometry of curves in Calabi-Yau 3-folds.

Tyler Jarvis I just want to thank you all for an excellent conference. This was certainly one of the best mathematics conferences I have attended.

I learned a lot and was also able to meet some people that are likely to prove very helpful to my research. Specifically, I have begun a new collaboration with Dan Edidin that seems likely to produce some interesting results in the near future.

List of Participants

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Chapter 10

Topics in Von Neumann Algebras (08w5093)

Mar 23 - Mar 28, 2008

Organizer(s): Juliana Erlijman (University of Regina), Hans Wenzl (University of California, San Diego)

The emphasis of the workshop was given to active areas in the theory of von Neumann algebras with connections to other fields as well as to these other fields themselves. Among the participants there were many leading researchers in the theory of von Neumann algebras, but also representatives from group theory, quantum computing and conformal field theory. In particular, a plenary speaker of the ICM, U. Haagerup, and several other invited speakers at various ICM conferences, including D. Bisch, N. Ozawa and R. Longo were among the participants. There were also many younger participants (including recent Ph.D.'s, graduate students, and a good representation of women) who had the opportunity to interact with these leaders. Participants expressed in numerous occasions that the workshop was very stimulating and allowed for fruitful discussions of joint projects. As perhaps the most striking example N. Ozawa was stimulated by the logician A. Tornquist to write a new paper which has already been posted. So we feel that the objectives for this workshop were fulfilled.

Short overview of the field and topics targeted in the workshop

Von Neumann algebras are algebras of bounded linear operators on a Hilbert space which are closed under the topology of pointwise convergence. If their center only consists of multiples of the identity, they are called factors. Von Neumann algebras were first studied in a series of papers by Murray and von Neumann in the 1930's, such as in [MvN]. Their motivation was to have a tool for studying quantum mechanics and representations of infinite groups. As it will be seen below, these are still some of the major driving forces in research related to von Neumann algebras, with exciting recent developments.

In order to better describe the structure of the workshop, we will roughly divide the recent activities in von Neumann algebras into the study of subfactors, the interplay between groups and factors, and other developments.

1. *Subfactors.* The study of subfactors was initiated by V. Jones in the 1980's by introducing an important invariant for them called the index, [J1]. Moreover, he proved a surprising and fundamental theorem on the set of possible index values and he produced an important class of examples called the Jones subfactors. This class of examples carried a representation of braid groups, and was later used to define link invariants, [J2]. This in turn led to invariants of 3-manifolds and to connections to conformal field theories, fusion categories

and quantum computing (see e.g. [Wi], [RT], [Wa], [We] and [F]). Some of these connections will be discussed below.

An important classification result for amenable subfactors of the hyperfinite II_1 factor was proved by S. Popa, [P1]. He showed that they can be reconstructed by what he calls the standard invariant; it is, however, still a wide open problem what values this standard invariant can take in general. The following topics are still very active areas in connection with subfactors, which were addressed in the workshop.

(a) *Conformal Field Theory and Subfactors*. Von Neumann algebras have appeared in algebraic quantum field theory for a long time, e.g. in the works of R. Haag, S. Doplicher, J. Roberts, R. Longo and others. More recently, a connection has also been established between Jones' subfactor theory and conformal field theory in the works by D. Evans, Y. Kawahigashi, R. Longo, A. Wassermann [Wa] and and others. Research in this direction has continued and has been reflected in talks by R. Longo on superconformal quantum field theory and by Y. Kawahigashi on super moonshine and operator algebras. Another talk by F. Xu dealt with mirror extensions, by which one can obtain a new net as 'mirror' from a given net.

(b) *Other constructions.* There are also constructions of subfactors via other methods. One of these yields the famous Haagerup subfactor, the irreducible subfactor of the hyperfinite II_1 factor of smallest known index > 4, [AH]. This subfactor was obtained from a list of possible standard invariants provided by U. Haagerup, [26]. It has been shown recently by M. Asaeda and S. Yasuda that only two standard invariants in these list actually do produce subfactors (which had been previously constructed in a joint paper of her with Haagerup). This result was presented at the Banff workshop.

(c) *Planar Algebras*. It is difficult to work directly with the standard invariant of a subfactor. A useful algebraic/combinatorial description of these invariants has been given by V. Jones in the context of planar algebras. New results in this context were presented in the workshop by D. Bisch about planar algebras of group-type subfactors and by V. Sunder. We also mention two talks here primarily dealing with the algebraic structure of subfactors, even though planar algebras do not explicitly appear in these results: In joint work with M. Izumi, P. Grossman gave a complete classification of quadrilaterals (i.e of subfactors with two intermediate subfactors whose intersection is the given subfactor). R. Burstein talked about a certain class of subfactors, constructed via Hadamard matrices, which turn out to be isomorphic to another class of subfactors constructed by D. Bisch and U. Haagerup by a completely different method.

(d) *Quantum Computing*. An approach for building quantum computers, going back to M. Freedman, is based on the theory of anyons; these are quasi-particles whose exchange statistics lies between bosons (phase $= 1$) and fermions (phase $= -1$). They can be studied in the framework of unitary topological quantum field theory and braid statistics, which are intimately related to the theory of subfactors. This approach and its connections to operator algebras were explained in the talk by Z. Wang. Moreover, E. Rowell talked about the role of unitary braid representations and of certain tensor categories in this field.

2. *Factors and groups.* One of the main problems in von Neumann algebras is the classification of II_1 factors. One can define an important class of examples of such factors from discrete groups acting on a measure space; this includes as a special case the group von Neumann algebra. One of the big questions in this context is how much the von Neumann algebra still remembers of the group from which it was constructed. Various invariants for II_1 factors have been introduced by A. Connes, e.g. [Co], and several deep results have been proved by him. He showed all the factors obtained from amenable groups are isomorphic to the hyperfinite II_1 factor. It is known that this factor is not isomorphic to the one obtained from a free group with n generators. It has been a longstanding unsolved problem to decide whether the factors obtained from the free groups with n and m generators respectively are isomorphic if n is not equal to m with both $n, m > 1$. This was one of the motivations for the creation of D. Voiculescu's free probability. There was another Banff workshop on free probability a few months prior to this one. So we shall concentrate on other developments in this context, primarily based on work by S. Popa and his collaborators.

The most exciting developments in the theory of von Neumann algebras in the last few years undoubtedly took place in connection with group theory. D. Gaboriau defined a notion of ℓ^2 Betti numbers for countable measure preserving equivalence relations in a Borel space, [Ga]. This proved a crucial tool in S. Popa's solution of a long-standing problem in von Neumann algebras, the construction of a II_1 factor with trivial fundamental group, [P2]. In addition Popa has continued proving exciting (super)rigidity results concerning group actions on probability spaces. More precisely, he shows for certain groups acting on probability spaces that an equivalence between their orbits already induces an equivalence between the groups themselves, e.g. [P3]. Popa's techniques have led to many new recent results in connections with von Neumann algebras coming from groups.

In particular, there are several new constructions of type II_1 factors with prescribed fundamental group. Talks about this were given by C. Houdayer and by S. Vaes (joint work with S. Popa), who use quite different approaches to tackle this problem.

N. Ozawa gave talks on his recent work [OP2] with Popa which contains several deep results on Cartan subalgebras for certain von Neumann factors. For instance, they show the nonexistence of Cartan subalgebras for the tensor product of a free group factor with a subfactor of any tensor product of free group factors, and they also show the uniqueness of the Cartan subalgebra (up to conjugacy) for certain measure space subfactors with respect to free group actions. These are consequences of a general result about the(non)existence of diffuse AFD sub von Neumann algebras in factors satisfying Haagerup complete metric approximation property. Further results in connection with discrete groups acting on measure spaces were presented in the talk by A. Ioana.

J. Peterson talked about von Neumann algebras closed under (Γ)-extensions, which leads to results on maximally injective subalgebras of von Neumann algebras. J. Asher gave a talk on an analog of the Kurosh subgroup theorem in the context of type III_1 factors.

There have been similarly exciting and related results within geometric group theory, e.g by Y. Shalom, N. Monod and A. Furman. We also had some interesting talks in this field:

R. Sauer talked about his joint work with U. Bader and A. Furman on l^1-orbit equivalence rigidity for hyperbolic lattices. Moreover, M. Pichot talked about Wise's non-Hopfian group and showed, among other things, that it has polynomial growth.

3. Other developments in von Neumann algebras. U. Haagerup gave a talk on the solution of the Effros-Ruan conjecture for bilinear forms on C^*-algebras. The methods in his joint work with M. Musat rely on classical type III von Neumann algebra techniques such as Tomita-Takesaki theory and properties of Powers factors, completely different to previous related results by Pisier and Shlyakhtenko. In another talk, Ken Dykema discussed a characterization of Connes' embedding problem in terms of a question of spectral distributions of a sum of certain self-adjoint elements in a II_1 factor.

We finally also mention two talks related to general classifications of von Neumann algebras. R. Sasyk shows (joint work with Tornquist) that von Neumann factors can not be classified using countable structure. G. Elliott presented his approach of studying pointed von Neumann algebras.

Presentation Highlights (following same thematic order as in the workshop schedule)

Day 1.

Speaker: **Narutaka Ozawa** (University of Tokyo)
Title: *On a class of II_1 factors with at most one Cartan subalgebra II*
Abstract: (Joint work with S. Popa.) We extend some of our previous result to a large class of discrete groups. This includes proving the non-existence of Cartan subalgebras for tensor products of a free group subfactor

with a subfactor Q of a tensor product of free group subfactors. We also show that several von Neumann algebras have at most one Cartan subalgebra. Here Haagerup's complete metric approximation property is still required.

Speaker: **Jesse Peterson** (University of California, Berkeley)
Title: *von Neumann subalgebras closed under (*Γ*)-extensions*
Abstract: Given a finite von Neumann algebra N, we will say that a diffuse subalgebra B is closed under (Γ)-extensions in N if whenever $P \subset N$ is a subalgebra with $P \cap B$ diffuse and $P' \cap N^\omega$ diffuse for some free ultrafilter ω then we have $P \subset B$. We show that if δ is a densely defined closable derivation into the Hilbert-Schmidt operators which is of the form $\delta(x) = [D, x]$, for some $D \in \mathcal{B}(L^2N)$ then $\overline{\ker(\delta)}$ is closed under (Γ)-extensions in N. In particular if $\overline{\ker(\delta)}$ is injective then it is maximal injective and we obtain generalizations of results of Popa and Ge on maximal injective subalgebras. Also by applying this result to derivations coming from group cocycles we show that if G is a countable discrete group with a proper ℓ^2-cocycle and if $H \subset G$ is an infinite maximal amenable subgroup then LH is maximal injective in LG.

Speaker: **Adrian Ioana** (University of California, Los Angeles)
Title: *On the subequivalence relations induced by a Bernoulli action*
Abstract: Let Γ be a countable group and denote by $\mathcal{S}$ the equivalence relation induced by the Bernoulli action $\Gamma \curvearrowright [0,1]^\Gamma$, where $[0,1]^\Gamma$ is endowed with the product Lebesgue measure. I will prove that for any subequivalence relation $\mathcal{R}$ of $\mathcal{S}$, there exists a partition $\{X_i\}_{i\geq 0}$ of $[0,1]^\Gamma$ with $\mathcal{R}$-invariant measurable sets such that $\mathcal{R}_{|X_0}$ is hyperfinite and $\mathcal{R}_{|X_i}$ is strongly ergodic (hence ergodic), for every $i \geq 1$. This is joint work with Ionut Chifan.

Speaker: **Jason Asher** (University of California, Los Angeles)
Title: *A Kurosh-Type Theorem for Type III Factors*
Abstract: We will present an extension of the Kurosh-Type Theorem of N. Ozawa to the case of the reduced free product of II_1 factors with non-tracial states. The argument will proceed via a generalization of S. Popa's intertwining-by-bimodules technique.

Speaker: **Zhenghan Wang**
Title: *Topological phases of matter: classification and application*
Abstract: Topological phases of matter are exotic states of matter with anyonic excitations such as the fractional quantum Hall (FQH) liquids. FQH liquids are described effectively by Witten's Chern-Simons theories. More general topological phases of matter are described by unitary TQFTs or unitary braided tensor categories. I will discuss the mathematical models for topological phases of matter, their emergence from electrons, classification and application to quantum computing.

Speaker: **Eric Rowell** (Purdue University)
Title:*Topological quantum computers: when universality fails*
Abstract: In the topological model for quantum computation, the computational power is controlled by the closed image of the braid group. Universal quantum computers correspond to dense images, while the weakest quantum computers correspond to finite images. We conjecture that finite images occur precisely when the categorical dimensions in the underlying braided category are square-roots of integers. I will present evidence for this conjecture and discuss its potential ramifications.

Day 2.

Speaker: **Roman Sauer** (University of Chicago)
Title:*l^1-orbit equivalence rigidity for hyperbolic lattices*
Abstract: (Joint work with Uri Bader and Alex Furman.) We say that two group actions are l^1-orbit equivalent if the corresponding cocycle satisfies a certain l^1-integrability condition. This l^p condition interpolates between the extreme cases $p = 0$ (usual orbit equivalence) and $p = \infty$ (implying quasi-isometry). We show that any group that is l^1-orbit equivalent to a lattice in $SO(n, 1)$ ($n > 2$) is also a lattice in the same Lie group, and the cocycle is cohomologous to a standard cocycle coming from this situation (i.e. it can be straightened). The methods involve a generalization of Thurston's proof of Mostow rigidity and new homological methods.

Speaker: **Mikaël Pichot** (Institut des Hautes Etudes Scientifiques (IHES))
Title: *On the Wise group*
Abstract: We will study D. Wise's non Hopfian group from an intermediate rank perspective and prove that it satisfies the Haagerup inequality (property RD), and in fact that it is of polynomial growth rank. This is joint work with S. Barre.

Speaker: **Cyril Houdayer** (University of California, Los Angeles)
Title: *Another construction of II_1 factors with prescribed countable fundamental group.*
Abstract: I will present another construction of such II_1 factors using free products of von Neumann algebras endowed with almost periodic states.

Speaker: **Dietmar Bisch** (Vanderbilt University)
Title: *The planar algebra of group-type subfactors*
Abstract: Haagerup and I introduced some 10 years ago a class of subfactors associated to outer actions of two finite groups. These subfactors play an important role in the theory, since they provide a very simple mechanism to construct irreducible subfactors whose standard invariant has infinite depth. We will review this construction and describe the planar algebra of these subfactors. We obtain natural IRF models in this way. This is joint work with Paramita Das and Shamindra Ghosh.

Speaker: **Roman Sasyk** (University of Ottawa)
Title:*On the (non)classification of factors*
Abstract: We show that the sets of factors of types II_1, II_∞, and III_λ, $0 \leq \lambda \leq 1$ on a separable Hilbert space are not classifiable using countable structures. Joint work with A. Tornquist.

Speaker: **Pinhas Grossman** (Vanderbilt University)
Title: *Pairs of Intermediate Subfactors*
Abstract: An intermediate subfactor is an algebra P in between two factors:$N \subset P \subset M$, where $N \subset M$ is an irreducible inclusion of factors with finite Jones index. For non-commuting pairs of intermediate subfactors, there is a rigidity to the inclusions which severely limits the number of possible configurations, in terms of the indices and the standard invariant. In particular, there are exactly seven non-commuting, irreducible quadrilaterals of factors whose sides have index less than or equal to 4. This is joint work with Masaki Izumi.

Day 3.

Speaker: **Uffe Haagerup** (University of Southern Denmark)
Title: *Solution of the Effros-Ruan conjecture for bilinear forms on C*-algebras*
Abstract: (Joint work with Magdalena Musat.) In 1991 Effros and Ruan conjectured that a certain Grothendieck type inequality for a bilinear form on a pair of C*-algebras holds if (and only if) the bilinear form is jointly completely bounded. In 2002 Pisier and Shlyakhtenko proved that this inequality holds in the more general setting of operator spaces, provided that the operator spaces in question are exact, in particular they proved the Effros-Ruan conjecture for pairs of exact C*-algebras. In a recent joint work with Magdalena Musat we prove the Effros - Ruan conjecture for general C^*-algebras (and with constant one), i.e. for every jointly completely bounded (jcb) bilinear form u on a pair of C^*-algebras A, B there exists states f_1, f_2 on A and g_1,g_2 on B, such that

$$|u(a,b)| \leq \|u\|_{jcb}(f_1(aa^*)g_1(b^*b) + f_2(a^*a)g_2(bb^*))$$

While the approach by Pisier and Shlyahktenko relied on free probability theory, our proof uses more classical operator algebra methods, namely Tomita Takesaki theory and special properties of the Powers factors of Type III_λ, $0 < \lambda < 1$.

Speaker: **Ken Dykema** (Texas A&M University)
Title: *Connes's embedding problem and Horn's inequalities*
Abstract: Connes's embedding problem asks whether every separable II_1-factor can be embedded in the

ultrapower of the hyperfinite II_1-factor; this is equivalent to asking whether every finite set in every II_1-factor has microstates. Bercovici and Li have related this to a question concerning the possible spectral distributions of $a+b$, where a and b are self-adjoint elements in a II_1-factor having given spectral distributions. We show that Connes' embedding problem is equivalent to a version of this spectral distribution question with matrix coefficients.

Speaker: **Stefaan Vaes** (Katholieke Universiteit Leuven) Title: *An action of the free group F_∞ whose orbit equivalence relation has no outer automorphisms*
Abstract: (Joint work with Sorin Popa.) We prove that there exist uncountably many stably orbit inequivalent, essentially free, ergodic, probability measure preserving actions of the free group with infinitely many generators such that their associated orbit equivalence relations have trivial outer automorphism group and trivial fundamental group.

Day 4.

Speaker: **Roberto Longo** (University of Rome Tor Vergata)
Title: *SUSY in the Conformal World*
Abstract: The talk concerns part of a recent joint work with S. Carpi and Y. Kawahigashi on the operator algebraic analysis of Superconformal Quantum Field Theory, with an initial step in the program of constructing Noncommutative Geometrical invariants for certain representations.

Speaker: **Feng Xu** (University of California, Riverside)
Title: *An application of mirror extension*
Abstract: Mirror extension is a general result about obtaining new nets as mirror of known ones. As an application of this result, in this talk I will discuss construction of new holomorphic conformal nets of central charge 24.

Speaker: **Richard Burstein** (University of California, Berkeley)
Title: *Subfactors Obtained from Hadamard Matrices*
Abstract: A subfactor may be obtained from a commuting square via iteration of the basic construction. For certain commuting squares coming from Hadamard matrices, the resulting subfactor may be described using the group construction of Bisch and Haagerup. We will show how this description allows us to find the principal graphs of these subfactors, and how it may lead to a full classification up to subfactor isomorphism.

Speaker: **Yasuyuki Kawahigashi** (University of Tokyo)
Title: *Super moonshine and operator algebras*
Abstract: We constructed an operator algebraic counterpart of the Moonshine vertex operator algebra with Longo before. Its automorphism group is the Monster group and its character is the modular elliptic j-function without the constant term. We now construct its "super" analogue for Conway's sporadic group Co_1, following work of Duncan for an enhanced super vertex operator algebra.

Speaker: **V.S. Sunder** (IMSc, Chennai)
Title: *Non-crossing partition $\simeq$ 2-cabled Temperley-Lieb*
Abstract: For each complex number $\delta \neq 0$, we consider a planar algebra whose space $NC_n(\delta)$ of 'k-boxes' has a basis consisting of non-crossing partitions of a set of $2k$ points, (usually thought of as being arrayed on two parallel lines, with k points on each line), and with multiplication and other planar algebra structure being defined almost exactly as in the case of the Temperley-Lieb planar algebra $TL(\delta)$. We show that this planar algebra $NC(\delta)$ is a C^*-planar algebra when $\delta > 4$. We do this by showing that $NC(\delta^2)$ is isomorphic to the so-called 2-cabling of $TL(\delta)$.

Speaker: **Marta Asaeda** (University of California, Riverside)
Title: *Non-existense of finite depth subfactors with certain small indices*
Abstract: (With S.Yasuda.) In 1991 Haagerup gave the list of graphs as candidates of principal graphs of subfactors with indices within $(4, 3+\sqrt{3})$. We prove that one of the parametrized series of the graphs are not realized as principal graphs except for the first two, using algebraic number theory.

Day 5.

Speaker: **George Elliott** (University of Toronto)
Title: Pointed von Neumann algebras

Speaker: **Narutaka Ozawa** (University of Tokyo)
Title: Cocycle super-rigidity and profinite actions
Abstract: (With Popa) First, I will briefly review the history of cocycle super-rigidity. Cocycle super-rigidity per se is a subject of ergodic theory, but I talk how von Neumann algebraic perspective helps in finding new examples of cocycle super-rigid actions, and present applications of the new examples to von Neumann algebras.

Scientific Progress Made

The meeting provided plenty of opportunity for participants to exchange ideas, some of which is expected to influence future publications. As a very concrete result, let us just mention a paper by Ozawa, posted at http://arxiv.org/abs/0804.0288 which was directly inspired by a question asked at BIRS by one of the participants, Asger Tornquist.

Final comments

As mentioned at the beginning, the workshop was very successful in bringing together many leading experts in von Neumann algebras as well as researchers from related areas. We think it provided an excellent reflection of the current exciting developments in this subject and its influences on/from other areas. This should be particularly helpful for the many younger researchers which attended our workshop.

We received positive comments and feedback about the meeting from many participants. So we believe that it was indeed stimulating and did contribute to further progress in our field.

List of Participants

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Asaeda, Marta (University of California, Riverside)
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Dean, Andrew (Lakehead University)
Dykema, Ken (Texas A&M University)
Dynov, Ivan (Max Planck Institute for Mathematics)
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Chapter 11

Elliptic and Degenerate Elliptic PDE, Systems and Geometric Measure Theory (08w5061)

Mar 30 - Apr 04, 2008

Organizer(s): David Cruz-Uribe (Trinity College), Steven Hofmann (University of Missouri-Columbia), Marius Mitrea (University of Missouri, Columbia), Salvador Perez Esteva (Universidad Nacional Autonoma de Mexico), Cristian Rios (University of Calgary), Eric Sawyer (McMaster University)

The workshop on Recent Developments in Elliptic and Degenerate Elliptic Partial Differential Equations, Systems and Geometric Measure Theory at BIRS was held from March 31 to April 4 of 2008. The workshop focused on the exciting recent advances in the theory of Elliptic, and Parabolic Partial Differential Equations with rough coefficients as well as equations and systems which fail to be elliptic in a traditional sense, due to various sources of degeneracy. Leading international researchers from related areas of expertise gathered at the BIRS Centre for a work week of scientific exchange. The participants consisted of mathematicians from Canada, United States, Mexico, France, Spain, Australia and China, they included some of the most distinguished mathematicians in the world as well as many of the top upcoming young researchers in the areas of interest on the workshop. There were great interactions both between senior and junior mathematicians and between experts in different areas that greatly benefited from the information gained and the contacts established. This kind of research interactions are crucial to the continuing development of the fields and the seeding of new approaches through the dissemination of techniques from different yet related disciplines. The combination of talks, informal discussions, scheduled social events, and the special environment of BIRS provided this opportunity. Because of the geographic diversity of the researchers in the field, bringing the participants together for the 5-day workshop strongly facilitate the dissemination of the most recent research ideas and results, which otherwise might not be possible. The atmosphere of the workshop and its surroundings may lead to new collaborations during the workshop and especially in the years following the workshop. Alan McIntosh (Centre for Mathematics and its Applications, Mathematical Sciences Institute, Australian National University, Canberra), one of the most prominent mathematicians in the field, personally testifies that ”this was not only an enjoyable workshop, the talks were of the highest order, and the mathematical discussions most helpful.”. The combination of the breadth and the cohesiveness of the field of Monge-Ampère type equations certainly has made the 5-day workshop at BIRS have significant impact on the field.

The workshop opened with a series of colloquium talks at an introductory level surveying the state of the art of important areas in Elliptic and Degenerate Elliptic PDEs. The plenary talks addressed specific topics and individual projects. The program also allocated time for short communications thereby maximizing the exposure opportunities for younger researchers that participated in the workshop.

Overview of the Topics

The mathematics of the Kato problem.

Given an elliptic second order operator in divergence form $\mathcal{L}$ with complex coefficients, the square root operator $\sqrt{\mathcal{L}}$ satisfies $\left\|\sqrt{\mathcal{L}}f\right\|_{L^2} \approx \|\nabla f\|_{L^2}$ for all f in $H^1(\mathbb{R}^n)$. The path originating from the very formulation of the conjecture and leading all the way to the recently obtained full solution of this major problem contains a wealth of innovative ideas and techniques, and opens new frontiers to explore [1]-[7]. Some of the themes orbiting around the Kato problem are: Heat Kernels, Evolutionary Equations, Operator Theory, Semigroup Theory, Functional Analysis, Functional Calculus, Holomorphic Calculus, Singular Integrals and Calderón-Zygmund theory, Riesz Transforms, and Carleson measure criteria (T1/Tb) for the solvability of boundary problems [2].

The degenerate Kato problem and related topics. It is natural to conjecture that the Kato square root problem could be generalized to operators with degenerate ellipticity, where the degeneracy is controlled by a weight in some Muckenhoupt class. Recent developments in this direction indicate that a suitable "Weighted Kato Conjecture" might indeed hold for certain degenerate elliptic operators. The battery of related questions arising in the context of the classical Kato problem can be phrased in the more general context when certain types of degeneracies are allowed. In this workshop we propose to discuss the state of the art of this area and explore the aforementioned issues.

Geometric measure theory and PDEs

The theory of uniformly rectifiable sets, and applications in elliptic and parabolic PDEs, and in the theory of quasiconformal mappings. Relationship between the geometry of a domain and the regularity of its harmonic measure. Free boundary regularity problems, singular sets. Following the ground-breaking work of Kenig-Toro on the regularity of the Poisson kernel in vanishing cord arc domains [9], and of David-Semmes on the singular integral operators and rectifiability [4], a naturally emerging direction is exploring the effectiveness of the method of layer potentials for BVPs in vanishing cord arc domains. Some of the participants in the workshop have already made substantial progress in this direction.

A priori regularity of solutions of subelliptic systems of equations

The Dirichlet problem. Systems with Infinite-degenerated ellipticity. Nash-Moser techniques, Campanato and Schauder methods are techniques originally developed to obtain a priori estimates and interior regularity for elliptic problems. These paradigms have evolved into more sophisticated, broad ranging, and powerful methods. Some examples are the treatment of quasilinear subelliptic systems satisfying Hormander's commutation condition (Xu and Zuily [16]), and recent generalizations to systems of the subelliptic regularity theorem by P. Guan [23].

Applications to Monge-Ampère equations

The n-dimensional Partial Legendre Transform (PLT) (Rios-Sawyer-Wheeden [15]) converts the Monge-Ampère (MA) equation into a system of equations. This is the first PLT-based technique to be successfully implemented to treat equations of MA type in dimensions higher than two since Alexandrov first used the PLT in the plane over half a century to that purpose. In this workshop recent applications of this technique to subelliptic and infinite degenerate MA equations will be presented. One goal is to explore possible generalizations of this approach to treat other degenerate nonlinear equations.

Presentation Highlights and Outcomes

In what follows we describe the reported outcomes from the meeting. This is not a comprehensive list of collaborations, ideas, and results developed as outcome of the activities held at the BIRS Centre during the week of the workshop, but just a sample of these scientific advancements. All participants were invited to contribute with their reports, what follows is the voices of those who answered.

1. Mikhail Safonov presented **new results,** even for the case $L = \Delta$.

   Theorem : A Oleinik-Hopf type lemma (Safonov 2008) Let $\Psi(\rho)$ be a non-negative, non-decreasing function on $[0, 1]$, such that
   $\Psi(0) = 0$ and $\Psi(1) < 1$, Denote

$$\Omega := \{x = (x', x_n) \in \mathbb{R}^n : |x'| < 1, \ \Psi(|x'|) < x_n < 1\},$$
$$\Gamma := \{x = (x', x_n) \in \mathbb{R}^n : |x'| < 1, \ \Psi(|x'|) = x_n\} \subset \partial\Omega.$$

   Let $n \times n$ matrices $a = [a_{ij}(x)]$ satisfy the uniform ellipticity condition, and let $b = [b_i(x)] \in \mathbb{R}^n$ be such that $|b| \in L^p(\Omega)$ with $p > n$. Let $u \in W^{2,n}_{loc}(\Omega) \cap C(\overline{\Omega})$ satisfy

$$u > 0, \quad Lu := (aD, Du) + (b, Du) = 0 \quad \text{in} \quad \Omega,$$

   and $u \equiv 0$ on Γ. Consider the quantities

$$I := \int_0^1 \frac{\Psi(\rho)\, d\rho}{\rho^2}$$

   and

$$0 \leq m := \liminf_{x_n \to 0^+} \frac{u(0, x_n)}{x_n} \leq M := \limsup_{x_n \to 0^+} \frac{u(0, x_n)}{x_n} \leq \infty.$$

   We claim: (i) If $I < \infty$, then $m > 0$. (ii) If $I = \infty$, then $m = 0$.
   Now consider the complementary domains, i.e. replace Ψ by $-\Psi$ in the definition of Ω and Γ.
   We claim: (i) If $I < \infty$, then $M < \infty$. (ii) If $I = \infty$, then $M = \infty$.
   Also, simple examples show that the above estimates for m and M may fail even for $\Psi \equiv 0$, when $Lu := \Delta + (b, Du)$ with $|b| \in L^n(\Omega)$.

2. Alan McIntosh presented his work done in collaboration with Pascal Auscher and Andreas Axelson, providing a direct proof of a quadratic estimate that plays a central role in the determination of domains of square roots of elliptic operators and, as shown more recently, in some boundary value problems with L^2 boundary data. The application to the Kato conjecture and to a Neumann problem was also developed. This quadratic estimate enjoys some equivalent forms in various settings. This gives new results in the functional calculus of Dirac type operators on forms.

Theorem (Auscher, Axelson, McIntosh 2008) Let n, m be positive integers, $\mathcal{H} = L^2(\mathbb{R}^n, \mathbb{C}^m)$ and D, B operators on $\mathcal{H}$ satisfying the requirements (H). Then one has the quadratic estimate

$$\int_0^\infty \left\| t^k BDI + t^{2k} BDBD)^{-1} u \right\|^2 \frac{dt}{t} \lesssim \|u\|^2, \qquad \text{for all } u \in \mathcal{H}.$$

H The following comprise the set of requirements (H):

- H1 The operator $D : \mathrm{D}(D) \longrightarrow \mathcal{H}$ is a homogeneous k^{th} order operator with constant coefficients.
- H2 D is self-adjoint.
- H3 D is strictly accretive on its range, i.e.

$$\left\| \nabla^k u \right\| \lesssim \|Du\|, \qquad \text{for all } u \in \mathrm{D}(D) \bigcap \overline{\mathrm{R}(D)}.$$

- H4 B is a bounded operator on $\mathcal{H}$.
- H5 B is strictly accretive on $\mathrm{R}(D)$: there is a constant $\delta > 0$ such that

$$\mathrm{Re}\,(BDu, Du) \geq \delta \|Du\|^2, \qquad \text{for all } u \in \mathrm{D}(D).$$

H6 (Off diagonal decay) For every Integer N there exists $C_N > 0$ such that

$$\left\|t^k BDI + t^{2k} BDBD)^{-1} u\right\|_{L^2(E)} \leq C_N \left[1 + \text{dist}\,(E,F)\,/t\right]^{-N} \|u\|$$

for all $t > 0$, whenever $E, F \subset \mathbb{R}^n$ are closed sets, $u \in \mathcal{H}$ satisfies support$u \subset F$.

3. Steve Hofmann and José M. Martell continue to work on *Extrapolation of Carleson measures and applications to divergence form elliptic operators*. Substantial progress was attained in this project during their meetings at the workshop [8].

4. Loredana Lanzani reported some progress was made during the workshop on her joint project with Ken Koenig: *Comparing the Szego ad Bergman projections on non-smooth planar domains*.

5. Michael Lacey, Eric Sawyer, and Ignacio Uriarte-Tuero continued their fruitful collaborations which sprouted in the previous months at the Fields Institute. While these authors were at the BIRS Centre they finalized important details on two major results. The paper [11] addresses an important question in quasi-conformal mapping. Astala famously showed sharp bounds for the distortion of Hausdorf dimension by quasi-conformal maps. Lacey,Sawyer, and Uriarte-Tuero show "a continuity in distortion" answering a question by Astala.
   In the paper [12], the same authors provide a novel characterization of two weight norm inequality for singular integrals. A fundamental question concerns the two-weight condition for the Hilbert transform. This work addresses the maximal truncations of the Hilbert transform.

   Abstract [11] (Lacey, Sawyer, Uriarte-Tuero 2008) We prove that the multiplier algebra of the Drury-Arveson Hardy space H_n^2 on the unit ball in $\mathbb{C}^n$ has no corona in its maximal ideal space, thus generalizing the famous Corona Theorem of L. Carleson in the unit disk. This result is obtained as a corollary of the Toeplitz Corona Theorem and a *new Banach space result*: the Besov-Sobolev space B_p^σ has the "baby corona property" for all $0 < \sigma < \frac{n}{p} + 1$ and $1 < p < \infty$.

   Abstract [12] (Lacey, Sawyer, Uriarte-Tuero 2008) Let and σ and ω be positive Borel measures on $\mathbb{R}^n$ and let $1 < p < \infty$. We characterize boundedness of certain maximal singular integrals $T_\natural$ from $L^p(\sigma)$ to $L^p(\omega)$ in terms of two testing conditions. The first applies to a restricted class of functions and is a strong-type condition,

$$\int_Q T_\natural(\chi_Q g\sigma)(x)^p \, d\omega(x) \leq C_1 \int_Q d\sigma(x), \qquad \text{for all } |g| \leq 1,$$

   and the second is a weak-type condition,

$$\int_Q T_\natural(\chi_Q f\sigma)(x) \, d\omega(x) \leq C_2 \left(\int_Q |f(x)|^p \, d\sigma(x)\right)^{\frac{1}{p}} \left(\int_Q d\omega(x)\right)^{\frac{1}{p'}},$$

   for all cubes Q in $\mathbb{R}^n$ and all functions $f \in L^p(\sigma)$ We also characterize the weak type two weight inequality in terms of the second condition.

6. David Cruz-Uribe, José M. Martell and Carlos Pérez worked on two projects while at BIRS. First, they continued to revise the manuscript for their book project, *Weights, Extrapolation, and the Theory of Rubio de Francia*. This research monograph is in two parts. The first part gives a new an extremely elementary proof of the classical extrapolation theorem of Rubio de Francia. Further, the authors have shown that this proof yields a number of powerful generalizations of extrapolation. The second part, further extends the ideas of their new proof to create a theory of extrapolation for two-weight norm inequalities. Though this has been done in the past, their approach is new and they are able to use their results to prove a number of new results for singular integrals, Riesz potentials, the dyadic square function, and the vector-valued maximal operator.

7. Cruz-Uribe, Martell and Pérez also discussed a new project: proving the Muckenhoupt conjecture for the two-weight, weak $(1,1)$ inequality for the Hilbert transform. In the early 1970's Muckenhoupt

conjectured that for any locally integrable, non-negative function u, there exists $C > 0$ such that for every $\lambda > 0$,

$$u(\{x \in \mathbb{R} : |Hf(x)| > \lambda\}) \leq \frac{C}{\lambda} \int_{\mathbb{R}} |f(x)| Mu(x)\, dx,$$

where H is the Hilbert transform and M is the Hardy-Littlewood maximal operator. Limited progress has been made on this problem to date, and there has been some uncertainty as to whether or not it is true. However, recent numerical work by H. Lepo (an undergraduate thesis student of Cruz-Uribe) suggests that this conjecture is true. Cruz-Uribe, Martell and Pérez discussed an early draft of Lepo's work and sketched some possible approaches to a proof of the conjecture.

8. Dorina Mitrea and Irina Mitrea initiated a collaboration [13] during the workshop which resulted in a paper that is now ready for publication. Let Ω be a bounded Lipschitz domain in $\mathbb{R}^n$ and let ν be the outward unit normal for Ω. For $\lambda \in [0, \infty]$, the Poisson problem for the Laplacian $\Delta = \sum_{i=1}^n \partial_i^2$ in Ω with homogeneous Robin boundary condition reads:

$$\begin{cases} \Delta u = f \quad \text{in} \quad \Omega, \\ \partial_\nu u + \lambda \text{Tr} u = 0 \quad \text{on} \quad \partial\Omega, \end{cases} \tag{11.1}$$

where $\partial_\nu u$ denotes the normal derivative of u on $\partial\Omega$ and Tr stands for the boundary trace operator. In the case when $\lambda = \infty$, the boundary condition in (11.1) should be understood as Tr $u = 0$ on $\partial\Omega$. The solution operator to (11.1) (i.e., the assignment $f \mapsto u$) is naturally expressed as

$$\mathbb{G}_\lambda f(x) := \int_\Omega G_\lambda(x, y) f(y)\, dy, \qquad x \in \Omega,$$

where G_λ is the Green function for the Robin Laplacian. That is, for each $x \in \Omega$, G_λ satisfies

$$\begin{cases} \Delta y G_\lambda(x, y) = \delta_x(y), \qquad y \in \Omega, \\ \partial_{\nu(y)} G_\lambda(x, y) + \lambda G_\lambda(x, y) = 0, \qquad y \in \partial\Omega, \end{cases}$$

where δ_x is the Dirac distribution with mass at x. We investigate mapping properties of the operator $\nabla \mathbb{G}_\lambda$ when acting on $L^1(\Omega)$. In this regard, weak-L^p spaces over Ω, which we denote by $L^{p,\infty}(\Omega)$, play an important role. The following theorem summarizes the regularity results obtained.

Theorem (Mitrea-Mitrea 2008) Let Ω be a bounded Lipschitz domain in $\mathbb{R}^n$ and fix $\lambda \in [0, \infty]$. Then

$$\nabla [G_\lambda(x, \cdot)] \in L^{\frac{n}{n-1},\infty}(\Omega) \qquad \text{uniformly in } x \in \Omega.$$

In particular,

$$\nabla \mathbb{G}_\lambda : L^1(\Omega) \to L^{\frac{n}{n-1},\infty}(\Omega) \qquad \text{is a bounded operator.}$$

9. David Cruz-Uribe and Cristian Rios continued their work on the Kato problem for degenerate elliptic operators. They made the final revisions on their paper *Gaussian bounds for degenerate parabolic equations* [5], in which they proved that if $\mathbf{A}$ is a real symmetric matrix that satisfies the degenerate ellipticity conditions

$$\begin{cases} \lambda w(x) |\xi|^2 \leq \text{Re} \langle \mathbf{A}\xi, \xi \rangle = \text{Re} \sum_{i,j=1}^n A_{ij}(x) \xi_j \bar{\xi}_i, \\ |\langle \mathbf{A}\xi, \eta \rangle| \leq \Lambda w(x) |\xi||\eta|, \end{cases}$$

where w satisfies the Muckenhoupt A_2 condition, and if $L_w = -w^{-1}\text{div}\mathbf{A}\nabla$, then the heat kernel of the operator e^{-tL_w} satisfies Gaussian bounds. They also began to prove that L^∞ complex perturbations of such matrices have the same property. The existence of Gaussian bounds plays a key role in proving a special case of the Kato problem for degenerate elliptic operators: proving that if $w \in A_2$,

$$\|L_w^{1/2} f\|_{L^2(w)} \approx \|\nabla f\|_{L^2(w)}.$$

Cruz-Uribe and Rios have been able to extend the groundbreaking proof of Auscher, *et al.* of the Kato problem for uniformly elliptic operators to the degenerate case assuming Gaussian bounds.

10. Sawyer and Rios finished the final details on paper describing the existence and regularity of radial solutions to Monge-Ampère equations. This work exhausts the final open problems on radial Monge-Ampère equations with right hand side vanishing to infinite order, moreover, generalized solutions are considered instead of classic solutions. The characterization of regularity is beautiful in its simplicity:

    Theorem (Rios and Sawyer 2008) Suppose that u is a generalized convex radial solution (in the sense of Alexandrov) to the generalized Monge-Ampère equation $\det D^2u = k(x, u, Du)$ with

    $$k(x, u, Du) = f\left(\frac{|x|^2}{2}, u, \frac{|\nabla u|^2}{2}\right)$$

    where f is smooth and nonnegative on $[0, 1) \times \mathbb{R} \times [0, \infty)$. Then u is smooth in the deleted ball $\mathbb{B}_n \setminus \{0\} = \{0 < |x| < 1\}$.

    Suppose moreover that there are positive constants c, C such that

    $$cf(t, 0, 0) \leq f(t, \xi, \zeta) \leq Cf(t, 0, 0) \tag{11.2}$$

    for (ξ, ζ) near $(0, 0)$. Let $\tau \in \mathbb{Z}_+ \cup \{\infty\}$ be the order of vanishing of $f(t, 0, 0)$ at 0. Then u is smooth at the origin if and only if $\tau \in n\mathbb{Z}_+ \cup \{\infty\}$.

This paper has been subsequently **accepted for publication**n at Proceedings of the AMS.

11. Sawyer and Rios also started a new project on regularity of solutions to degenerate Monge-Ampère equations. Building on a method due to Caffarelly, subsequently applied by Daskalopoulos, and O. Savin to characterize regularity and type of solutions to the degenerate Monge-Ampère **in the plane** $\det D^2u = |x|^\alpha$, with $\alpha > -2$, there is hope to generalize these results to higher dimensions via the n-dimensional partial-Legendre transform of Rios-Sawyer-Wheeden, and the use of some new (yet to be established) a priori regularity results for quasilinear equations with some special structure.

Final Conclusions

The workshop on Recent Developments in Elliptic and Degenerate Elliptic Partial Differential Equations, Systems and Geometric Measure Theory at BIRS was a great success. Every single participant expressed their individual delight with their experience at the workshop, and in particular there were numerous testimonials of admiration for the modality in which the BIRS Centre enables and promotes scientific exchange – distinctly between mathematicians – by providing an environment brilliantly designed for such purpose. The outcomes from this workshop will not only be measured in the several papers and preprints already existing and coming in the near future, but more importantly in the long term collaborations and projects that germinated from this propitious gathering of top researchers in related areas of interest.

One of the factors that was instrumental in the success of this particular workshop was the low rate of scheduled talks in relation to unscheduled social time. The organizers took special care in allowing for plenty of free discussion sessions and social activities. The fact is that top scientists use ”spare time” for brain-storming of ideas, and allowing the time and space for this phenomenon brought about the most fruitful exchanges. The scheduled talks started moving the ideas to the front of the scene, and the free time afterwards was effectively used to push forward new problems and projects; with great results already materialized and many more to come.

As a final remark, there was an unanimous feeling by the whole body of participants and organizers that it would be in the best interests of the field to offer continuation workshops at regular intervals of time. The discipline of Partial Differential Equations is continuously evolving and there is no doubt that revisiting the experience at two or three year intervals would multiply the fruits of scientific advances already in motion thanks to the powerful inspirational opportunity offered by the BIRS Centre.

List of Participants

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Chapter 12

Geometric flows in Mathematics and Physics (08w5110)

Apr 13 - Apr 18, 2008

Organizer(s): Gerhard Huisken (Max-Planck-Institute for Gravitational Physics), Todd Oliynyk (Monash University), Eric Woolgar (University of Alberta)

Overview of the Field

The workshop on Geometric Flows in Mathematics and Physics was held 13–18 April 2008. The area is presently quite active. This was the second such workshop, the first having been held at the Albert Einstein Institute in Potsdam in November 2006. Participants in the BIRS workshop co-organized two subsequent workshops on the topic in Europe in the Autumn of 2008 and will hold another in 2009.

Cross-disciplinary interest in geometric flows is not new. Much of this interest first arose in general relativity. Geroch proposed what became known as the inverse mean curvature flow in the early 1970s as a way to address the positive mass conjecture, now a theorem. Eventually, in the late 1990s, Huisken and Ilmanen were successful in applying this approach to prove a conjecture of Penrose supporting the cosmic censorship hypothesis. The Calabi flow also arose in relativity in the study of Robinson-Trautman metrics.

Other geometric flows were known to be important in the physics of quantum field theory and string theory. Both the mean curvature flow and the Ricci flow arise as approximations to renormalization group flow in quantum field theory. It is therefore of little surprise that the spectacular development of the mathematics of Ricci flow in this decade, much of it due to Perelman's work in completing Hamilton's approach of applying the Ricci flow to prove the Poincaré conjecture, has generated much interest and a good deal of activity amongst physicists.

Presentation Highlights

The workshop opened with the mathematics of the Ricci flow. In the first talk, Huai-Dong Cao gave an introduction to and summary of much of the recent progress in the Ricci flow and Kähler-Ricci flow. Cao was able to present recent advances in a way that was comprehensible to the diverse audience. This was very helpful to all, especially the physics side of the audience, and was an excellent way to open the meeting. We then moved on to two shorter in-depth talks. Lei Ni discussed ancient Type I solutions of the Ricci flow. Miles Simon then described Ricci flow for nonsmooth metrics. He considered non-negatively curved metric spaces which arise as limits of smooth Riemannian manifolds (M_i, g^i), $i \in N$, whose Ricci curvature is bigger than $-1/i$, whose diameter is less than d_0 (independent of i), and whose volume is bigger than $\nu_0 > 0$ (independent of i). He showed that a solution to Ricci flow of such a space exists for a short time, that the solution is smooth for $t > 0$, and has $\mathrm{Ricci}(g(t)) \geq 0$ and $\mathrm{Riem}(g(t)) \leq c/t$, $t \in (0, T)$ for (for some constant $c(\nu_0, d_0, n)$). This allows him to classify the topological type and the differential structure of the limit manifold.

The first afternoon was occupied with talks by physicists. Holzegel and Warnick described their joint work (also joint with Schmelzer). First Holzegel introduced some basic concepts of Euclidean quantum gravity and Black Hole Thermodynamics and explained how the Ricci flow can be used as a tool to address questions arising in this subject. Warnick then described numerical simulation of a Ricci flow connecting 4-dimensional Euclidean Taub-NUT and Taub-Bolt geometries considered as infilling a homegeneously squashed 3-sphere with fixed boundary metric. The flow may develop a singularity in finite time, which is resolved using a surgery. Bakas described how the Calabi flow on a 2-sphere, which arises as the Einstein equation for a Robinson-Trautman metric in General Relativity, describes a non-equilibrium process in the fluid induced on the boundary of a perturbed Kottler spacetime in a box. The final talk of the first day was given by Carfora, who spoke about the nice properties of the linearized conjugate Ricci flow, and the application of this to deformed initial data sets in Einstein cosmology.

Tuesday morning consisted of lectures on the renormalization group (RG) in quantum physics and string theory models. Dan Friedan, one of the inventors of the field, gave an introduction to the subject, stressing how ancient solutions of the Ricci flow define good Quantum Field Theories. He was followed by David Morrison, who brought the audience up to date on supersymmetric and string theoretic aspects. Jack Gegenberg spoke on the fixed points of RG flow with the full complement of fields present in heterotic string theory, including a tachyon field. These fixed points include all 8 Thurston model geometries. In the afternoon, V Suneeta spoke about the stability of Anti-de Sitter spacetime under RG flow. Xianzhe Dai described his work with Li Ma on asymptotically locally Euclidean Ricci flows and the evolution of mass. P Miao discussed his recent work with H Bray in which they use mean curvature flow to find an inequality relating the mass and the so-called capacity of a Riemannian manifold. The last talk of the day was by J-F Li on quermassintegral inequalities.

Wednesday morning Robert Bartnik spoke on his work on the ellipticity of so-called geometric boundary conditions for Ricci curvature operators. This is expected to be very important for the case of Ricci flow on manifolds with boundary. An important question it to find elliptic boundary conditions for such a Ricci flow. It appears that requiring the induced metric and mean curvature to match along the boundary will work. T Lamm then described approximation methods for solutions to geometric variational problems, such as harmonic maps and Willmore surfaces. Jeff Streets spoke on his Yang-Mills-Ricci flow and connection Ricci flow, which is related to RG flow in string theory with an anti-symmetric B-field. There were no talks scheduled for the afternoon.

Thursday morning was primarily concerned with the mathematics of flows other than the Ricci flow. Natasa Sesum described her recent results, obtained with Daskolopoulos and Hamilton, on ancient, convex, closed solutions to the curve shortening flow. She then described her work on a class of extrinsic curvature flows that generalize the curve shortening and mean curvature flows. Stephen Anco then spoke on his work on Hamiltonian integrability.

Maria Athanassenas opened the afternoon session with a talk on the volume-preserving mean curvature flow. This is the mean curvature flow of a bounding hypersurface, normalized so that the enclosed volume is constant. For an axisymmetric configuration with sufficiently large enclosed volume, the flow exists for all time and converges. Athanassenas has been able to show that, conversely, pinching off occurs when the enclosed volume is sufficiently small. She and a student are exploring the intermediate region. Jan Metzger then discussed his work with Lars Andersson on marginally trapped surfaces. These are surfaces that provide a quasi-local definition of the global concept of a black hole horizon in general relativity. He presented an existence theorem for such surfaces in the presence of suitable barriers and discussed the application of the existence theorem to prove an area bound for outermost marginal surfaces. This implies that a certain subclass of marginal surfaces is compact which in turn yields the existence of the unique outermost marginal surface. The final talk of the workshop was given by Felix Schulze, who considered convex symmetric, lens-shaped networks that evolve under curve shortening flow. He showed that the enclosed convex domain shrinks to a point in finite time. Furthermore, after appropriate rescaling, the networks converge to a self-similarly shrinking network, which he showed to be unique in an appropriate class.

Outcome of the Meeting

One of the most important aspects of these meetings has been that mathematicians and physicists have been able to identify common areas of interest. One example has been ancient solutions of the Ricci flow. In 3-dimensions, these play an important role in understanding singularities of the Ricci flow, so that surgery can be implemented. But in any dimension, ancient solutions allow physicists to define good quantum field theories. A second outcome has been that the number of physical applications of geometric flows appears to be growing. An example of this is the application to black holes described in the talks of Holzegel and Warnick.

The meeting succeeded in stimulating a good deal of ongoing research. The organizers are aware of at least two ongoing collaborations that began at the workshop, as well as two additional workshops in the autumn which were inspired by our meeting.

The organizers' own work was advanced at this meeting. We were able to collaborate on a geometric flows approach to a conjecture of Bartnik regarding the definition of quasi-local mass in relativity, and also to begin discussions on a possible approach on another physics conjecture, the generalized positive mass conjecture of Horowitz and Myers.

In each of these collaborations, both mathematicians and physicists are playing a role. That is, we think, the most important outcome of the meeting. It has opened avenues of communication between the two disciplines in what is presently a rapidly evolving area.

List of Participants

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Chapter 13

Dynamics of structured populations (08w5031)

Apr 20 - Apr 25, 2008

Organizer(s): Thomas Hillen (University of Alberta), Frithjof Lutscher (University of Ottawa), H. Thieme (Arizona State University), Pauline van den Driessche (University of Victoria)

Overview of the Field

Overview

In order to accurately describe and fully understand the dynamics of populations, one needs to consider the different stages and functions of individuals as well as their spatial distribution. It is particularly challenging to model and analyze the interplay between stage structure and movement ability. The resulting mathematical equations are in the form of systems of (partial) differential equations, functional differential equations, integro-differential equations, difference equations or integral equations.

This 5-day workshop provided a unique opportunity to bring together specialists from different fields to discuss recent progress in the qualitative analysis of structured population models, with regards to pattern formation, front propagation, and bifurcation phenomena. Special attention was given to the applications in spread and control of epidemic diseases, invasion and persistence in ecological systems as well as in biomedical and cancer modeling.

Objectives

A standard method in the mathematical modeling of populations and their interactions is to model the populations as whole entities and derive equations for all relevant classes. This method typically leads to systems of ordinary or partial differential equations. While their exploration continues, the qualitative behavior of these models and their relevance to biological applications is fairly well understood. Ongoing biological research provides us with more detailed insight into the structure of populations and the individual behavior of its members. To include these biological details into more refined models is a chance and a challenge.

For example, the larval stages in mosquitoes can be included into a new model for West-Nile Virus, the social order in wolf packs can be included into models for home-range formation, or the cell reproduction cycle can be included into tumor growth and treatment models. Typical structure variables are age, size, stage, function, spatial location, genotype, or phenotype. A combination of one or more of these structure variables into a model leads to systems of reaction-diffusion equations, integro-difference and integro- differential equations, integral equations, matrix models, hyperbolic and parabolic partial differential equations, and stochastic processes. The methods for analyzing these structured population models are based on linear algebra, dynamical system theory, and the theory of ordinary and partial differential equations.

During this workshop we focused on three main topics of structured population modeling:

1. Theory of structured populations
2. Spatial models
3. Epidemiology and diseases

Theory of structured populations

Population structures result from the simple fact that individuals are different with respect to age, stage, size, gender, and location. Structure can also be generated by the involvement of many species like host, vector and parasite in an epidemic model or of multiple parasite strains. Structured population models are a suitable intermediate between abundance models and agent-based models. The conference presented an update on the development of an encompassing theory which occurred during the last 25 years. This theory is based on linear and nonlinear functional analysis, notably the theory of dual operator semigroups and their nonlinear perturbation. It allows a relatively easy study of stationary population states, their stability, and the bifurcation of other stationary states or periodic solutions. The bifurcation is intimately linked to mathematical or biological threshold parameters like the spectral bound (or radius in discrete time) of the linearized system or a basic reproduction number. Different reproduction numbers seem to be possible depending on the biological emphasis though they share the same threshold characteristics. Fortunately convenient graph-theoretic methods are available to calculate the reproduction numbers if there are finitely many distinct individual stages.

The use of the general theory was illustrated in discussing evolutionary trends in endophyte metapopulation models. Structured population models have the advantage to make important population dynamic parameters explicit, and the sensitivity of the model dynamics to these parameters becomes an important and sometimes daunting task. In stage-structured models the sensitivity analysis can be performed through novel approaches based on matrix calculus.

Spatial models

Since the 1970's, the classical models for spatial spread of populations in the form of reaction-diffusion equations have been studied widely and applied successfully to many different questions in biology. However, their applicability to certain biological systems is limited and new approaches are needed. Alternative models in the form of hyperbolic transport equations or parabolic/hyperbolic Fokker-Planck equations structure the population into velocity classes and describe how individuals change velocity. These models have received much attention, and their relationship to the classical reaction-diffusion models is fairly well understood through scaling and moment closure methods.

Another recent development in modeling spatial spread of populations is to incorporate different compartments for different modes of movement or even a compartment for non-moving individuals. These models capture biologically diverse phenomena such as seeds being transported by wind and by birds, animals and cells stopping their movement to reproduce, and proteins in the cell nucleus undergoing binding-unbinding events with immobile cell structures. Mathematically speaking, these structured models come in the form of integro-differential or integro-difference equations (with mixed dispersal kernels), integral equations, and as systems of coupled partial and ordinary differential equations. It is known that dividing the population into compartments with different movement characteristics can significantly alter the models predictions, e.g., regarding invasion speeds and stability.

While there is an overwhelmingly rich qualitative mathematical theory available for reaction-diffusion equations, a similarly complete theory for these alternative structured models is only just emerging. One focus of this workshop was on novel developments of the qualitative theory of spatially structured population models. Advances in this area help in the choice of the most appropriate model for different applications in biology, such as the dynamics of the immune system, the epidemic spread of an infectious disease, and the invasion of microbes.

Epidemiology and diseases

The transmission characteristics of newly emerging diseases, such as SARS, West Nile Virus, and AIDS, are quite different from the local periodic outbreaks of "classical" infectious diseases, such as childhood diseases, and new models and methods are discussed to describe and analyze these outbreaks. Spatial heterogeneity is an important factor to consider in the spread of many diseases, e.g., influenza. Models for realistic vaccination schedules usually require the inclusion of the population age structure, in particular if antiviral doses are limited. Infection-age is a crucial structural variable in models for the emergence and spread of antibiotic-resistant bacteria, be it in the treatment of tuberculosis or the prevention of hospital-acquired infections.

When no vaccine is available (e.g., SARS) control by isolation and/or quarantine can be built into a model. In particular, in light of the threats of terrorism, there is an increased need to understand and to model spatial spread of epidemics as well as optimal vaccination strategies and control. Among other things, this modeling requires a blending of different mathematical techniques and the embedding of these epidemic models into a more general class of structured population models, as they have been discussed at our workshop.

Mathematical modeling in medicine has become a major focus of research and has contributed new insights into medical processes on the individual, cellular and intra-cellular level. The techniques and analytical methods, originally developed in the context of population dynamics, are now being extended to medical applications. For example, transport equations play a role for the conduction of nervous impulses, hyperbolic models are used to model movement of leucocytes, and reaction-diffusion equations are used to model embryonal development, wound healing, and angiogenesis in cancer. The relevant population structures include the cell reproduction cycle, the circadian rhythm, the age of an organ or tissue and the stages in cell development (for example six stages are involved in the modeling of stem cell differentiation into blood cells). Again, ordinary and partial differential equations and integro-differential equations are the major tools for biomedical modeling. Questions of interest include pattern formation (in development), persistence (in cancer) and control (in diseases and in the immune system). During this workshop we emphasized the extension of the existing mathematical modeling methods to biomedical applications. We focused on new questions and therapies that make use of structured population modeling, for example taking account of the cell reproduction cycle in chemotherapy treatment planning. Furthermore, we discussed modeling and implications of resistant bacterial strains.

Presentations of Recent Developments

Some participants were selected to give either 20 or 40 minute talks, which were grouped into sessions according to the three overarching themes of the workshop. One outstanding full-hour lecture was given by Karl Hadeler on past, present and future research on transport equations and quiescent states. The workshop allowed younger researchers and postdocs to present their results and experienced researchers to present an overview of their work. All the presentations were of very high quality and stimulated interesting discussions, some leading to new collaborations. Speakers and abstracts of contributed talks are listed below in alphabetical order:

Lora Billings
ADE in multi-strain disease models
As we increase our resources to fight disease, pathogens become more resilient in their means to survive. One example is antibody-dependent enhancement (ADE), a phenomenon in which viral replication is increased rather than decreased by immune sera. We study the complex dynamics induced by ADE in multi-strain disease models and investigate the effects of vaccine campaigns. In particular, we study the consequences of using single-strain vaccines, which would increase the virulence in other infections.

Thanate Dhirasakdanon
A sharp threshold for disease persistence in host metapopulations
A sharp threshold is established that separates disease persistence from the extinction of small disease outbreaks in an SEIRS type metapopulation model where the travel rates between patches can depend on disease prevalence. The threshold is formulated in terms of a basic replacement ratio (disease reproduction number), R_0, and, equivalently, in terms of the spectral bound of a transmission and travel matrix. Since frequency-

dependent (standard) incidence is assumed, the threshold results do not require knowledge of asymptotic behavior of disease-free dynamics. As a trade-off, for $R_0 > 1$, only uniform weak disease persistence is shown in general, while uniform strong persistence is proved for the special case of constant recruitment of susceptibles into the patch populations. For $R_0 < 1$, Lyapunov's direct stability method shows that small disease outbreaks do not spread much and eventually die out. (joint work with H.R. Thieme and P. van den Driessche)

Hal Caswell
Some new sensitivity analyses of matrix population models
Sensitivity analysis of growth rates in linear structured population models is well-developed and frequently used. Sensitivity analysis of other demographic properties, and of nonlinear models, is not as well understood. I will present some new approaches, based on matrix calculus, that make the analyses easy. With examples, of course.

Odo Diekmann
How to miss a key point for 25 years, but see it at last?
The real contents of the lecture would be: how to represent the state of a structured population? Answer : by way of the history of the population birth rate and the history of the environmental interaction variables (even though logic suggests to use a distribution over the state space of individuals). Motivation: with this choice of p-state space the sun-star theory of delay equations applies (and so a wealth of results comes for free).

Kevin Flores
Modeling the Progression of Malignancy in Cancer
There is strong biological evidence for the selection of cells with malignant phenotypes in the progression of many cancers. Selection of a phenotype is associated with particular molecular or genetic abnormality and an extracellular environment that makes such an alteration favorable. In this talk we propose 2 structured models of such a scenario in 2 structurally distinct cancers. We first describe the simplest example of this mechanism of selection in a model of Chronic Myelogenous Leukemia, where the selection is artificially imposed by the drug Gleevec and the selection is for resistant phenotypes. We then describe a model of Colon Cancer progression, where cell differentiation and cycle time are taken into account using distinct differentiation classes and cycle-age structure, respectively; we will hypothesize that this model can be used to describe the selection for p53 gene mutants under competition for oxygen and show how it can be used to model cell cycle specific chemotherapy.

Cindy Greenwood
Stochastic effects in SIR modeling
A number of stochastic effects in the SIR epidemic model are important even when populations are large, e.g. bimodality of epidemic size distributions, stochastically sustained oscillations in numbers of infective individuals. I have recently written a book chapter on this.

Mats Gyllenberg
Ecology and evolution of symbiosis in structured metapopulations
We present a model for symbionts in plant host metapopulation. Symbionts are assumed to form systemic infection throughout the host and pass into the host seeds, but also to reproduce and infect new plants by spores. Thus, we study a metapopulation of qualitatively identical patches coupled through seeds and spores dispersal. Symbionts that are only vertically inherited cannot persist in such a uniform environment if they lower the host's fitness. They have to be beneficial in order to coexist with the host if they are not perfectly transmitted to the seeds, but evolution selects for 100 fidelity of infection inheritance. In this model we want to see in what way mixed strategies (both vertical and horizontal infection) affect the coexistence of uninfected and infected plants at equilibrium; also, what would evolution do for the host, for the symbionts and for their association. We present a detailed classification of the possible equilibria with examples. The (in)stability of the steady states is investigated using resent results by Diekmann, Gyllenberg & Getto (SIAM J. Math. Anal. 2007). This talk is based on joint work with Diana Preoteasa.

K.P. Hadeler

Transport Equations and Quiescent States

Moving organisms perform complicated walks which can be described by transport equations modeling changing velocity, turning events etc. On a larger/longer scale, such movements appear as diffusion. Several mathematical problems appear quite natural: How do the known results on reaction diffusion equations translate into transport equations? How to get diffusion approximations to transport equations and perhaps a hierarchy of intermediate approximating equations.

Transport equations can be seen in the wider framework of coupled systems (velocity states are coupled by turning events) and (some) diffusion approximations can be seen as singular perturbation problems. Also dynamics with quiescent phases fit into this framework of coupled systems (quiescence may appear as absence of motion or absence of any non-trivial dynamics). For systems with quiescent phases an outline of an emerging coherent theory is given.

Fred Hamelin

A differential game theoretical analysis of mechanistic models for territoriality

In this paper, elements of differential game theory are used to analyze a spatially explicit home range model for interacting wolf packs. The model consists of a system of partial differential equations whose parameters reflect the movement behavior of individuals within each pack and whose solutions describe the patterns of space-use associated to each pack. By controlling the behavioral parameters in a spatially-dynamic fashion, packs adjust their patterns of movement so as to find a Nash-optimal balance between spreading their territory and avoiding conflict with hostile neighbors. On the mathematical side, the game let appear some of the few singularities never observed in nonzero-sum games. From the ecological standpoint, one recognizes in the resulting evolutionarily stable equilibrium a buffer-zone, or a no-wolf's land where deers are known to find refuge. Territories overlap arises as a singular solution. Scent-marking is not yet incorporated into the model. (joint with Mark Lewis)

Alan Hastings

Persistence of structured populations

Many populations are structured by space or stage. We derive a biologically interpretable persistence condition for these systems using ideas from M-matrices. We show that persistence of such a population consisting of subpopulations depends on whether the sum of the reproductive gains through all possible closed, between-patch reproductive paths through multiple generations, relative to the shortfall in self-persistence in each path, exceeds unity. This provides the basis for evaluating connectivity and habitat heterogeneity to understand marine reserve design, the collapse of marine fisheries and other conservation issues and understanding of the dynamics of structured populations. We extend these results to look at conditions for growth rates other than 1 (persistence), and for continuous time models. We also consider particular applications of these results.

Frank Hilker

Epidemiological models with Allee effect

Infectious disease models have traditionally focused on epidemics that run over a relatively short time scale. The host population size can therefore be assumed constant. This talk addresses host populations with a strong Allee effect (i.e., there is a critical threshold size below which population growth is negative). Endemic diseases which lead to a reduction in population size could drive the host below the Allee threshold and thus to extinction. The interplay between infection and demographics can lead to a rich dynamical behaviour, including tristability, limit cycle oscillations and homoclinic bifurcations. Due to the model's structural simplicity, it is amenable to phase plane analysis. The bifurcation behaviour is investigated by numerical continuation. Implications for disease control and conservation management are discussed.

Petra Klepac

Matrix models for stage-classified epidemics

Petra Klepac, Hal Caswell, Michel Neubert

The demographic time-scale is usually very different from the epidemic time-scale, so most models focus either on demographic or epidemic questions. But most infectious diseases affect different stages of the host population in a different way, so the model should incorporate both realistic demographic and epidemic detail. To allow for demographic detail in each epidemic compartment, we have constructed a matrix model by generalizing the vec-permutation matrix approach to spatial models, developed by Hunter and Caswell, to a model that classifies individuals by demographic stage and epidemiological status. We find that the combined matrix model changes the dynamics of its building blocks; a simple demographic model and the basic SIR model, and show how to do sensitivity analysis for such a model.

Mark Lewis
First passage time: insights into animal movement
Hannah W. Mckenzie, Mark A. Lewis, and Evelyn H. Merrill
Movement plays a role in structuring the interactions between individuals, their environment, and other species. First passage time is a novel way of understanding the effect of the landscape on animal movement and search time. In the context of animal movement, first passage time is the time taken for an animal to reach a specified site for the first time. We derive a general first passage time equation for animal movement that can be connected with empirical data. This equation is related to the Fokker-Planck equation, which is used to describe the distribution of animals in the landscape. To illustrate the first passage time method we consider three examples. First we show how territorial behavior affects the time required for a red fox to locate prey throughout its territory. Second, we discuss the effect of two different searching modes on the functional response and show that random searching leads to a Holling type III functional response. Third we show how detailed GPS data for wolf movement can be coupled to a first passage time model and used to assess the impact of linear habitat features such as roads on the time taken to locate prey. First passage time analysis provides a new tool for studying the influence of animal movement on ecological processes.

Pierre Magal
P-gp transfer and acquired multi-drug resistance in tumors cells
Pierre Magal, Frank Le Foll, Jennifer Pasquier, Glenn Webb, Peter Hinow
Multi-Drug resistance for cancer cells has been a serious issue since several decades. In the past, many models have been proposed to describe this problem. These models use a discrete structure for the cancer cell population, and they may include some class of resistant, non resistant, and acquired resistant cells. Recently, this problem has received a more detailed biological description, and it turns out that the resistance to treatments is due in 40 of cancers to a protein called P-glycoprotein (P-gp). Moreover it has been proved that P-gp can be transferred from cell to cell by an osmotic phenomenon. This transfers turn to be responsible for the acquired resistance of sensitive cells. The goal of this talk is to introduce this problem, and to present a cell population dynamic model with continuous P-gp structure.

Andrew Nevai
Sluggish susceptibles and the endemic equilibrium in three related disease models
I will compare and contrast properties of the endemic equilibria in three related SIS disease models. In each model, suspectibles move slower than infectives through spatially heterogeneous habitats.

Shigui Ruan
Travelling Wave Solutions in Multi-group Age-Structured Epidemic Models
Age-structured epidemic models have been used to describe either the age of individuals or the age of infection of certain diseases and to determine how these characteristics affect the outcomes and consequences of epidemiological processes. Most results on age-structured epidemic models focus on the existence, uniqueness, and convergence to disease equilibrium of solutions. In this paper we investigate the existence of travelling wave solutions in a deterministic age-structured model describing the circulation of a disease within a population of multi-groups. Individuals of each group are able to move with a random walk which is modelled by the classical Fickian diffusion and are classified into two subclasses, susceptible and infective. A susceptible individual in a given group can be criss-cross infected by direct contact with infective individuals of possibly any group. This process of transmission can depend upon the age of the disease of infected individuals. The goal of this paper is to provide sufficient conditions that ensure the existence of travelling wave solutions for the age-structured epidemic model. The case of two population groups is numerically investigated which applies to the criss-cross transmission of certain sexual transmission diseases and feline immunodificiency virus (FIV). (Based on a joint paper with Arnaut Ducrot and Pierre Magal)

Sebastian Schreiber

Persistence of structured populations in random environments

I will present preliminary results on necessary and sufficient criteria for the existence of a positive stationary distribution for discrete time models of the form $x(t+1) = A(\xi(t), x(t))x(t)$ where $A(\xi(t), x(t))$ is a $k \times k$ non-negative matrix depending on the current vector of population densities $x(t)$ and a stationary process $\xi(t)$. Applications to models of spatially structured and stage structured populations will be given. This work is in collaboration with Michel Benaïm.

Hal Smith

Models of Virulent Phage Growth with application to Phage Therapy

We modify existing models of bacteriophage growth on an exponentially growing bacterial population by including (1) density dependent phage attack rates and (2) loss to phage due to adsorption to both infected and uninfected bacteria. The effects of these modifications on key pharmacokinetic parameters associated with phage therapy are examined. More general phage growth models are explored which account for infection-age of bacteria, bacteria-phage complex formation, and decoupling phage progeny release from host cell lysis.

Rebecca Tyson

Modelling the Dynamics of the Canada Lynx and Snowshoe Hare Population Cycle

The population cycle of the Snowshoe Hare (SH) has been a focus of scientific interest for the past century. These populations are characterized by striking high amplitude multi-year cycles with a period of 8-11 years. For many years, the SH cycle was thought to be a classical predator-prey interaction between the hare and the lynx. Existing models have shown the importance of the predator-prey interaction, and have approximately captured many traits of the cycle. None however, have been able to simultaneously capture all of the five main cycle characteristics, namely the maximum population, minimum population, cycle amplitude and cycle period for both the lynx and hare. In particular, models generally predict minimum hare densities that are much higher than those observed in the field. Our first objective is to develop a model of the lynx-hare population dynamics that generates cycles with realistic boreal values for all five cycle probes mentioned above. We then use this model to investigate possible sources of the difference in dynamics between northern and southern hare populations: the northern populations exhibit large multiannual cycles, while the southern populations exhibit little to no cycling. In particular, we study the effect of generalist predation and of habitat fragmentation.

Hans Weinberger

A multi-age-stage fish model

I have been looking at the application of some recent work with Nanako Shigesada and Kohkichi Kawasaki to a multi-age-stage fish model. The idea is to model the situation envisioned by Ricker by a reaction-diffusion system in which there is predation of the juveniles by the adults when the adult population is large. One finds that the system is partially cooperative, in the sense that is is cooperative when the population densities are small, but not when they are large. This fact leads to spreading results of the kind introduced by H.R. Thieme in a 1979 paper on epidemic models. Everything works nicely for the 2-stage model, and I have begun to think about the corresponding 3-stage model with eggs in addition to juveniles and adults.

Xiaoqiang Zhao

Spreading Speeds and Traveling Waves for Non-monotone Integrodifference Equations

The invasion speed is a fundamental characteristic of biological invasions, since it describes the speed at which the geographic range of the population expands. The theory of spreading speeds and monostable traveling waves for monotone semiflows has been well developed in such a way that it can be applied to various discrete- and continuous-time evolution equations admitting the comparison principle. However, there are only a few works on spreading speeds for non-monotone biological evolution systems.

In this talk, I will report our recent research on a class of non-monotone discrete-time integrodifference equation models. We obtain a set of sufficient conditions for the existence of the spreading speed, and the existence and nonexistence of traveling waves. It turns out that the spreading speed is linearly determinate and coincides with the minimal wave speed of traveling waves.

Huaiping Zhu
Modeling the West Nile Virus with corvids and non-corvids
There have been mathematical modeling studies for the West Nile virus among mosquitoes and avian species. In all of the existing models, the avian species were treated as one family. Also for the first several years since its first appearance in North America, the dead birds, especially the dead American crows due to the infection of the virus were used as an indication of the virus activity in a given region. I will first introduce and summarize the existing models and related results. The surveillance data for West Nile virus in southern Ontario, Canada, suggests that corvids and non-corvids have different infection-induced rates. By taking corvids and non-corvids as multiple-reservoirs hosts and mosquitoes as vector, we propose a single-season ordinary differential equations model to model the transmission dynamics of WNV in the mosquito-bird cycle. The eight-dimensional system of differential equations can have up to 2 positive equilibria. We will study the local stability and bifurcations of the model. The existence of the backward bifurcation gives a further sub-threshold condition beyond the reproduction number for the control of the virus. The existence of the backward bifurcation also suggests that the West Nile virus activity in a given region is initial-size dependent. The result of this study also suggests that even though the dead American crow may not be seen in a given region, there might be still a possibility of an outbreak due to the existence of the non-corvids as a reservoir.

Scientific Progress and Open Questions

The presentations stimulated lively discussions. These discussions helped to clarify the interaction of space, stage, and time scales. The different approaches that the participants presented allowed for a synthesis of different concepts and methods. Out of these discussions emerged new research challenges (see list below). In addition to the scheduled program, participants spontaneously organized two breakout session:

- Discussion on R_0 in stage-structured models. This discussion clarified similarities and differences in threshold values in ecological and epidemiological models.
- Discussion of spatial disease with Allee effect. Importance of demographic factors in epidemic models. Discussion of the strong and weak Allee effect, its mechanistic underpinning and its dynamic consequences (e.g. disease cycles, invasion fronts).

List of Open Problems:

1. Theory of Structured Populations
   (a) Unified approach (in which all the classical approaches of linearization and stability analysis work)
   (b) Role and calculation of R_0
   (c) Apply sensitivity results and find patterns in biological systems
   (d) Include stochasticity with large deviations
   (e) Blending the abstract and concrete for equations with infinite delay.
   (f) Investigate the effect of quiescent dynamics on the qualitative behavior of a dynamical system
2. Spatial Models
   (a) Include stochasticity in spread models
   (b) Rate of convergence for traveling waves
   (c) Traveling waves and spread rates for nonmonotone systems
   (d) Advance and retreat of population fronts in systems with multiple equilibria
3. Epidemiology and Diseases

(a) Including several serotypes
(b) Vaccination policy when secondary infection can be more harmful
(c) Seasonal forcing in stochastic systems with periodic solutions
(d) How does the disease transmission term influence the dynamics
(e) Final size distribution when R_0 is close to one
(f) What is the probability of a disease going extinct after the first outbreak ?
(g) Phage treatment models
(h) Vertical transmission in WNV models
(i) Backwards bifurcations in epidemic models: what features give rise to them ?
(j) Including demographic functions in epidemic models

Outcome of the Meeting

The workshop fostered new contacts, and collaborations. Participants learned about new techniques. Young researchers had the opportunity to meet experienced colleagues and receive valuable feedback. Mutual future collaborative research visits and workshops were envisioned and discussed. Many participants expressed the wish to continue the spirit of this workshop in future meetings. To demonstrate the impact of the meeting we list some quotes from a survey collected from the participants.

- *For the first time, I truly started to grasp the connections between matrix models and continuous models, epidemic models and predator prey models, delay equations and stage structured models.*
- *Everyone of the workshop was supportive and willing to share their experience and ideas with the more junior researchers.*
- *I am in the process of looking for a postdoc. This was a terrific experience to know what other opportunities there are for research and collaboration in the future. I learned about analytic methods about structured populations, sensitivity analysis, and to formulate age structured models as delay equations.*
- *I began two new projects, resulting from meeting people whom I would not have otherwise met.*
- *I received many useful commends from others after my talk which will improve my future modelling efforts.*
- *I received excellent feedback on first passage time problems (discussed ellipticity of operators and nonlinear averaging of stochastic process) ... will result in improved revision of two current papers.*
- *This is a very valuable meeting for me - my first broad acquaintance with this community.*
- *Increased my overview, which is helpful, among other things, for editorial work.*
- *I am a PhD student and this was my first scientific meeting ever. The research presented is overwhelming, and I am very impressed how friendly and supportive the participants are.*
- *I got into contact with possible future postdocs and arranged possible co-supervision of graduate students.*

The meeting has given impulse to an area that covers topics in mathematics as well as in field biology and that is significant for resource management and preservation and for disease prevention and control. From a strictly mathematical point of view, population dynamics as presented here provides new results and questions in particular in the qualitative analysis of ordinary and partial differential equations, difference equations and stochastic processes. We thank BIRS for this great opportunity and for outstanding hospitality.

List of Participants

Arino, Julien (University of Manitoba)
Billings, Lora (Montclair State University)
Boldin, Barbara (University of Helsinki)
Caswell, Hal (Woods Hole Oceanographic Institution)
Cushing, Jim (University of Arizona)
Desjardins, Sylvie (University of British Columbia, Okanagan)
Diekmann, Odo (Universiteit Utrecht)
Flores, Kevin (Arizona State University)
Gong, Jiafen (University of Alberta)
Greenwood, Priscilla (Cindy) (Arizona State University)
Guo, Hongbin (York University)
Gyllenberg, Mats (University of Helsinki)
Hadeler, Karl (Arizona State University)
Hamelin, Frederic (University of Alberta)
Hastings, Alan (University of California, Davis)
Hilker, Frank (University of Alberta)
Hillen, Thomas (University of Alberta)
Klepac, Petra (Penn State University)
Kot, Mark (University of Washington)
Lewis, Mark (University of Alberta)
Lutscher, Frithjof (University of Ottawa)
Ma, Junling (University of Victoria)
Magal, Pierre (University of LeHavre)
Martin, Jonathan (University of Alberta)
Neubert, Michael (Woods Hole Oceanographic Institution)
Nevai, Andrew (The Ohio State University)
Ruan, Shigui (University of Miami)
Schreiber, Sebastian (University of California, Davis)
Seo, Gunog (University of Washington)
Smith, Hal (Arizona State University)
Thanate, Dhirasakdanon (Arizona State University)
Thieme, H. (Arizona State University)
Tyson, Rebecca (University of British Columbia, Okanagan)
van den Driessche, Pauline (University of Victoria)
Watmough, James (University of New Brunswick)
Weinberger, Hans (University of Minnesota (Prof. Emeritus))
Zhao, Xiaoqiang (Memorial University of Newfoundland)
Zhu, Huaiping (York University)

Chapter 14

Nonlocal operators and applications (08w5102)

Apr 27 - May 02, 2008

Organizer(s): Cyril Imbert (University Paris-Dauphine, CEREMADE), Antoine Mellet (University of British Columbia), Regis Monneau (École nationale des ponts et chaussées)

Introduction

One of the main objectives of this workshop was to present a state of the art of current research on non-local operators. Over the last few years, there has been a lot of interests for such operators, and much progress have been made by mathematicians working in many different areas. The goal of this workshop was thus to bring together those mathematicians and encourage interactions between different areas of mathematics.

Our interest for such models is motivated by the wide range of applications, and the flourishing of new mathematical tools and results, stimulated by the theory of (local) elliptic operators. This workshop has permitted to bring together mathematicians to present the most recent trend on this topic.

Scientific activities

We now wish to present the scientific activities that took place during this meeting. In the first subsection, we explain how those activities were organized. In the remaining of the section, we describe the results presented by speakers in their talks. Six main topics were treated: non-local moving fronts, fractal Burgers equations, non-linear stochastic differential equations, mean-field and kinetic equations, non-linear elliptic equations, reaction-diffusion equations. Several talks also discussed problems coming from applications such as oil extraction and genetic evolution.

Organization

Scientific activities consisted in 21 talks and 10 informal discussion sessions. There were two one hour talks and a 25 minute talk in the morning and two or three 25 minute talks in the afternoon. There were also two informal discussion sessions in the afternoon, one before the talks and another one after them. See the tabular below.

	Monday	Tuesday	Wednesday	Thursday
09:00 - 10:00	Vasseur	Méléard	Souganidis	Perthame
10:30 - 11:30	Cardaliaguet	Woyczynski	Roquejoffre	Dolbeault
11:30 - 12:00	Peirce	Jourdain	Informal discussion	Mouhot
01:30 - 02:30	Informal discussion	Informal discussion	Free afternoon	Informal discussion
02:30 - 03:00	Informal discussion	Silvestre		Informal discussion
03:00 - 03:30	Droniou	Gentil		Alibaud
04:00 - 04:30	Sire	Schwab		Karch
04:30 - 05:00	Informal discussion	Monteillet		Margetis
05:00 - 06:00	Informal discussion	Informal discussion		Informal discussion

One hour talks were given by senior researchers and short talks were given by either senior researchers or younger mathematicians. Two PhD students (Schwab and Monteillet) and two young mathematicians[1] (Sire and Alibaud) gave short talks. We would like to mention that several PhD students had planed to come and finally could not make it because of job interviews in France or difficulties with visa (Coville, El Hajj, Forcadel).

Non-linear elliptic equations

- A. Vasseur. *Regularity of solutions to drift-diffusion equations with fractional Laplacian.*
- L. Silvestre. *Some regularity results for integro-differential equations.*
- R. Schwab. *Periodic Homogenization of Nonlinear Integro-Differential Equations*

Non linear elliptic and parabolic equations involving nonlocal operators arise naturally in various frameworks. A well known example of such an equation is the so called quasi geostrophic equation which was presented in A. Vasseur's talk. These equations enjoy many properties of the usual elliptic and parabolic equations, though the nonlocal character of the problem introduces new, sometime unexpected difficulties. In his talk, L. Silvestre generalize the notion of fully nonlinear equation to the nonlocal setting. This is a work in collaboration with L. Caffarelli, who has been one of the main actor in the recent trend in studying the properties of nonlocal elliptic equation. They are able to extend the usual definition of Extremal operators and viscosity solutions to integro-differential equations and establish the main properties of these equations. R. Schwab, is then interested in the homogenization of such equations. His result extends the recent result of L. Caffarelli, P. Souganidis and L. Wang to the nonlocal framework.

The quasi geostrophic equation was introduced by Constantin and Wu in 1999 as a toy model for the study of possible blow-up in 3D fluid dynamics. It is a non-local non-linear equation for the temperature $\theta : \mathbb{R}^2 \to \mathbb{R}$:

$$\begin{aligned} &\partial_t \theta + u \cdot \nabla\theta = -\Lambda\theta, \\ &u = R^\perp \theta \end{aligned} \tag{14.1}$$

with the operator $\Lambda = (-\Delta)^{1/2}$ is defined by $\widehat{\Lambda\theta} = |\xi|\widehat{\theta}$ and where $R^\perp$ denotes the orthogonal of the Riesz transform. Other nonlocal operators can be consider, the most natural choices being other powers of the Laplace operator: $\Lambda = (-\Delta)^\alpha$ with $\alpha \in (0, 1)$. The case $\alpha = 1/2$ is usually refer to as the critical case.

Together with Luis Caffarelli, A. Vasseur proves that the solutions of the drift-diffusion equation

$$\partial_t \theta + u \cdot \nabla\theta = -\Lambda\theta$$

are locally Holder continuous for L^2 initial data and under minimal assumptions on the drift u. As an application they show that solutions of the quasi-geostrophic equation (14.1) with initial L^2 data and critical diffusion $(-\Delta)^{1/2}$, are locally smooth for any space dimension. The main difficulty is to obtain Hölder regularity. The method is inspired by the celebrated proof of E. De Giorgi for C^α regularity of the solutions of elliptic equation with bounded measurable coefficients.

[1] They had a position less than two years ago.

Over recent years, there has been a lot of interest from the mathematical community for non-local operators, and many of the well known properties of standard elliptic and parabolic equations have been extended to non local ones. In that direction, Luis Caffarelli and Luis Silvestre study fully nonlinear integro-differential equations. These are the non local version of fully non-linear elliptic equations of the form $F(D^2u, \nabla u, u, x) = 0$. Typical examples are the ones that arise from stochastic control problems with jump processes.

We first recall that linear integro-differential operators have the form

$$Lu(x) = \int_{\mathbb{R}^n} (u(x+y) - u(x) - \chi_B(y)\nabla u(x) \cdot y)K(y)dy$$

where the most typical case is

$$K(y) = \frac{1}{|y|^{n+\sigma}}$$

corresponding to the fractional Laplacian. In stochastic control problems with jumps processes it is classical to deal with nonlinear equations of the form

$$0 = lu(x) := \sup_{\alpha} L_\alpha u(x).$$

¿From two-player stochastic games we would get even more complicated equations of the form

$$0 = lu(x) := \inf_{\beta} \sup_{\alpha} L_{\alpha\beta} u(x).$$

These equations form basic examples of fully nonlinear integro-differential equations.

In order to study these equations, we need to generalized of the notion of uniformly ellipticity for fully nonlinear nonlocal equations. This, as explained in L. Silvestre's talk, can be done using the Pucci extremal operators $M_\sigma^\pm$ defined by

$$M_\sigma^+ u(x) = \sup_{\lambda a(y) \leq \Lambda \ a(y)=a(-y)} (2-\sigma) \int (u(x+y) - u(x)) \frac{a(y)}{|y|^{n+\sigma}} dy$$

and a similar definition for M_σ^-.

Then, a nonlocal operator l is said to be uniformly elliptic of order σ if

$$M_\sigma^- v(x) \leq l(u+v)(x) - lu(x) \leq M_\sigma^+ v(x)$$

(σ is always in $(0, 2)$).

L. Caffarelli and L. Silvestre are then able to obtain results analogous to the Alexandroff estimate, (Krylov-Safonov) Harnack inequality and $C^{1,\alpha}$ regularity for uniformly elliptic equations. Interestingly, as the order of the equation approaches two, in the limit the estimates become the usual regularity estimates for second order elliptic partial differential equations.

Since those nonlocal equations have similar properties as the local ones, it seems natural to investigate their behavior under various classical perturbation limits. In his PhD thesis work, R. Schwab investigate the homogenization limit of such equations. The recent work of L. Caffarelli, P. Souganidis and L. Wang for the homogenization of fully non-linear equations of elliptic and parabolic type introduced a new approach to obtain homogenization result in stationary ergodic media. In his talk, R. Schwab shows that the method can be adapted to a somewhat general class of nonlinear, nonlocal uniformly "elliptic" equations. Motivated by the techniques of the homogenization of fully nonlinear uniformly elliptic second order equations by L. Caffarelli, P. Souganidis and L. Wang, he shows how a similar obstacle problem can be used to identify the effective equation in the nonlocal setting.

Reaction-diffusion equations

- J.-M. Roquejoffre. *Free boundary problems for the fractional Laplacian.*
- Y. Sire. *Rigidity results for elliptic boundary reaction problems.*

Reaction-diffusion equations are important in many area of applied mathematics involving phase transition. In view of the recent progress in understanding the behavior of nonlocal elliptic operators, it seems natural to extend to such operators some of the well known results of the theory of elliptic equations. This is one of the goal of J.-M. Roquejoffre and Y. Sire in their respective talks. Both of them rely heavily on the extension formula of L. Caffarelli and L. Silvestre which allows us to rewrite fractional Laplace operators as boundary operator for degenerate (local) elliptic operators. This formula, which first appeared in 2005 has generated a lot of new development in the field and the works presented below are good examples.

One of the most studied stationary free boundary problem is Bernoulli problem, which consists of a elliptic equation sets in the positivity set of the solution:

$$\Delta u = 0 \text{ in } \{u > 0\}$$

and a free boundary condition

$$|\nabla u|^2 = 1 \text{ on } \partial\{u > 0\}$$

where the unknown function u is non-negative.

This problem arises in the modeling of flame propagation as the limit of the singular reaction problem

$$\Delta u = \beta_\delta(u)$$

where β_δ is an approximation of the Dirac mass. The same free boundary problem also appears in heat flux minimization, as the Euler Lagrange equation for the minimization of the non continuous functional

$$\int |\nabla u|^2 + \chi_{\{u>0\}} dx.$$

The study of such problems is very delicate because of the lack of a priori regularity or the free boundary $\partial\{u > 0\}$. The first regularity results go bak to the early 80's with the works of Alt-Caffarelli and Alt-Caffarelli-Friedman.

In his talk, J.-M. Roquejoffre presented some recent work with L. Caffarelli and Y. Sire concerning a non-local version of this famous problem. In this problem, the Laplace equation is replaced by a fractional Laplace equation:

$$(-\Delta)^s u = 0 \text{ in } \{u > 0\}.$$

In that case, the appropriate free boundary condition (which correspond to the natural Neuman condition for fractional Laplace operators) is

$$u(x) \sim A[(x - x_0) \cdot \nu(x_0)]^s$$

for any $x_0 \in \partial\{u > 0\}$, where $\nu(x_0)$ denotes the inward unit normal vector to $\partial\{u > 0\}$. This problem can be seen as the limit for equations of the form

$$(-\Delta)^s u = -\beta_\delta(u)$$

which arise in physic as a first attempt to take into account non local effects in the modeling of reaction-diffusion phenomena.

L. Caffarelli, J.-M. Roquejoffre and Y. Sire investigates the variational formulation of this problem and strongly rely on the extension formula of Caffarelli-Silvestre. They are able to obtain the main result in the theory, namely the optimal regularity of the minimizer ($u \in \mathcal{C}^s$)), the hölder growth away from the free boundary and the positive density of $\{u > 0\}$ and $\{u = 0\}$ along the free boundary. This implies in particular that blow-up limits have non-trivial free boundaries and that free boundaries cannot form cusps. However, it leaves as an open question a very classical property of the free boundary for the usual Bernoulli problem: Does the free boundary have finite $(n - 1)-$Hausdorff measure?

Finally, they investigate the behavior of minimizers in the neighborhood of the regular free boundary points (differentiability points) and show that indeed, u satisfies

$$u(x) \sim A[(x - x_0) \cdot \nu(x_0)]^s$$

where A is a universal constant. The set of differentability points can be proved to be dense in the free boundary, but further regularity results, as in the usual Bernoulli problem are still, for the most part, open problems.

De Giorgi's famous conjecture concerns some symmetry properties of the solution of equations of the form

$$(-\Delta)u = f(u) \text{ in } \mathbb{R}^n$$

with $f(u) = u^3 - u$. The conjectures claims that if u is an entire solution such that

$$|u| \leq 1$$

and

$$\frac{\partial u}{\partial x_n} > 0$$

(where $x = (x, x_n) \in \mathbb{R}^N$), then, at least for $n \leq 8$, the level sets of u must be hyperplanes.

The problem originates in the theory of phase transition and is so closely connected to the theory of minimal hypersurfaces that it is sometimes referred to as the "version of Bernstein problem for minimal graphs".

Since the work of Nassif Ghoussoub and Changfeng Gui in 1998, which proved the conjecture in dimension 2, there has been a lot of activity trying to establish the conjecture in all dimensions.

E. Valdinocci and Y. Sire attempted to investigate a similar conjecture for boundary phase transition problems, which can easily be reformulated as a nonlocal reaction-diffusion problem:

$$(-\Delta)^s u = f(u) \text{ in } \mathbb{R}^n.$$

Following the extension formula established by Caffarelli and Silvestre, this equation can be rewritten as

$$-\operatorname{div}(y^a \nabla u) = 0 \text{ in } \mathbb{R}^{n+1}$$

and

$$-y^a \partial_y u = f(u) \text{ at } y = 0.$$

Y. Sire describes a technique based on a geometric Poincare-type inequality which allows to get some symmetry results for bounded stable solutions of boundary reaction problems in low dimension.

This technics relies on the use of the second variation and the notion of stable solutions. The idea to use the second variation to get fine control on the level sets of the solution goes back to Steinberg-Zumbrum and was used, in particular, by Farina-Scienzi and Valdinocci for the usual E. Valdinocci and Y. Sire show how to apply this technique to elliptic degenerate quasi-linear equations set in the half-space. As a consequence of Caffarelli-Silvestre formula, one gets some rigidity properties of solutions for the corresponding nonlocal equations involving fractional powers of the laplacian.

Non-local moving fronts

- P. Cardaliaguet. *Front propagation with non-local terms.*
- A. Monteillet. *Convergence of approximation schemes for non-local front propagation equations.*
- P. E. Souganidis. *Non-local approximations of moving interfaces.*

Three speakers presented results concerning non-local moving interfaces: P. Cardaliaguet, A. Monteillet and P. E. Souganidis. Contributions of P. E. Souganidis to the field of moving interfaces are fundamental. The reader is referred to his survey paper [32] which contains many important references on this topic. P. Cardaliaguet [15] is one of the first mathematician who developed tools for studying in a very general setting interfaces whose geometric law is non-local. A. Monteillet is a PhD student of P. Cardaliaguet.

P. E. Souganidis presented results concerning non-local approximations of moving interfaces. A moving interface can be defined by considering a family $K = \{K(t)\}_{t\in[0,T]}$ of compact subsets of $\mathbb{R}^N$:

$$\forall x \in \partial K(t), \forall t \geq 0, \quad V(x,t) = f(x, t, \nu_{x,t}, A_{x,t}, K) \tag{14.2}$$

where

- $V(x,t)$ is the normal velocity of a point x of $\partial K(t)$ at time t
- $\nu_{x,t}$ is the unit exterior normal to $K(t)$ at $x \in \partial K(t)$
- $A_{x,t} = \left[\frac{\partial \nu^i_{(x,t)}}{\partial x_j}\right]_{ij}$ is the curvature matrix of $K(t)$ at $x \in \partial K(t)$
- $K \mapsto f(x,t,\nu_{x,t},A_{x,t},K)$ is a non-local dependence in the whole front K (up to time t).

Equation (14.2) is referred to as the geometric law of the moving interface. Such evolution equations appear in several areas: cristal growth, elasticity, biology, finance, shape optimization design, image processing... For these problems, existence and uniqueness of classical solutions can be obtained by methods of differential geometry (Huisken, Escher-Simonnet, ...) However the front (often) develops singularities in finite time. Hence, two important problems are: on one hand, to define the front after the onset of singularities and, on the other hand, to study its properties.

P. E. Souganidis explained that when one expects the geometric inclusion principle to hold true, generalized moving interfaces $\{K(t)\}_{t\in[0,T]}$ can be defined in several ways. In particular, it can be defined

- either by using the level set method which consists in representing the set $K(t)$ as the zero level set of a function $u(t,\cdot)$. The geometric law (14.2) is translated into a geometric partial differential equation and this equation is studied by using viscosity solution theory;
- or by using a geometric formulation such as in [7]; loosely speaking, this approach consists in considering a smooth test front that is contained in (resp. contains) the generalized front. If this test front evolves with a speed that is smaller (resp. greater) than the one of the generalized front, then it has to stay inside (resp. outside) the generalized front as time increases.

For local evolutions of the form

$$\forall x \in \partial K(t), \forall t \geq 0, \quad V_{x,t} = f(x,t,\nu_{x,t},A_{x,t})$$

Evans and Spruck [23], Chen, Giga and Goto [17] have defined notion of generalized solution by using the level set approach and techniques of viscosity solutions. Similar but more geometric approaches have been developed by Soner [31], Barles, Soner and Souganidis [5], Belletini and Novaga [8], Barles and Souganidis [7]...

After recalling these definitions and classical results, P. .E. Souganidis considered two non-local approximations of moving interfaces: Bence-Merriman-Osher (BMO) schemes and rescalings of solutions of reaction-diffusion equations. He presented results corresponding to two working papers, one with L. Caffarelli and one with C. Imbert. As far as BMO schemes are concerned, he explained that if the Gaussian kernel is replaced with kernels which decay slowly at infinity (as a proper power law), then either mean curvature flow or "fractional" mean curvature flow are obtained at the limit, depending on the decay rate of kernels. He explained that classical BMO schemes can be seen as Trotter-Kato approximation of rescaled reaction-diffusion equations in the classical case. Hence, it can be proved that mean field equations associated with stochastic Ising models with long range interactions can be rescaled in order to prove that, on one hand, mean curvature flows can be obtained at the limit [22, 5] and on the other hand, fractional mean curvature flows can be obtained (working paper).

P. Cardaliaguet presented results related to flows with and without inclusion principle. We recall that a geometric flow satisfies the inclusion principle if, at initial time, a front $\mathcal{O}_1$ is included in another front $\mathcal{O}_2$, this inclusion is preserved by the flow. A typical example of inclusion preserving flows is the one associated with the following geometric law

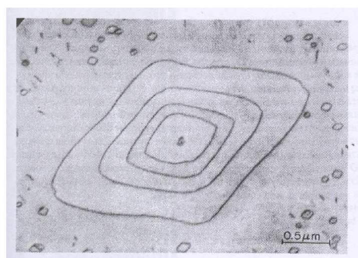
$$V_{x,t} = 1 + \lambda |\nabla u|^2$$

where u is the solution to

$$\begin{cases} -\Delta u = 0 & \text{in } K(t) \setminus S \\ u = 1 & \text{on } \partial S \\ u = 0 & \text{on } \partial K \end{cases}$$

Cardaliaguet explained that this flow can be interpreted as a gradient flow for the Bernoulli problem. In [16], a notion of sub- and super-flow is defined by using (smooth) test fronts. Such an idea first appeared in [7] where a geometric formulation of moving interfaces is developed in order to be able to solve singular perturbation problems arising in the phasefield theory of reaction-diffusion equations. Moreover, an inclusion principle is proved in [16] and a generic uniqueness result is obtained. Moreover, a link with the energy of the problem is presented; it is related to the definition of minimizing movements in the spirit of the seminal paper of De Giorgi, Marino and Tosques [18]. As far as flows without inclusion principle are concerned, Cardaliaguet presented a general existence result obtained with G. Barles, O. Ley and A. Monteillet [4]. Precisely, a generalized moving interface is constructed here by the level set method (see above). He also presented the first uniqueness result for a Fitzhugh-Nagumo type system [4]. Finally, he presented existence result for dislocation dynamics (see Figure 14).

Figure 14.1: Dislocation line



A. Monteillet presented results about approximation schemes for computing the weak solution constructed in [4]. More precisely, he considered a general class of stable, monotone and consistent schemes in order to be able to apply the fundamental result of Barles and Souganidis [6] which can be adapted to the non-local geometric equation studied in [4] by using a new stability result of Barles [3].

Mean-field and kinetic equations

- J. Dolbeault. *Mean field models in gravitation and chemotaxis.*
- I. Gentil. *A Lévy-Fokker-Planck equation: entropies and convergence to equilibrium.*
- C. Mouhot. *Some properties of non-local operators from collisional kinetic theory.*

Dolbeault'stalk was intended to provide an overview of some results of mean field theory, mostly in case of an attractive Poisson law. He first presented some stability results for stationary solutions of the gravitational Vlasov-Poisson model [20]. Connection with drift-diffusion equations were obtained in a diffusion limit. As a side result, he presented some results and conjectures on the two-dimensional Keller-Segel model, which share properties which are similar to gravitational models, but for which the mass is a critical parameter [14]. He then presented some results for a three-dimensional flat model of gravitation, showed the existence of solutions stationary with high Morse index and state some conjectures about their stability [19].

Gentil presented results related to a Lévy-Fokker-Planck equation

$$\begin{cases} \partial_t u = \mathcal{I}[u] + \mathrm{div}(u \nabla V) & x \in \mathbb{R}^d, t > 0, \\ u(0,x) = u_0(x) & x \in \mathbb{R}^d \end{cases}$$

where u_0 is non-negative and in $L^1(\mathbb{R}^d)$ and V is a given proper potential for which there exists a nonnegative steady state. The operator $\mathcal{I}$ is a Lévy operator

$$\mathcal{I}[u](x) = \mathrm{div}\,(\sigma \nabla u)(x) - b \cdot \nabla u(x) + \int_{\mathbb{R}^d} (u(x+z) - u(x) - \nabla u(x) \cdot z h(z)) \nu(dz)$$

with parameters (b, σ, ν) where $b = (b_i) \in \mathbb{R}^d$, σ is a symmetric semi-definite $d \times d$ matrix $\sigma = (\sigma_{i,j})$ and ν denotes a nonnegative singular measure on $\mathbb{R}^d$ that satisfies

$$\nu(\{0\}) = 0 \quad \text{and} \quad \int \min(1, |z|^2)\nu(dz) < +\infty;$$

h is a truncature function and we fix it on this article: for any $z \in \mathbb{R}^d$, $h(z) = 1/(1 + |z|^2)$.

The starting point of this work is a paper by Biler and Karch [10] where an exponential decay towards the equilibrium u_∞ in L^p norm is proved by assuming, loosely speaking, that $\sigma \neq 0$. Moreover, the rate of convergence seemed not to be optimal. In order to get such an exponential decay, they study the following family of entropies: for any nonnegative function f,

$$\mathrm{Ent}^{\Phi}_{u_\infty}(f) := \int \Phi(f)\, u_\infty dx - \Phi\left(\int f u_\infty dx\right).$$

where Φ is a convex function. In particular they prove that the equilibrium state u_∞ is an infinite divisible law and that entropies are Lyapunov functions for the Lévy-Fokker-Planck equation.

Gentil explained that the main contributions of [24] are the following results:

- if $\int_{|z|\geq 1} \ln|z|\nu(dz) < +\infty$, there exists an equilibrium state u_∞ (even if $\sigma = 0$); it is also proved that it is an infinite divisible law;
- the energy associated with the Φ-entropy is explicitely computed; it looks like the Dirichlet form associated with $\mathcal{I}$ with respect to the measure $u_\infty(x)dx$;
- under additional assumptions on Φ and ν, the entropy decays exponentially fast; in particular, an optimal exponential rate is obtained.

C. Mouhot presented results related to collisional kinetic (integro)-differential equation

$$\partial_t f + v\nabla_x f + F \cdot \nabla_v f = Q(f, f) \tag{14.3}$$

where Q is the collision operator; it is local in t, x.

The operator Q is local for linear Fokker-Planck equations, but it is bilinear and integral for collisional dilute gases (Boltzmann) or plasmas (Landau). There are many interesting issues involving these non-local operators (Cauchy, regularity, asymptotic behavior, derivation, hydrodynamic limit,...). Here the speaker focused on the case of Boltzmann collision operators with singular kernel (long-range interactions) (with Landau operator as a limit) in the linearized setting.

The spatially homogeneous non-linear case has be studied a lot see the papers of Funaki, Goudon, Villani, Lions, Méléard, Desvillettes, Graham, Fournier, Guérin,... about the Cauchy problem, the regularity of solutions, the study of grazing collision limit *etc.* But there are fewer works in the spatially inhomogeneous case and the linearized problem; see the papers of Alexandre, Alexandre-Villani (and Chen-Desvillettes-He for the Landau equation). The linearized study is crucial for stability issues.

Mouhot next recalled the definition of the linearized operator. The normalized Maxwellian equilibrium is the function $M(v) = e - |v|^2$. If now f in (14.3) is chosen under the form $M + Mh$, the following linearized Boltzmann operator appears: $L(h) = M^{-1}[Q(Mh, M) + Q(M, Mh)]$ with $h(v) \in L^2(M)$. An explicit formula of L is given now

$$Lh(v) = \frac{1}{4}\int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} (h(v') + h(v'_*) - h(v) - h(v_*))B(|v - v_*|, \sigma)M(v_*)dv_* d\sigma$$

where $v' = \frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma$ and $v'_* = \frac{v+v_*}{2} - \frac{|v-v_*|}{2}\sigma$. The physical important case is the case where $B = \Phi(|v - v_*|)b(\cos\theta)$ with b a power-law and $\cos\theta = \sigma \cdot (v - v_*)/|v - v_*|$.

Here are the important properties of this operator.

- L is symmetric on the Hilbert space $L^2(M)$.

- It is non-positive (linearized H theorem):

$$D(h) = -(h, Lh) = \frac{1}{4}\int_{v,v_*,\sigma} |h' + h'_* - h - h_*| BMM_* \geq 0\,.$$

- Its null space $N(L)$ is $(d+2)$-dimensional and spanned by the collisional invariants $1, v_1, ..., v_d, |v|^2$.

Therefore important question of the existence of a spectral gap: positive distance isolating 0 from the remaining part of the spectrum. After recalling a lot of previous results (Hilbert 1912, Carlman 1957, Grad 1962, Wang-Chang and Uhlenbeck 1970, Bobylev 1988, Pao 1974, Caflisch 1980, Degond-Lemou 1997, Lemou 2000, Guo 2002 *etc*), the speaker stated the main theorem of his talk.

Theorem 1 ([30]) *Assume* $B = \Phi(|v - v_*|)b(\cos\theta)$ *with*

$$\Phi(z) \geq C_\Phi z^\gamma, \quad b(\cos\theta) \geq b_0(\sin\theta/2)^{-(d-1)-\alpha} \text{ for } \theta \sim 0\,.$$

Then

- $\forall \epsilon > 0$*, there exists* $C_{B,\epsilon} > 0$ *(constructive proof) such that*

$$D(h) \geq C_{B,\epsilon} \|h - \Pi(h)\|_{L^2_{\gamma+\alpha-\epsilon}}(M)$$

where Π *denotes the orthogonal projection on* $N(L)$.

- *There exists* $C_{B,0} > 0$ *(non constructive proof) such that*

$$D(h) \geq C_{B,0} \|h - \Pi(h)\|_{L^2_{\gamma+\alpha}}(M)\,.$$

From non-linear stochastic differential equations to non-linear non-local evolution equations

- B. Jourdain. *Non-linear SDEs driven by Lévy processes and related PDEs.*
- S. Méléard. *Stochastic approach for some non-linear and non-local partial differential equations.*
- W. A. Woyczynski. *Non-linear non-local evolution equations and their physical origins.*

In Woyczynski'stalk, the physical and biological problems leading to non-linear and non-local evolution equations were reviewed and the outstanding problems in this area discussed.

His talk was divided into five parts. In the first one, he presented a model for describing the growth of an interface. This model involves a non-linear non-local diffusion equation. He also presented numerous examples from physical sciences where distributions associated with α-stable Lévy processes appear. For instance, "at the atomic level, there is no reason to assume automatically that surface diffusion is Gaussian"; he illustrated this point by showing some molecular dynamics calculations [29].

The third part of his talk was devoted to fractal conservation laws and fractal Hamilton-Jacobi-KPZ equations. Results concerning fractal conservation laws are presented Subsection 14 below. The results for fractal Hamilton-Jacobi-KPZ equations were obtained with G. Karch [28]. The equation at stake in this paper is the following one

$$\partial_t u = (-\Delta)^{\alpha/2} u + \lambda |\nabla u|^q$$

where λ is a real number. As a matter of fact, more general Lévy operators are considered in the paper but we present the results in this framework for the sake of clarity. The case $\lambda > 0$ corresponds to the deposition case; indeed, it is proved that if $\lambda > 0$, then the total mass $M(t) = \int_{\mathbb{R}^d} u(t,x)dx$ increases as time t increases. In the case $\lambda < 0$, $M(t)$ decreases and we say that we are in the evaporation case. In the deposition case, the existence of a limit of $M(t)$ as $t \to +\infty$ is discussed; it depends on the non-linearity exponent q. In any case, as long as $M(t)$ has a finite limit M_∞ as $t \to +\infty$, it is proved that $u(t)$ behaves like the fundamental solution of the fractional heat equation times M_∞.

The case of the strongly non-linear problems analogous to the classical porous medium equation requires further attention here. Some limitations, such as nonexistence of global solutions for general non-local diffusion-convection mean field models will be indicated.

Recent results on the interplay between the strength of the “anomalous” diffusive part and ”hyperbolic” non-linear terms will be presented in the case of fractal Hamilton-Jacobi-KPZ equations (see [28] and the joint working paper with B. Jourdain, S. Meleard, G. Karch, and P. Biler).

Méléard’s talk was a survey describing various stochastic approaches for non-linear and non-local equations, in terms of interpretation, existence and uniqueness, regularity and particle approximations of the solution of the equation. She explained why it is in a certain sense easier, in a probabilistic point of view, to study non-local non-linearity.

In the first part of the talk, she briefly recalled the link between some non-linear Fokker-Planck partial differential equations and stochastic differential equations which are non-linear in the sense of McKean and are driven by a Brownian motion. Jourdain developed this part in his talk; see below. S. Méléard recalled the particle approximation result deduced from this stochastic interpretation. she generalized this approach to a non-linear partial differential equation with fractional Laplacian and show how it is related with a non-linear jump process.

In a second part, she considered kinetic equations known as (spatially homogeneous) Fokker-Planck-Landau equations [25] (see also J. Fontbona). She showed that the probabilistic interpretation involves a non-linear stochastic differential equation driven by a space-time white noise. She used this interpretation to define an easily simulable stochastic particle system and prove its convergence in a pathwise sense, to the solution of the Landau equation.

B. Jourdain first recalled how existence for a stochastic differential equation (SDE for short) non-linear in the sense of McKean implies existence for the associated non-linear Fokker-Planck partial differential equation. In the case where the driving Lévy process is square integrable and the diffusion coefficient is Lipschitz continuous, B. Jourdain explained how to prove existence and uniqueness for the SDE by a fixed-point approach. He also exhibited strong rates of convergence of approximations by interacting particle systems as the number of particles tends to infinity. When either the integability properties of the Lévy process or the smoothness assumption on the diffusion coefficient are relaxed, weak existence for the SDE is obtained by weak convergence of the particle systems.

Fractal conservation laws

- N. Alibaud. *Fractional Burgers equation.*
- J. Droniou. *A numerical approximation of the solutions to fractal conservation laws.*
- G. Karch. *Large time asymptotics of solutions to the fractal Burgers equation.*

Four talks (the three previous ones and the one of W. A. Woyczynski, see above) were related to the study of Fractal conservation laws in one space variable

$$\begin{cases} \partial_t u + \partial_x(f(u)) + (-\Delta)^{\alpha/2} u = 0 & t > 0, x \in \mathbb{R}\,, \\ u(0,x) = u_0(x) & x \in \mathbb{R}\,, \end{cases} \tag{14.4}$$

where f is a non-linear flux function and $(-\Delta)^{\alpha/2}u$ is the fractional Laplacian.

We recall that the fractional Laplacian is defined as follows: for all Schwartz function ϕ,

$$(-\Delta)^{\alpha/2}\phi = \mathcal{F}^{-1}(|\xi|^\alpha \mathcal{F}\phi)$$

where $\mathcal{F}$ denotes the Fourier transform. There also exists an integral representation of the fractional Laplacian: for all $\phi \in C^{1,1} \cap L^\infty$, $x \in \mathbb{R}$,

$$(-\Delta)^{\alpha/2}\phi(x) = -c(\alpha)\int (u(x+z) - u(x) - Du(x)\cdot z\mathbf{1}_B(z))\frac{dz}{|z|^{1+\alpha}}$$

where $\mathbf{1}_B(z)$ denotes the indicator function of the unit ball of $\mathbb{R}$ and $c(\alpha) > 0$ is a constant which only depends on α.

An important special case of (14.4) is the fractal Burgers equation which corresponds to the case $f(u) = u^2/2$.

$$u_t + uu_x + (-\Delta)^{\alpha/2}u = 0 \tag{14.5}$$

with $\alpha \in (0, 2)$.

Before reviewing the results presented during the workshop about (14.4), we would like to mention that all the important results known for this equation were proved by people attempting the workshop. As far as existence and uniqueness of a solution is concerned, a first study was done in a framework of fractional Sobolev spaces and Morrey spaces [9, 11]. Next, solutions were studied in a L^∞ framework in [21]. In particular, it is proved in the case $\alpha > 1$ that there exists a smooth solution of (14.4) as soon as f is Lipschitz continuous and u_0 is bounded.

As far as fractal conservation laws are concerned, W. A. Woyczynski focused on results about the asymptotic behavior of solutions are obtained in [12, 28] in the case where $f(u) = |u|^{r-1}u$ and the physical origin of the equation [26]. He explained that $r_C = 1+(\alpha-1)/d$ is a critical non-linearity exponent. When $r > r_C$, then the solution u of (14.4) for such f's behaves the one where $f \equiv 0$ (with the same initial datum). It is even possible to get second-order asymptotics. When $r = r_C$, there exists a unique source solution U and the long time behaviour of u can be described by using U [28].

Alibaud explained that in the case $\alpha \leq 1$, the analyis developed in [21] in a L^∞ framework do not apply. In particular, shocks can occur even with smooth initial data u_0 [2] and weak solutions are not unique; see the working paper by Alibaud and Andreianov (Besançon, France). This is the reason why it is necessary to define entropy solutions [1] by using the integral representation of the fractional Laplacian.

Karch presented results about the large time behavior of solutions of the Cauchy problem for (14.5) supplemented with the initial datum of the form

$$u_0(x) = c + \int_{-\infty}^{x} m(dy)$$

with $c \in \mathbb{R}$, m being a finite (signed) measure on $\mathbb{R}$. If $\alpha \in (1, 2)$, the corresponding solution converges toward the rarefaction wave *i.e.* the unique entropy solution of the Riemann problem for the nonviscous Burgers equation [27]. On the other hand, using a standard scaling technique one can show that equation (14.5) with $\alpha = 1$ has self-similar solutions of the form $u(x,t) = U(x/t)$. These profiles determine the large time asymptotics of solutions to the initial value problem with $\alpha = 1$. If $\alpha \in (0, 1)$, the Duhamel principle allows us to show that the non-linear term is asymptotically negligible and the asymptotics is determined by the linear part of equation (14.5). These results will be contained in a working paper by C. Imbert and G. Karch.

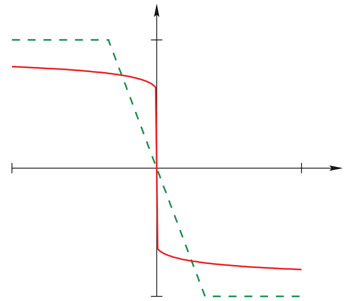
Droniou presented a method to compute numerical approximations of solutions of (14.4). The conservation law is discretized using classical monotone upwind fluxes (either 2-points fluxes, or higher order methods such as MUSCL), and the discretization of the fractal operator is based on its integral representation. He gave a few elements on the analysis of this scheme, and he provided numerical results showing behaviors of the solution (such as shock or speed of diffusion) which have been predicted in the literature on theoretical study of fractal conservation laws. See for instance Figure 14 for a numerical simulation of the appearence of shocks [2].

Applications

- A. Peirce. *Hydraulic Fractures: multiscale phenomena, asymptotic and numerical solutions.*
- B. Perthame. *Adaptive evolution; concentrations in parabolic PDEs and constrained Hamilton-Jacobi equations.*

Some of the talks more directly described direct applications of nonlocal operators. This is in particular the case of A. Peirce's talk, in which he describe a model for studying propagation of hydraulic cracks. After introducing the problem of Hydraulic Fracture and providing examples of situations in which Hydraulic Fractures are used in industrial problems, A. Peirce presented some numerical method for solving the governing equations, for which very few rigorous properties are known.

Figure 14.2: Initial condition (in green) and solution (in red) at time $T = 0.5$ and $\alpha = 0.3$



Hydraulic fractures (HF) are a class of tensile fractures that propagate in brittle materials by the injection of a pressurized viscous fluid. Natural examples of HF include the formation of dykes by the intrusion of pressurized magma from deep chambers. HF are also used in a multiplicity of engineering applications, including: the deliberate formation of fracture surfaces in granite quarries; waste disposal; remediation of contaminated soils; cave inducement in mining; and fracturing of hydrocarbon bearing rocks in order to enhance production of oil and gas wells.

The governing equations in 1-2D as well as 2-3D models of Hydraulic Fractures involve a coupled system of degenerate nonlinear integro-partial differential equations as well as a free boundary Namely, the width of the fracture $w(x, t)$ satisfies

$$\partial_t w = \partial_x (w^3 \partial_x p)$$

where the pressure p is given by

$$p - \sigma_0 = (-\Delta)^{1/2}(w).$$

This equation is satisfied inside the fracture itself, i.e. for $|x| \leq l(t)$. It is a non local diffusion equation (the pressure law is nonlocal) of order 3. At the tip of the fracture ($x = \pm l$), we must have

$$w(\pm l, t) = 0 \qquad w^3 \partial_x p = 0.$$

A. Peirce then demonstrates, via re-scaling the 1-2D model, how the active physical processes manifest themselves in the HF model and show how a balance between the dominant physical processes leads to special solutions.

He then discussed the challenges for efficient and robust numerical modeling of the 2-3D HF problem including: the rapid construction of Greens functions for cracks in layered elastic media, robust iterative techniques to solve the extremely stiff coupled equations, and a novel Implicit Level Set Algorithm (ILSA) to resolve the free boundary problem. The efficacy of these techniques with numerical results can be demonstrated.

Living systems are subject to constant evolution through the two processes of mutations and selection, a principle discovered by Darwin. In a very simple, general and idealized description, their environment can be considered as a nutrient shared by all the population. This alllows certain individuals, characterized by a ’phenotypical trait’, to expand faster because they are better adapted to the environment. This leads to select the ’best fited trait’ in the population (singular point of the system). On the other hand, the new-born population undergoes small variance on the trait under the effect of genetic mutations. In these circumstances, is it possible to describe the dynamical evolution of the current trait?

In a work based on collaborations with O. Diekmann, P.-E. Jabin, S. Mischler, S. Cuadrado, J. Carrillo, S. Genieys, M. Gauduchon and G. Barles, B.Perthame study the following mathematical model which models such dynamics:

$$\begin{cases} \partial_t n = d\partial_{xx} n + n(1 - \phi \star n), \quad 0 \leq x \leq 1, \\ n(t,0) = n(t,1), \qquad \partial_x n(t,0) = \partial_x n(t,1) \\ n(0,x) = n_0 \geq 0 \end{cases}$$

where the convolution kernel ϕ satisfies

$$\phi \geq 0, \quad \int \phi = 1, \quad \phi = 0 \text{ in } \mathbb{R} \setminus [-b, b].$$

Then it can be shown that an asymptotic method allows them to formalize precisely the concepts of monomorphic or polymorphic population. Then, we can describe the evolution of the 'best fitted trait' and eventually to compute various forms of branching points which represent the cohabitation of two different populations.

The regime under investigation correspond to letting the small parameter ϵ go to zero in

$$\begin{cases} \partial_t n = \epsilon \partial_{xx} n + \frac{1}{\epsilon} n(1 - \phi \star n), \quad 0 \leq x \leq 1, \\ n(t,0) = n(t,1), \qquad \partial_x n(t,0) = \partial_x n(t,1) \\ n(0,x) = n_0 \geq 0 \end{cases}$$

This leads to concentrations of the solutions and the difficulty is to evaluate the weight and position of the moving Dirac masses that desribe the population. It can be shown however, that a new type of Hamilton-Jacobi equation, with constraints, naturally describes this asymptotic.

Outcome of the meeting

This meeting brought together mathematicians with a common interest for nonlocal operators to present their latest results on the topic. Besides the great quality of the talks (see above), this meeting has also given the opportunity for people to meet and exchange ideas on this subject. Many participants have taken advantages of the informal discussion sessions to work together. We know that several new collaborations were started during the meeting, and we think that this is an indication that BIRS is extremely important to the mathematical community.

List of Participants

Alibaud, Nathael (Université Montpellier 2)
Capella, Antonio (Universitat Bonn)
Cardaliaguet, Pierre (Université de Bretagne Occidentale)
Cowan, Craig (University of British Columbia)
Dolbeault, Jean (University of Paris Dauphine)
Droniou, Jerome (Universite Montpellier 2)
Gentil, Ivan (Universite of Paris-Dauphine)
Ghoussoub, Nassif (BIRS)
Imbert, Cyril (University Paris-Dauphine, CEREMADE)
Jourdain, Benjamin (Ecole Nationale des Ponts et Chausses)
Karch, Grzegorz (Uniwersytet Wroclawski)
Margetis, Dionisios (University of Maryland)
Meleard, Sylvie (Ecole Polytechnique)
Mellet, Antoine (University of British Columbia)
Monteillet, Aurelien (University of Brest)
Moradifam, Amir (University of British Columbia)
Mouhot, Clément (Centre National de la Recherche Scientifique & Université Paris-Dauphine)
Patrizi, Stefania (Sapienza Università di Roma)
Peirce, Anthony (University of British Columbia)
Perthame, Benoit (Laboratoire J. L. Lions, University Pierre et Marie Curie)
Roquejoffre, Jean-Michel (Universite Paul Sabatier Toulouse III)
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Souganidis, Panagiotis (University of Chicago)
Vasseur, Alexis (University of Texas at Austin)
Vovelle, Julien (Pacific Institute for the Mathematical Sciences, Unité Mixte Internationale)
Woyczynski, Wojbor (Case Western Reserve University)

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Chapter 15

Climate Change Impacts on Ecology and the Environment (08w5054)

May 04 - May 09, 2008

Organizer(s): Charmaine Dean (Simon Fraser University), Sylvia Esterby (University of British Columbia Okanagan), Peter Guttorp (University of Washington), Jim Zidek (University of British Columbia)

Aims and Scope

The purpose of the proposed workshop is to engage climate change researchers in the scientific enterprise of developing novel methods for addressing these problems. It is envisioned that the proposed workshop would build upon collaborative initiatives already conceived through the environmetrics collaborative research group. Gaps in methodological developments will be identified, for example, methods for isolating the species and ecosystems most vulnerable to climate change. In addition, some techniques discussed will cross several of the themes, for example, detection of changes when observations are available at several spatial and temporal scales. This workshop will also play the important role of providing opportunity for discussion of timelines and progress toward the goals identified in the collaborative research group application on “Georisk and climate change” by these organizers and will provide a forum for interim reporting on research objectives of that collaborative research group. It is envisaged that this workshop will bring together researcher in diverse scientific fields. It will also have a strong focus on student participation, bringing together students working in this area in a unique networking opportunity including both environmental and statistical sciences.

Presentation Highlights

Presentations covered most of the planned topics by a mix of subject area researchers and statistical scientists. Speakers included both junior and senior investigators. Discussions were lively as the records of the three roundtable discussion sessions, included below demonstrate. These records present a number of important current issues, challenges and research directions. Their depth derives in part from of the wide range of expertise of the meeting’s participants.

Francis Zwiers, Director of the Climate Research Division, Environment Canada and co-winner of the Nobel Prize as a member of the IPCC panel, led things off. He gave a very informed, clear introduction to climate modeling. His presentation prepared the participants for a novel feature of the meeting on its second day when Myles Allen gave an interactive tutorial via Internet link from the UK. This worked extremely well, something that bodes well for the future when the organizers of this meeting plan to establish multi-centre graduate programs based at least partly on multi-centre simulcasts of lectures to be given at one centre and transmitted to the others.

Quite a number of talks focussed the climate models that have become so central to establishing a foundation for analyzing scenarios of climate change. Speakers explored the problems of differential scaling of measurement and models, of downscaling and of quantifying the uncertainty in the outputs of ensembles of such models. How are appropriate and meaningful measures of their spread to be computed?

Speakers from the UK imparted an international flavour to the meeting. They gave an overview of problems associated with monitoring climate to detect change on the one hand, and detecting impacts of change on the other.

Some of the presentations covered theory, others applications achieved through collaborative research. This gave the meeting variety and provided a profitable exchange of ideas between "producers" and "consumers" of statistical methods.

One planned topic not adequately covered was agroclimate risk management. Although that topic was linked into the Environmetrics CRG, it was to have been funded by the NICDS rather than PIMS. Although two papers were given on this topic, research was retarded due to a long delay in the start-up of funding, a result of NICDS's lengthy and time-consuming renewal application process.

The facilities provided by BIRS are generally excellent and they contributed much to the success of the meeting.

Best Practices approaches for characterizing, communicating, and incorporating scientific uncertainty in decision-making

Chair and Recorder: Jim Zidek

Peter Guttorp introduced the topic of the discussion paper, noting that he is organizing a future meeting on the topic of this session. Furthermore he noted that the US Climate Change Science Program is drafting a number of synthesis documents, each subject to public review and amendment on the basis of input received. Statisticians have been involved in writing the report but most of the authors are decision analysts. Tilmann Gneiting then introduced the report by going through a summary of its sections and highlighting selected issues found in them. Discussion followed on the following main themes:

1. Characterizing uncertainty
2. Defining probability, chance and likelihood
3. Combining expert opinion
4. The role of uncertainty in decision-making
5. Communicating uncertainty

Theme 1. Characterizing uncertainty

Surprises
The minimax approach in decision analysis captures the natural behavior of humans faced with the prospect of deeper uncertainty.

Communicating uncertainty
How you express uncertainty depends on the purpose and with whom you are communicating. For example,

standard error has long been used as a measure of uncertainty about parameter estimates. Odds seem a basic language of uncertainty.

IPCC report
IPCC has done a good job and has been overly open and honest - opposite of exaggerated. Two ways of describing uncertainty - one calibrated by chance, the other based on likelihood. Chance, likelihood are however undefined.

Expert opinion
Some evidence shows uncertainty to be highly under-estimated, based on range of expert opinion.

Ensemble uncertainties
We need to revisit ensembles and start our assessment "from the ground up" in order to understand and characterize these uncertainties. In particular, we need to characterize the intrinsic uncertainty of the model components. However sensitivity analysis has a key role to play; model outputs may not be sensitive to the way uncertainties of some of those components are characterized. At the same time interactions may mean that sensitivity to one component may well depend on the level of another. From some perspectives these issues hardly matter - the issues of major concern will not be much affected by how uncertainty of these ensembles is expressed. Yet from others it does. After all plans are now being made about how to manage change and uncertainty would play into those plans such as adopting more efficient light bulbs or building sea walls.

In any case, as Myles Allen noted, much more planning needs to go into the design of ensembles instead of simply relying on the ones that come to hand, in order to address these issues. Myles Allen's grey error bands are not the same as confidence bands. For one thing, the builders of these models try to bring their models into line with those already available, making them "dependent" if regarded as outcomes of an experiment - the result: unduly narrow uncertainty bands.

Major research problem: Find valid ways of characterizing the uncertainty of ensembles.

Assessment of climate model uncertainty
Regional instead of global climate models may be useful in assessing uncertainties if they can be extrapolated to adjoining regions for comparisons of results.

Theme 2. Defining probability, chance and likelihood

Popular misconceptions
The general population does not understand probability let alone second order probability (probability expressing uncertainty about probability). Moreover when confronted by a variety of scenarios or possibilities as in climate projections, they will be perceived as equally likely.

Second order probabilities
Although second order probabilities are probabilities on uncertain probabilities, the result is quite complicated. However, there may well be a "philosophical" if not technical reason for preserving the distinction. However, communicating probability could then include the challenge of explaining the difference between first and second order probabilities.

Keeping a unified front
We do not all agree about how probability should be defined. However, advantages, including political advantages, will accrue from presenting a unified face in communicating uncertainty via probability, since credibility will be lost if we do not. In fact from a cynical point of view, such divisions will be seized on by nay-sayers and politicians with an agenda.

Chance

Its hard to know what true meaning to attach to “chance” in the context of climate, owing to such thing as the complexity of the analysis, models, and the numerous types of uncertainties that obtain.

Expectation instead of probability?
Whittle bases his book on the notion of “expectation” rather than “probability”, pointing to the importance of the form in which we communicate random outcomes. For example, “expected amount of precipitation” might be more informative than the “probability of precipitation”, the latter giving the sort of information the public might better use. [At the same time probability is an expectation (of a 0 - 1 variable).] In his tutorial, Myles Allen distinguished between “expected” vs “average” weather. The loaded dice seems an excellent metaphor and could well be used to communicate this idea. For climate, it’s the expected degree of change that matters.

Behavioural definition
Probability has a behavioural interpretation. Yet generally people overestimate small probabilities. Moreover, assessments can be irrational as when, following Sep 11 people stopped flying to a steadily declining degree as time wore on.

Relative frequency definition
“One life - one replication” means the relative frequency definition of probability is challenging. But repeatedly running probabilistic simulation models could provide relative frequency estimates in some situations even in “one-off” events like climate change. The value of such estimates will depend on the credibility accorded to the science built into the model.

Theme 3. Combining expert opinion

Although the report generally gives a “academic” survey of relevant work, its coverage is weak on work and issues on combining expert opinion, in spite the great importance these days of multi-agent decision theory. In particular, scientific panels are becoming increasingly important, the IPCC being a particularly noteworthy example. The Delphi method is mentioned but more on its practical implementation in group decision-making needs emphasis. When that process does lead to multi-agent convergence to convergence, the result can be more a product of “group think” rather than the exchanging of information. When that convergence does not take place beliefs will need to be combined (normative methods have been published for doing this) or a joint decision made (theories for doing this also exist).

A particular problem arises from the deliberately mixed disciplines of panel members. That can mean that components of a big decision problem are being assessed by individuals with varying levels of expertise leading to the need to weight their views according (and this can be done by the methods alluded to above). In general, the multi - agent problem has three levels. In the first, the group attempts to reach a consensus. If not controlled, as it is in the Delphi method, such things as group-think and psycho-dynamics can denigrate the contribution of individual experts and bias the outcome in favor of the dominant experts. At the next level in the so-called “team approach”, the group is assumed to have a common objective (utility function), as in the case of a jury in Savage’s classic on the foundations of decision analysis. Then the goal becomes that of combining the beliefs of the agents into a single prior distribution. [See Genest, C. and Zidek, J.V. (1986). “Combining probability distributions: a critique and an annotated bibliography.” Statistical Sciences, 1:114-148 for possible solutions.] More generally, the multi - agent problem becomes a group decision problem where the group must come to a joint decision, for example, an agreed upon standard. [See Weerahandi, S. and Zidek, J.V. “Elements of multi-Bayesian decision theory.” Ann. Statist., 11:1032-1046, (1983).] Numerous papers have been written on this problem in the contexts of computer science.

Theme 4. The role of uncertainty in decision-making

Uncertainty plays a variety roles in decision-making. In particular, in an adversarial context, it can be exploited to argue in favor of maintaining the status quo. The report should therefore include advice on how the process of decision-making should be structured, especially when the level of uncertainty is high, to help insure a sensible outcome. In particular, in a multi-agent situation, emphasis should be placed on an “estimation approach” rather than a “hypothesis testing approach”; the latter will likely lead to non-rejection of the hypothesis.

Theme 5: Communication of uncertainty

Experts on communicating uncertainty need to be educated. That leads to the need for programs that do just that for such people as journalists, stakeholders, scientists and the general public. Australia has started a new project to educate politicians and journalists with scientists going out in teams to do that. The report under discussion tends to focus on analysis rather than communication. What is needed to ensure an honest expression of uncertainty? How can one compensate for the tendency nowadays for people to discount reported uncertainty on the cynical assumption that it has been inflated by hyperbole in the first place?

Important need: The education of both communicators of uncertainty and their audiences.

Climate Change and Impacts on Forest Disturbances

Chair: Dave Martell; Recorder: Douglas Woolford

The majority of the discussion can be grouped into the following main themes:

1. Dynamical systems models
2. Statistical/Quantitative methods for comparing maps
3. Simulation models and scaling issues
4. State space modelling and ecosystem modelling

Theme 1. Dynamical systems models

A different approach to the statistical models proposed in the workshop would to use dynamical systems models. However, these are currently fit using expert opinion/judgement and there appears to be a lack of statistical methodology for fitting in such models. As a result of this discussion, John Braun volunteered to give a brief presentation on related work where he has been fitting a dynamical systems process to fire data using results from experimental lab fires to fit parameters to the Prometheus fire growth model. In addition, he has been incorporating randomness into this model via smoothing/sampling of residuals.

Ron Smith has also done some work on model fitting related to fire data, indicating that there are several methods available that depend on the complexity of the model in question. The reference is “Managing Uncertainty in Complex Models” (MUCM) out of the UK.

A hot area is using the Kalman filter to change a complex deterministic model into another type of model. This allows one to bring in statistics to improve upon the current model. Other related work is the convergence of the Kalman filter and convergence of dynamical systems with random perturbations, noting that these two topics can be united. In general this is “easy” when the model is relatively simple (i.e., consists of a few differential equations), but becomes more difficult as the model complexity increases. Regardless as to whether or not a model can be fit, there are still questions of identifiability and goodness of fit testing. There also does not appear to be a robust method for sensitivity analysis for dynamical models.

Theme 2. Statistical/Quantitative methods for comparing maps

A common issue in forestry is the comparison of maps. For example, foresters may develop burn probability maps (i.e., a colour-coded, pixel-based map or the probability that a pixel will burn) under various scenarios/models. Foresters are looking for proper statistical methods for comparing maps. It was noted that this is a very active field of research in meteorology called “object-based verification”. A possible reference is a special issue on forecast verification in Meteorological Applications that appeared sometime around early 2007.

Theme 3. Simulation models and scaling issues

Although there appears to be a push to build big simulation models, significant issue remain. In particular, scaling problems and compensating errors remain common. Furthermore, there have been instances where, upon further statistical analysis, large simulation models have been reduced to significantly simpler simulation models. However, simulation models, regardless of model complexity, are attractive to policy builders, since they perceive them as being easier to understand than a statistical model. A well-written critique comparing a simulation model to a related statistical model might be useful.

There are other issues with simulation models. A key issue is extrapolation, since, in many cases a simulation / dynamical-systems model can be somewhat useless when one hopes to extrapolate. The underlying hope is that if a physical model fits past data correctly, then it might produce a reasonable forecast in the future.

Theme 4. Incorporating randomness into deterministic models

A topic that was discussed more than once was the idea of incorporating randomness into deterministic models. A method for this was introduced by John Braun during his talk (for more details see Theme 1 above). In general, models for complex simulations likely only provide a limited amount of information, since some data will be masked or unmeasured. A possible solution would be to use models which sample from a set of possible solutions. That is, one can incorporate randomness into a deterministic model by varying the initial conditions. However, in this case a “uniform” assumption for sampling is probably wrong. Hence, one needs a method for determining if one is sampling from the ensemble of models/conditions correctly. Another method for incorporating randomness would be via conversion of differential equations in a model to stochastic differential equations.

Climate Change Impacts in Ecology: Science and Government Policy

Chair: Rick Routledge; Recorder: Sylvia Esterby

The chair provided a list of issues that have emerged repeatedly (provided below) and opened the session with the suggested focus for the discussion: identifying high-priority statistical, scientific, and policy issues requiring further research. Most of the discussion was concerned with informing policy, drawing on experience in the UK, the United States and Canada.

An example: species at risk
Science question: Probability of extinction for a species at risk
Policy limitation: difficulty of getting a species on the endangered list

Policy making process
US example, Ozone Panel (Clean Air Act)

- Panel made up of external scientists
- Panel and EPA staff have clear roles and do not interact
- Open public consultation, largely interest groups

- Means of contributing is well-defined, with clear limitations
- Administrator makes final ruling

It was noted that this is the process for a panel operating under an Act. A different process applies if a panel addresses an issue not under an Act, and an example of an ecological panel operating very differently was mentioned.

UK process

- Peer review of government commissioned work
- Public participation through interest groups, with limits
- EU standards apply and must be approved across member countries
- UK example of air pollution standards - work to bring EU protocol in line with UK's previously developed protocols

In Canada the process seems less clearly defined. More is done internally by departmental scientists.

Other observations related to taking uncertainty into account in policy making:

- Policy makers find the less definitive approach of statistics difficult to embrace
- Uncertainty and a statistical approach presents difficulty for policy makers who want clear direction for helping them make decisions
- Precautionary principle allows action to be taken under uncertainty
- Europe is ahead of US and Canada in applying the precautionary principle

Models and communicating uncertainty:
How can we build models that allow for surprises (unanticipated events, future change in physical processes)

- Attempts to put surprise term in Bayesian models have not been successful
- Would mixture models work?
- Appears to be an open question

Maps are often problematic

- Visual nature makes them a powerful tool
- Should have "error bars" since we know all predictions are uncertain
- Challenge is how to present just the right amount of information. The case of probabilistic forecasting, described earlier in the workshop, provides an example where this question has been carefully considered

Clarity on what different groups understand uncertainty to be is important in all cases.

Some Issues that have Emerged Repeatedly

Chair and Recorder: Rick Routledge

1. Quantitative research challenges
   (a) Assessing uncertainty in:
      i. Evidence on emerging trends
      ii. Inference on causal relationships (attribution)
      iii. Forecasts of potential impacts
   (b) Strategies for:
      i. Assessing impacts that may already be underway
      ii. Predicting future impacts
      iii. Combining more precise, extensive, physical data with less accurate, consistent, and rigorous biological data
      iv. Drawing inferences from a combination of (i) deterministic, primarily physical, and often larger-scale models, and (ii) data on biological systems typically operating in a more restricted geographic scale
      v. Dealing with severely skewed distributions
      vi. Handling informal censoring of non-occurrences
      vii. Designing monitoring networks
      viii. Improving the associated statistical analyses (with emphasis on spatio-temporal modeling, nonparametric smoothing, additive modeling, quantile regression, and repeated illustrations of the value of innovative approaches)
      ix. Fostering long-term consistency in labour-intensive monitoring systems
      x. Developing and assessing indices of environmental health
      xi. Designing meaningful and measurable objectives
2. Communication and policy issues
   (a) Creating meaningful summaries for informing public discussion and policy making
   (b) Methods for conveying estimates of uncertainty
   (c) Management strategies under uncertainty
      i. Adaptive management
      ii. Precautionary principle

List of Participants

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Chapter 16

Locally Symmetric Spaces (08w5056)

May 18 - May 23, 2008

Organizer(s): Stephen Kudla (University of Toronto), Juergen Rohlfs (Katholische Universitaet Eichstaett), Leslie Saper (Duke University), Birgit Speh (Cornell University)

The setting

A locally symmetric space is the quotient $\Gamma\backslash X$ of a globally symmetric space $X = G/K$, where G is a non compact reductive Lie Group with maximal compact subgroup K and where Γ is a discrete subgroup of G. Locally symmetric spaces are important in geometry, analysis, and as well as in number theory. We considered at the conference both arithmetic and non-arithmetic subgroups Γ as well as compact and non-compact locally symmetric spaces $\Gamma\backslash X$.

The topics covered at the conference belong to

- compactifications,
- differential geometry and topology, and
- arithmetic.

Techniques and results from all these areas were represented.

Background material

Several developments in different fields over the past few years made this an opportune time for this workshop.

Compactifications

When X/Γ is non-compact, various compactifications (often singular) have been introduced to address different problems in geometry and number theory. The construction and relationship between various compactifications has become more clear through the work of several mathematicians, particularly Borel, Goresky, Ji, and Zucker.

Various types of cohomology associated to these compactifications are important in number theory. The relation between the L^2-cohomology and the intersection cohomology of the Baily-Borel compactification is important for Langlands's program and was resolved by Looijenga and Saper-Stern. The further relationship between this and the weighted cohomology of the (less singular) reductive Borel-Serre compactification was settled by Goresky, Harder, and MacPherson. The analogous theorem for the intersection cohomology of the reductive Borel-Serre compactification was a conjecture of Rapoport which was established by Saper. More recently the relation between the space of L^2-harmonic forms and the intersection cohomology of the reductive Borel-Serre compactification was determined by Saper in a general context. The presence of the reductive Borel-Serre compactification in recent work shows its ubiquity.

A topological problem concerning locally symmetric spaces which has received a fair bit of attention is the problem to determine if a cycle class of a locally symmetric subvariety is a nontrivial cohomology class; see for example the work of Bergeron, Clozel, Rohlfs-Speh, Speh-Venkataramana, and Venkataramana. This problem is related on the one hand to the difficult problem of determining the restriction to a semisimple subgroup H of an irreducible representations of G as in the work of Kobayashi-Oda and on the other hand to the arithmetic problem of period integrals with respect to H of automorphic representations where special values of L-functions also play a role. Another interesting and important problem, where similar techniques are useful, are non-vanishing results for cup products of cohomology classes such as those of Bergeron and Venkataramana.

Differential geometry and topology

Important geometric invariants of locally symmetric spaces which have been considered are the analytic torsion and the related length spectrum of closed geodesics, as well as the special values of the geometric theta functions; in particular we note the work of Deitmar, Juhl, and Rohlfs-Speh. In this context, invariants of non-arithmetic subgroups are also of great interest as in the work of Bunke, Olbricht, and Leuzinger.

Arithmetic

The application of locally symmetric spaces to arithmetic involves a great deal of analysis. One of the main problems in analysis on locally symmetric spaces is the study of the spectrum of the Laplace operator on the space X/Γ. A very well-known spectral problem is to obtain a lower bound on the spectrum of the Laplacian. For GL_n, the Ramanujan conjecture is equivalent to such a bound. For $n = 2$, the best bound is due to Shahidi and Kim. In the general case, substantial work has been done by P. Sarnak and his collaborators. The techniques used here are L-functions and the lifting of automorphic representations.

Another source of interesting analytic problems is connected to the Arthur-Selberg trace formula. Particularly notable here is the recent work of W. Müller on the spectral side of the Arthur-Selberg trace formula and his results about Weyl's law for the cuspidal spectrum.

Other connections to number theory also play an important role in the study of locally symmetric spaces. This can be seen for example in the work of Ash, Bruinier, Clozel, Emerton, Hanamura, Harder, Kudla, Mahnkopf, Rapoport, Rohlfs, Schwermer and Speh. Conjectures of Langlands, Tate, Beilinson and others are the driving force behind these developments which involve Hecke eigen-functions, L-functions, special values of L-functions, special points of varieties, modular symbols, mixed motives, Chow groups, and K-theory.

The conference

The conference was attended by 31 scientists from all over the world. There were 17 talks, each of one hour, covering recent developments in the field. One goal of the workshop was to give an opportunity for young researchers to learn more about the different aspects of the field, the different methodologies, and the many open problems. With around half the participants being young researchers, this goal was well achieved. Another goal was to stimulate new developments, possibly involving interactions of researchers from different areas. The format of the conference, with sufficient unstructured time for informal discussions, allowed this goal to be achieved as well. Mathematical discussions, both formal and informal, in the common room continued far into the night.

Abstracts of talks (in alphabetical order)

Speaker: *Yves Benoist* (University of Paris, South)
Title: Effective equidistribution of S-integral points on symmetric varieties

Abstract: Let S be a finite set of places of a global field K. We describe counting and equidistribution results for the S-integral points on a symmetric variety defined over K. We give also an upper bound for the error term in characteristic 0. This joint work with Hee Oh is based on a polar decomposition of p-adic symmetric spaces.

Speaker: *Mathieu Cossutta* (University of Paris, 7)
Title: Asymptotics of L^2-Betti numbers in congruence coverings of some arithmetically defined locally symmetric varieties.
Abstract: Let $G/\mathbb{Q}$ be an algebraic group and $X = G(\mathbb{R})/K$ the associated symmetric space. The aim of my talk is to give some new informations on $b_{i,2}(\Gamma(p^n)\backslash X)$ when n goes to infinity for a large family of groups G, in the direction of conjectures formulated by Xue and Sarnak. Our proof is based on theta correspondence. For example when G = Sp_{2g}, the primitive holomorphic cohomology appears only in degree $r(2gr)$ for r an integer between 1, . . . , g. We then obtain that for $g \leq \frac{5}{4}p + 1$:

$$\begin{aligned} &\mathrm{Vol}(\Gamma(p^n)\backslash X)^{\frac{2r}{g+1}(1-\frac{r(r+1)}{g(g+1)})-\epsilon} \\ &\qquad \ll_\epsilon \dim H^{r(2g-r),0}_{\mathrm{prim},2}(\Gamma(p^n)\backslash X, \mathbb{C}) \\ &\qquad \ll_\epsilon \mathrm{Vol}(\Gamma(p^n)\backslash X)^{\frac{2r}{g+1}(1+\frac{r(r-1)}{g(g+1)})+\epsilon} \end{aligned}$$

Speaker: *Anton Deitmar* (University of Tübingen)
Title: Automorphic forms of higher order
Abstract: The present talk presents an attempt to study them in the general context of higher order invariants and cohomology. It is shown that for arithmetic groups, higher order cohomology can be computed as $(\mathbf{g}, K)$-cohomology, even using functions of moderate growth. It is, however, an open question whether the higher order analogue of Franke's theorem holds, which states that the cohomology can be computed using automorphic forms. An action of the Hecke algebra is introduced in which the Hecke operators are bounded operators. Questions about their spectral decomposition are raised.

Speaker: *Jens Funke* (New Mexico State University)
Title: Special cohomology classes arising from the Weil representation
Abstract: The Weil representation is a well-known tool to study arithmetic and cohomological aspects of orthogonal groups. We construct certain special cohomology classes for orthogonal groups O(p, q) with coefficients in a finite dimensional representation and discuss their automorphic and geometric properties. In particular, these classes are generalizations of previous work of Kudla and Millson and give rise to Poincare dual forms for certain special cycles with non-trivial coefficients in arithmetic quotients of the associated symmetric space for the orthogonal group. Furthermore, we determine the behavior of these classes at the boundary of the Borel-Serre compactification of the associated locally symmetric space. As a consequence we are able to obtain new non-vanishing results for the special cycles. This is joint work with John Millson.

Speaker: *Jayce Getz* (Princeton University)
Title: Twisted relative trace formulae with a view towards unitary groups
Abstract: (joint work with E. Wambach) We introduce twisted relative trace formulae and provide tools to relate them to relative trace formulae modeled on the relative trace formula introduced by Jacquet and Lai. As an application, we consider the analogue for odd rank unitary groups of the work of Harder, Langlands and Rapoport on modular curves embedded in Hilbert modular surfaces.

Speaker: *Harald Grobner* (University of Vienna)
Title: Regular and residual Eisenstein cohomology classes for inner forms of symplectic groups
Abstract: Let G be a semisimple Lie group with maximal compact subgroup K and arithmetic congruence subgroup Γ. The locally symmetric space $\Gamma\backslash G/K$ carries interesting arithmetic information encoded in its cohomology groups $H^*(\Gamma\backslash G/K)$. One of the major tasks in understanding this cohomology is to understand a certain subspace $H^*_{Eis}(\Gamma\backslash G/K)$, called Eisenstein cohomology. We will focus on the case of inner forms of the symplectic group Sp_n and try to give an overview of interesting phenomena which one encounters in the search of a description of $H^*_{Eis}(\Gamma\backslash G/K)$. If time permits, we will present completely new results.

Speaker: *Lizhen Ji* (University of Michigan)
Title: Borel extension theorem and Mostow strong rigidity
Abstract: An important result for the Baily-Borel compactification of Hermitian locally symmetric spaces is the Borel extension theorem for holomorphic maps from the punctured disk into the Hermitian locally symmetric spaces. We discuss an analogue for the Deligne-Mumford compactification for the moduli space of curves. Then we will discuss the Mostow strong rigidity for mapping class groups of surfaces (or equivalently the moduli spaces of curves) and outer automorphism groups of free groups. We will also discuss non-isomorphism results between three closely related groups: lattice subgroups of Lie groups, mapping class groups, and outer automorphisms of free groups.

Speaker: *Christian Kaiser* (Max Planck Institute for Mathematics, Bonn)
Title: Irreducibility of Galois representations associated to automorphic forms of multiplicative groups of skew fields over function fields
Abstract: This is work in progress. Not all details have been checked yet. Let D be a skew field of degree d over some global field of characteristic p. Under some ramification constraint on D, Lafforgue and Lau associated to an automorphic representation π of $D^\times$ a d-dimensional Galois representation $\sigma(\pi)$ with the same L-functions as π. If π is (almost everywhere) tempered it is conjectured that $\sigma(\pi)$ is irreducible. We prove this conjecture in some cases. The main tool, which may be of independent interest, is an uniformization theorem for the moduli space of $\mathcal{D}$-shtukas of rank one at a point $(0,\infty) \in X \times X$ with $\mathrm{inv}_0 D = \frac{1}{d}$ and $\mathrm{inv}_\infty D = -\frac{1}{d}$ by a product of two copies of Drinfeld's upper half space Ω^d. Using results of Boyer and Dat on the cohomology of Ω^d and its coverings one concludes for skew fields D which have invariant $\frac{1}{d}$ and -$\frac{1}{d}$ at some different places (and under some more constraints). Using simple cases of the Jacquet-Langlands conjecture one can reduce many cases to this special situation.

Speaker: *Toshiyuki Kobayashi* (University of Tokyo)
Title: Restriction of unitary representations of real reductive groups
Abstract: Branching problems ask how an irreducible representation of a group decomposes when restricted to its subgroup. Having an observation of bad features of branching problems in a general non-compact setting even for real reductive symmetric pairs, I will discuss how to find a nice setting for branching problems, and give an upper estimate on multiplicities. If time allows, some applications are also presented.

Speaker: *Bernhard Kroetz* (Max Planck Institute for Mathematics, Bonn)
Title: Globalization of Harish-Chandra modules
Abstract: We will explain short and simple proofs of the globalization theorems of Casselman-Wallach and Kashiwara-Schmid. The work is partly joined with Joseph Bernstein and partly with Henrik Schlichtkrull.

Speaker: *Enrico Leuzinger* (University of Karlsruhe)
Title: Reduction theory for arithmetic and mapping class groups
Abstract: Reduction theory is concerned with the construction of (coarse) fundamental domains for groups acting properly discontinuously. I will describe a remarkable analogy between (a version of) reduction theory for arithmetic groups and corresponding results for mapping class groups. As an application I will discuss asymptotic cones for locally symmetric spaces and moduli spaces.

Speaker: *Joachim Mahnkopf* (University of Vienna)
Title: Traces on Hecke algebras and p-adic families of modular forms
Abstract: We prove that any modular eigenform f of level $\Gamma_1(Np)$, finite slope and weight k_0 can be placed into a p-adic family of modular eigenforms f_k of the same level and slope and weight k varying over all natural numbers which are sufficiently close to k_0 in the p-adic sense. Here, the term p-adic family means that a p-adic congruence between two weights k and k_0 entails a certain p-adic congruence between the corresponding eigenforms f_k and f_{k_0}. We also prove that the dimension of the slope subspace of the space of modular forms of weight k does not depend on the weight as long as we consider weights k which are sufficiently close to each other in the p-adic sense. Both these statements are predicted by the Mazur-Gouvea conjecture, which has been proven by Coleman. Our proof of these statements, which is completely different from Coleman's proof, is based on a comparison of (topological) trace formulas.

Speaker: *Werner Mueller* (University of Bonn)
Title: The Arthur trace formula and spectral theory on locally symmetric spaces

Abstract: In this talk I will discuss various applications of the Arthur trace formula to spectral theory on locally symmetric spaces. I will also discuss analytic problems related to the trace formula which need to be settled for further applications.

Speaker: *Martin Olbrich* (University of Luxembourg)
Title: Extending the realm of Patterson's conjectures
Abstract: This talk is concerned with analysis and spectral geometry of certain rank 1 locally symmetric spaces of typically infinite volume, namely geometrically finite ones. Geometrically finite spaces without cusps correspond to convex co-compact discrete groups. In 1993, Patterson formulated two conjectures concerning convex co-compact groups acting on real hyperbolic spaces. The first conjecture relates invariant currents supported on the limit set to the cohomology of the locally symmetric space, while the second gives a description of the singularities of Selberg's zeta function in terms of objects supported on the limit set. Both conjectures are now proved for many cases. We shall discuss how the conjectures should be modified in order to make sense for arbitrary geometrically finite locally symmetric spaces of rank 1. Already the inclusion of noncompact spaces of finite volume into the picture is an interesting and nontrivial task.

Speaker: *Gopal Prasad* (University of Michigan)
Title: Lengths of closed geodesics and isospectral locally symmetric spaces
Abstract: I will give an exposition of my recent work with Andrei Rapinchuk in which we have introduced a new notion of "weak commensurability" of Zariski-dense subgroups. Weak commensurability of arithmetic subgroups of semi-simple Lie groups turns out to have very strong consequences. Weak commensurability is intimately related to the commensurability of the set of lengths of closed geodesics on, and isospectrality of, locally symmetric spaces of finite volume (and with nonpositive sectional curvatures). Using our results we are able to answer Marc Kac's famous question "Can one hear the shape of a drum?" for compact arithmetic locally symmetric spaces. Our proofs use algebraic number theory, class field theory, and also some results and conjectures from transcendental number theory.

Speaker: *Andras Vasy* (Stanford University)
Title: Scattering theory on symmetric spaces
Abstract: I will explain how methods from N-body scattering can be used to analyze the resolvent of the Laplacian and spherical functions on globally symmetric spaces (joint work with Rafe Mazzeo), and ongoing work with Rafe Mazzeo and Werner Mueller to extend the framework to locally symmetric spaces.

Speaker: *Dan Yasaki* (University of Massachusetts)
Title: Spines for Q-rank 1 groups
Abstract: Let $X = \Gamma\backslash D$ be an arithmetic quotient of a symmetric space associated to a semisimple algebraic group defined over $\mathbb{Q}$ with $\mathbb{Q}$-rank n. A result of Borel and Serre gives the vanishing of the cohomology of X in the top n degrees. Thus one can hope to find a Γ-equivariant deformation retraction of D onto a set D^0 having codimension n. When such a set exists, it is called a spine and is useful for computing the cohomology of X. Spines have been explicitly computed in many examples, and the general existence is known for groups associated to self-adjoint homogeneous cones. I will describe my work on the existence of spines for groups of $\mathbb{Q}$-rank 1.

Mathematical outcomes

The new results which have been presented can be roughly described by the following groups of key words:

- globalization theorems la Casselmann–Wallach, restriction of representations to subgroups, length spectrum of geodesics, scattering theory, discrete spectrum of the Laplace operator
- construction of cohomology classes for $\Gamma\backslash X$ by geometric and representation theoretical methods, new invariants for classical modular forms, retracts of $\Gamma\backslash X$, liftings and relative trace formula
- compactifications and rigidity, also for mapping class groups or groups of outer automorphisms of free groups
- p-adic modular forms, Galois representations

Most of the talks are reports on work in progress. The interested reader is encouraged to contact the speakers about preprints. Hence we refer in the bibliography only to some papers which give a first view on the field.

List of Participants

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Chapter 17

Emerging Statistical Challenges in Genome and Translational Research (08w5062)

Jun 01 - Jun 06, 2008

Organizer(s): Jennifer Bryan (University of British Columbia), Sandrine Dudoit (University of California, Berkeley), Jane Fridlyand (Genentech Inc.), Darlene Goldstein (Ecole Polytechnique Federale de Lausanne), Sunduz Keles (University of Wisconsin, Madison), Katherine S. Pollard (University of California, Davis)

Overview of Genome-scale Data Analysis

Modern high-throughput technologies are changing the face of biomedical and life science research. Biological research is moving from a hypothesis-driven focus on single genes and proteins to a high-throughput, discovery-driven strategy. Integrating the vast amounts of ever-changing types of data collected to study complicated entities, such as protein complexes and regulatory networks, requires an interdisciplinary approach.

The field of high-dimensional biology comprises several areas that are fueled by technological advances and require rigorous statistical and computational analysis. In each, there are high-dimensional multivariate data that are similar in nature. Background for these topics is given here.

Statistical Genomics and Regulation of Gene Expression

Quantitative traits are biological variables that are measured on a continuous (typically positive) scale. Examples include physical properties (e.g. height, weight, time to an event), molecular biomarkers (e.g. levels of mRNA, microRNA, protein or glycan), and chemical profiles (e.g. drug or metabolite concentrations). These traits tend to vary among individuals in a population. The observed trait variation results from genetic variation between individuals in the population. A region of the genome associated with variation in a quantitative trait is called a quantitative trait locus (QTL).

Single nucleotide polymorphism (SNPs) are a simple and prevalent source of genetic polymorphism in the human genome. SNP genotyping and haplotyping technologies are producing massive amounts of SNP data. One challenge faced by researchers is how to relate such multimillion dimensional genotypic profiles to biological and clinical phenotypes, such as disease and drug reaction. Analysis of the emerging complex data requires comprehensive statistical methodologies capable of dealing with challenging issues such as power, censoring, and causality.

Cancer Genomics

Translational aims are of paramount importance in current biomedical research. Recently, the National Cancer Institute has awarded a number of grants to generate an atlas of genomic and genetics features in cancers. While the ultimate aim is to improve cancer patient treatment, two major statistical complications arise. The first involves using high-dimensional patient data for predictions (e.g. response to standard or experimental therapies, time to recurrence). This problem falls into the class of *prediction statistical approaches*. The second involves identification of druggable markers of response to treatment, recurrence, progression or early detection. This can be viewed as a *variable selection problem*. We note that these two issues are tightly linked.

The statistical challenges include study design, building predictors based on heterogeneous cohorts, dealing with the small ratio of sample size (hundreds) to the number of variables (hundreds of thousands), multiple testing issues, computationally efficient classification, exploration of the interaction space of the variables, and handling the diverse data types in a unified rather than ad hoc manner.

Genome-scale data are also at the forefront of research into targeted therapeutics and individualized medicine. Pharmacogenomics deals with the influence of genetic variation on drug response in patients, and is overturning the “one size fits all” paradigm of drug development and treatment. Better understanding of an individual’s genetic makeup may be a key element of the prescribed therapeutic regime. This multidisciplinary field combines traditional pharmaceutical sciences with large scale data and meta-data on genes, proteins, and SNPs.

The realization of the promise of personalized molecular medicine will require the efficient development and implementation of novel targeted therapeutics. The goal will be to deliver the right drug to the right patient at the right time at the right dose. This effort will require a integration of information from the DNA, RNA and protein level into predictors of which patients are likely to respond to particular therapies. The overall likelihood of response to particular drugs represents the interaction between predictors of sensitivity with predictors of resistance. Efficient clinical trials testing these precepts will require the development and implementation of novel trial designs. It is likely that the size of Phase I and II trials will need to be increased to allow the identification and validation of molecular markers at the same time as the initial evaluation the toxicity and efficacy of targeted therapeutics. This will come with the advantage of being able to deliver targeted therapeutics to enroll a much smaller population of patients selected for the likelihood to respond in phase III trials accelerating the approval of effective targeted therapeutics.

However, data analysis can be difficult due to limitations in the present state of knowledge regarding the relevant signaling pathways, as well as to high noise levels inherent in such data. New statistical developments here have the potential to play an important role in further progress toward individualized medicine.

High-Throughput Biotechnologies

Recent technological advances enable collection of many different types of data at a genome-wide scale, including: DNA sequences, gene and protein expression measurements, splice variants, methylation information, protein-protein interactions, protein structural information, and protein-DNA binding data. These data have the potential to elucidate cellular organization and function. There is now a trend for quantitative genome-wide phenotyping, with several large-scale studies currently being carried out with these new technologies: e.g. large collections of deletion mutants, cells or organisms undergoing RNA interference (RNAi). Studies of disease processes in humans often include patient clinical data and covariates as well.

Revolutionary breakthroughs in genomic technologies are enabling both the measurement of trait variation (especially molecular phenotypes) and the assaying of millions of genetic markers for large QTL studies. Microarrays, high-throughput (“next generation”) sequencing, and mass spectrometry have revolutionized the field of quantitative genetics. In particular, single nucleotide polymorphism (SNP) chips have enabled genome-wide studies of genetic variation in panels of thousands of individuals. Next generation sequencing technologies (e.g. Illumina, Roche 454, SOLiD) have increased the quantity of DNA sequence data that can be produced in a laboratory by several orders of magnitude. The savings in time and cost mean that in the not very distant future it will be feasible to collect entire genome sequences of individual humans and model organisms. Advances in mass spectrometry are enabling researchers to accurately measure the concentrations of proteins (proteomics) and small molecules (metabolomics) in samples, expanding the collection of molecular phenotypes that researchers can use to understand a biological process, such as a particular disease.

Each technology involves computational, mathematical, and statistical issues regarding data acquisition, processing, analysis and subsequent interpretation. Statisticians have already contributed immensely to improvements in low- and high-level analyses of genomic data, e.g. generated by microarrays. Continued interdisciplinary research is crucial to achieving a high level of methodological success for analyzing these newer data types, which will only gain in importance.

Data Integration

Fundamentally sound quantitative methods for combining the very heterogeneous data types described above are required in order to give researchers power to uncover meaningful biological relationships, enabling further understanding, targeted follow-up, and efficient use of resources.

Genomic studies differ from traditional epidemiological or clinical trials in several important respects. One obvious difference is that the number of variables measured in genomic studies is usually in the thousands per sample, rather than the perhaps tens for a clinical trial. Microarray study sample sizes are also typically much smaller, putting additional impetus on effective data integration methods.

In a clinical trial, the overall goal is primarily to obtain a combined estimate treatment effect. Genomic studies more often focus on combining evidence supporting the role of a gene or to rank evidence for a large number of genes. In contrast to the estimation scenario, in this case it may be advantageous rather than harmful to draw upon multiple, heterogeneous sources. Heterogeneity should tend to increase robustness of inferences, thereby enhancing the generalizability of study conclusions. The effects of within-study bias might also be reduced, as we would expect different biases in different studies.

The possibilities for combining information across studies can be viewed as occurring along a spectrum of levels of analysis, moving roughly from combination of least to most “processed” quantities – that is, in order of decreasing information content: pooling raw or adjusted data, combining parameter estimates, combining transformed p-values, combining statistic ranks, or combining test decisions.

Findings learned *jointly* from multiple, diverse data types are likely to lead to new insights that are not as readily discovered by the analysis of just one type of data. So far computationally straightforward, mainly correlative approaches have been applied in gene expression and copy number analyses for combining study results. It seems clear, though, that traditional meta-analytic methods are not very straightforwardly applied to the problem of combining data of different types, the most obvious impediment being lack of a common parameter across a mix of letter-based (sequence), categorical (SNP), ordinal (methylation, protein expression) and continuous (expression and copy number) data types. More sophisticated approaches include hierarchical Bayesian models and variations on correlation-based approaches. However, integrating multiple data types in an automated, quantitative manner remains a major challenge. This frontier is so novel that challenges appear at even the most fundamental levels of analysis: identifying the biologically relevant questions arising from data integration; specifying applicable statistical models and corresponding parameters.

Recent Developments and Open Problems

The technological advances outlined above provide unprecedented opportunity for understanding the genetic basis and molecular mechanisms of disease, as well as normal biological function. At the same time, these large and complex data sets are posing serious challenges. We outline some of these, with some comments on progress in the field and open questions.

Handling Massive SNP and Phenotype Data Sets

The scale of current data sets, which far exceeds that of earlier genomic technologies such as early gene expression microarrays, generates tough computational and algorithmic problems related to data storage, normalization, and modeling. With so many variables measured in each experiment – and in light of mounting evidence that complex phenotypes (e.g. common diseases) are the result of interactions between a large number of genetic and environmental variables – methods (for multiple testing, modeling, prediction) that properly and powerfully account for correlation between genomic variables are essential.

Multiple QTLs

Most quantitative traits are controlled by the combination of multiple different QTLs, each making a contribution to observed variation in the trait. There is great interest in identifying QTL locations, quantifying their effects on the trait, and understanding their modes of interaction (e.g. additive, multiplicative, or more complex). These biological questions can be addressed with statistical models and testing procedures. The scale and complexity of quantitative genetics data sets demands rigorous statistical methods for assessing power, modeling interactions, and accounting for multiple comparisons.

Confounding

Population structure can lead to genetic associations with quantitative traits that are not causal. This confounding is particularly a concern in studies that measure many phenotypes and markers, because it is very likely that a data set will include at least a few spurious associations.

Currently and historically, quantitative genetics is facilitated by controlled breeding and/or knowledge of population history and structure. Minimizing confounding by non-genetic factors through these experimental strategies helps reduce noise in trait data and to remove false associations caused by population structure. Several speakers pointed out the importance of such study designs and reported on results from studies of gene expression (Sunduz Keles) and metabolomics (Katherine Pollard) traits measured on controlled experimental crosses.

Another approach to this problem is to undertake specific genetic manipulations and measure their effects on a trait (or traits) of interest. Studies are now being conducted on huge panels of organisms in which distinct (combinations of) genes have been knocked out, or knocked down (e.g. by RNA interference). 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. Elizabeth Conibear's poster illustrated this approach and presented a large knock-out data set.

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.

John Ngai discussed biological insights into the workings of the vertebrate olfactory system gained by molecular, genomic, and computational approaches. He presented results of two studies carried out in his laboratory that utilized genome-wide approaches to identify genes involved in different aspects olfactory development.

Sunduz Keles pointed out that in a typical study with many phenotypes and many genetic markers (e.g. expression QTL (eQTL) studies), most markers are not associated with variation in most traits. This sparsity allows one to massively simplify the statistical problem by either filtering out or down-weighting the contributions of most loci. She presented a sparse partial least squares (sPLS) method based on a sparse prediction model.

Ru-Fang Yeh presented analysis issues for DNA methylation data from bead arrays. Aberrant cytosine methylation in CpG dinucleotides is associated with silencing of tumor suppressor genes in many cancers. Methylation status can be assessed using specialized microarrays. Yeh extends her methods developed for SNP array genotyping to make dichotomized methylation calls and derive associated confidence measures as an alternative for the manufacture-recommended metric, relative intensity ratio, and also developed a likelihood ratio test and a model-based clustering algorithm based on the underlying beta distribution for differential methylation and clustering analysis. These methods were illustrated on applications to cancer data.

Jenny Bryan presented several novel statistical approaches for both low-level and high-level analysis (normalization, clustering, growth curve modelling) of high-throughput phenotyping data from model organisms such as yeast.

Aseem Ansari presented results on the comprehensive binding preferences of polyamides against the entire sequence space of a typical 10bp binding site. He also described a new method for visualizing DNA binding data, called a Specificity Landscape. A Specificity Landscape displays the relative affinity of a particular binding molecule for every DNA sequence assayed simultaneously. Specificity Landscapes were shown to accurately represent DNA sequence motifs with interdependent positions with high confidence.

Katherine Pollard noted that in many cases classical models for trait distributions (e.g. the normal model) are not appropriate with molecular phenotypes, which often have skewed or even discrete distributions, some times with point masses at zero. She presented several non-parametric methods for QTL mapping that avoid potentially incorrect distributional assumptions.

Karl Broman reviewed the traditional approach to multiple QTL mapping in which each genomic position is tested individually and then the family of tests is adjusted for multiple testing. He then argued that this problem is better viewed as one of model selection, and proposed a penalized likelihood method for simultaneously considering multiple loci. His method has better power than the traditional approach and also allows for the investigation of interactions.

Ingo Ruczinski discussed the problem of missing data and genotyping errors, which arise when the genotyping algorithms indicate that the confidence in certain genotype estimates is low. He presented several approaches to halding missing data and genotype uncertainties, and demonstrated that accounting for genotype uncertainty can be crucial when inferring possible copy number variants. The noveloty of this approach includes joint modeling of genotype calls and copy number, and in addition, integrating confidence estimates of the genotype calle and copy number estimates. The results presented in the talk demonstrated the superiority of the joint approach in terms of the accuracy of the genotype and copy number calls as shown on HapMap data. Although he focused on association studies, the methods may also be useful for QTL analysis.

Mark van der Laan presented a general maximum likelihood based approach targeting a user supplied parameter of the data generating distribution. This approach results in locally efficient estimators fully tailored for the parameter of interest, which have been shown to be more robust than maximum likelihood estimators. The method was illustrated in several applications: HIV drug resistance, detecting binding sites in the regulatory region of the yeast genome, breast cancer response to treatment and SNP association in case-control studies.

Adam Olshen presented the circular binary segmentation (CBS) technique for identifying regions of abnormal copy number. This has important ramifications in cancer, where progression often involves alterations in DNA sequence copy number. Multiple microarray platforms now facilitate high-resolution copy number assessment of entire genomes in single experiments. This technology is generally referred to as array comparative genomic hybridization (array CGH). The first published version of CBS was criticized for being slow. He present a methods for greatly speeding up the procedure. He also has shown approaches to recent copy number applications, including allele-specific copy number, clonality, and copy number variation. As in the talks of Ruczinski and Broman, the advantage of performing joint rather than unidimensional estimation of allele-specicifc copy number becomes apparent since join estimation allows making use of the summary constraint on the two alleles copy number number. Moreover, Adam discussed an interesting issue of clonality detection especially useful when one wants to distinguish between secondary primary and metastatic cancers. The clinical distinction is frequently vague; however, the ensuing treatment is dependent on the conclusion: a more aggressive treatment if metastasis, same treatment if secondary primary. Olshen has shown how copy number from paired samples could be used to distinguish these two situations.

Franck Picard considered joint analysis of multiple array CGH profiles. Most current segmentation methods can deal with one CGH profile only, and do not integrate multiple arrays, whereas array CGH microarray technology are becoming widely used to characterize chromosomal defaults at the cohort level. Picard presented a new statistical model to jointly segment multiple CGH profiles based on linear models. This strategy turns out to be very powerful for the joint segmentation of multiple profiles, as well as for the joint characterization of aberration types (status assignment of regions based on the cohort). The computational difficulties of simultaneous estimation are addressed using such tricks as model estimation with CART and linear programming. Overall, linear models offer a unified framework for the joint analysis of multiple CGH profiles.

Annette Molinaro presented a new experimental and analytical methodology to obtain enhanced estimates which better describe the true values of DNA methylation level throughout the genome, giving a model-based estimate of the absolute and relative DNA methylation levels. This model has been successfully applied to evaluate DNA methylation status of normal human melanocytes compared to a melanoma cell strain. Importantly, the model-derived DNA methylation estimates simplify the interpretation of the results both at single-loci and at chromosome-wide levels. This feature should make the method more accessible to life scientists.

Mark Segal extends random forests (ensembles of decision trees) to multivariate responses and illustrates their use on several yeast microarray experiments, including cell cycle, and various stresses. Segal demonstrates that random forest derived covariate importance measures more reliably identify key regulators compared to relying on a single tree. Further, utilizing the proximity matrix from the forest output to cluster genes into homogeneous groups based on both motifs and expression values, Segal showed that the multivariate response random forest effectively reveals high-order motif combinations that influence gene expression patterns, thereby obviating the need for examining the entire combinatorial space of all motif pairs.

Jason Lieb described a number of projects, including identifying DNA-encoded regulatory elements and exploring how targeting and transcriptional output relate to each other in a simple developmental context for yeast.

Terry Speed reported on a case-study of qRT-PCR normalization, using principal components analysis for data quality assessment and normalization. He also considered the more general question of how to assess the effectiveness of a normalization method in the absence of other data (e.g. calibration data) and discussed a framework for quality assessment. This work has implications for other data types, such as microarrays.

Simon Tavaré described a high-throughput sequencing technology that replaces cloning and sequencing of bisulfite-treated DNA to identify DNA methylation patterns in single cells. The technology can be used to reconstruct ancestral information about stem cells and their lineages, and also applied to study tumour evolution.

Keith Baggerly Discussed the difficulties in predicting response to chemotherapy based on microarray data. The usual approach is to define a gene expression signature of drug sensitivity. In establishing the signatures, it would be preferred to use samples from cell lines, as these can be grown in abundance, tested with the agents under controlled conditions, and assayed without poisoning patients. Recent studies have suggested how this approach might work using a widely-used panel of cell lines, the NCI60, to assemble the response signatures for several drugs. Unfortunately, ambiguities associated with analyzing the data have made these results ambiguous and difficult to reproduce. Baggerly described methods to make the analyses more reproducible, so that progress can be made more steadily.

Neil Hayes discussed clinical experience in the genomic classification of lung cancer. He described an in-depth analysis of three independent lung cancer cohorts demostrating reproducibility of the gene-expression based signatures for known clinical subtypes and also for survival. The approaches presented were exemplary in terms of the study design, care with the classifier building and clear conclusions.

Pratyaksha (Asa) Wirapati looked at leveraging the accumulating public data to carry out combined analysis of data from multiple cancer studies by using hierarchical modeling for detection of differential gene expression, prediction, and cluster analysis. He presented a framework to modify standard single set microarray data analysis methods to accommodate datasets from multiple studies.

Gordon Mills gave an introduction to the topic of personalized medicine and a systems approach. Studies show that patients with the same type of cancer can have very different outcomes, even with the same treatment. Now physicians and researchers are developing personalized medicine treatment plans for each patient based on the molecular markers of their tumor. Systems biology is the study of the emergence of functional properties that are present in a biological system but that are not obvious from a study of its individual components. Systems biology is a data-driven process requiring comprehensive databases at the DNA, RNA, and protein level to integrate systems biology with cancer biology. Combining these patient and model-based databases with the ability to interrogate functional networks by a systematic analysis using siRNA libraries and chemical genomics provides an ability to link in silico modeling, computational biology, and interventional approaches to develop robust predictive models applicable to patient management. In describing the types of studies being carried out, he also emphasized the clinical needs for methodological development. He discussed some specific examples of utilization of diverse sources of data to identify specific genomic and genetic alterations which would make a cell susceptible to PI3K inhibitors. PI3K inhibitors are designed to attack a true heartland of cancer pathway and are being developed by nearly every company developing oncology drugs.

Jian-Bing Fan, from Illumina, discussed his company's development of technologies that address the scale of experimentation and the breadth of functional analysis required to achieve the goals of molecular medicine. There are array-based technologies for: SNP genotyping, copy number variation detection, DNA methylation studies, gene expression profiling, and low-multiplex analysis of DNA, RNA, and protein. These serve as tools for disease research, drug development, and the development of molecular tests in the clinic.

Steffen Durrinck followed on with the recent technological advances in high-throughput transcriptome sequencing, For the last decade microarrays have been the major technology used to study gene expression. Despite their popularity, microarrays have known limitations such as cross-hybrization, probe affinity effects, availability for sequenced genomes only, and limited ability to study alternative transcription. Recent advances in sequencing technologies have significantly reduced the cost of sequencing, making it possible to now use sequencing for transcriptome studies. Because sequencing of transcriptomes on this scale is new there is a tremendous need for development of statistical and computational methods, for example to convert sequence data into exon and transcript-level expression measurements and to study differential transcript expression when comparing samples.

Hongyu Zhao gave an introduction to gene signaling pathways and showed how hierarchical models can be applied to the problem of signal transduction pathway analysis from single cell measurements. In contrast to measurements based on aggregated cells, e.g. gene expression analysis from microarrays, single cell-based measures provide much richer information on the cell states and signaling networks. The modeling framework allows pooling of information from different perturbation experiments, and network sparsity is explicitly modeled. Inference is based on Markov Chain Monte Carlo. Results from a simulation study demonstrate the effectiveness of this hierarchical approach, and the approach was also illustrated on experimentally-derived data.

Tim Hughes described efforts by his lab to determine the binding preferences of as many individual mouse transcription factors as possible, by determining binding specificity using a microarray technique. Mapping the complete spectrum of protein-DNA interactions is important for understanding global gene regulation and to fully decoding the genome and interpreting its evolution. The data accumulated thus far reveal a landscape of DNA sequence preferences, with many proteins exhibiting what appear to be multiple binding modes. Since the binding preferences correlate with conserved protein sequence features, the mouse data can be used to predict relative binding sequences in other species.

Rafael Irizarry presented a method that can accurately discriminate between expressed and unexpressed genes based on microarray data, thereby defining a unique “gene expression bar-code” for each tissue type. This method enables direct quantification of expression levels (rather than just relative expression between two samples) is also likely to contribute to better quantitative phenotyping for QTL studies. The method has been assessed using the vast amount of publicly available data sets, performing well in predicting normal versus diseased tissue for three cancer studies and one Alzheimer’s disease study. The bar-code method also discovers new tumor subsets in previously published breast cancer studies that can be used for the prognosis of tumor recurrence and survival time. The bar-code approach to classification and discovery might also improved in various ways, for example by optimizing the simple detection method and distance calculations, or by expanding it to include microarray platforms in addition to the Affymetrix array types on which it has been developed.

Joaquin Dopazo described the bioinformatic challenges of casting genomic data into biological concepts, with the ultimate goal of providing a functional interpretation of experimental results. This is often done now by using functional enrichment methods on a gene list resulting from the experiment. Because the gene list requirements may be too stringent, there is a loss of power to detect the relationships of interest. The assumption that modules of genes related by relevant biological properties, and not the genes alone, are the real actors of the cell biology dynamics, leads to the development of new procedures implicitly closer to systems biology concepts. Some advantages and difficulties with these systems approaches were described.

Yee Hwa (Jean) Yang presented work on identification of candidate microRNA using matched mRNA-miRNA time course data. This is an example of using data from multiple technologies to address a biological question. Here, integration of the different data types was used to reduce the number of candidate genes to follow up. Also discussed were some of the technical difficulties with matching diverse data types.

Darlene Goldstein discussed work using the relatively recent technology of glycan arrays, used to study the biological roles for oligosaccharides. Glycomics represents another strategy for biomarker discovery. Some applications in HIV and cancer using glycomics were also described. She closed the meeting with highlighting some of the common and recurring themes in high-throughput life science research.

Open Questions and Outlook for the Future

There remain several open areas of research in the domain of genome-scale data analysis; we outline some of these here.

Statistical Issues for Genome-scale Data

Major issues in all genome-scale data analyses are the high dimensionality (although sometimes sparse) and multiple testing problem. Although the sparse partial least squares approach shows promise, it (like all PLS methods) lacks a rigorous theoretical framework. Sunduz Keles presented some preliminary theoretical results, but more work is needed in this area. The use of nonparametric models for trait data can be appropriate, but the performance of these models versus the better understood parametric approaches requires further study.

Several of the methods presented in this meeting account for the effects of multiple loci on (single) phenotype (trait or disease) expression. Taking this approach to the next level, one could also consider multivariate phenotypes being jointly analyzed with respect to multiple loci. It would be interesting to evaluate whether additional power might be gained by combining information across traits. Katherine Pollard presented a Hidden Markov Model that attempts to do this type of pooling, but initial simulation studies indicated relatively poor performance in terms of identifying the location of QTLs. The underlying model needs some refinement to better capture the relevant system characteristics.

Genomics of Human Disease

One general area of great importance is the genomics of human disease. Some aspects for which statistical and computational problems remain to be addressed include: identification and analysis of appropriate intermediate and endpoint phenotypes, reliable systematic discovery of disease-associated polymorphisms and pathways, appropriate and powerful study designs in genome-wise linkage and association studies, models for mechanistic studies of disease-associated genetic variants, models incorporating gene-environment interactions, study designs and sample sizes which allow reliable detection of genetic effects, and the translational step between information obtained from these studies toward therapies of clinical usefulness at either the group or individual (personalized medicine) level.

The area of personalized medicine presents a number of statistical challenges. In searching for markers that distinguish people who will respond to a given treatment, the multiplicity problem comes greatly into play. With hundreds of thousands of tests being carried out, the potential for false positives is huge. Further statistical research is needed in model selection, particularly in development and characterization of procedures based on data-snooping, examination of the signal-noise patterns occurring in the various high-throughput technologies, and assessment of bias-variance tradeoff and overfitting. Evaluation of the stability and reproducibility of results should help to reduce the chance that false positive results are erroneously followed up in subsequent studies.

Models that leverage the dependence structures in genomic data will be particularly useful, since a dimensionality reduction should result in higher power. It might also be more interpretable and biologically relevant to focus on groups of genes rather than single genes. A common method for interpretation of results is a two-step approach in which genes of interest are initially selected based on analysis of experimental data, and then in a second, independent step the enrichment of these genes in biologically relevant terms is analyzed (e.g. using Gene Ontology data). It should be more powerful to consider groups of genes and functional knowledge in an initial modeling step so that the association of the sets of genes can be tested directly. There are many complications associated with this type of approach, but more work in this direction could prove to be fruitful.

In the area of biomarker discovery and translational research, the variety and ready availability of very high-dimensional data types is still waiting to be exploited effectively. It may also be the case that different diseases will require different modeling approaches to address specific problems. As an example, there are very different issues when considering breast cancer and ovarian cancer. Breast cancer is a relatively common disease while ovarian cancer is much more rare, so that sample size issues will be different. There is no screening available for ovarian cancer, and cases are most often detected only when the disease is in the advanced stages. Thus, unlike in the case of breast cancer, there is little material available to detect some of the early changes associated with the disease. It therefore seems that more targeted approaches will be required to search for biomarkers for diseases like ovarian cancer.

Data Integration

There remain several open statistical problems in the joint analysis of data across different studies. One primary problem is as basic as getting such a project started. If we consider the spectrum of analyses outline above, it would seem preferable to combine more informative data (i.e. closer to raw than highly processed data). However, obtaining the appropriate raw data is not always very straightforward, even with databases containing publicly available data. For example, clinical data are usually excluded from these, due to legal and/or patient privacy concerns. However, without such clinical information, it is not possible to analyze data for association with these outcomes. Improved sharing mechanisms for primary data are needed. Until this situation improves, though, it might be possible to use a missing data-EM framework for inference based on processed information that is more readily available.

Enhanced networking and sharing databases will also benefit the advancement of personalized medicine, as there will be more data to mine and hence more reliable inference should be possible. Methods for integrated analysis of heterogeneous data will depend on the types of data available, and whether it is raw or summarized. This area remains wide open for innovative applications of statistics.

List of Participants

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Chapter 18

Mathematical and Numerical Methods for Free Energy Calculations in Molecular Systems (08w5074)

Jun 15 - Jun 20, 2008

Organizer(s): (Christophe Chipot (Universite Henri Poincare, CNRS), Eric Darve (Stanford University)

Introduction, objectives and motivations

Eric Darve and Chris Chipot

This workshop was concerned with recent mathematical methods for modeling molecular systems, with an emphasis on proteins and biological molecules. Even though the field of molecular modeling is quite mature, we are still very far from the level of maturity seen in computational fluid dynamics where simulation of aircraft or engines are almost routine and play an integral part in the design process. On the contrary for molecular modeling, there is still a significant gap between what simulations can predict and phenomena of interest to biologists and experimentalists. The basic difficulty is the range of time scales involved. Simulations require a time step of 1 femto second (10^{-15} sec) while typical molecular events (e.g. protein folding) take place on a time scale of milli second (10^{-3} sec). Consequently the development of novel mathematical and numerical methods to bridge this gap is sorely needed. The contributions in this workshop are roughly divided between techniques which reduce the computational cost and techniques which estimate or control the approximation error and the statistical error. We have asked a few participants to summarize discussions and presentations on different topics. There are 13 sections in this report organized as follows.

Section 18: dynamics of collective variables. Most simulations are typically interested in only a small set of variables, sometimes called observables, collective variables, order parameter or reaction coordinate. This section considers the problem of building effective equations in terms of these resolved variables, in which the other variables are averaged out by some procedure.

Section 18: adaptive methods. Changes in the conformation of proteins happen on a long time scale because of large energy barriers separating metastable basins. This time scale issue can be overcome in some situations by biasing the system so that transition states are sampled more often.

Section 18: modeling probability density functions. it is well known that in free energy calculations, the tail of distributions makes large contributions to the final answer. This leads in general to large sampling errors. This can be addressed by modeling the probability density function.

Section 18: thermostats. Despite being a well-studied topic, generating NVT ensembles using a thermostat is still an active area of research. The open problems are: how is it possible to generate an NVT ensemble while perturbing as little as possible NVE trajectories? How can one control the accuracy and ergodicity of NVT simulations?

Section 18: non-equilibrium methods. Most quantities of interest are defined in the NVT ensemble. It has been shown by Jarzynski and others that simulations out of equilibrium, i.e. which sample an ensemble different from the canonical ensemble, can still yield exact results in the NVT ensemble. In a number of cases, these methods can be computationally advantageous.

Section 18: transition path sampling. A powerful technique to simulate systems with rare transition events is to do transition path sampling in which only paths that transition between 2 metastable states are considered. It has been shown that many properties of the system can be reconstructed from such paths.

Section 18: algorithmic bias. This section considers the effect of errors due to numerical integration and other approximations.

Section 18: transition pathway with swarms of trajectories. The mean free energy path can be used to rapidly estimate the free energy, the reaction rate and approximate the reaction coordinate. These paths can be obtained from the string method with swarms of trajectories, a technique pioneered by Roux.

Section 18: optimizing free energy calculations. Controlling the different sources of errors, systematic and statistical, is essential to predict the accuracy of calculations. This discussion covers various aspects of this problem.

Section 18: optimal bias. Related to the previous section, the design of an optimal biasing potential to reduce the computational cost is considered.

Section 18: enhanced sampling. Tuckerman has created an original method to speed-up sampling of phase-space based on a change of variable.

Section 18: statistical error control. Despite its fundamental importance, the question of assessing the effective size of the sample set is not completely understood. Given a set of samples, to what number of statistically independent samples is it equivalent?

Section 18: committor function. The rigorous way to define a reaction coordinate is to use the committor function which is the probability at a given point in phase-space to reach the product states before the reactant states. Mathematical properties of the committor function are considered.

Effective dynamics of collective variables

Eric Darve and Frèdèric Legoll

Coarse grained stochastic models

One of the most difficult challenge of molecular dynamics simulations of proteins is the existence of multiple time scales in the system ranging from femtosecond (10^{-15}) bond vibrations to milli-second conformational changes (e.g., insertion of protein in a phospholipid membrane or unbinding of a ligand from a pocket). Even though computers are getting faster, it is evident that brute force computation will ultimately not be able to bridge this time scale gap. Instead more efficient numerics are required. In many systems, it is possible to identify some order parameters of interest. These parameters characterize the state of the system in some suitable sense, for example they could measure the progress of an ion moving through an ion channel or the distance between a ligand and the active site of a protein. These variables will be called collective variables (CV) in this report. The CVs are not in general slow variables but they are associated with rare events during which the protein moves from one metastable basin to another. Even though the event may be rare, the transition process itself may take place rapidly.

Several contributions during this workshop were related to this topic, including J. Izaguirre who discussed the appropriate choice of CV based on normal modes of proteins, and E. Darve and F. Legoll who presented two different approaches for deriving reduced stochastic equations in terms of the CVs only. These methods address the challenge above in two different ways. By producing a reduced set of equations, they reduce the cost of the time integration by orders of magnitude. In addition, these techniques can lead to the formulation of appropriate Fokker-Planck equations. The solution of these Fokker-Planck equations then allows predicting all the time scales of interest in the system, including time scales which may extend by orders of magnitude the length of time covered by the simulations. For example, Darve demonstrated that data from 200 nanosecond of molecular dynamics simulations can be used to predict reaction rates and exit time in the millisecond range.

Effective stochastic dynamics of collective variables

By construction, the free energy $A(z)$ characterizes the equilibrium distribution of the CVs. It allows determining equilibrium quantities, but its relation to dynamical information (such as time correlations, or kinetics) is only approximate. In some cases, the free energy barrier can be related to the reaction rate but this is often only a crude approximation.

Several techniques have been presented in the workshop to derive stochastic equations for the CVs which correctly reproduce certain dynamical properties. The solution of this modeling problem depends on the criterion considered to assess the quality of the reduced dynamics. The dynamics should be *ergodic* with respect to $\exp(-\beta A(z))\,dz$. A weak dynamical requirement is that, at each time t, the *law of* ξ is close to the law of $\xi(q_t)$ in the full system (here, q_t denotes the full system evolution and $\xi(q)$ is the CV). A stronger requirement is that the *autocorrelation functions* are well reproduced. This amounts to asking that the probability distribution function (pdf) of ξ, as a function of space and time, be close to the pdf of $\xi(q_t)$ in the full system. This next implies the correct reproduction of residence times, a quantity of paramount importance. An even stronger requirement is that the *trajectory* $t \mapsto \xi(t)$ is close to $t \mapsto \xi(q_t)$ in the full system. This, however, is probably only achievable in certain cases, such as when the CVs are slow variables.

Darve discussed a method based on the Mori-Zwanzig projection [1]. In this approach, the evolution of the CVs, $d\xi_t$, is decomposed as the sum of a drift term (the potential of mean force), a memory kernel (non-Markovian contribution) and a fluctuating term dR_t. The essential property of this decomposition is that the drift and memory kernel are functions of $\xi(\tau)$, $0 \le \tau \le t$, only, and the conditional average of dR_t is zero:

$$\mathbb{E}\big[dR_t \,|\, \xi(q) = \xi^*\big] = 0.$$

In addition, Darve showed how a Fokker-Planck equation for the CVs can be derived. One of the difficulty of this approach is that computing the memory kernel requires in principle solving a partial differential equation, called the orthogonal dynamics equation, in dimension $6n+1$ where n is the number of atoms in the system. However Darve derived a different approach based on sampling the system using a long trajectory which does not require solving the orthogonal dynamics equation. This makes this calculation possible even for large systems with many atoms. Numerical examples were shown where for example the memory kernel due to water molecules surrounding the protein was computed from molecular dynamics data.

Legoll showed how to use conditional expectations applied directly to the Langevin equation to obtain a reduced dynamics. Starting from the overdamped Langevin equation for the full system,

$$dq_t = -\nabla V(q_t)\,dt + \sqrt{2k_BT}\,dW_t,$$

it is easy to write a dynamics for $\xi_t = \xi(q_t)$, essentially using a chain rule argument:

$$d\xi_t = \nabla\xi(q_t)\cdot dq_t + \text{Ito term} = b(q_t)\,dt + \sigma(q_t)\,dW_t,$$

for some drift function $b(q)$ and diffusion function $\sigma(q)$. This dynamics depends on the evolution of the full system, and not only on the CV. It is hence unclosed. A simple way to close it is to average the right hand side over all configurations of the system (weighted with the Boltzmann-Gibbs measure) that correspond to the current CV value. This leads to

$$d\xi_t = \overline{b}(\xi_t)\,dt + \overline{\sigma}(\xi_t)\,dW_t,$$

where $\overline{b}(\xi^*) = \mathbb{E}\big[b(q)\,|\,\xi(q) = \xi^*\big]$, and a similar definition for $\overline{\sigma}(\xi)$. Computing $\overline{b}(\xi)$ and $\overline{\sigma}(\xi)$ can be done in a similar way as for free energy computations. Depending on some explicit criteria, this effective dynamics was shown to be related to the free energy (with $\overline{b}$ being the potential of mean force). An analysis of the accuracy of this dynamics was also proposed. Some simple numerical examples were used to illustrate the practical feasibility of this approach and its accuracy.

Adaptive methods

Chris Chipot and Tony Lelièvre

Adaptive schemes belong to a class of methods that has recently emerged, in which, either the force or the potential is continuously updated to enhance the exploration of a free-energy along a specific order parameter, ξ, or combination thereof.

In the adaptive biasing force (ABF) approach of Darve and Pohorille [2], the thermodynamic force along ξ is evaluated in unconstrained simulations coupled with an adaptive algorithm which subtract the position-dependent average force from the instantaneous force, hence yielding a uniform sampling along ξ. The remarkable efficiency of this approach, compared to other, either adaptive or non-adaptive algorithms, is due to the fact that forces, in contrast with probabilities, are local properties and, therefore, can be updated efficiently without the need to explore the remainder of the configurational space. On Monday, Andrew Pohorille introduced a novel formulation of the ABF method, in which Darve *et al.* show how the same information can be obtained from first derivatives with respect to the order parameters and time only [3], which greatly simplifies implementation of this method for ξ that are complex functions of Cartesian coordinates.

The same day, Tony Lelivre presented a mathematical viewpoint on adaptive methods for free energy computations, with an emphasis on the ABF approach. A unified approach for adaptive methods was proposed, and a demonstration of the convergence properties of the method was outlined [4, 5]. That ABF, and other adaptive schemes, enhance sampling along a chosen order parameter, ξ, but not along orthogonal, possibly strongly coupled degrees of freedom — which is conducive to quasi nonergodicity scenarios, constitutes the main motivation for the development of a novel approach that combines ABF and replica-exchange-like methods. In this parallel implementation of ABF method, a selection mechanism associated to a birth–death process is proposed. Preliminary computations on toy models were presented.

On Thursday, Celeste Sagui introduced a new approach, differing markedly from ABF and coined adaptively biased molecular dynamics (ABMD). This method [6], aimed at the computation of the free energy surface along a reaction coordinate, relies on non-equilibrium dynamics. It belongs to the general category of umbrella sampling methods with an evolving biasing potential. The ABMD method has several useful features, including a small number of control parameters, and an $\mathcal{O}(t)$ numerical cost with molecular dynamics time, t. As noted by Sagui, it naturally allows for extensions based on multiple walkers and replica exchange, where different replicas can have different temperatures and/or collective variables — in line with an earlier comment by Andrew Pohorille, that free-energy methods can be combined seamlessly to enhance both their accuracy and convergence properties.

On Friday, Chris Chipot returned to the ABF method, emphasizing through a variety of case examples, that convergence of the free-energy calculation is rapidly reached if ξ is fully decoupled from other, slowly relaxing degrees of freedom. Unfortunately, under most circumstances, reaction coordinates are modeled by surrogate, usually one-dimensional order parameters. By and large, order parameters that depart from the true reaction coordinate yield convergence issues that hamper uniform sampling along ξ [7, 8].

Modeling probability distribution functions

Andrew Pohorille

One of the oldest and most frequently used approaches to calculating free energies is the free energy perturbation (FEP) method. This approach relies on computing potential energy difference, ΔU, between two systems, say 0 and 1. Then, the corresponding free energy difference, ΔA, is calculated from the expression:

$$\Delta A = -\ln\langle \exp\{-(\Delta U)\}\rangle_0 \tag{18.1}$$

where $\langle \ldots \rangle_0$ denotes an average over the ensemble 0 and energy units of kT are used.

Since ΔA is evaluated as the average of a quantity that depends only on ΔU, it can be expressed as a one–dimensional integral over energy difference:

$$\Delta A = -\ln \int \exp(-\Delta U)\; P_0(\Delta U)\, d\Delta U \tag{18.2}$$

where $P_0(\Delta U)$ is the probability distribution of ΔU sampled for system 0.

An inspection of this equation points to difficulties with simple implementations of FEP. The integrand is the product of $P_0(\Delta U)$ sampled in simulations and the exponential Boltzmann factor. The latter weights the probability distribution towards low, poorly sampled values of ΔU, which in turn might significantly reduce statistical precision of estimated ΔA.

A considerable effort has been expended to improve efficiency and reliability of FEP. This effort has been concentrated, with significant success, on optimization of stratification strategies and proper choices of the reference state with respect to the target state [9]. An alternative, or perhaps more appropriately, complementary approach is to model $P_0(\Delta U)$ either as an analytical function [10] or a series expansion [11, 12] whose adjustable parameters are determined primarily from the well sampled region of the function. For this relatively new approach, both types of functions were considered during the workshop.

A series expansion discussed during the workshop was in terms of Gram-Charlier polynomials, which are the products of Hermite polynomials and a Gaussian function:

$$P_0(\Delta U) = \sum_{n=0}^{\infty} c_n \varphi_n (\Delta U) \tag{18.3}$$

where c_n is the n–th coefficients of the expansion and ϕ_n is the n–th normalized Gram–Charlier polynomial and related to the n–th Hermite polynomial by:

$$\varphi_n(x) = \frac{1}{\sqrt{2^n \pi^{1/2} n!}} H_n(x) \exp\left(-x^2/2\right) \tag{18.4}$$

In general, this approach is difficult to apply because reliability of the $P_0(\Delta U)$ deteriorates away from the well sampled region. A remedy is to carry out both "forward" and "backward" (from state 1 to state 0) simulations and exploit the relation between the corresponding probability distributions:

$$P_1(\Delta U) = \exp(\Delta A) \exp(-\Delta U) P_0(\Delta U) \tag{18.5}$$

The key to the success of this approach is to determine the optimal order, N, of the expansion 18.3. If the expansion is truncated too early, some terms that contribute importantly to $P_0(\Delta U)$ are lost. On the other hand, terms above some threshold carry no information, and only add noise to the probability distribution. Both the optimal N and the corresponding coefficients c_n can be determined using a Bayesian approach [11]. So far, this procedure was applied only to synthetic data, but yielded highly promising results even in the most challenging cases.

An alternative model for $P_0(\Delta U)$ discussed during the workshop is an analytical function sometimes called the "universal" probability distribution function (UPDF) [13] . It has been suggested that this function describes well statistical properties of global quantities in a broad class of finite–size, equilibrium or non-equilibrium systems characterized by strong correlations and self–similarity. UPDF takes the following form [13, 10]:

$$P(y) = Ke^{a[b(y-s)-e^{b(y-s)}]} \tag{18.6}$$

where a, b and shift s are adjustable parameters, and K is the normaization constant. Here, $y = (\Delta U - \langle \Delta U \rangle_0)/\sigma$, so that the distribution has zero mean and a unit variance. UPDF was successfully used to model $P_0(\Delta U)$ obtained from alchemical transformations involving an anion, adenosine and a fatty acid [10]. It is, however, not clear whether it obeys eq. 18.5

Even though modeling probability distribution has not been utilized nearly as extensively as some other techniques for improving efficiency of FEP calculations, it appears to be a highly promising area for further research. Initial applications of this technique lead to a conclusion that it can considerably improve estimates of ΔA. Furthermore, it can be readily combined with other techniques for improving FEP calculations. The method also has drawbacks. The physical underpinnings for choosing a model distribution are, so far, not very strong, which in turn makes its range of applicability and error estimates somewhat uncertain. Further theoretical and application studies on this approach are warranted.

Symplectic integrators and thermostats

Ben Leimkuhler

The emphasis in molecular dynamics is shifting to problems involving transient dynamics, and the flow of energy from one part of a system (one set of variables) to another. There is now widespread agreement that for challenging problems such as polymers and bio-macromolecules the long timescales (relative to the shortest vibrational periods) and complexity of boundary interactions that must be incorporated to generate useful data in realistic computational time mean that the typical system must be modelled in a pre-equilibrium state.

Computational methods are needed for the multiscale molecular simulation setting. As examples, methods have been proposed recently for computing free energy along a reaction coordinate [16, 17] which rely on forcing the molecular system into infrequently visited domains to study slowly-unfolding transitions. A crucial part of these calculations is the computation of averages or time-correlation functions of a system subject to imposed constraints or initialization enforced as part of the modelling framework. The local equilibration/dynamics problem is nontrivial, so implementing these methods (which effectively require us to equilibrate the system in regions of rapid dynamical transition) is itself a major task.

Molecular dynamics is chaotic with differences between nearby trajectories doubling in magnitude every several hundred steps. In typical simulations, trajectory errors invariably grow to the size of the system. This means that traditional numerical analysis, based on accurate approximation of trajectories, offers little to explain the effectiveness of MD. The pragmatic explanation for the usefulness of MD comes from the geometric integration theory, and, in particular, the backward error analysis which tells us that we may(approximately) view the numerical solution as the exact solution of a perturbed dynamical system, with its own associated statistical mechanics[14].

Thermostats generate step sequences that can be, for some choices of parameters, modest perturbations of Hamiltonian dynamical trajectories. Although both dynamics-based and stochastic thermostats are found to be useful for MD simulation, robust ergodic sampling, especially for systems with strong harmonic components, appears to require a random perturbation. Strongly ergodic processes may control temperature well, but at the price of modifying diffusion rates. Such defects are easily seen for Langevin dynamics with even modest damping (collision) coefficient, when used in systems involving liquid water, in that the diffusion of energy from the OH bond stretch is corrupted. On the other hand, if the collision coefficients are further reduced, the dynamics may be recovered but at the expense of tight control of kinetic energy. There is no practical and general way to tune Langevin dynamics so that all diffusive processes of a complex macromolecular system are simultaneously accurately modelled while the thermodynamic averages are correctly and rapidly recovered. With F. Theil (Warwick) and E. Noorizadeh (U. of Edinburgh) we have proposed new ergodic schemes which incorporate a modified weak stochastic perturbation of dynamics [18]. The ergodicity of these methods can be analyzed by studying the regularity properties of the associated Fokker-Planck operator.

Thermostatting challenges are even more dramatic in the setting of nonequilibrium modelling. When one dynamics or numerical procedure is switched off and another switched on, the effects may be dramatic. Not only does every Hamiltonian system have its own natural measure, but the numerical integrators themselves perturb this ensemble [14]. Initial conditions that are "well equilibrated" for a certain ensemble may not be when an integrator is engaged with a large timestep, leading to unstable initial perturbation, re-equilibration, and a temperature shift. This difficulty can be addressed by use of adaptive dynamical thermostats which smoothly incorporate stronger perturbations to control the simulation only where needed [15].

Non-equilibrium methods

Chris Jarzynski

Nonequilibrium estimates of equilibrium free energy differences are well known to exhibit poor convergence, for reasons analogous to the poor convergence of traditional, equilibrium-based perturbation methods. Specifically, the dominant contribution to the quantity being calculated typically comes from either rarely visited regions of phase space (in the case of equilibrium perturbation), or from very rare, low-dissipation trajectories (nonequilibrium methods). During the Tuesday morning session, Jarzynski described a general strategy for improving the convergence of nonequilibrium-based estimates of equilibrium free energy differences [20]. This strategy involves non-physical terms that are added to the equations of motion, and are represented by a parameter-dependent *flow field* $\mathbf{u}(\mathbf{z};\lambda)$ that acts on the phase space coordinates $\mathbf{z}$. While the method is in principle valid for any choice of flow field (subject to modest boundary conditions), the efficiency of the free energy estimate is improved only if the flow field effectively "escorts" the system along a near-equilibrium trajectory, thus reducing dissipation and therefore improving convergence. The strategy was illustrated using two simple models – a one-dimensional toy system, and a Lennard-Jones fluid excluded from a spherical cavity – but its application to more complicated, realistic systems remains a challenge.

During the Tuesday afternoon session, Ytreberg discussed the estimation of binding affinities using exponentially averaged nonequilibrium work values. The system under consideration was a calixarene-benzene complex. Calixarenes are cyclic oligamers that form a basket-like shape, and are of interest as potential nano-sensors. In the studies described by Ytreberg, non-equilibrium unbinding simulations were performed using harmonic forces, analogous to atomic force spectroscopy. During the simulation a harmonic spring is imagined to be attached to the benzene, which is initially bound non-covalently inside the calixarene pocket. The other end of this spring is then pulled away from the (fixed) calixarene. As in similar studies involving protein-ligand binding affinities [21], the estimation of ΔG is made challenging by the presence of the surrounding solvent. Ytreberg was nevertheless able to obtain accurate estimates of the equilibrium unbinding free energy differences using nonequilibrium trajectories.

The theoretical foundations of nonequilibrium free energy estimation methods are a number of rigorous *work relations*. These pertain to the statistical mechanics of systems driven away from thermal equilibrium by the external manipulation of a mechanical – or in the case of simulations, "alchemical" – work parameter. On Wednesday morning, Stoltz presented careful mathematical analyses of several issues related to nonequilibrium work relations. Among the results he discussed was an extension of such relations to the case of reaction coordinates rather than alchemical parameters [22]. This is of considerable importance in the context of biomolecular simulations, in which a Lagrange multiplier approach is often used to project the dynamics onto a submanifold representing a given value of the reaction coordinate (as in the RATTLE and SHAKE algorithms). For nonequilibrium simulations in which the projection scheme is used to "drag" the reaction coordinate through a range of values, Stoltz discussed the appropriate definition of work, and how the distribution of work values can be used to reconstruct the equilibrium free energy profile (potential of mean force) along the reaction coordinate. Stoltz also discussed a method for sampling *paths*, when the underlying dynamics are stochastic [23], and a strategy for avoiding degeneracies of the exponential weights that are responsible for the poor convergence of nonequilibrium free energy methods.

During the final session, on Friday morning, Geissler's talk focused on the optimization of nonequilibrium free energy methods, and on a comparison with the efficiency of traditional methods based on importance sampling. Among the results he described was the recent idea of using "bad dynamics" to get good free energy estimates, by performing simulations with large time steps [24]. Such time steps result in trajectories that inaccurately integrate the underlying equations of motion. However, as long as a volume-conserving algorithm (such as Verlet) is used, the exponentially averaged work values will converge to the correct ΔG. This is established rigorously using an analogy between nonequilibrium dynamics and mappings between phase space ensembles. Geissler also discussed a path-sampling method for deterministic (typically, Hamiltonian) dynamics, originally developed in the context of transition path sampling. This approach takes advantage of local linearization of trajectories to overcome the difficulty associated with the exponential divergence of highly chaotic trajectories.

Transition path sampling

Peter Bolhuis

Rare events are ubiquitous in nature. The nucleation of crystals, the folding of proteins, and many chemical reactions are examples of processes that take place on time scales much longer than the molecular vibrations. This separation of timescales makes a straightforward molecular dynamics simulation very inefficient for the computation of the mechanism and kinetics of such processes. The timescale gap is due to a high free energy barrier between the initial and final state. To overcome these high free energy barriers many computational techniques employ a biasing potential along an a priori defined collective variable/order parameter approximating the reaction coordinate. For the calculation of the kinetic rate constant one can correct the transition state theory estimate based on the free energy barrier, with a so-called transmission coefficient. However, the choice of an order parameter that does not capture the reaction coordinate correctly might result in an underestimated free energy barrier, the observation of severe hysteresis, and a statistically poor estimate of the transmission coefficient. Trajectory based simulation methods aim to alleviate this problem by focusing on the unbiased dynamic pathways connecting the initial and final state. The transition path sampling (TPS) method performs a Monte Carlo importance sampling of trajectory space. The basic concept is to generate a new trial trajectory from an existing valid trajectory using for instance the highly efficient shooting algorithm, and accept or reject that pathway according to a criterion that preserves detailed balance. The collection of paths harvested provides unbiased insight into the mechanism of the reaction. Committor analysis of this path ensemble yields the transition state ensemble, and, by likelihood maximization, the best possible reaction coordinate. Furthermore, by a reversible transformation of the ensemble of paths that connect the initial and final state to one that only starts the initial state, one can compute the rate constant. To do so the efficient transition interface sampling (TIS) method introduces an order parameter along which a set of interfaces is constructed, and expresses the rate constant as the product of the effective positive flux through the interface close to the initial state and so-called interface crossing probabilities. For diffusive processes partial paths turned out to be sufficient, and led to the partial path transition interface sampling method (PPTIS) (which is related to the Milestoning method of Elber and coworkers). Using PPTIS and TIS one can, besides the rate constant, also obtain the free energy along the order parameter directly.

Notwithstanding their advantages, the TPS and (PP)TIS algorithms still suffer from two drawbacks: (1) They rely on the absence of any long-lived intermediate states between the initial and final state. (2) Due to the fact that for the shooting algorithm a new trial path resembles to a large extent the previous path, multiple reaction channels separated by a high barrier in between are not sampled efficiently. In my contribution to this workshop I discussed solutions to both these problems. For the first problem our group developed a multiple state transition path sampling (TPS) approach in which it is possible to simultaneously sample pathways connecting a number of different stable states [26]. Based on the original formulation of TPS we have extended the path ensemble to include trajectories connecting not just two distinct stable states but also any two states defined within a system. The multiple state TPS approach is useful in complex systems exhibiting a number of intermediate stable states that are interconnected in phase space. Combining this approach with transition interface sampling one can also directly obtain an expression for the rate constants of all possible transitions within the system. I illustrated the approach on a simple 2D Langevin potential.

The second problem can be addressed by combining the TIS method with the replica exchange concept [27]. The basic idea is to perform many TIS simulations (replicas) in parallel, each at a different interface, and regularly allow for exchange between the interface ensembles, based on a detailed balance criterion. The replica exchange TIS (RETIS) method does allow for sampling multiple channels, as during a RETIS simulation a path slowly diffuses along the interfaces, and can choose another channel during this diffusion, thus enhancing sampling dramatically. I showed how by including both the backward and forward reaction the corresponding rate constants, as well as the free energy barrier follow from a single simulation. I illustrated the method on a two dimensional potential using Langevin dynamics.

Shadowing and algorithmic bias

Bob Skeel and Stephen Bond

Even if our model for the molecular system is exact, computational resources limit the simulation length, which introduces statistical error when computing ensemble averages. Additionally, molecular dynamics, unlike Monte Carlo, simulations give biased results due to the use of numerical integrators. This applies whether the dynamics is deterministic or stochastic; this discussion considers only the deterministic case.

In molecular dynamics (MD) it is assumed that time averages of “physically meaningful functions” do not depend on a detailed description of the initial conditions, which is a consequence of the ergodic hypothesis. Due to the chaotic nature of the underlying equations of motion, it is impossible to construct an exact trajectory over a long time interval. Hence, it is remarkable that there exist numerical integrators that can approximately preserve the correct invariant density for very long durations, in particular, symplectic integrators such as Verlet.

There are three ways in which temporal discretization introduces bias into averages. First, the finite step size, Δt, modifies the dynamics in a systematic way, with an effect that can be expressed as an asymptotic expansion in powers of Δt. Second, discretization may affect ergodicity [36], which is particularly problematic since it cannot be easily detected or corrected. Third, it introduces energy drift, particularly for nonsymplectic integrators like Nosé-Hoover schemes [14].

The presentation by Stephen Bond addresses the first of these concerns. It describes practical methods for estimating and correcting bias in averages computed from molecular dynamics simulation. Variations of this idea have been explored by several authors including Bond [28, 14, 29], Leimkuhler [14], and Reich [33]. Assuming ergodicity, the error in a MD average can be bounded by the sum of bounds on the statistical and truncation error. The statistical error decays at a rate proportional to $1/\sqrt{\tau}$, where τ is the simulation time. On the other hand, the truncation error is asymptotically proportional to Δt^r, where r is the order of accuracy of the numerical integrator.

The dependence of the computed average on step size is observed only when the simulation is long enough, otherwise statistical error dominates. Bond and Leimkuhler observed up to one percent error in the induced temperature in NVT molecular dynamics simulations based on the Nosé thermostat [14]. Cuendet and van Gunsteren found a much more severe bias in constant pressure simulations due to the use of the virial in the computation of system pressure [30]. In their study, they found that a one percent error in temperature could cause the induced pressure to be off by a factor of 5 to 14.

When a symplectic integrator is applied to a Hamiltonian system, the result is a modified Hamiltonian system which is nearly exactly conserved by the numerical integrator. For example, it can be shown that the Verlet method conserves $H(x,p) = \frac{1}{2}p^{\mathsf{T}}M^{-1}p + U(x)$, to second-order accuracy over long time intervals, where M is a mass matrix and U is the potential energy. However, the modified Hamiltonian $H_{2,\Delta t}(x,p) = H(x,p) + \Delta t^2(\frac{1}{12}p^{\mathsf{T}}M^{-1}U_{xx}M^{-1}p - \frac{1}{24}\nabla U^{\mathsf{T}}M^{-1}\nabla U)$ is preserved to fourth-order accuracy. Estimates of such modified Hamiltonians can be computed at almost no additional cost [28, 35, 31, 34].

The impact of discretization error on MD time averages is to cause the sampling to be from the invariant distribution (or ensemble) of the modified system. Since the effect of discretization error is known, it can be corrected for, resulting in higher-order averages from a single MD simulation. Specifically, samples from the modified distribution can be reweighted to get an estimate from the desired distribution [14, 29]. An alternative approach is to estimate a correction using an analytical estimate of the effect of a Hamiltonian perturbation on time averages [36].

Finally, it might be noted that an estimate of sampling bias is also useful for improving the efficiency of hybrid Monte Carlo methods [32, 34].

Applications made possible by novel free-energy methods

Benoît Roux

Great advances have been made to tackle the difficult problem of finding transition pathways in molecular systems, notably by the "string method" of Maragliano et al [37]. The string method has some analogies with previous approaches to determine reaction paths based on energy minimization [38] and the "path integral" formulation of Elber et al. [39, 40]. In this method, the string represents the transition pathway as a chain of "states" or images, in the multi-dimensional space of collective variables $\mathbf{Z}$. Among all the possibilities, the transition path that is the most representative is found when the system evolves along the maximum probability transition path (MPTP) [37]. The main property of the MPTP is that a system starting somewhere along the path must evolve on average in a manner that is tangential to the path. We have exploited those ideas into a robust and efficient computational scheme that we call the "string method with swarms-of-trajectories"[41].

Briefly, we determine the most probable transition path by evolving the chain of states from the systematic drift of swarm-of-trajectories initiated from each $\mathbf{Z}(0)$. Evolution during a time τ of a system started at $\mathbf{Z}$ leads to many random positions $\mathbf{Z}(\tau)$, but on average the system systematically drifts by $\langle\Delta\mathbf{Z}\rangle = \langle\mathbf{Z}(\tau) - \mathbf{Z}(0)\rangle$, while remaining along the path (that is why it is the most likely path). The dynamics of the swarms is used to estimate the systematic average drift $\langle\Delta\mathbf{Z}\rangle$ of each image in a time τ in the collective variable space $\mathbf{Z}$. The algorithm can robustly deal with several hundred variables, though the final answer is not expected to strongly depend on the specific choice of collective variables (as long as the subspace is sufficiently large). In previous tests [41], we have used torsional angles and inter-residue distances. It is also possible to use the Cartesian position of a subset of protein atoms (e.g., the Cα and Cβ). The iterative process for relaxing and improving an initial guess for the transition pathway consists of 5 steps, which should be repeated iteratively until convergence is reached. The iterative process is illustrated schematically in Figure 1 of ref [41].

We have also been able to exploit the optimized path to efficiently calculate the free energies and transition rates within the framework of a Markov state model [42]. This has some similarities with the "Milestoning" of Ron Elber [43, 44]. The method consists in computing the transition probabilities Pij between neighboring substates i and j along the path by running swarms of unbiased trajectories, each initially thermalized within a substate i, and then measure the conditional probability to reach substate j after a coarse-grained lagtime τ. The full relaxation of the system is then determined from the eigenvalue spectrum of the full Markov process, which can be evaluated for different value of the lagtime τ. Within this framework, it is possible to estimate the error in the mean first passage time using techniques from Bayesian inference, and develop an adaptive sampling strategy based on the error predictions to guide the design of swarms-of-trajectories, so that the best possible Markov model can be efficiently obtained.

The "string method with swarms-of-trajectories" [41] and the discrete Markov state model [42] are key methodologies that we plan to use to investigate inactivation and gating in ion channels. All the methodological developments described above will lead to freely distributed scripts and code to treat large conformational transitions quantitatively that many other labs will use.

Optimizing the design of free-energy calculations

David Kofke

Free energy calculations cover a broad range of methods and applications, and there is no single approach that one might take to their optimization. Nevertheless it is possible to identify the important issues to consider when undertaking such a calculation.

The first question to address is the choice of the basic method to use. These may be generally categorized into work-based methods (free-energy perturbation, Jarzynski's non-equilbrium work averaging, Bennett's method, thermodynamic integration, etc.) and histogram-based methods (Ferrenberg-Swendsen, WHAM, expanded ensembles, etc.); recently transition-matrix methods have emerged which bridge these approaches. The choice of which to use depends to some degree on what types of free energy calculations are desired (*e.g.* a single difference along a path versus many differences from a common reference state), as well as more parochial effects such as personal preference or the availability of coded methods for the system of interest. As of now there is no clear evidence indicating the superiority of one approach over all others. This situation holds because it is difficult to generalize the problem, and because the factors affecting the performance of the various methods are still a subject of active research.

For most methods there are options to choose with respect to the number and definition of systems that bridge two given systems of interest, or which characterize the space of the parameter(s) of interest. So for a given method these options present additional variables for optimization. Then, given all of this, there remain additional choices about how to process and interpret the data that are gathered.

Optimization can emphasize either the precision of the result (e.g. statistical errors) or its accuracy (e.g. bias or systematic errors). For very long sampling M, bias vanishes as M^{-1}, while the standard error decreases more slowly, as $M^{-1/2}$. However for small sampling the bias may be quite significant. Optimization of precision proceeds through minimization of a variance. Many approaches have been developed in this manner, and progress is still being made. Shirts and Chodera for example presented a poster describing a general Bayesian approach for optimizing the precision of free-energy averages taken over a range of states. Formal optimization with respect to accuracy is much more difficult to accomplish. Methods for detecting bias and optimizing to minimize it are still under development. It seems that the key consideration is the relation between the phase spaces of the systems of interest. Kofke argues that it is necessary to have a phase-space subset relation between pairs of systems in which direct free-energy calculations are performed, at least when using work-based methods. He has proposed the relative entropy as a useful metric for identifying the phase-space relations between a pair of systems, and he has used this to formulate a scaled sampling parameter that can indicate whether sufficient sampling has been performed to ensure that the bias in the estimate is reduced to an acceptable level. The subset criterion can then be applied as a qualitative guide when formulating stages for multistage sampling. There is still much to learn however. Geissler has evidence that the phase-space subset requirement does not necessarily apply when finite-time non-equilibrium work calculations are conducted. There are also questions remaining about how to optimize quantitatively the number and definition of intermediate stages when designing multistage free-energy calculations.

Thermodynamic integration is a widely used technique that does not suffer from the same type of systematic error as other work-based methods. Instead, systematic error can arise from the use of too-few quadrature points in the calculation, and this depends on the nature of the free-energy surface. For simple free-energy landscapes, thermodynamic integration can present the optimal method (e.g., only one calculation is needed if the free-energy is constant, only two if it varies linearly, etc). However it is difficult to know a priori the shape of the free-energy integration path, so it is difficult to make general prescriptions for optimizing the calculation. Evidence for sufficient integration steps would be of the kind examined for standard quadrature applications, i.e., removing some of the data points and seeing whether it affects the result. Vanden Eijnden demonstrated a novel approach of this type for integration in a multidimensional space.

Histogram-based approaches did not receive much attention in the discussion of methods. Emerging issues in relating to this methodology are focused on the type of basis functions used to represent the probability function being measured. Pohorille and Vanden Eijnden both raised this question to some extent in their presentations.

Optimum bias in free-energy calculations

Thomas Woolf

The calculation of a relative free energy difference depends on critical choices involving sampling, computer time, sophistication of the model system, desired level of accuracy, and the total-time needed for making the calculation. All of these interconnected parts of a calculation involve both rational thinking and the making of estimates for how much of an effect the decision will make on the final calculation.

One method to speed-up the route to an estimated free energy difference is the use of biasing functions. Similar to their first introduction within the Monte Carlo community, these biasing functions can provide a dramatic speed-up in the total time to completion and provide an increased statistical accuracy, through a reduction in the variance of the relative free energy estimate. Since the correction for the bias is applied at the time of making the biased step, the results are unbiased estimators for the free energy.

An advantage of constructing a biasing function is that it can be applied in either the framework of equilibrium free energy methods or within the framework of the non-equilibrium methods first developed by Chris Jarzynski. In either of these situations, the biasing approach, along with its correction, can improve sampling efficiency and accuracy from several times to several orders of magnitude, depending on the problem and the set of conditions used in the initial, unbiased, calculation.

Since 1997, our group has pursued a variant of importance sampling that we've titled "Dynamic Importance Sampling". In this route a molecular dynamics algorithm is defined that enables variance reduction methods to be applied to sampled trajectories. The set of trajectories can then be used to defined kinetics between two states and thus both relative reaction coordinates, as well as free energy differences.

In a post-processing step, considerations of biasing can also prove to be very effective, in providing a fast route to analysis of error and to determination of a converged answer. This is shown through the fitting of non-Gaussian distributions to the work events of a non-equilibrium simulation. Our analysis of this work distribution suggests that a universal probability distribution, developed by Bramwell and Pinton (and suggested to us by Gavin Crooks) fits the distributions very well. This enables the computation of relative free energy differences even with minimal overlap and is related to, but improves on the methods first developed by Bennett. In a more complete formulation we have labeled these approaches overlap and funnel sampling and the idea is to focus the simulation effort on the maximal overlap between the two end states.

In the most recent work on biasing methods, we have been extending ideas developed under the name of Kullback-Leibler or Cross-entropy. These approaches focus on the information available during the simulation and suggests that a variance reduced answer for the optimal biasing function does exist. It can be found by the method of iteration and is the sampling route that provides the most accurate answer with the smallest variance. We are continuing to work on ways to improve convergence to an optimal biasing estimator, since robust routes to finding this would significantly aid the rapid and accurate determination of relative free energy differences.

Enhanced sampling for free-energy calculations

Mark Tuckerman

One of the computational grand challenge problems is the development of methodology capable of sampling conformational equilibria in systems with rough energy landscapes. If met, many important problems, most notably protein structure prediction, could be significantly impacted. In my presentation, I discussed a new approach [45, 46] in which molecular dynamics is combined with a novel variable transformation designed to warp configuration space in such a way that barriers are reduced and attractive basins stretched. The fundamental idea can be illustrated by considering a single particle of mass m moving in a one-dimensional double-well potential $V(x)$ with minima at $x = \pm a$ and a barrier of height $V^\ddagger$. If $kT \ll V^\ddagger$, then barrier-crossing in a thermostatted molecular dynamics or Monte Carlo calculation will be rare. Thus, consider the classical canonical partition function for this system is

$$Q = \frac{1}{h}\int dp\, dx\, \exp\left\{-\beta\left[\frac{p^2}{2m} + V(x)\right]\right\} \tag{18.7}$$

where h is Planck's constant. Since the partition is simply an integral over the phase space, we are free to change variables of integration. Since the potential $V(x)$ is a "rough" function of x, we introduce a change of variables from x to $u = f(x)$ with the goal of smoothing out the roughness but without altering any of the thermodynamic or equilibrium properties of the system. A choice for $f(x)$ that accomplishes this is

$$u = f(x) = -a + \int_{-a}^{x} dy\, e^{-\beta\tilde{V}(y)} \tag{18.8}$$

where $\tilde{V}(x)$ is an arbitrary potential energy function. Note that, since $f(x)$ is a monotonically increasing function of x, the inverse $x = f^{-1}(u) = g(u)$ exists. Introducing this transformation into the canonical partition function gives

$$Q = \frac{1}{h}\int dp\, du\, \exp\left\{-\beta\left[\frac{p^2}{2m} + V(g(u)) - \tilde{V}(g(u))\right]\right\} \tag{18.9}$$

Since the difference $V(g(u)) - \tilde{V}(g(u))$ now appears in the partition function, it is clear that the optimal choice for $\tilde{V}(x)$ is $\tilde{V}(x) = V(x)$ for $x \in [-a, a]$ and $\tilde{V}(x) = 0$ for $|x| > a$. With this choice, the difference potential $V - \tilde{V}$ will have no barrier. Thus, by performing thermostatted molecular dynamics with the Hamiltonian $H(p, u) = p^2/2m + V(g(u)) - \tilde{V}(g(u))$, sampling efficiency can be significantly enhanced. The new scheme is denoted REPSWA for REference Potential Spatial Warping Algorithm.

Note that the new method rigorously preserves equilibrium properties while leading to very large enhancements in sampling efficiency. The performance of the method was demonstrated on long polymer chains and simple protein models and was shown to significantly outperform replica-exchange Monte Carlo [57, 58] with only one trajectory [46]. The implementation of REPSWA to polymers and biomolecules involves the application of the aforementioned transformation scheme to the backbone dihedral angles. The latter are a useful set of collective variables that, in part, determine the relevant conformational space of this class of molecules. The comparison between REPSWA, hybrid Monte Carlo [49] and paralle tempering for an all-atom 50-mer alkane chain is shown in Fig. 18.1 below. The figure shows, with one trajectory, REPSWA is able to visit more minima on the potential energy surface than either hybrid Monte Carlo or parallel tempering with ten optimally chosen replicas.

Statistical error control

Daniel Zuckerman

Although significant efforts by many investigators are directed at developing improved sampling schemes for molecular systems, the field lacks a standard method for assessing sampling. Without the ability to quantitatively assess sampling, we cannot judge methodologies objectively. Prof. Zuckerman therefore chose to present research on a method to quantify sampling quality in terms of the "effective sample size" (defined below). The fully automated and "blind" approach simultaneously determines approximate physical states which may be useful in other analyses.

Dr. Zuckerman addressed the question, "To what number of statistically independent configurations is a given ensemble equivalent?" The answer is the effective sample size. In physical terms, this approach is similar to estimates based on dividing the total simulation time by a correlation time. Yet unless the system is well understood in advance, the most important correlation times can be very difficult to determine.

The Zuckerman group compared fluctuations observed in a simulation of unknown quality to those expected for an ideal simulation - consisting of N fully uncorrelated and properly distributed configurations.

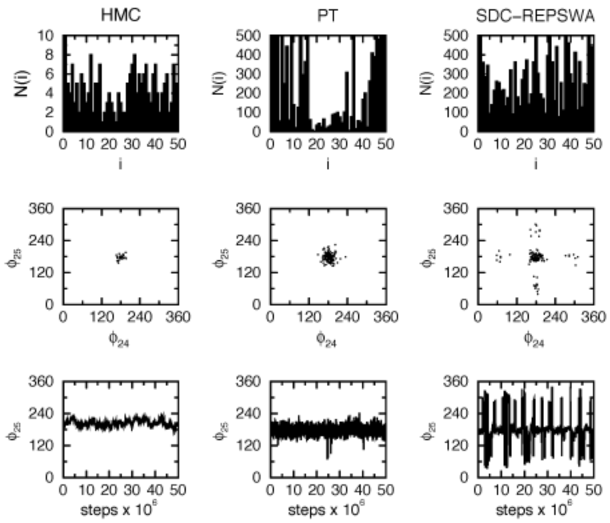

Figure 18.1: Comparison is made for HMC, PT with 10 replicas, and REPSWA in their sampling efficiency of the conformational space of the a 50-mer alkane chain. Top: N(i), number of barrier crossing events for each torsional dihedral i, found in a 5×10^7 MC step trajectory. One crossing event of a dihedral angle corresponds to any transition between gauche $(\phi = 60°/300°)$ and trans $(\phi = 180°)$ conformers. Middle: Ramachandran plot of the central dihedral angles (ϕ_{24}, ϕ_{25}). Bottom: Value of the central dihedral (ϕ_{25}) as a function of the MC steps.

The comparison permits determination of the value of N governing the fluctuations in the ensemble of unknown quality (see Lyman and Zuckerman, J. Phys. Chem. B 111:12876-12882, 2007). Such a comparison was realized by dividing configuration space into many small regions using a Voronoi procedure. For a region i with population pi, ideal simulation leads to an easily calculable variance as a function of N. This ideal variance provides the basis for the comparison.

The results obtained by Dr. Zuckerman's research group show that such a procedure provides very reliable and accurate estimates of sample size for dynamical trajectories (from MD, Langevin, or dynamical MC).

What about physical states? During the sample-size determination, the small regions of configuration space are grouped together based on whether their occupancy sequences during a dynamical simulation are correlated. This step is critical for reliably estimating sample size, but it also turns out to be a blind and automated method for determining approximate physical states. In systems where the physical states were known a priori, Dr. Zuckerman's group found that the combined regions corresponded quite closely to these known states.

Although the procedure described above is applicable only to dynamical simulations, non-dynamical simulations can be analyzed based on variances in the populations of physical states determined from one or more dynamical simulations of the same system.

The hope is that such a procedure, or a related one, could be used by the community as an objective measure of sample quality - and therefore of sampling methods. The efficiency of a sampling method can be assessed quite simply by calculating the computer cost per independent configuration.

Applications of committor functions for free-energy calculations

Eric Van den-Eijnden

Important processes such as allosteric transitions in biomolecules, gating in ion channels, conformation changes in enzymes leading to ligand binding, nucleations events during phase transformation, etc. arise on a time scale which is way beyond what is accessible by brute force molecular dynamics (MD) simulations. The reason is that these processes are rare reactive events which only arise when the system manages to find its way through dynamical bottlenecks in phase-space to escape from the region where it is initially confined.

A major issue in computational chemistry is to deal with these rare reactive events and this requires first to identify the right statistical descriptors for these events. Much in the same way as an equilibrium trajectory is only informative through the lens provided by the framework of equilibrium statistical mechanics, the question is what are the equivalent for the reactive trajectories of objects like the Boltzmann-Gibbs? Here by reactive trajectories we mean the pieces of a long ergodic trajectory $x(t)$ with $t \geq 0$ during which it goes from the reactant state to the product state. Identifying these statistical descriptors is a prerequisite to any computational work aimed at describing the mechanism of rare reactive events.

Recently, a framework termed transition path theory (TPT) has been introduced to describe the statistical properties of the reactive trajectories [50, 51, 52]. Let us briefly recall the main results of TPT. We denote by A and B the product and the reactant state, respectively, and by R the set of times during which the trajectory is reactive, i.e. $t \in R$ if $x(t)$ is out of A and B, it visited last the reactant state A rather than the product state B, and it will go next to B rather than A. Two fundamental objects to describe the mechanism of the reaction are: (i) the probability density of the reactive trajectories, *i.e.* the density defined as

$$\rho_R(x) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \delta(x - x(t)) 1_R(t) dt \tag{1}$$

and (ii) the probability current of the reactive trajectories, i.e. the vector field defined as

$$j_R(x) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \dot{x}(t) \delta(x - x(t)) 1_R(t) dt \tag{2}$$

Here $1_R(t) = 1$ if $t \in R$ and $1_R(t) = 0$ otherwise: this factor is included in (1) and (2) to prune out of the time-averages all the times during which the trajectory is not reactive. TPT gives explicit formulas for $\rho_R(x)$ and $j_R(x)$ but before giving those, let us recall what these objects mean. The probability density $\rho_R(x)$ is self-explanatory. The current $j_R(x)$ is a somewhat more subtle quantity but it is also the most informative about the mechanism of the reaction. $j_R(x)$ gives the average velocity of the reactive trajectories at point x and so this current can be interpreted pretty much as we would interpret the (averaged) velocity field of a fluid flow, with the states A and B playing the role of fluid source and sink, respectively. In particular, the flow lines of the current (*i.e.* the curves along which the local tangent vector is $j_R(x)$) characterize the average way the reactive trajectories flow from A to B, and its integral on any surface gives the probability flux of reactive trajectories though this surface (and so the surface integral of $j_R(x)$ on any dividing surface gives the total flux, i.e. the rate of the reaction). Taken together these objects permit to identify the preferred channels for the reaction.

TPT gives explicit expressions for $\rho_R(x)$ and $j_R(x)$. In the context of a system governed by the over-damped dynamics, these are

$$\rho_R(x) = Z^{-1} e^{-\beta V(x)} q(x)(1 - q(x)) \tag{1$'$}$$

and

$$j_R(x) = Z^{-1} e^{-\beta V(x)} \nabla q(x) \tag{2$'$}$$

Similar expression can be given for a system with inertia governed, say, by the Langevin equation. Here $V(x)$ is the potential, β is the inverse temperature, and $Z = \int e^{-\beta V(x)} dx$. The function $q(x)$ entering $(1')$ and $(2')$ is a key object of the theory: it is the committor function, i.e. the function whose value at point x gives the probability that a trajectory initiated from x reaches first the product state B rather than the reactant state A. The isosurfaces of $q(x)$ foliate the configuration space between A and B and give a precise measure of the advancement of the reaction. This means that $q(x)$ not only can be used as a reaction coordinate but, owing to the role that this function plays in the expressions for $\rho_R(x)$ and $j_R(x)$, that it is the *best reaction coordinate among all*. The current $j_R(x)$, especially, shows how much information about the mechanism of the reaction can be extracted from the specific reaction coordinate $q(x)$ (and how much more than what conventional wisdom attributes to a reaction coordinate). It also shows that the concept of a reaction coordinate can be reconciled with that of using one or more specific paths to explain the reaction: such paths can e.g. be defined as the center of the reaction tubes carrying most of the flux of the reactive trajectories (assuming of course that such tubes exist, i.e. the reaction does indeed occur via localized channels).

In view of all this, the central question in the study of rare reactive event becomes how to calculate the committor function in some approximate way and identify the tubes carrying most of the flux of the reactive trajectories. Much in the same way as the Boltzmann-Gibbs distribution can be sampled more efficiently by modifying the dynamics appropriately (e.g. by using umbrella sampling, parallel tempering, Wang-Landau, etc.), the same is true for the committor function: infinitely many different type of dynamics have the same committor, and, hence, reactive trajectories with identical statistical properties. This property suggests to find one for which sampling of $q(x)$ is easier. One approach in this direction is the string method, developed in [53, 54, 37], but it certainly is not the only possible one.

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Chapter 19

Emerging Directions in String Theory (08w5059)

Jun 22 - Jun 27, 2008

Organizer(s): Robert Myers (Perimeter Institute), Hirosi Ooguri (California Institute of Technology), Washington Taylor (Massachusetts Institute of Technology), Mark Van Raamsdonk (University of British Columbia)

Overview of the Field

Of all scientific endeavors, string theory has perhaps the grandest ambitions: to explain all known matter and forces in the universe in a single unified framework. In the most optimistic scenario, string theory would explain all properties of the elementary particles and the forces between them, the physics of the big bang which led to the universe we observe, the nature of the mysterious dark matter and dark energy required to explain the observed large-scale properties of our universe, and the detailed physics of black holes, perhaps the most mysterious objects in our present universe. Remarkably, it is already clear that string theory provides a rich enough framework to accomplish all of these objectives. However, there is an enormous amount to be understood at both the technical and conceptual levels before it can be decided whether string theory provides a satisfactory description of our universe.

Open Questions

At the time of the conference, some of the interesting questions discussed included

- What are the allowed compactifications of string theory to four dimensions? What are the possibilities for the low-energy effective theory that emerges from a string compactifications?
- How can we understand the microstates that give rise to the entropy of various types of black holes in string theory?
- What can we say about string theory on time dependent backgrounds? Does string theory make any predictions about the physics in the early universe that could be checked by present-day cosmology experiments?
- Can we find a proof of or convincing evidence for the conjectured dualities between gauge theories and string theory in certain backgrounds. Can we exactly solve string theory is certain cases such as the free string limit of type IIB string theory on $AdS^5 \times S^5$. Correspondingly, can we compute the exact

spectrum of maximally supersymmetric Yang-Mills theory in the planar limit? Is the planar theory exactly integrable?

- Can we learn new lessons about quantum gravity using low-dimensional toy models that can be solved exactly?
- Can we embed inflationary cosmology in string theory? Does string theory provide alternatives to inflation that solve the horizon, flatness, and monopole problems and produce the observed scale-invariant spectrum of fluctuations? Does string theory predict primordial cosmic strings, and if so, what are the observable signatures?
- Can we use gauge-theory / gravity duality to learn about real-world systems such as hot QCD, superconductors, or other condensed matter systems?

Presentation Highlights

The presentations by participants included talks on all of these subjects. Below, we provide a summary of the talks:

Allan Adams - "non-relativistic AdS/CFT"
Building on our earlier work and that of Son, we construct string theory duals of non-relativistic critical phenomena at finite temperature and density. Concretely, we find black hole solutions of type IIB supergravity whose asymptotic geometries realize the Schroedinger group as isometries. We then identify the non-relativistic conformal field theories to which they are dual. We analyze the thermodynamics of these black holes, which turn out to describe the system at finite temperature and finite density. The strong-coupling result for the shear viscosity of the dual non-relativistic field theory saturates the KSS bound.
Katrin Becker - "Torsional Heterotic Geometries"
New heterotic torsional geometries are constructed as orbifolds of T^2 bundles over $K3$. The discrete symmetries considered can be freely-acting or have fixed points and/or fixed curves. We give explicit constructions when the base $K3$ is Kummer or algebraic. The orbifold geometries can preserve $N = 1, 2$ supersymmetry in four dimensions or be non-supersymmetric.
Robert Brandenberger - "Status of String Gas Cosmology"
String gas cosmology is a string theory-based approach to early universe cosmology which is based on making use of robust features of string theory such as the existence of new states and new symmetries. A first goal of string gas cosmology is to understand how string theory can effect the earliest moments of cosmology before the effective field theory approach which underlies standard and inflationary cosmology becomes valid. String gas cosmology may also provide an alternative to the current standard paradigm of cosmology, the inflationary universe scenario. Here, the current status of string gas cosmology is reviewed.
Jan de Boer - "Black hole quantization"
N=2 supergravity in four dimensions, or equivalently N=1 supergravity in five dimensions, has an interesting set of BPS solutions that each correspond to a number of charged centers. This set contains black holes, black rings and their bound states, as well as many smooth solutions. Moduli spaces of such solutions carry a natural symplectic form which we determine, and which allows us to study their quantization. By counting the resulting wavefunctions we come to an independent derivation of some of the wall-crossing formulae. Knowledge of the explicit form of these wavefunctions allows us to find quantum resolutions to some apparent classical paradoxes such as solutions with barely bound centers and those with an infinitely deep throat. We show that quantum effects seem to cap off the throat at a finite depth and we give an estimate for the corresponding mass gap in the dual CFT. This is an interesting example of a system where quantum effects cannot be neglected at macroscopic scales even though the curvature is everywhere small.
Oliver DeWolfe - "Nonsupersymmetric brane vacua in stabilized compactifications"
We derive the equations for the nonsupersymmetric vacua of D3-branes in the presence of nonperturbative moduli stabilization in type IIB flux compactifications, and solve and analyze them in the case of two particular 7-brane embeddings at the bottom of the warped deformed conifold. In the limit of large volume and long throat, we obtain vacua by imposing a constraint on the 7-brane embedding. These vacua fill out continuous spaces of higher dimension than the corresponding supersymmetric vacua, and have negative effective

cosmological constant. Perturbative stability of these vacua is possible but not generic. Finally, we argue that anti-D3-branes at the tip of the conifold share the same vacua as D3-branes.

Jacques Distler - "General F-Term Gauge Mediation"

In a model-independent formalism of gauge mediation, Meade, Seiberg, and Shih have shown that hidden sector effects are captured by two-point correlation functions of the gauge current superfields and that, generically, many of the characteristic features of gauge mediated SUSY breaking do not survive. We review the general story, particularly the way that the correlators enter the low-energy effective action and give rise to soft-breaking terms. We then specialize to the case where there is a small parameter, F/m^2, where m is the mass scale characterizing the hidden sector, and F is the strength of the SUSY breaking. To leading nontrivial order in this small parameter, we show that many of the classic predictions of gauge mediated SUSY breaking are recovered.

Ben Freivogel - "A bound on lifetimes of string theory vacua"

Recent work has suggested a surprising new upper bound on the lifetime of de Sitter vacua in string theory. The bound is parametrically longer than the Hubble time but parametrically shorter than the recurrence time. We investigate whether the bound is satisfied in a particular class of de Sitter solutions, the KKLT vacua. Despite the freedom to make the supersymmetry breaking scale exponentially small, which naively would lead to extremely stable vacua, we find that the lifetime is always less than about $exp(10^(22))$ Hubble times, in agreement with the proposed bound.

Ori Ganor - "On S-duality and Chern-Simons"

We propose a relation between the operator of S-duality (of N=4 super Yang-Mills theory in 3+1D) and a topological theory in one dimension lower. We construct the topological theory by compactifying N=4 super Yang-Mills on a circle with an S-duality and R-symmetry twist. The S-duality twist requires a selfdual coupling constant. We argue that for a sufficiently low rank of the gauge group the three-dimensional low-energy description is a topological theory, which we conjecture to be a pure Chern-Simons theory. This conjecture implies a connection between the action of mirror symmetry on the sigma-model with Hitchin's moduli space as target space and geometric quantization of the moduli space of flat connections on a Riemann surface.

Jaume Gomis - "M2-branes and Bagger-Lambert theory"

We show that by adding a supersymmetric Faddeev-Popov ghost sector to the recently constructed Bagger-Lambert theory based on a Lorentzian three algebra, we obtain an action with a BRST symmetry that can be used to demonstrate the absence of negative norm states in the physical Hilbert space. We show that the combined theory, expanded about its trivial vacuum, is BRST equivalent to a trivial theory, while the theory with a vev for one of the scalars associated with a null direction in the three-algebra is equivalent to a reformulation of maximally supersymmetric 2+1 dimensional Yang-Mills theory in which there a formal SO(8) superconformal invariance.

Sean Hartnoll - "Towards an ads/cmt correspondence, part I"

Chris Herzog - "Towards an ads/cmt correspondence, part II"

We show that a simple gravitational theory can provide a holographically dual description of a superconductor. There is a critical temperature, below which a charged condensate forms via a second order phase transition and the (DC) conductivity becomes infinite. The frequency dependent conductivity develops a gap determined by the condensate. We find evidence that the condensate consists of pairs of quasiparticles.

Petr Horava - "Quantum Gravity at a Lifshitz Point"

We present a candidate quantum field theory of gravity with dynamical critical exponent equal to z=3 in the UV. (As in condensed matter systems, z measures the degree of anisotropy between space and time.) This theory, which at short distances describes interacting nonrelativistic gravitons, is power-counting renormalizable in 3+1 dimensions. When restricted to satisfy the condition of detailed balance, this theory is intimately related to topologically massive gravity in three dimensions, and the geometry of the Cotton tensor. At long distances, this theory flows naturally to the relativistic value z=1, and could therefore serve as a possible candidate for a UV completion of Einstein's general relativity or an infrared modification thereof. The effective speed of light, the Newton constant and the cosmological constant all emerge from relevant deformations of the deeply nonrelativistic z=3 theory at short distances.

Dan Kabat - "Timescales and local probes of BTZ black holes"

First we review the description of local bulk operators in Lorentzian AdS in terms of non-local operators in the boundary CFT. We discuss how bulk locality arises in pure AdS backgrounds and how it is modified at finite N. Next we present some new results on BTZ black holes: local operators can be defined inside the horizon of a finite N BTZ black hole, in a way that suggests the BTZ geometry describes an average over black hole microstates, but with finite N effects resolving the singularity.

Matthew Kleban - "When Do Worlds Collide?"

We extend our previous work on the cosmology of Coleman-de Luccia bubble collisions. Within a set of approximations we calculate the effects on the cosmic microwave background (CMB) as seen from inside a bubble which has undergone such a collision. We find that the effects are always qualitatively similar–an anisotropy that depends only on the angle to the collision direction–but can produce a cold or hot spot of varying size, as well as power asymmetries along the axis determined by the collision. With other parameters held fixed the effects weaken as the amount of inflation which took place inside our bubble grows, but generically survive order 10 efolds past what is required to solve the horizon and flatness problems. In some regions of parameter space the effects can survive arbitrarily long inflation.

Emil Martinec - "Matrix models of tachyonic vacua"

Alex Maloney - "Aspects of three dimensional gravity"

We consider pure three-dimensional quantum gravity with a negative cosmological constant. The sum of known contributions to the partition function from classical geometries can be computed exactly, including quantum corrections. However, the result is not physically sensible, and if the model does exist, there are some additional contributions. One possibility is that the theory may have long strings and a continuous spectrum. Another possibility is that complex geometries need to be included, possibly leading to a holomorphically factorized partition function. We analyze the subleading corrections to the Bekenstein-Hawking entropy and show that these can be correctly reproduced in such a holomorphically factorized theory. We also consider the Hawking-Page phase transition between a thermal gas and a black hole and show that it is a phase transition of Lee-Yang type, associated with a condensation of zeros in the complex temperature plane. Finally, we analyze pure three-dimensional supergravity, with similar results.

Rob Myers - "The fast life of holographic mesons"

We use holographic techniques to study meson quasiparticles moving through a thermal plasma in $N = 2$ super-Yang-Mills theory, with gauge group $SU(N_c)$ and coupled to N_f flavours of fundamental matter. This holographic approach reliably describes the system at large N_c, large 't Hooft coupling and $N_f/N_c << 1$. The meson states are destabilized by introducing a small quark density n_q. Spectral functions are used to examine the dispersion relations of these quasiparticles. In a low-momentum regime, the quasiparticles approach a limiting velocity which can be significantly less than the speed of light. In this regime, the widths of the quasiparticles also rise dramatically as their momentum approaches a critical value q_{crit}. While the spectral functions do not display isolated resonances for $q > q_{crit}$, the dispersion relations can be extended into this high-momentum regime by studying the dual quasinormal modes. A preliminary qualitative analysis of these modes suggests that the group velocity rises to the speed of light for $q >> q_{crit}$.

Joseph Polchinski - "Matrix Models for Black Holes and Cosmology"

We study various matrix models with a charge-charge interaction as toy models of the gauge dual of the AdS black hole. These models show a continuous spectrum and power-law decay of correlators at late time and infinite N, implying information loss in this limit. At finite N, the spectrum is discrete and correlators have recurrences, so there is no information loss. We study these models by a variety of techniques, such as Feynman graph expansion, loop equations, and sum over Young tableaux, and we obtain explicitly the leading $1/N^2$ corrections for the spectrum and correlators. These techniques are suggestive of possible dual bulk descriptions. At fixed order in $1/N^2$ the spectrum remains continuous and no recurrence occurs, so information loss persists. However, the interchange of the long-time and large-N limits is subtle and requires further study.

Aninda Sinha - "Quantum corrections to eta/s"

We consider corrections to the ratio of the shear viscosity to the entropy density in strongly coupled non-abelian plasmas using the AdS/CFT correspondence. In particular, higher derivative terms with the five-form RR flux, which have been ignored in all previous calculations, are included. This provides the first reliable calculation of the leading order correction in the inverse 't Hooft coupling to the celebrated result $eta/s = 1/4pi$. The leading correction in inverse powers of the number of colours is computed. Our results hold very generally for quiver gauge theories with an internal manifold L_{pqr} in the holographic dual. Our analysis implies that the thermal properties of these theories will not be affected by the five-form flux terms at this order.

Marcus Spradlin - "Scattering amplitudes and Wilson loops in N=4"
We use the leading singularity technique to determine the planar six-particle two-loop MHV amplitude in N=4 super Yang-Mills in terms of a simple basis of integrals. Our result for the parity even part of the amplitude agrees with the one recently presented in arXiv:0803.1465. The parity-odd part of the amplitude is a new result. The leading singularity technique reduces the determination of the amplitude to finding the solution to a system of linear equations. The system of equations is easily found by computing residues. We present the complete system of equations which determines the whole amplitude, and solve the two-by-two blocks analytically. Larger blocks are solved numerically in order to test the ABDK/BDS iterative structure.
Alessandro Tomasiello - "New and old AdS_4 vacua in string theory"
We find the gravity duals to an infinite series of $N = 3$ Chern-Simons quiver theories. They are AdS_4xM_7 vacua of M-theory, with M_7 in a certain class of 3-Sasaki-Einstein manifolds obtained by a quotient construction. The field theories can be engineered from a brane configuration; their geometry is summarized by a "hyperKaehler toric fan" that can be read off easily from the relative angles of the branes. The singularity at the tip of the cone over M_7 is generically not an orbifold. The simplest new manifolds we consider can be written as the biquotient $U(1)$
$U(3)/U(1)$. We also comment on the relation between our theories and four-dimensional N=1 theories with the same quiver.
Brian Wecht - "Torsion and SUSY Breaking"
We identify the auxiliary fields in the hypermultiplets of type IIB string theory compactified on a Calabi-Yau manifold, using a combination of worldsheet and supergravity techniques. The SUSY-breaking squark and gaugino masses in type IIB models depend on these auxiliary fields, which parametrize deformations away from a pure Calabi-Yau compactification to one with NS-NS 3-form flux and $SU(3) \times SU(3)$ structure. Worldsheet arguments show that such compactifications are generically globally nongeometric. Our results, combined with earlier results for type IIA compactifications, imply that these deformations are the mirrors of NS-NS 3-form flux, in accord with work from the supergravity point of view. Using the worldsheet current algebra, we explain why mirror symmetry may continue to hold in the presence of fluxes breaking the symmetries (e.g., (2,2) SUSY) on which mirror symmetry is typically taken to depend. Finally, we give evidence that nonperturbative worldsheet effects (such as worldsheet instantons) provide important corrections to the supergravity picture in the presence of auxiliary fields for Kahler moduli.
Johannes Walcher - "Tadpole cancellation in the topological string"
We study the topological string on compact Calabi-Yau threefolds in the presence of orientifolds and D-branes. In examples, we find that the total topological string amplitude admits a BPS expansion only if the topological charge of the D-brane is equal to that of the orientifold plane. We interpret this as a manifestation of a general tadpole cancellation condition in the topological string that is necessary for decoupling of A- and B-model in loop amplitudes. Our calculations in the A-model involve an adapted version of existing localization techniques, and give predictions for the real enumerative geometry of higher genus curves in Calabi-Yau manifolds. In the B-model, we introduce an extension of the holomorphic anomaly equation to unoriented strings.
Timo Weigand - "(Non-)BPS (Multi-)Instantons"
We study non-perturbative effects in four-dimensional N=1 supersymmetric orientifold compactifications due to D-brane instantons which are generically not invariant under the orientifold projection. We show that they can yield superpotential contributions via a multi-instanton process at threshold. Some constituents of this configuration form bound states away from the wall of marginal stability which can decay in other regions of moduli space. A microscopic analysis reveals how contributions to the superpotential are possible when new BPS states compensate for their decay. We study this concretely for D2-brane instantons along decaying special Lagrangians in Type IIA and for D5-branes instantons carrying holomorphic bundles in Type I theory.

Outcome of the meeting

The meeting was extremely successful. All talks were well attended, and there was intense discussion and collaboration between participants. Participants were encouraged to use the blackboard for talks, and this led to a very informal and collaborative atmosphere. In addition to the regular talks, there was much discussion about a new proposal by Aharony, Bergman, Jafferis and Maldacena for a non-perturbative definition of

M-theory on $AdS^4 \times S^7$ in terms of a supersymmetric Chern-Simons matter theory. Discussions at the conference led to published work on this subject, including the paper arXiv:0807.1074 by Gomis, Rodriguez-Gomez, Van Raamsdonk, and Verlinde. The BIRS conferences on string theory are gaining recognition as some of the most productive and enjoyable forums for scientific discussion in the field.

List of Participants

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Chapter 20

Recent Progress in Two-Dimensional Statistical Mechanics (08w5084)

Jun 29 - Jul 04, 2008

Organizer(s): Richard Kenyon (Brown University)

Statistical mechanics is a diverse and active field, treating problems coming from the areas of physics, probability, computer science, and even biology. The main goal of this workshop was to study the mathematical side of statistical mechanics, and in particular two-dimensional problems, many of which are well-known and classical but few of which are really well-understood even today.

As we can see from the descriptions of some of the talks below, there is still definite and exciting progress being made on the old problems of statistical mechanics from the mid-20th century (see talks of Kotecky, Nienhuis, Ciucu, Imbrie). But also there are many new directions and problems being studied as well (see descriptions of talks by Peres, Hoffman, Sheffield, Borcea).

The classical two-dimensional models: percolation, the Ising model, loop-erased random walks, polymers, random tiling models, random packings, are all idealized models of physical reality, dealing with the organization of large numbers of atoms or particles; these particles are interacting only locally but forming large-scale structures. It is this "local-to-global" organizational principle which makes these problems so intriguing and important. While highly idealized, these models nonetheless have the two key features of, on the one hand, being mathematically treatable and on the other, retaining some of the structure of natural organizational phenomena.

Our focus at this workshop was to discuss current research on these paradigmatic models, as well as hear about new ideas and models of focus in recent years.

Let me briefly discuss the major open problems in this area. Historically the Ising model was the first "exactly solved" model to exhibit a phase transition. This model is just a measure on the space $\{1, -1\}^G$ where G is a graph, usually the square grid in the plane. This measure weight configurations with an exponential factor according to the number of nearest neighbors with the same spin. If the interaction is large, there is a coherence in the system: the correlation of spins between far-away vertices does not decay towards zero but instead remains bounded away from zero. If the interaction is small, then there is no such long-range order. There is a critical value of the interaction parameter at which this behavior changes. If we sit exactly at the critical value, moreover, something remarkable happens: the system has a scale-invariance, in the sense that large structures survive on all scales. One in fact knows how to rescale the lattice, so that the mesh size goes to zero, and get a nontrivial continuous process in the limit, called the scaling limit. This continuous process is not very well understood mathematically, but it is known to have some conformal invariance properties. For example it is suspected that the boundaries of spin-domains (domains of constant spin) are, in a well-defined sense in the scaling limit, fractal curves which can be described by the so-called SLE process.

There are many other two-dimensional models which exhibit the same kind of conformally-invariant scaling limit behavior. The first model for which we had a rigorous proof is the dimer model on $\mathbf{Z}^2$, (also called domino tiling model). However this proof and the proofs for other similar models are all quite difficult and, indeed, give only partial results. We would like to develop tools to handle conformally invariant limits in greater generality—but at present these are lacking.

Conformal invariance aside, the problem of phase transitions is also tantalizing and often seemingly intractable. A classical example, maybe the more important example, is the hard-disk model in the plane. If you pack αN^2 disks randomly in an $N \times N$ box, for small α the typical configuration (using just normalized Lebesgue measure on the configuration space) appears to be unordered and quite random. However there is a critical α beyond which the system "crystallizes" and you will typically see the presence of long-range order in the form of a nearly-hexagonal packing of disks. Unfortunately this critical point is not known, and indeed nobody has any good methods to say anything quantitative about this model. The recent paper [1] is the first interesting mathematical foray into this model, and it is hoped that we'll see more results in the near future.

Individual talks

Bernard Nienhuis discussed **percolation** on a family of geometric "rhombic" planar graphs. Here the goal is to obtain exact formulas for certain connection probabilities under simple geometric constraints. It is remarkable that under these constraints (called "Z-invariant lattices" by Baxter) one can determine through various commutation relations the leading eigenvector of the "transfer operator". This allows Nienhuis and coauthors to determine exact formulas for various connection probabilities and connection correlations. While many aspects of percolation in 2D are now understood, almost all of these are qualitative. There are few quantitative—i.e. exact— probabilities known. It is clear that this is important work and it remains to be seen how this will change our point of view on percolation: perhaps we can foresee a complete analytic solution someday to the standard questions probabilists ask about this model. For example, can one use these techniques to compute exact long-range connection probabilities for standard edge percolation on the grid? It would seem that this is a distinct possibility.

Roman Kotecky talked about his work on the antiferromagnetic 3-state **Potts model** (3-colorings of the grid). This is another classical statistical mechanics model, first studied by Lieb in the 1960's. Kotecky gives a computer-aided proof of an old conjecture on the co-existence of multiple Gibbs states in the two-dimensional square grid at low temperature.

Omer Angel discussed weak limits of graphs and an extension of the Szemeredi regularity lemma to sparse graphs. While not strictly two-dimensional, this is in a certain sense a theorem about random geometries, which is the subject of intense research in statistical mechanics and modern physics. Angel's theorem is that a bounded degree graph can be decomposed into pieces which are "almost uniform" in the sense that they resemble **random graphs** in a well-defined way.

Mihai Ciucu talked about defects in **dimer models**, see [2], showing how classical conjectures of Fisher and Stephenson from the 1960's about the behavior of defects can be proved, using modern combinatorial techniques, in certain symmetric cases. With increasing generality of his examples he seems to be zeroing in on the general case. The main conjecture is that the two holes behave like charged particles, in the sense that the number of dimer covers with single-hole defects at v_1 and v_2 depends only on the Euclidean distance from v_1 to v_2 (up to sub-leading order corrections).

Chris Hoffman studied a model of random two-complexes, built from a complete graph by gluing in random triangles. He proves a phase transition as the density of triangles increases, in which the fundamental group of the resulting complex becomes trivial. This is related to a result of Gromov who studied random presentations of groups (in which there is again a phase transition as the number of relators increases). Hoffman's problem is also a natural higher-dimensional generalization of the Erdös-Renyì random graph problem. There are many interesting questions in this area: most importantly, can one understand the structure of the fundamental group near the critical point?

John Imbrie discussed work with David Brydges [1] relating the **hard sphere gas** (really the simplest, and perhaps the most important, "unsolved" model in statistical mechanics) in dimension d and branched polymers in dimension $d + 2$. His talk was an introduction to techniques from Gaussian variables applied to combinatorics.

There were a number of talks on SLE, the Stochastic Loewner Evolution. This is a process which connects the models of discrete two-dimensional statistical mechanics with their continuum limits (scaling limits) in the (ubiquitous) case when these have some conformal invariance properties [3]. Michael Kozdron spoke about a computation involving the intersection of an SLE curve with a semicircle; this is a computation needed to compute properties of the diameter of an SLE curve, useful for understanding the geometry of SLE. His talk was quite pedagogical and it was useful to see how one can do explicit computations with SLE.

David Wilson discussed joint work with Richard Kenyon on the connection probabilities in “groves”, or **spanning forests** on planar graphs, relating them to pairing probabilities for multiple $SLE(2)$ paths and multiple $SLE(4)$ paths in the same domain. Spanning forests are classical objects, but tools are still being developed to understand them, particularly for planar graphs. These connection probabilities are analogous to the connection probabilities that Nienhuis discussed (see above), but for the spanning tree model rather than percolation.

Greg Lawler also spoke on SLE-related question, that of Brownian excursion measures and loop measures. He showed how to define the random-walk loop measures, and their limits, the Brownian loop soup measures. These are object of fundamental interest but also useful for relating the various SLE measures amongst themselves.

A third SLE talk was by Robert Masson, a recent PhD, who showed how one can compute the expected length of a **loop-erased walk** (LERW) from the knowledge that the LERW measure converges to an $SLE(2)$. This gives an alternative method of relating discrete models with continuous analogues.

Julien Dubedat was also connecting SLE with stat mech: attempting to define a “partition function” for SLE, which would somehow relate it more closely to the partition function of some underlying discrete model.

Scott Sheffield discussed a continuum version of Liouville quantum gravity, which is a measure on random metrics on surfaces, arising as a limit of uniform measure on planar triangulated graphs. New breakthoughs in SLE, and study of the Gaussian free field have yielded these unexpectedly simple connections between basic discrete objects (like random triangulations) and their continuum limits. This result opens new avenues for connections between statistical mechanics on discrete lattices and their continuum analogues.

Yuval Peres discussed two simple two-dimensional probability models, the rotor-router and IDLA (internal diffusion-limited aggregation). proving limit shape theorems for them. While not directly related to stat mech, these probability models are solved using familiar techniques and can be related through somewhat complicated bijections with spanning tree models.

Julius Borcea, who was a participant at a concurrent BIRS event, gave a talk on zeroes of multivariate polynomials, showing how certain operators on polynomials preserve zero-free regions. These results are useful in proving some classical theorems of statistical mechanics on the location of zeroes of partition functions, for example for the **Ising model** and Potts model (e.g. the Lee-Yang Theorem, the Heileman-Lieb Theorem and generalizations).

Mirjana Vuletic discussed a generalization of the classical Macmahon’s function for counting **plane partitions**. Her results use new tools of Schur functions and Fock space formalism to old combinatorial problems, including this particular problem, originally proved in the 1900’s by Macmahon but on which present-day research is still ongoing.

Problem sessions

Another feature of the workshop was a sequence of discussion/problem sessions focussing on a small number of open problems. On the first day of the workshop we spent some time presenting open problems and then narrowed the list down by vote to four open roblems that we would focus on in groups during the week. These problems were:

1. Conformal restriction measures (presented by Greg Lawler): can one classify conformally-invariant measures on closed subsets of the disk which satisfy the “conformal restriction property”?

2. Determinantal processes (presented by Richard Kenyon): can one characterize in any simple way those matrices which are the kernels of (not necessarily Hermitian) determinantal processes?

3. Dimer covers with two singularities (presented by Mihai Ciucu) Ciucu proposed a model of random dimer covers of random planar graphs with two holes. Can one say anything about the dependence of the partition function on the locations of the holes in such a general setup?

4. Packings of noncrossing horizontal and vertical unit segments (proposed by Richard Kenyon) Is there a way to estimate or otherwise calculate the partition function of the model in the limit of high density?

We spent several sessions discussing strategies of attack for these problems.

In conclusion this was a very successful workshop: there seem to be many new tools people are using to attack old (and new) problems of statistical mechanics, and we had good opportunities to present new methods and discuss applications of them. I feel that what makes statistical mechanics such a unique and exciting field is this diversity of methods: it can be attacked with techniques from many different part of mathematics, and as a result one sees structures in mathematics lying "across" the present (human-imposed) boundaries of different mathematical disciplines.

List of Participants

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Chapter 21

The Biology-Combinatorics Interface: Addressing New Challenges in Computational Biology (08w5069)

Jul 06 - Jul 11, 2008

Organizer(s): David Bremner (University of New Brunswick), Anne Condon (University of British Columbia), Ken Dill (Universtiy of California, San Francisco), Ron Elber (University of Texas at Austin), Arvind Gupta (MITACS), Ladislav Stacho (Simon Fraser University)

Overview of the Field

Math and biology have a long history together [6], beginning with the work of Mendel and Darwin. Today, combinatorics and discrete mathematics are key tools for genome sequencing alignment and assembly, Markov modeling of RNA sequences, gene expression haplotyping, phylogeny construction, and biomolecular statistical mechanics and protein structure modeling.

Now, on the horizon, are the new and bigger challenges posed by systems biology. Systems biologists are interested in models at various levels, from the microscopic (genes, protein structures, and signaling pathways) to the macroscopic (metabolic and genetic circuits, cells, organs, organisms, and populations). Mathematics is poised to help to understand emergent large-scale properties from properties of smaller subsystems, in ways that less quantitative modeling cannot. A key goal is ultimately a quantitative theory of biological cells that begins with the folding, structures and binding of proteins and the regulation of genes, and scales up to the properties of full metabolic and genetic networks, and to the evolutionary dynamical processes that lead to them.

Structure of the Workshop

The BIRS workshop on the *Biology-Combinatorics Interface* brought together bio-scientists, discrete mathematicians, and some researchers with a foot in both camps. Rather than look back at recent work in (discrete) mathematical biology, the goal was to look forward and to try to better understand the emerging challenges in systems biology, and how the tools of discrete mathematics can be brought to bear on these challenges. Because of this outlook, the workshop was organized into 3 phases. We began with a sequence of advanced tutorials to help explain the relevant systems biology. In the second phase we held a series of roundtable discussions to help better define mathematical problems. Finally, roughly the last two days of the workshop were dedicated to smaller working groups taking a more in-depth look at the problems developed in the first two phases.

Recent Developments and Open Problems

Recent developments are captured in the next section — Presentation Highlights. Open problems are presented in the next two sections — Presentation Highlights and Scientific Progress Made.

Presentation Highlights

Because of the format of our workshop, there were relatively few talks. It speaks to the quality of the presentations that the parallel workshop on Rigidity and Biology chose to attend almost all of our talks. We also attended several of their presentations; in fact the interaction between the two workshops could be characterized as one of the presentation related highlights.

Ken Dill

Ken Dill described some general unsolved problems at the interface of combinatorics and biology, described below.

Proteins & RNA molecules: predicting structures, stabilities, conformational changes, aggregation, rates, higher structures, loop modeling, interactions with ligands or biomolecules, mechanisms & motions. The key issue is that proteins are chain molecules with large numbers of degrees of freedom that must be searched by computer to find globally optimal states, but there are complex steric constraints (the chain cannot pass through itself – Hamilton walks, not random walks – and these problems are particularly acute for compact states, like the native states of proteins, which are the biologically important structures). An important problem is how to enumerate the relevant states efficiently by computer. Solving these problems is important for drug discovery in the pharmaceutical and biotech industries.

Zipping and assembly is a mechanism involving fast conformational searching for protein structures. Proteins and RNA molecules fold on funnel-shaped energy landscapes. These landscapes themselves help proteins search through their exponential search spaces with high efficiency.

Cells: characterize network topologies & traffic, flows, and robustness. Biochemical reactions inside biological cells are arranged as networks of molecules that take up substrates from some nodes and pass along products to other nodes. Problems in cell biophysics require understanding these networks and the flows of biochemicals along them. These flows are generally quite nonlinear, and there are many of them, coupled to each other. Mathematical methods are needed to better understand their global properties.

Evolution: How do networks arise? What are properties of fitness landscapes? Advantages of modularity, hierarchy? Cancer - a disease of evolution? How do pathogens become drug-resistant? Not only do we need to better understand the biochemical networks of biological cells, but it is also important to know how those networks evolved from simpler networks, as one species evolves from another. This is important for understanding the unity of life, but it is also of great practical importance. Cancer is a disease in which cells in the body evolve away from their canonical states and structures and become renegade. Cancer is called somatic cell evolution: it involves not the evolution of a species over long evolutionary time scales, but the evolution of a few cells in the body over the body's lifetime.

Nano- bio- tech: Make new structure: as scaffolds, drugs, delivery vehicles, biomaterials, test-tubes-in-a-cell, imaging agents. Biology provides powerful design principles for making functional machines on the nano size scale. However, to build machines on this scale requires overcoming Brownian and entropic forces. To better understand these forces requires better combinatorial techniques to understand the complexity of such systems – the entropies of protein chains, the diffusion of particles subject to constraints, the random navigation of particles through highly confined cell interior regions.

Paul Higgs

Paul Higgs spoke on the problem of evolution in a *pre-DNA World*. Several *RNA World conjectures* exist, the weaker being that RNA acted as a precursor to DNA and proteins for replication and catalysis. Models of growth by self-replication and by catalysis (for example in a “lipid world”) can show heredity without using polymers for information storage, but the question of how evolution can occur remains. One hypothesis that is both biologically interesting and poses interesting questions of mathematical modelling and simulation is the notion of *vesicles* or autocatalytic set of molecules.

Ron Elber

One of the striking observations of modern structural biology is the relatively small number of experimentally-determined families of structures (about a thousand) that capture a significant portion of the empirically-known and much larger sequence space (several millions). The large capacity of protein structures (folds) to sequences motivates research along two directions. The first, which is perhaps more practical, is the modeling of protein structures from sequences based on similarity of the target sequence to another sequence for which the structure is known (homology). The second is an attempt to understand the ”history” of sequence-structure relationships and analyze sequence evolution taking into account changes in the stability of protein structures upon mutations.

In the workshop we focused on the second item. To investigate the impact of stability on evolutionary processes we need to consider the options open to a mutating sequence. The protein mutant may be more or less stable than the native, it may unfold, or it may flip to a different structure.

The first question that was discussed concerned sequence capacity. Namely, how many sequences fit a particular fold and have energy lower than the energy of the native sequence? The capacity sets an upper bound on the evolvability of a protein fold. Besides stability there are other factors that impact mutability of a sequence. These factors include conservation of active site residues, of protein- protein interactions, of required flexibility, etc. We discussed randomized algorithms that sample sequences that fit a fold efficiently and allow for quantitative estimates of the capacity. It was found that the number of sequences accessible to a fold is exponential in the sequence length. The vast number of accessible sequences should be contrasted with the even (exponentially) larger number of possible sequences. Interestingly protein capacity correlates with protein mutation rates as observed empirically [2], supporting the idea that stability influences biological changes. Fold stability may provide a zero order model for molecular evolution.

Another intriguing view of protein evolution is the possibility that a protein sequence that folds into a particular family of structures flips into another family following a single amino acid change. Some experimental evidence is available that supports this idea [1] We discussed construction of a network of sequence of flow in which folds are nodes and weighted edges represent flow of sequences between structures. Hubs in the network are identified as structures rich in beta sheet.

Jie Liang

One of the most important topics in molecular biology is understanding the relationship between the sequence of amino acids in a protein and the resulting folded structure and function of the protein. Dr. Jie Liang presented recent work on using sequence (and hence evolutionary) information to understand geometric structure, and conversely, on extrapolating from known structure information to study evolutionary processes.

Proteins have many voids and pockets, which can be computed (identified and measured) through the aid of alpha complex and pocket algorithms. Identification of particular pockets as biologically important is challenging, since compact self-avoiding random walks exhibit similar behaviour to proteins. For enzymes, Dr. Liang explained that searching using sequence information, augmented by Markov model based processes had achieved success both in solving the resulting surface similarity problems and in distinguishing evolutionary factors from those related to physical folding stability.

A second issue related to protein evolution is the construction of protein fitness function important for protein design. The task is to develop a global fitness function that can discriminate correct protein sequence from unmatchable sequences for all known proteins structures simultaneously. Dr. Liang presented nonlinear potential function of Gaussian kernels. The resulting fitness landscape can be used to study protein evolution.

Christine Heitsch

An RNA molecule is a linear biochemical chain which folds into a three dimensional structure via a set of 2D base pairings known as a nested secondary structure. Reliably determining a secondary structure for large RNA molecules, such as the genomes of most viruses, is an important open problem in computational molecular biology. Dr. Heitsch discussed combinatorial results which yield insights into the interaction of local and global constraints in RNA secondary structures and suggest new directions in understanding the folding of RNA viral genomes.

Ján Maňuch, Ladislav Stacho, Arvind Gupta

The HP model for protein folding has been proposed in mid 80s as a simplification of complex interactions among protein molecules. The main problem is to understand the processes and determine the folds of proteins that minimize total free energy. To simplify the problem, the protein is laid out on a 2D lattice with each monomer occupying exactly one square and neighboring monomers occupy neighboring squares. The free energy is minimized when the maximum number of non-neighbor hydrophobic monomers are adjacent in the lattice. Even in its simplest version this problem is NP-complete.

In many applications such as drug design, we are actually interested in the inverse problem to protein folding: *protein design*. Again, most of the known research concentrates on the 2D and 3D designs in the HP model. Surprisingly, the complexity of this problem is not known, however it is generally believed that all interesting versions will be NP-complete. Recently research concentrated on designs based on domino like structures. Here the required design is composed of small base structures and it is done so that the resulting fold will have a minimum free energy. In 2D this method gives solutions that approximate required shapes arbitrary closely and in 3D such solutions are knows for a large classes of shapes. The main unsolved problem remains to prove the stability of the solutions, i.e. to prove that the folds will be unique in addition to their minimality. The stability of solutions is proved only for very basic shapes in both 2D and 3D cases.

Recently, an interesting refinement of the HP model, in which the cysteine and non-cysteine hydrophobic monomers are distinguished and SS-bridges which two cysteines can form are taken into account in the energy function. In 2D variant of this model with the additional assumption of two distinct SS-bridges types (that cannot interact between each other) it is possible to prove the stability of many solutions that can be used to approximate any structure. The main open question remains the stability of solutions when only one type of SS- bridges is used. In 3D variant stability still cannot be guaranteed and only results possible are that we get only few folds that are somehow structurally close to each other. The challenge remains to tweak these solutions so that stability is guaranteed.

Joint RNA Session

During the joint RNA session, participants from the Biology-Combinatorics Interface workshop and the Rigidity, Flexibility and Motion workshop met for a joint session on RNA structure. Jack Snoeyink described the computational challenges that arise in inferring RNA backbone conformations from NMR or X-ray crystallography data. The challenges arise because of the many possible dihedral angles per residue in the RNA sequence. Anne Condon described computational problems that arise in predicting RNA secondary structure. These include the high complexity of recognizing pseudoknotted structures, and the challenges in improving accuracy of both pseudoknot free and pseudoknotted structure predictions.

Scientific Progress Made

Evolutionary Capacity of Proteins

Inspired by the talk of Ron Elber, David Bremner and Jie Liang discussed how to construct simple exact models for the evolutionary capacity of known protein structures. By abstracting spatial information into a graph, and considering a simple hydrophobicity based energy model, exact and asymptotic bounds on the number of sequences that are a "good fit" to a given structure can be computed.

Energy barriers in RNA secondary structure

Topological Results

Christine Heitsch, Paul Higgs and David Bremner considered the barrier height problem for RNA molecules [3, 5]. They investigated the existence of a transition path between any two RNA configurations where the energy of each move does not exceed some pre-determined threshold. Prior results [4] show that this is indeed possible in the most abstract situation. Preliminary results include that this extends to arbitrary balanced binary sequences of n 0's and n 1's; it turns out that every such sequence has a complete nested folding with n noncrossing $(0, 1)$ and $(1, 0)$ pairs, and that any two such foldings are connected by some minimal energy path of local moves. They are now considering the situations where the binary sequence is unbalanced and where only base pairings in the source or target structure are allowed. They will also investigate the problem of enumerating the number of possible foldings.

Computational Complexity

Problem worked on at the workshop: understanding the computational complexity of calculating energy barriers in RNA secondary structure pathways.

Context: RNA structures are determined largely by pairings of bases in the RNA molecules, with A's binding to T's and C's binding to G's. Given enough time, RNA molecules will fold to their minimum free energy (MFE) structures. There are many algorithms available that aim to predict MFE structures. However, the accuracy of such algorithms is still quite poor, suggesting that perhaps a molecule gets trapped in a locally optimal structure, from which there is a high energy barrier to the MFE structure. For this reason, it's interesting to calculate the energy barrier between two RNA secondary structures. Additionally, knowing the energy barrier can shed light on the pathway of structures formed by a molecule before it reaches it stable (MFE) structure.

Currently, the best methods for calculating the energy barrier between two RNA secondary structures are heuristic in nature, and it is an open problem whether the barrier can be calculated efficiently. To understand the complexity of calculating energy barriers, we cast the problem in a simple setting, and investigate whether the resulting simplified problem is in P or is NP-complete. We look at many problem variations.

Defining folding pathways: Let S be a secondary structure, and let —S— be the number of base pairs in secondary structure S. A secondary structure can be represented as an arc diagram, in which the bases of the molecule are arrayed along a horizontal line and arcs connect two paired bases. For this reason, we refer to base pairs as arcs. A structure is pseudoknotted if two base pairs cross.

A direct path P from secondary structure S to secondary structure S' is a sequence $S = S_0, S_1, \ldots S_t = S'$ of structures, each obtained from the previous one either by (i) removing an arc which is in S or (ii) adding an arc which is in S' and does not cross any arc of S which has not yet been removed.

The energy barrier of path P is

$$\max_{1 \leq k \leq t} |S| - |S_k|$$

The energy change of path P is $|S| - |S'|$.

One problem we considered is the Pseudoknot Free Folding Problem:

Given: S and S', which are two pseudoknot free secondary structures, and a positive integer k.

Question: Is there a direct path from S to S' with energy barrier at least k?

This problem does not allow intermediate arcs to be introduced along the path from S to S', by definition of direct path. A related problem, the Pseudoknotted Folding Problem is defined similarly, except that S and S' may be pseudoknotted. This problem is somewhat artificial, because the secondary structures S and S' may be pseudoknotted, yet when adding arcs of S', they are not allowed to cross those in S.

While we were unable to resolve the complexity of the pseudoknot free version of the problem, we did make progress during the workshop in showing that the pseudoknotted version is NP-hard.

Step self-assembly

Self-assembly is an autonomous process by which small simple parts assemble into larger and more complex objects. Self-assembly occurs in nature, for example, when atoms combine to form molecules, and molecules combine to form crystals. It has been suggested that intricate self-assembly schemes will ultimately be useful for circuit fabrication, nano-robotics, DNA computing, and amorphous computing. To study the process of self-assembly we use the Tile Assembly Model proposed by Rothemund and Winfree [7]. This model considers the assembly of square blocks called "tiles" and a set of glues called "binding domains". Each of the four sides of a tile can have a glue on it that determines interactions with neighbouring tiles. The process of self-assembly is initiated by a single seed tile and proceeds by attaching tiles one by one.

During the meeting we have discussed an extension of the basic tile model to step self-assembly as suggested by Ken Dill. In this extension, several sets of tiles are used. In each step one tile set is applies on the growing structure, which grows as long as possible. When the growth stops, the current tile set is washed away and a new tile set is applied on the structure. In this way, it is possible to build a square of size $2N + 1 \times 2N + 1$ in N steps using only 2 sets of tiles each having a constant number of tiles. This is true even at temperature 1 and when all neighboring tiles of the assembled square are connected by a glue. For comparison, using the original model to assemble $2N + 1 \times 2N + 1$ square in the same setting would require $(2N + 1)^2$ distinct tiles.

Outcome of the Meeting

The increasingly quantitative nature of biology is most readily evidenced in molecular genomics. To ensure rapid progress, matching the most appropriate mathematical techniques to specific problems is essential. This workshop was a major step in this direction. Outcomes can generally be grouped as follows:

1. Identify key problems amenable to combinatorial treatment. These range from understanding biomolecular molecular structures, build models for cellular processes such as signalling and network topologies, evolution and its role in disease and building nanotechnological structures using biomolecules.

2. New collaborations formed which should lead to rapid progress on a number of specific problems as outlined in Section 5.

3. Preliminary plans for continued and expanded collaborations. The main organizers are exploring possibilities to launch future meetings that bring together an expanded group of scientists.

A typical reaction from a participant was from mathematician Christine Heitsch

> The workshop was an exciting opportunity to interact with people interested in both discrete mathematics and molecular biology. I learned a lot about combinatorial models for protein structures, and had many stimulating conversations about RNA folding. I'm looking forward to future opportunities to interact with workshop participants, and hope that some of these connections will develop into research collaborations.

This reinforces the organizers' view that there are many interesting interactions to study between discrete and combinatorial mathematics and biology. One option we may explore is application to BIRS for *Research in Teams* programs to speed up progress on specific problems.

List of Participants

Bremner, David (University of New Brunswick)
Bruinsma, Robijn (University of California Los Angeles)
Condon, Anne (University of British Columbia)
Dill, Ken (Universtiy of California, San Francisco)
Elber, Ron (University of Texas at Austin)
Evans, Patricia (Faculty of Computer Science, University of New Brunswick)
Gupta, Arvind (MITACS)
Heitsch, Christine (Georgia Institute of Technology)
Higgs, Paul (McMaster University)
Liang, Jie (University of Illinois at Chicago)
Manuch, Jan (Simon Fraser University)
Meyer, Irmtraud (University of British Columbia)
Rafiey, Arash (Simon Fraser University)
Sneppen, Kim (Niels Bohr Institute University of Copenhagen)
Stacho, Ladislav (Simon Fraser University)
Stoll, Christine (Simon Fraser University)
Thachuk, Chris (University of British Columbia)
Winfree, Erik (California Institute of Technology)

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Chapter 22

Rigidity, Flexibility, and Motion: Theory, Computation and Applications to Biomolecules (08w5104)

Jul 06 - Jul 11, 2008

Organizer(s): Walter Whiteley (Department of Mathematics and Statistics York University), Maria Kurnikova (Carnegie Mellon University), David Richardson (Duke University Medical Center), Jack Snoeyink (University of North Carolina, Chapel Hill), Michael Thorpe (Arizona State University)

Overview of the Field

Following from work on the genome, the focus is shifting to protein and RNA structure and function. Much of the function of a biomolecule is determined by its 3-D structure (shape) and motions (often in combination). While static structures of many new proteins is being determined by x-ray crystallography and by nuclear magnetic resonance techniques (work represented by several invitees),understanding the function of biomolecules requires understanding of conformational changes of these structures in time, e.g. dynamics. Therefore much interest has been focused recently in experimental and computational approaches to study dynamics of biomolecules on different timescales ranging from femtoseconds (local vibrations) to motions on the micro-to millisecond timescale (large-scale motions). In other words, the emphasis now is to describe a biomolecule in an ensemble of appropriate conformations rather than just as a single, static structure. In this context the impact of other contacts such as ligands (drugs), or binding of other proteins, RNA, DNA etc. to the multidimensional energy landscape need to be addressed. It is apparent that experimental approaches yield important but limited information. Computational approaches have to play a crucial role in this goal. Computer modeling of possible motions; the conformational accessible space, unfolding pathways; multiple configurations with different biological functions and paths between these are just some of the objectives of current computational geometry and applied mathematics.

The mathematical theory of rigidity, and related techniques from geometric constraint theory (CAD, robotics), are tools for such computer modeling, and the development of fast algorithms. Applications of such techniques to protein flexibility have been expanding over the last ten years [8, 22, 21, 24, 25]. The core mathematical theory has also been evolving in multiple ways, through the work of mathematicians and computer scientists [7, 10, 26] . A short summary of the state of the art for combinatorial analysis of rigidity includes three problems:

(a) the general problem of predicting whether a graph, build in 3-space as a bar and joint framework, will be rigid or flexible, for almost all realizations, is a long-standing problem, going back at least to James

Clerk Maxwell.

(b) the general problem of predicting whether a graph built with vertices as rigid bodies, and edges as hinges, in 3-space, will be rigid or flexible for almost all choices of lines for the hinges, has a simple combinatorial solution and an efficient algorithm (a result of Tay and Whiteley, extending the basic theorem of Tay) [20, 26];

(c) the general problem of frameworks extracted from covalent bonds of molecular structures (with fixed angles at the bonds) is covered by the algorithms of (b) (the Molecular Framework Conjectures) although it is a special class of frameworks under (a) [21, 25]. Recent experimental and theoretical work provides strong evidence for these conjectures, and the proof has recently been announced [16]. The implementations of this approach provides fast combinatorial algorithms for modeling and predictions (see flexweb.asu.edu).

Work in computational geometry (represented by other participants) has investigated the computational complexity of a variety of algorithms and questions around folding and unfolding chains, polygons and other simplified models that would relate to proteins [12, 18]. This includes the recent solution of the Carpenters' Rule Problem (can a plane linear linkage, laid out with out crossings, always be straightened in the plane without any crossing during the motion?), which combined computational geometry with results in rigidity theory [3, 19, 18]. Work on linkages in 3-space confirms that the 3-D problem is significantly harder, but also indicates that some results can be obtained. The computational modeling of molecular motions involves problems such as ring closure and inverse kinematics, which are central to robotics. Work in robotics has studied the kinematics of larger scale structures subject to geometric constraints, using probabilistic road map algorithms and other sampling techniques. These have recently been extended to combine rigidity decomposition and probabilistic road maps (see the material at parasol.tamu.edu/foldingserver/), and key people from this work are among the invitees.

In computational biophysics and biochemistry, there are web implementations of several algorithms [e.g. FIRST available at flexweb.asu.edu] for modeling the rigidity and initial flexibility of biomolecules as frameworks to which this mathematical theory applies [21, 22]. These models incorporate rigidity features, including the Molecular Framework Conjecture. These algorithms are fast enough to be used as preliminary screening in areas such as ligand docking in drugs [12] as well as some simulations of unfolding pathways. Motions simulated over larger time-scales are also being developed, using programs such as ROCK (also on flexweb). A single static image, plus a rigidity simulation generated an ensemble of conformations similar to the ensemble of conformations generated from NMR data. Key people in these simulations and comparisons participated, along with others who are exploring related computational methods. Other methods, such as Gaussian Network Models (also fast and simple) and Molecular Dynamics Simulations (slow but with more detail) also offer predictions. It is important to compare these methods and search for ways to refine and combine them; some of the organizers and invitees are working on these problems. Significant and suggestive initial results have been obtained, but much work remains.

The mathematical and computational models have become more sophisticated, offering qualitative and quantitative predictions for the behaviour of biological complexes. Meanwhile, dynamics measured using X-ray crystallography, NMR [15, 23, 27], fluorescence and other experimental techniques are expanding. We are now entering a period of comparison of predictions with experimental observations, which is challenging at all levels. What motions does the experimental data measure (and on what time scale)? How do different measurements compare? What properties of the mathematical models correlate with measurements? What role to other mathematical models and assumptions play in generating the experimental evidence deposited in sites such as the Protein Data Bank? What is the reliability of data and the scope of the models. Among the organizers and the invitees, we have some leading experts in this area, who will assist with the vital task of grounding the models in the best evidence from experiment, both as a caution and a stimulation to the computational and mathematical modelers.

Of course, such intensive work on modeling stimulates new mathematical problems, which has generated progress on existing unsolved problems. Work in rigidity has always engaged collaborations with other disciplines, including material science, physics, engineering, and now biology and chemistry. The organizers and invitees include representatives from many of these fields who are already collaborating with mathematicians. Each of these fields is in rapid evolution, due both to new theoretical results and to new experimental techniques that modify our assumptions and raise new questions. The work is increasingly interdisciplinary and the workshop proposal reflects that reality. Any major mathematical progress will have potential impact within mathematics and with work in these other fields.

The July 20004 BIRS Workshop 04w5017: Modeling Protein Flexibility and Motions, offered an unusually interdisciplinary gathering of people from these diverse communities. This workshop was a continuation of the first workshop, though as a half sized group - with restricted numbers and a sharper focus.

Recent Developments and Open Problems

At the time the workshop was held, the Molecular conjecture was an important unsolved problem. Since the workshop, a manuscript has circulated, and the consensus is that this conjecture has been confirmed [16]. This completes the basis for the FIRST algorithm (flexweb.asu.edu) and supports the ongoing application of these 'generic' techniques to determine the first-order rigidity of molecular models extracted from the protein structures.

In the period prior to the workshop, there was significant progress on global rigidity in the plane - and there was a major unsolved general problem of further characterizing generic structures (including molecules) which are globally rigid in 3-space. During the workshop, some significant conjectures were generated, and important new results are presented below.

Presentation Highlights

We held several joint sessions with The Biology-Combinatorics Interface: Addressing New Challenges in Computational Biology 08w5069. In the first two days we held four joint lectures, giving an overview of the problems each group was addressing - and laying the groundwork for further informal conversations during the five days.

One of these survey talks, by Michael Thorpe, covered a range of methods from rigidity analysis and finite motion simulation, and a range of applications including zeolite (a crystaline like material), modeling protein dynamics and and virus capsids and symmetry. The lecture is available at the BIRS web site for viewing and downloading.

Maria Kurnikova presented a biochemistry tutorial, including a focus on stability vs instability (a recurring theme after this talk) and insights from Molecular Dynamics Simulation (MDS).

Walter Whiteley led off a discussion of current problems - potential areas for work during the workshop. In the remaining periods, we mixed talks with working sessions, to enable people to engage in more detailed conversations to share work and to develop more refined questions and conjectures. One special feature of our workshop was the number of hands on models, and materials for constructing additional models. These were used during talks, within working groups and in the evenings in the common room. These models were essential to clarifying points and exploring possibilities - as people gathered around tables and explored situations such as the possible 'flips' for structures which were rigid, but not 'stable' (see below).

In the context of our visual and kinesthetic exploration of examples, we participated as subjects in an ongoing research project of Natasha Meyers, an Anthropologist of Science at York University. With our informed consent, Natasha observed and collected field notes on how people in such an interdisciplinary environment communicated and interacted. In addition, Natasha gave a one hour talk about her prior work on interactions between supervisors and graduate students who were constructing 3-D models of proteins, as well as some larger questions for her ongoing research. Overall, these interactions provided an additional awareness of how we communicated, and what situations lead to confusion or to clarity for people coming from diverse intellectual communities.

With a number of senior graduate students participating, we ensured that each of them had an opportunity to present and to receive feedback about fruitful directions and additional methods which could be applied to their work. Areas for such follow-on discussions included the interactions of symmetry and rigidity, and the exploration of periodic structures (real and mathematical zeolites), as well as flatness of substructures as an additional feature which altered the rigidity of structures. These themes engaged a substantial number of the participants - and the further exchanges among those participants have continued since this workshop.

Derek Wilson presented particular protein modeling challenge - Acylphosphatase from Sulfolobus Solfataricus (Sso AcP) [**?**]. We were given HD Exchange data (colored by a convention) on two conformations of a molecule. The challenge was to consider mathematical techniques, including rigidity analysis for individual conformations or for an ensemble of conformations from the Protein Data Bank, and generate a 'comparable' coloring / prediction of which parts were 'rigid' and which were 'flexible' (variable). This discussion integrated with our growing awareness of communication issues / variations, so that on the last day we held a discussion on ways of color coding measures of 'flexibility' both as detected in diverse samples of biological data and in mathematical simulations.

In Thursday, we had another pair of talks shared by the two workshops: Mary Condon on RNA Secondary Structure and David Richardson and Jack Snoeyink on RNA tertiary structure.

Before the workshop and throughout the week, a wiki site was used to post a number of conjectures and open problems. There were regular updates, including posting of presentations and revised conjectures. This was quite fruitful and continued to be available for some months following the workshop.

Scientific Progress Made

As anticipated, there was substantial interaction around the use of the words *rigid*, *flexible* and *stable* in the various disciplines. Over the week, through examples and explorations, there was a refined consensus that:

1. flexible as used in generic rigidity, and in molecular discussions, described a configuration with a continuous path of variation in shape.

2. stable, as used in molecular descriptions, coincided with *global rigidity* in the discussions of mathematicians and computer scientists - particularly for generic configurations (or configurations where small variations did not change the global rigidity). This generally coincides with redundant rigidity, where removing one constraint still leaves rigidity (see the next item);

3. minimal infinitesimal matched up with what biochemists and biophysicists would call fluctuating, or having small range floppy nodes.

One of the key examples, explored with models and with mathematical theories was the five-fold ring - which is generically globally rigid (and redundantly rigid) and occurs in the basic structure of proline - the unusual amino acid which is rigid rather than flexible across the carbon bonds between amide plates.

From this analysis, there were two threads of further discussion. (A) A recognition that in 'coloring' flexibility, it was at least important to use three colors: red, for flexible; grey, for minimally infinitesimally rigid; and blue for redundantly rigid / stable. Of course the flexible and the redundantly rigid could be further colored to show 'degrees' but comparisons might well only be possible across fields with these three categories. (B) It was important to develop a more complete mathematical and computational theory for stability (global rigidity). This was evident in the extensive entries on the wiki for conjectures and problems around global rigidity, and in the progress made to generate new conjectures and begin work on verifying these conjectures and extending methods for further work.

In the second thread, a conjecture was developed, by Tibor Jordan Meera Sitharam, and Walter Whiteley, that a generic body bar framework is globally rigid if and only if it is redundantly rigid. As the section below indicates, this conjecture has been proven, using methods explored during the workshop and extended afterwards. This conjecture extends to the claim that a generic molecular framework is globally rigid if and only if it is redundantly rigid. This further conjecture remains unsolved, but is now more accessible because of the results for body-bar frameworks.

Work continued on how symmetry (a common feature of families of proteins, such as dimers) impacts the rigidity of the corresponding framework model and the underling molecule. This was a topic first explored during the prior 2004 workshop, and has become an important area of mathematical work, combining mathematical rigidity and the representation theory of groups. Some further collaborative work was developed (see below for a resulting paper) and topics for continuing exploration were listed. These topics played a valuable part in the recently completed thesis of Bernd Schulze [17]. Further recent specific connections to protein modeling are mentioned below.

Outcome of the Meeting

There was substantial overlap with with two day workshop immediately following this five day workshop, both in terms of participants and in terms of topics / conjectures / collaborations. With that in mind, several of the resulting collaborations and papers will reasonably be reported in both reports.

As mentioned above, one theme which rose in importance through the preparations for the workshop, the conjectures posted on the wiki site, and discussions of what 'stability' in biochemistry translated to in mathematics, and the mathematical discussions was Global Rigidity. One outcome was the conjectures for body bar frameworks linking redundant rigidity with global rigidity, generically. This core conjecture is confirmed in the paper of Connely, Jordan and Whiteley [5]. From this result, there are natural questions of extensions to molecular structures - so there is an extended Global Rigidity conjecture for molecular structures: a generic molecular model is globally rigid if and only if it is redundantly rigid. We note that there are fast algorithms for redundant rigidity, encoded in programs such as FIRST at flexweb.asu.edu.

The paper above was based on some extensions of the prior stress matrix methods for confirming global rigidity in all dimensions. An other paper flowing from the workshop, by Connelly and Whiteley [6], confirmed projective transformations and coning as as a valuable methods for global rigidity, also giving a mathematical basis for transferring results on global rigidity to other metrics, such as spheres, hyperbolic geometry, and even broader metrics built on the shared projective geometry of the structures.

On the impact of symmetry on rigidity / flexibility, continuing discussions in several informal sessions during the workshop generated the core results which are in the paper [11], authored by Simon Guest, Bernd Schulze and Walter Whiteley. This extension of prior results for bar and joint frameworks of [4] to more general frameworks suggests that versions for molecular structures are within reach. Since that time, the thesis of Bernd Schulze [17] has clarified a number of issues, and generated new results which have potential applications back to molecules. This work is also ongoing.

The discussion generated by an example brought by the biochemist Derek Wilson provided some ideas of mathematical / computational models which could potentially address the data given. As a result, a new collaboration of Adnan Sljoka (mathematics graduate student) and Derek Wilson (biochemistry) on explicit ways of incorporating ensemble information in the mathematical theory to give a plausible account / prediction of the observed HD data for .... . This collaboration has continued, forming part of Ph.D. thesis work of Adnan Sljoka, and a draft paper is being polished for submission.

The presentation of Adam Watson on his Ph.D. work on Flatness and Rigidity demonstrated situations where some simple geometry not detected in the usual counts gave additional flexibility to a structure. The ensuing discussion laid the seeds for further correspondence on when symmetry was sufficient to induce the corresponding flatness, again an extra situation not detected even in the symmetry adapted counts of [4, 11]. There are plans to present these connections in a joint paper of Adam Watson, Bernd Schulze, and Walter Whiteley.

It is clear that, overall, the workshop supported new collaborations, and supported the developed of all the graduate students who participated. In the summer of 2009, a workshop in Budapest provided follow up for a number of the mathematical topics which arose during this five day workshop and the follow-on two day workshop.

List of Participants

Chubynsky, Mykyta (University of Ottawa)
Connelly, Robert (Cornell University)
Degraff, Adam (Arizona State University)
Gao, Jie (SUNY Stony Brook)
Guest, Simon (University of Cambridge)
Jackson, Bill (Queen Mary College (London))
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Kurnikova, Maria (Carnegie Mellon University)
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Myers, Natasha (York University)

Palfi, Villo (Eotvos University)
Richardson, David (Duke University Medical Center)
Ross, Elissa (York University)
Schulze, Bernd (York University)
Servatius, Brigitte (Worcester Polytechnic Institute)
Servatius, Herman (Clark University)
Shai, Offer (Tel-Aviv University)
Sitharan, Meera (University of Florida)
Sljoka, Adnan (York University)
Snoeyink, Jack (University of North Carolina, Chapel Hill)
Szabadka, Zoltan (Eotvos Universite)
Tama, Florence (University of Arizona)
Thorpe, Michael (Arizona State University)
Watson, Adam (Queen Mary, University of London)
Whiteley, Walter (Department of Mathematics and Statistics York University)
Wilson, Derek (York University)

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Chapter 23

Multi-View and Geometry Processing for 3D Cinematography (08w5070)

Jul 13 - Jul 18, 2008

Organizer(s): Rémi Ronfard (Xtranormal Technology and INRIA Rhone-Alpes), Gabriel Taubin (Brown University)

By 3D cinematography we refer to techniques to generate 3D models of dynamic scenes from multiple cameras at video frame rates. Recent developments in computer vision and computer graphics, especially in such areas as multiple-view geometry and image-based rendering have made 3D cinematography possible. Important applications areas include production of stereoscopic movies, full 3D animation from multiple videos, special effects for more traditional movies, and broadcasting of multiple-viewpoint television, among others. The aim of this workshop was to bring together scientists and practitioner who have contributed to the mathematical foundations of the field, as well as those who have developed working systems. There were 20 participants from Canada, the United States, Europe and Asia. A total of 20 talks of length 30 minutes were presented during the five-day workshop.

A book comprising extended versions of these presentations is currently under production, and will be published by Springer-Verlag in 2010 [3].

Overview of the Field

The name 3D cinematography is motivated by the fact that it extends traditional cinematography from 2D (images) to 3D (solid objects that we can render with photorealistic textures from arbitrary viewpoints) at the same frame rate. A first workshop on 3D Cinematography took place in New York City in June 2006 jointly with the IEEE Conference on Computer Vision and Pattern Recognition [1]. Selected speakers from this workshop were invited to write extended papers, which after review were published as a special section in IEEE Computer Graphics and Applications [2]. At the time some prototypes had demonstrated the ability to reconstruct dynamic 3D scenes in various forms and resolutions. Various names were used to refer to these systems, such as virtualized reality, free-viewpoint video, and 3D video. All of these efforts were multi-disciplinary. These advances had clearly shown the promises of 3D cinematography systems, such as allowing real-time, multiple-camera capture, processing, transmission, and rendering of 3D models of real dynamic scenes. Yet, many research problems remained to be solved before such systems can be transposed from blue screen studios to the real world.

Recent Developments and Open Problems

This second workshop on 3D Cinematography was focused on summarizing the progress made in the field during the two years subsequent to the first workshop, and in particyular on real-time working systems and applications, with an emphasis on recent, realistic models for lights, cameras and actions. Indeed, 3D cinematography can be regarded as the geometric investigation of lights (how to represent complex lighting, how to relight, etc.); cameras (how to recover the true camera parameters, how to simulate and control virtual cameras, etc.); and actions (how to represent complex movements in a scene, how to to edit, etc.). From a geometric viewpoint, it is a hard problem to represent complex, time-varying scenes and their interactions with lights and cameras. One important question wxplored in this workshop was - what is the dimensionality of such scenes ? Space decomposition methods are popular because they provide one approximate answer, although not of very good quality. It has become increasingly evident that better representations are needed. Several partial solutions are proposed in the workshop papers, illustrated with examples. They include wavelet bases, implicit functions defined on a space grid, etc. It appears that a common pattern is the recovery of a controllable model of the scene, such that the resulting images can be edited (interaction). Changing the viewpoint is only one (important) aspect. Changing the lighting and action is equally important. Recording and representation of three-dimensional scenes. This is at the intersection of optics, geometry and computer science, with many applications in movie and entertainment technology. Note that the invention of cinema (camera and projector) was also primarily a scientific invention that evolved into an art form. We suspect the same thing will probably happen with 3D movies. This will still be based on optical systems. But computers have since replaced the mechanics. What motivates our field ? Build 3D cameras (record the scene) and 3D projectors (display the scene); Important addition - build 3D editing suites, to interact with the scene in NOVEL ways (edit the scene).

Presentation Highlights

Towards 4D Capture and 6D Displays: Mask for Encoding Higher Dimensional Reflectance Fields

Presented by Ramesh Raskar, MIT Media Lab This talk describes a capture method that samples 4D reflectance field using a 2D sensor and a display method that encodes 6D reflectance field on 2D film for subsequent viewing. They capture the 4D reflectance field using a lightfield camera. The lightfield camera used optical spatial heterodyning to multiple sub-aperture views inside a camera. They describe reversible modulation of 4D light field by inserting a patterned planar mask in the optical path of a lens based camera. They reconstruct a 4D light field from a 2D camera image without any additional lenses as required by previous light field cameras. The patterned mask attenuates light rays inside the camera instead of bending them, and the attenuation recoverably encodes the ray on the 2D sensor. Their mask-equipped camera focuses just as a traditional camera might to capture conventional 2D photos at full sensor resolution, but the raw pixel values also hold a modulated 4D light field. The light field can be recovered by rearranging the tiles of the 2D Fourier transform of sensor values into 4D planes, and computing the inverse Fourier transform. The lightfield is captured with minimum reduction in resolution allowing a 3D encoding of depth in a traditional photo. They display 6D reflectance field using a passive mask (2D film) and additional optics. Traditional flat screen displays (bottom left) present 2D images. 3D and 4D displays have been proposed making use of lenslet arrays to shape a fixed outgoing light field for horizontal or bidirectional parallax. They present different designs of multi-dimensional displays which passively react to the light of the environment behind. The prototypes physically implement a reflectance field and generate different light fields depending on the incident illumination, for example light falling through a window. They discretize the incident light field using an optical system, and modulate it with a 2D pattern, creating a flat display which is view *and* illumination-dependent. It is free from electronic components. For distant light and a fixed observer position, they demonstrate a passive optical configuration which directly renders a 4D reflectance field in the real-world illumination behind it. Combining multiple of these devices they build a display that renders a 6D experience, where the incident 2D illumination influences the outgoing light field, both in the spatial and in the angular domain. Possible applications of this technology are time-dependent displays driven by sunlight, object virtualization and programmable light benders / ray blockers without moving parts.

Skeleton Cube: Estimating Time-Varying Lighting Environments

Presented by Takashi Matsuyama, Kyoto University, Japan This is joint work with T. Takai, and S. Iino.

Lighting environments estimation is one of important functions to realize photometric editing of 3D video; lighting can give various effects on 3D video. In his talk, Matsuyama proposed the Skeleton Cube to estimate time-varying lighting environmens: e.g. lightings by candles and fireworks. A skeleton cube is a hollow cubic object and located in the scene to estimate its surrounding light sources. For the estimation, video of the cube is taken by a calibrated camera and then observed self shadows and shading are analyzed to compute 3D distribution of time-varying point light sources. Matsuyama's team developed an iterative search algorithm for computing the 3D light source distribution. Several simulation and real world experiments showed its effectiveness.

Smooth and non-smooth wavelet basis for capturing and representing light

Presented by Dana Cobzas, University of Alberta, Canada Indirectly estimating light sources from scene images and modeling the light distribution is an important, but difficult problem in computer vision. A practical solution is of value both as input to other computer vision algorithms and in graphics rendering. For instance, photometric stereo and shape from shading requires known light. With estimated light such techniques could be applied in everyday environments, outside of controlled lab conditions. Light estimated from images is also helpful in augmented reality in order to consistently relight an artificially introduced object. While algorithms that recover light as individual point light sources work for simple illumination environments, it has been shown that a basis representation achieves better results for complex illumination. In her talk, Cobzas proposed a light model that uses Daubechies wavelets and a method for recovering light from cast shadows and specular highlights in images. She assumes that the geometry is known for part of the scene. In everyday images, one can often obtain a CAD model of man-made objects (e.g. a car), but the rest of the scene is unknown. Experimentally, she has tested her method for difficult cases of both uniform and textured objects and under complex geometry and light conditions. She evaluated the stability of estimation and quality of scene relighting using smooth wavelet representation compared to a non-smooth Haar basis and two other popular light representations (a discrete set of infinite light sources and a global spherical harmonics basis). She demonstrated good results using the proposed Daubechies basis on both synthetic and real datasets. This is joint work with Cameron Upright and Martin Jagersand.

Accurate Camera Calibration from Multi-View Stereo and Bundle Adjustment

Presented by Yasutaka Furukawa, University of Illinois at Urbana-Champaign The advent of high-resolution digital cameras and sophisticated multi-view stereo algorithms offers the promises of unprecedented geometric fidelity in image-based modeling tasks, but it also puts unprecedented demands on camera calibration to fulfill these promises. In this talk, Furukawa presents a novel approach to camera calibration where top-down information from rough camera parameter estimates and the output of a publicly available multi-view-stereo system on scaled-down input images are used to effectively guide the search for additional image correspondences and significantly improve camera calibration parameters using a standard bundle adjustment algorithm. The proposed method has been tested on several real datasets, including objects without salient features for which image correspondences cannot be found in a purely bottom-up fashion; and image-based modeling tasks, including the construction of visual hulls where thin structures are lost without this additional step of re-calibration procedure. This work was funded by Industrial Light and Magic, for applications in movie special effects.

Large scale multiview video capture

Presented by Bennett Wilburn, Microsoft Research Asia Wilburn discussed issues in large scale multiview video capture, with football matches as a motivating example. He briefly reviewed existing multiview video capture architectures, their advantages and disadvantages, and issues in scaling them to large environments. Then he explained that today's viewers are accustomed to a level of realism and resolution which is not feasibly achieved by simply scaling up the performance of existing systems. He surveyed some methods for extending the effective resolution and frame rate of multiview capture systems. He explored the implications of real-time applications for smart camera design and camera array architectures, keeping in mind that real-time performance is a key goal for covering live sporting events. Finally, he commented briefly on some of the remaining challenges for photo-realistic view interpolation of multi-view video for live, unconstrained sporting events.

Capturing Live Action for 3D Cinema

Presented by Paul Beardsley, Disney Research Zurich Image capture for live-action 3D cinema is traditionally done using a pair of stereo cameras which provide the left-eye and right-eye sequences that will be projected on the cinema screen. This constrains artistic control of 3D effects because decisions about stereo parameters - such as choice of baseline and vergence - are made during shooting, and cannot easily be manipulated afterwards. Beardley‘s talk described Disney’s current work on a heterogeneous sensor array composed of a cinematographic camera, support cameras, and depth sensors, to shoot live action 3D cinema. The post-production process allows a user to specify a pair of virtual stereo cameras viewing the original scene, with synthetic generation of the left-eye and right-eye images of the virtual rig. Thus stereo parameters, and hence the 3D effects that will be perceived by the viewer in the completed movie, cease to be a fixed and irrevocable choice made when shooting and are instead opened up to artistic control during post-production.

Introducing FTV

Presented by Masayuki Tanimoto, University of Nagoya, Japan Tanimoto described a new type of television named FTV (Free viewpoint TV). FTV is an innovative visual media that enables us to view a 3D scene by freely changing our viewpoints. FTV is based on the ray-space method that represents one ray in real space with one point in the ray-space. By using this method, Tanimoto and his team constructed the world’s first real-time FTV system including the complete chain from capturing to display. He also developed new type of ray capture and display technologies such as a 360-degree mirror-scan ray capturing system and a 360 degree ray-reproducing display. He believes FTV will be widely used since it is an ultimate 3DTV, a natural interface between human and environment, and an innovative tool to create new types of content and art.

3D Video: Generation, Compression and Retrieval

Presented by Kiyo Aizawa, University of Tokyo, Japan In his talk, Aizawa explained the issues relating with compressing and broadcasting 3D video, which is a sequence of 3D models. 3D video reproduces a real moving object and provides free view point functionality. Differing to CG animation, models in the sequence of 3D video varies in the number of their vertices, connectivities, etc. Together with NHK and ATR in Japan, Aizawa developped specific compression methods for improving the quality of capture and reproduction of 3D video.

FTV with Free Listening-Point Audio

Presented by Masayuki Tanimoto In this talk, Tanimoto presented novel media integration of 3D audio and visual data for FTV with free listening-point audio. He captures the multi viewpoint and listening-point data, which are completely synchronized, by camera array and microphone array. This experiment demonstrates that it si possible to generate both free viewpoint images and free listening-point audio simultaneously.

The filming and editing of stereoscopic movies

Presented by Larry Zitnick, Microsoft Research, Redmont, USA The editing of stereoscopic movies, in which two views are shown to a user to provide the illusion of depth, leads to a variety of novel challenges. For instance when creating cuts between scenes, it is generally desirable to maintain a consistent vergence angle between the eyes. This may be accomplished by careful filming or in post-production using a variety of techniques. In this talk, Zitnick discussed basic video editing tasks in the context of stereoscopic movies, as well as more complex techniques such as the "Hitchcock effect", fade cuts and effects unique to stereoscopic movies.

Binocular cinematography: 3-D movies for the human eyes

Presented by Frederic Devernay, INRIA, France Most often, what is referred to as 3-D movies are really stereoscopic (or binocular) motion images. In stereoscopic motion images, two 2-D movies are displayed, one for the left eye and one for the right eye, and a specific device guarantees that each eye sees only one movie (common devices are active or passive glasses, parallax barrier displays or lenticular displays). 3-D content can be displayed as stereoscopic motion images, but the movie itself does not hold 3-D content, thus the name binocular cinematography. Although shooting a stereoscopic movie seems to be as simple as just adding a second camera, viewing the resulting movie for extended durations can lead to anything from a simple headache to temporary or irreversible damage to the oculomotor function. Although the film industry pushes the wide distribution of 3-D movies, visual fatigue caused by stereoscopic images should still be considered as a safety issue. In his talk, Devernay described the main sources of visual fatigue which are specific to viewing binocular movies, which can be identified and classified into three main categories: geometric differences between both images which cause vertical disparity in some areas of the images, inconsistencies between the 3-D scene being viewed and the proscenium arch (the 3-D screen edges), and discrepancy between the accommodative and the convergence stimuli that are included in the images. For each of these categories, he proposes solutions to either issue warnings during the shooting or correct the movies in the post-production phase. These warning and corrections are made possible by the use of state-of-the-art computer vision algorithms.

From 3D Studio Production to Live Sports Events

Presented by Adrian Hilton, University of Surrey In his talk, Hilton reviewed the challenges of transferring techniques developed for multiple view reconstruction and free-viewpoint video in a controlled studio environment to broadcast production for football and rugby. Experience in ongoing development of the iview free-viewpoint video system for sports production in conjunction with the BBC will be presented. Production requirements and constraints for use of free-viewpoint video technology in live events will be identified. Challenges presented by transferring studio technologies to large scale sports stadium will be reviewed together with solutions being developed to tackle these problems. This highlights the need for robust multiple view reconstruction and rendering algorithms which achieve free-viewpoint video with the quality of broadcast cameras. The advances required for broadcast production also coincide with those of other areas of 3D cinematography for film and interactive media production.

Photo-realistic Rendering from Approximate Geometry

Presented by Marcus Magnor, TU Braunschweig, Germany For 3D cinematography from sparse recording setups, estimating full 3D geometry of the dynamic scene is essential. If the geometry model and/or camera calibration is imprecise, however, multi-view texturing approaches lead to blurring and ghosting artifacts during rendering. In his talk, Magnor presented novel on-the-fly GPU-based strategies to alleviate, and even eliminate, rendering artifacts in the presence of geometry and/or calibration inaccuracies. By keeping the methods general, they can be used in conjunction with many different image-based rendering methods and projective texturing applications.

New Methods for Video-based Performance Capture

Presented by Christian Theobalt, Stanford University, Max Plank Institute Performance capture means reconstructing models of motion, shape and appearance of a real-world dynamic scene from sensor measurements. To this end, the scene has to be recorded with several cameras or, alternatively, cameras and active scanning devices. In this talk, Theobalt presented his recent work on mesh-based performance capture from a handful of synchronized video streams. His method does without a kinematic skeleton and poses performance capture as mesh deformation capture. In contrast to traditional marker-based capturing methods, the approach does not require optical markings and even allows to reconstruct detailed geometry and motion of a dancer wearing a wide skirt. Another important feature of the method is that it reconstructs spatio-temporally coherent geometry, with surface correspondences over time. This is an important prerequisite for post-processing of the captured animations. Performance capture has a variety of potential applications in visual media production and the entertainment industry. It enables the creation of high quality 3D video, a new type of media where the viewer has control over the camera's viewpoint. The captured detailed animations can also be used for visual effects in movies and games. Theobalt briefly talked about ways to post-process the captured data such that they can be modified with off-the-shelf animation software.

Dense 3D Motion Capture from Synchronized Video Streams

Presented by Yasutaka Furukawa, University of Illinois at Urbana-Champaign In his talk, Furukawa described a novel approach to nonrigid, markerless motion capture from synchronized video streams acquired by calibrated cameras. The instantaneous geometry of the observed scene is represented by a polyhedral mesh with fixed topology. The initial mesh is constructed in the first frame using the publicly available PMVS software for multi-view stereo. Its deformation is captured by tracking its vertices over time, using two optimization processes at each frame: a local one using a rigid motion model in the neighborhood of each vertex, and a global one using a regularized nonrigid model for the whole mesh. Qualitative and quantitative experiments using seven real datasets show that this algorithm effectively handles complex nonrigid motions and severe occlusions.

Automatic Virtual Cinematography

Presented by Remi Ronfard, Xtranormal, Montreal, Canada Current research in 3D cinematography is concerned with automating the tasks of placing cameras and lights in a virtual world to create cinematic shots and editing of those shots into a movie. This has applications in *real-time cinematography* for computer games and *scripted cinematography* for movie pre-production. Focusing on the latter case, Ronfard presented a quick overview of both traditional and virtual cinematography, including script analysis, shot selection, camera placement and editing, and discussed the issues and opportunities facing this new research area.

New Directions for Active Illumination in 3D Photography

Presented by Douglas Lanman, Brown University, USA In his talk, Lanman presented recent work on novel 3D capture systems using active illumination at Brown University. Specifically, he focused on two primary topics: (1) Multi-Flash 3D Photography and (2) Surround Structured Illumination. Extending the concept of multi-flash photography, Lanman demonstrates how the surface of an object can be reconstructed using the depth discontinuity information captured by a multi-flash camera while the object moves along a known trajectory. To illustrate this point, Lanman presented experimental results based on turntable sequences. By observing the visual motion of depth discontinuities, surface points are accurately reconstructed - including many located deep inside concavities. The method extends well-established differential and global shape-from-silhouette surface reconstruction techniques by incorporating the significant additional information encoded in the depth discontinuities. Lanman continued his discussion by exploring how planar mirrors can be used to simplify existing structured lighting systems. In particular, he described a new system for acquiring complete 3D surface models using a single structured light projector, a pair of planar mirrors, and one or more synchronized cameras. He projects structured light patterns that illuminate the object from all sides (not just the side of the projector) so that he is able to observe the object from several vantage points simultaneously. This system requires that projected planes of light be parallel, and so he constructed an orthographic projector using a Fresnel lens and a commercial DLP projector. A single Gray code sequence is used to encode a set of vertically-spaced light planes within the scanning volume, and five views of the illuminated object are obtained from a single image of the planar mirrors located behind it. Using each real and virtual camera, he is able to recover a dense 3D point cloud spanning the entire object surface using traditional structured light algorithms. This configuration overcomes a significant hurdle to achieving full

360x360 degree reconstructions using a single structured light sequence by eliminating the need for merging multiple scans or multiplexing several projectors.

Hierarchical Model for Capturing and Texturing of 3D Models from 2D Images

Presented by Martin Jagersand, University of Alberta, Canada Jagersand described a three scale hierarchical representation of scenes and objects, and explained how this representation is suitable for both computer vision capture of models from images and efficient photo-realistic graphics rendering. The model consists of (1) a conventional triangulated geometry on the macro-scale, (2) a displacement map, introducing pixelwise depth with respect to each planar model facet (triangle) on the meso level. (3) A photo-realistic micro-structure is represented by an appearance basis spanning viewpoint variation in texture space. To demonstrate the three-tier model, Jagersand implemented a capture and rendering system based entirely on budget cameras and PC's. For capturing the model, he uses conventional Shape-From-Silhouette for the coarse macro geometry, variational shape and reflectance estimation for the meso-level, and a texture basis for the micro level. For efficient rendering the meso and micro level routines are both coded in graphics hardware using pixel shader code. This maps well to regular consumer PC graphics cards, where capacity for pixel processing is much higher than geometry processing. Thus photo-realistic rendering of complex scenes is possible on mid-grade graphics cards. He showed experimental results capturing and rendering models from regular images of humans and objects.

3D Video of Human Action in a Wide Spread Area with a Group of Active Cameras

Presented by Takashi Matsuyama, Kyoto University, Japan 3D video is usually generated from multi-view videos taken by a group of cameras surrounding an object in action. To generate nice-looking 3D video, the following three constraints should be satisfied simultaneously: (1) the cameras should be well calibrated, (2) for each video frame, the 3D object surface should be well covered by a set of 2D multi-view video frames, and (3) the resolution of the video frames should be enough high to record the object surface texture. From a mathematical point of view, it is almost impossible to find such camera arrangement and/or camera work that satisfy these constraints. Moreover, when an object performs complex actions and/or moves widely, it would be a reasonable way to introduce active cameras to track the object and capture its multi-view videos; otherwise a large number of (fixed) cameras are required to capture video data satisfying the constraints. Then, the fourth constraint is imposed: (4) the group of active cameras should be controled in real time so that each video frame satisfies the above three constraints. In his talk, Matsuyama described a *Cellular Method* to capture 3D video of human action in a wide spread area with a group of active cameras. The problem to find the camera work that satisfies the above four constraints is formulated as an optimization process and then an algorithm to find an optimal solution is presented with experimental results. This is joint work with H. Yoshimoto, and T. Yamaguchi.

Multi-View Stereo beyond the Lab Setting

Presented by Michael Goesele, TU Darmstadt, Germany Goesele presented a multi-view stereo algorithm that addresses the extreme changes in lighting, scale, clutter, and other effects found in large online community photo collections and other data sets not captured specifically for reconstruction purposes. The basic idea of the algorithm is to intelligently choose images to match, both at a per-view and per-pixel level. Goesele demonstrates that such adaptive view selection enables robust performance even with dramatic appearance variability. The stereo matching technique takes as input sparse 3D points reconstructed from structure-from-motion methods and iteratively grows surfaces from these points. Optimizing for surface normals within a photo-consistency measure significantly improves the matching results. While the focus of the approach is to estimate high-quality depth maps, it can also be extended to merge the resulting depth maps into compelling scene reconstructions. Goesele demonstrated the algorithm on standard multi-view stereo data sets and on casually acquired photo collections of famous scenes gathered from the Internet. This is joint work with Brian Curless, Hugues Hoppe, Noah Snavely and Steve Seitz.

Scientific Progress Made

The next frontier is the synthesis of virtual camera movements along arbitrary paths extrapolating cameras arranged on a plane, a sphere, or even an entire volume. This raises difficult issues. What are the dimensions of the allowable space of cinematographic cameras that professional cinematographers would want to synthesize? In other words, what are the independent parameters of the virtualized cameras that can be interpolated from the set of existing views? Further, what is the range of those parameters that we can achieve using a given physical camera setup? Among those theoretically feasible parameter values, which are the ones that will produce sufficient resolution, photorealism, and subjective image quality? These questions remain open for future research in this new world of 3D cinematography.

Outcome of the Meeting

A book comprising extended versions of this workshop presentations is currently under production, and will be published by Springer-Verlag in 2010 [3]. This book will also include an introductory survey of the field, and an extensive list of references.

List of Participants

Aizawa, Kiyo (University of Tokyo)
Beardsley, Paul (Disney Research Zurich)
Birkbeck, Neil (University of Alberta)
Cobzas, Dana (University of Alberta)
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Chapter 24

Integrated Hydrogeophysical Inversion (08w5051)

Jul 13 - Jul 18, 2008

Organizer(s): Laurence Bentley (University of Calgary), Andrew Binley (Lancaster University), Ty Ferre (University of Arizona)

Overview of the Field

Managing groundwater resources and remediating contaminated groundwater require mathematical models to predict groundwater fluxes, quantify groundwater volumes and chemical transport. The models require definition of the physical system geometry, boundary conditions and specification of the values of parameters such as hydraulic conductivity. All of these parameters always are known with significant uncertainty because data are limited in space and time and often also have uncertainty associated with them. Hydrologic targets of primary focus for the meeting will be the rates and pathways of water flow, chemical transport and degree of water storage in the subsurface. These processes are dynamic and occur at a wide range of spatial scales. Also, as with most subsurface hydrologic processes, spatial heterogeneity of the hydraulic properties must be accounted for in quantitative analysis. Typically, the challenge for quantifying these processes lies in a severe lack of temporal and spatial to describe complex systems. Geophysical methods based on physical principles including electrical, electromagnetic, seismic, nuclear magnetic resonance, and gravity have been used to assess hydrologic parameters and processes. Geophysical methods are useful because properties such as electrical conductivity can be correlated to hydrogeologic parameters such as moisture content and hydraulic conductivity Typically, the challenge for geophysical interpretation lies in the underconstrained nature of the data sets, leading to uncertain interpretations. Coupled with limitations to the petrophysical models that relate the measured properties to the properties of interest to hydrologists, this often results in geophysical data that are only qualitatively useful for hydrologic analyses.

During the 1980s and 1990s, major advances in the field of hydrogeologic parameter estimation and hydrogeolocial inverse analysis were made by workers such as Mary Hill ([9]), Richard Cooley [1], [2]) and Jesus Carrera ([3], [4], [5]). However, the field has not experienced major progress in recent years, mainly due to the limited spatial data density and limited frequency of measurements. At the same time, improvements in geophysical data acquisition technology and computational capacity have lead to a new generation of geophysical instrumentation that produce much more higher quality data than in the past. Relevant examples are commercial ground-penetration radar units and multichannel electrical resistivity recording systems. Similarly, near surface geophysical inverse methods have seen major advancements in recent years through the work of researchers such as Doug Oldenberg ([10], [11]), M.H. Loke ([13], [14]), Bill Daily, Andy Binley and Doug LaBrecque ([6]). More recently there has been interest in the development of algorithms that permit the joint-inversion of multiple geophysical data; examples targeted in hydrogeophysics include those of Gallardo, Meju ([8]), Linde ([12]) and others.

Geophysical data also suffer from data sparsity and regularization methods are commonly used to stabilize the inversions at the cost of smoothing the resulting images. It has long been recognized that geophysical data could provide spatially dense data that has the potential to reduce problems associated with hydrogeologic data sparsity, and, in recent years, attempts have been made to constrain hydrological inversion with geophysical inverse results. However, recent work by Fred Day-Lewis, Kamini Singha, Andrew Binley and others ([7]) have shown that the most common approaches suffer from variations in geophysical image resolution through space and time. This body of work points to joint inversion of hydrogeological and geophysical data. The partial differential equations that describe hydrogeological processes provide a constraint on the feasible states of the petrophysical parameters that influence geophysical data and the geophysical data along with petrophysical relationships provide a dense set of data that can constrain feasible hydrogeological parameters and state.

Finally, the use of hydrogeophysical inversion is in its infancy. Some of the definitions and terminology is yet to be standardized. It still is not clear how hydrogeophysical fits into overall project work flow. These and other issues were the focus of the 5 day workshop

Hypothetical Case Studies

Since every individual case study has unique features, the workshop participants designed hypothetical case studies. The objective was to look at aspects of hydrogeophysical inversion in a holistic manner, from project design to processing and interpretation procedures. Each of three hypothetical case studies had unique aspects and it was anticipated that general principles would arise that were common to the design of the three hypothetical case studies. Following the discussion surrounding the hypothetical case approaches, definitions , an overall framework and a set of priority research directions were proposed. The three hypothetical case studies were motivated by real challenges or geological situations that various individuals attending the workshop were being faced with. The three studies were an unconfined aquifer storage and recovery study, a confined aquifer storage and recovery study and a watershed scale characterization study.

Unconfined Aquifer Storage and Recovery (Group: Ty Ferre, Tim Johnson, Ian Knowles, Sander Huisman, Larry Bentley)

There is growing recognition of the need to store water for public use in underground storage facilities. In the Southwestern United States, in particular, the use of unconfined aquifers for ASR facilities offers several advantages. First, water can be applied directly at the ground surface and allowed to infiltrate, greatly reducing operating costs compared to injection. Second, infiltration through a thick (100-200 ft) unsaturated zone provides initial filtration and opportunities for aerobic degradation. Third, mixing with groundwater of marginal quality can extend the volume of potable water for public use.

Given the importance of the water supply for public health and safety, above ground ASR facilities are seen as a potential target for terrorist activities. Specifically, the large scale and often relatively remote location of ASR facilities can leave them susceptible to intentional contamination. Therefore, we recognize that it is important to have procedures in place to respond to such an event. The primary challenge in responding to contamination is predicting the time required for the contaminated water to reach a recovery well and the expected concentrations of the contaminant in the recovered water. We seek proposals to develop practical methods to predict these quantities. In this initial stage, the methods will be designed for a specific but unnamed ASR facility. But, the method should be transferable to other unconfined ASR facilities.

Site description

The study site is located in the center of an alluvial valley in the basin and range province of the southwestern United States. Sediments are interbedded lenses with textures ranging from fine sand to gravel. Buried stream channels are common in the region, but their presence or locations are unknown for the site. Caliche layers may form or may have formed, leading to very low permeability layers in the upper 10 m. Geological, hydrologic, and petrophysical properties are available from one continuous core that was collected when drilling a borehole in the center of the infiltration basin. The background depth to the water table is approximately 33 m. The infiltration pond dimensions are approximately 460 m by 180 m. Very accurate records of inflow volume, water level in the pond, and atmospheric conditions are available over the past two

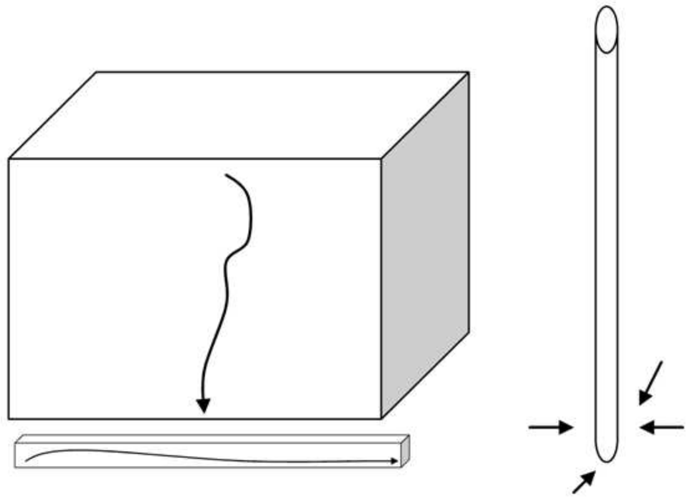

Figure 24.1: Conceptual model for transport and capture of aquifer storage water.

years of operation. The facility is flooded for three weeks then allowed to drain for one week. Once drained, the surface is scraped to remove any biological clogging layers. In addition, the facility is allowed to drain for two months for annual maintenance, including more intensive surface scraping. The water table elevation is monitored in the pumped well (located 450 m from the nearest point of the basin) and in a single, metal cased 2? diameter monitoring well located in the center of the basin. Only natural tracers may be used and no radioactive or otherwise hazardous methods may be employed. The maximum height of the water table mound at the center of the basin is approximately 5 meters. Annual potential evapotranspiration is approximately 1.0 m. Precipitation is approximately 0.3 m; 60

The budget is large after all, we are Homeland Security.

Proposed solution

The key prediction of interest is the concentration in the recovery well as a function of time. This response can be used to infer the maximum expected concentration, which may determine whether any remedial action is necessary. The response will also define the time of first arrival, which determines the urgency of a response. Finally, the response will define the residence time of the contaminant in the system. We will provide probabilistic break through curves that could be used for risk-based decision-making.

We conceptualize the problem as having three related parts: percolation and solute transport through the unsaturated zone; predominantly lateral flow and solute transport through the aquifer; and mixing of infiltrated water and groundwater during capture by the well. The conceptual model is shown in Figure 1:

It is currently not feasible to condition a fully heterogeneous three-dimensional saturated-unsaturated flow model at this scale. Therefore, we propose a staged investigation to define the simplest acceptable conceptual model.

Our first level analysis is based on the expected dilution of the infiltrated water by mixing during capture by the well. We propose to conduct a major anion end member mixing analysis to determine the time-varying dilution of the input water in the extraction well. To minimize the impact of reactions in the vadose zone, we will use samples collected immediately below the water table in the monitoring well located within the pond. This analysis requires that the major anion composition of the ambient groundwater is different than that of the water pumped from the recovery well.

Our analysis of the unsaturated flow and transport begins with a classification of the important processes controlling flow and transport. Our baseline assumption is that the medium can be represented as homogeneous with effective hydraulic properties. We will consider the impacts of heterogeneity through ensemble parameter estimation. We will then investigate the importance of two structural complications: dipping layers and discrete channels. We hypothesize that the plan view recharge patterns from each of these classes will have important differences. The general expected patterns for homogeneous, dipping, and discrete feature classes are shown schematically in Figure 2 A, B and C, respectively with the outline of the recharge basin

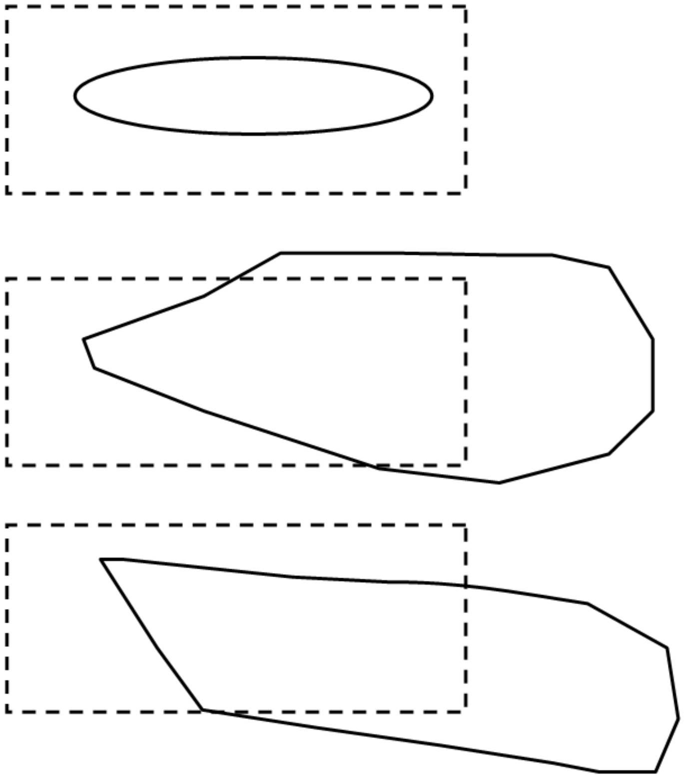

Figure 24.2: Recharge patterns for A. Homogeneous unsaturated zone, B. Unsaturated zone with a dipping aquitard layer and C. Fracture causing preferential flow path. The dashed line indicates the infiltration basin.

overlain as a dashed line.

Initially, we will collect ERT data to assess the importance of dipping layers and buried channels. We will use two orthogonal lines that cross the pond to identify dipping layers. We will use ERT lines around the boundary to identify flow beyond the boundaries of the pond due to channelized flow. ERT data would be collected at the end of the extended period of drainage and during the first ponding event following this period. We expect that dipping layers will result in dry regions below the updip end of a layer and wetter regions below the downdip end. This should result in relatively continuous changes in electrical conductivity along one or both of the lines placed within the basin. Time varying, localized changes in electrical conductivity along one of the boundary lines would indicate channelized flow. If we find that dipping layers are likely present we would use higher resolution time lapse ERT, GPR, or refraction seismics depending upon the conditions. Similarly, if channels are present, we would design a similar survey to better define their geometry.

Once we have classified the likely dominant flow processes we will generate multiple realizations of hydrologic and petrophysical model parameter values that honor the unsaturated flow conceptualization and the available geophysical data and the parameter value ranges seen in the core. For each realization, we will predict the geophysical responses corresponding with the geophysical observations. We will use DREAM to define the likelihood of each parameter set based on their consistency with the geophysical data, defined as a weighted misfit of the predicted and measured geophysical responses weighted by the inverse of the measurement error for each measurement type.

Once we have our parameter sets defined we will predict the pattern of recharge. We will then formulate a probability-weighted recharge pattern based on the ensemble of realizations. We will use this predicted recharge patterns to choose locations for four additional monitoring wells. We will conduct temperature tracer injection tests in each pair of the new monitoring wells to estimate the saturated zone transport parameters between each pair of monitoring wells. In addition, we will install a fiber optic distributed temperature sensing (DTS) cable along one of the wells and electrodes along the other wells.

Once the wells are installed, we will conduct a hot-water-infiltration experiment. We will monitor the advance of the wetting front using simple resistance measurements made with the electrodes. Simultaneously, we will use the DTS measurements to infer the transport parameters above the wetting front. We will use the wetting front measurements to further refine the vadose zone model likelihood assessment. Then we will update our recharge estimations based on the updated vadose zone models.

We will conduct slug tests in each of the monitoring wells to get local hydraulic conductivity estimates. We will conduct a pumping test in the recovery well, monitoring head in the monitoring wells as well as time-lapse gravity and SP data. We will interpret these measurements simultaneously in the coupled hydrogeophysical framework described above to infer the larger scale transmissivity, storativity, and specific yield values. Specifically, we will assume all transport and hydraulic properties are isotropic in the saturated zone with the exception of hydraulic conductivity. We will generate realizations that include a range of anisotropy ratios (in two horizontal directions) and we will test which of these ratios best predicts the SP and gravity data. The gravity data will help to constrain estimates of the specific yield and to test for anisotropy.

Our final step is to use the predicted recharge in space and time from each of the accepted unsaturated zone models together with observations in all of the monitoring wells during a ponding event and the inferred T, S, Sy, and anisotropy ratio values from pumping and slug tests to condition an inverse model of the saturated zone. This model will use Knowles? inverse approach to provide better estimates of the spatial distributions of T and S. This is repeated for each conditioned parameter set and associated recharge distribution.

We will produce independent estimates of the transport parameters in the unsaturated and saturated zones. We will also produce an ensemble of associated petrophysical and hydraulic parameters in the unsaturated zone and hydraulic parameters in the saturated zone. We will use each member of the ensemble of parameter sets to predict a breakthrough curve in the recovery well. These breakthrough curves, with associated likelihoods, will be used to produce a probability weighted breakthrough curve. These responses can be used to assess the risk posed by a contamination event in an infiltration pond.

Confined aquifer storage and recovery

(Group: Partha Roth, Mike Cardiff, Burke Minsley, Jonathan Ajo-Franklin, Andreas Kemna)

Problem Description

Aquifer storage and recovery has been proposed as a means for storing excess treated freshwater in Kuwait for subsequent use as an emergency water supply, as well as meeting variable seasonal demands. Injection of freshwater (100ppm) will occur at a rate of 1000 cubic meters/day into a confined saline aquifer (6000ppm). Initial pilot tests will use one injection/recovery well, but full production would involve a grid of up to 30 wells over an area of nearly 100km2. Success of this project relies on the ability to recover the maximum possible volume of freshwater with salinity less than 1500ppm. Some of the relevant scientific questions to be answered include:

1. What measurements can be made to help guide the optimal placement of injection & recovery wells? 2. How can the advancement of the freshwater plume effectively be monitored over time? 3. Can loss of freshwater through high permeability zones or fractures in the confining layer be detected? 4. What is the maximum storage period that can be achieved?

Background hydrogeology

The relevant hydrogeologic units for the Tertiary sedimentary sequence in Kuwait are shown below.

Because its confining nature, as well as clogging problems with pumping in the Kuwait Group, the ASR experiment is planned in the Dammam Formation. Due to its karstic nature, the transmissivity in the Dammam Formation is variable, but shows a general decreasing trend towards the northeast. The silicified topmost part of the Dammam Formation, in conjunction with the basal shaley/clayey layers of the Kuwait Group, form an aquitard that separates the Dammam Aquifer from the overlying Kuwait Group Aquifer, though hydraulic continuity is maintained possibly through fractures that are present in the top part of the Dammam Formation. The anhydritic Rus Formation and the basal shales of the Lower Members of the Dammam Formation act as an aquitard, separating the underlying Umm Er-Radhuma Aquifer from the Dammam Aquifer.

Some primary considerations for controlling the fate of the freshwater plume include: - secondary porosity due to fracture flow/karst within the Dammam aquifer - fractures or breaks in the aquitard separating the Dammam/Kuwait Group formations - buoyancy of the freshwater plume due to the salinity contrast *Research deliverables*

Figure 24.3: Aquifer storage and recovery experiment.

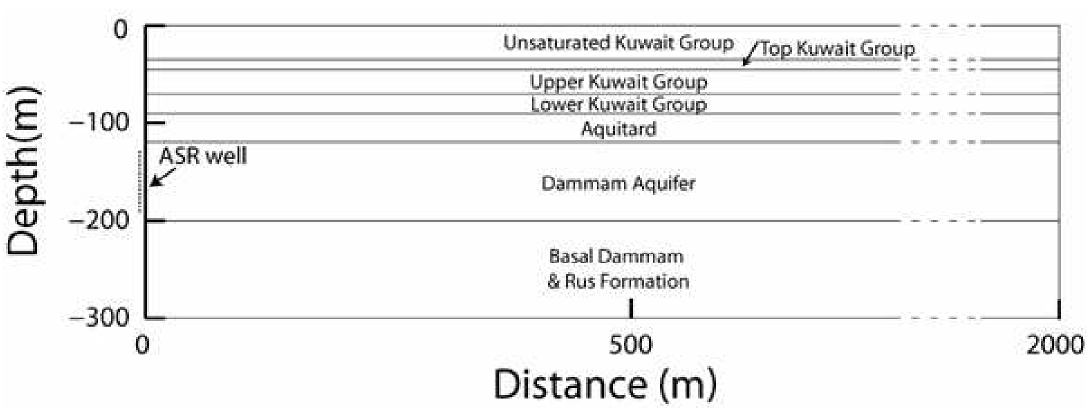

Figure 24.4: Site Geology.

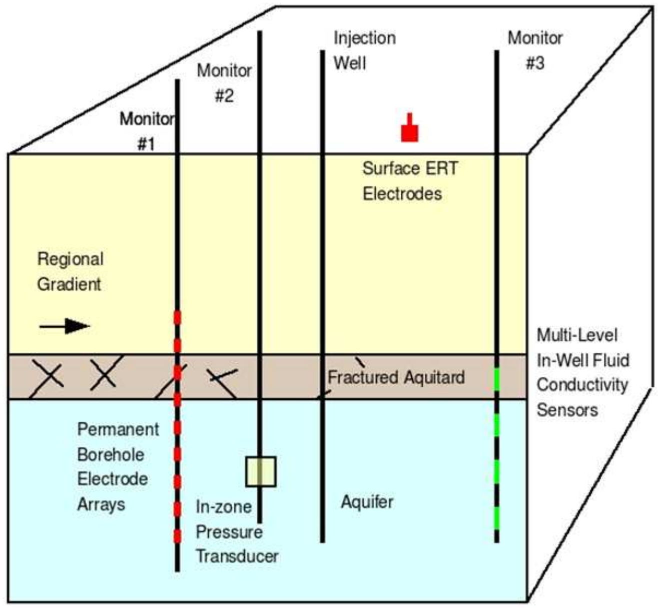

Figure 24.5: ASR Geometry.

The timeframe of the proposed research project is three years. Within this period, the pilot injection and recovery experiment will take place in conjunction with the proposed hydrogeophysical research. The end result of this study should be a report that provides guidance for the full-scale ASR project (100km2 scale), which addresses the following topics: - what is the optimal design for placement/operation of injection and recovery wells that will allow for a maximum storage period and ability to recover water less than 1500ppm? - a proposed methodology for monitoring losses of injected freshwater - developing a future strategy for long-term hydrogeophysical monitoring of aquifer storage and recovery projects

Program outline

Phase I Baseline geophysical surveys; Joint structural inversion of baseline geophysical data Phase II Site infrastructure development; Petrophysical core, construct hydrogeologic model, optimal survey design for time-lapse surveys Phase III Acquisition of optimal baseline geophysical survey Phase IV Acquire repeat surveys during injection/storage/recovery phases; Hydrogeophysical inversion, utilize forward modeling and inversion to implement design of full-scale ASR project

Phase I: Baseline hydrogeophysical characterization - ERT/SIP - CSEM - 2x 2D seismic lines to obtain structural information - Pump test at injection well Phase Ib: Joint structural inversion of baseline geophysical data - Joint inversion/interpretation of geophysical datasets for baseline characterization, primarily for structural information

Phase II: Site infrastructure development - Drill monitoring wells (x3) - Acquisition of core from monitoring wells - Logging – ?traditional? (neutron, density, gamma, conductivity, deviation) – fracture-oriented (acoustic televiewer, dipole sonic) – NMR to obtain permeability – Installation of borehole assemblie – Casing with ERT electrodes – Multi-level packers with conductivity sensors – In-aquifer pressure transducers

Phase IIb: Petrophysical core measurements & analysis - Permeability - Relationships between bulk conductivity & salinity - SIP of core

Phase IIc: Construct site hydrogeologic model for pilot experiment - Incorporate all information to date into hydrogeologic model - Simulate pilot injection experiment

Phase IId: Optimal survey design for timelapse geophysical experiments - Geophysical method resolution/uncertainty study based on hydrogeologic simulation - Select spatial sampling regime - Frequencies for CSEM

Phase III: Acquisition of pre-injection geophysical surveys (using optimal design) followed by initiation of injection

Phase IV: Acquire repeat surveys during injection/storage/recovery phases - Surveys at end of injection (month 3), end of storage phase (month 10), end of recovery phase (month 15)

Phase IVb: Hydrogeophysical inversion - Demonstrate ability to track the progress of freshwater injection and possible losses through confining unit or preferential flowpaths

Phase V: Utilize forward modeling & inversion to implement design of full-scale ASR project

Watershed (Group: Andrew Binley, Klaus Holliger, Niklas Linde, Jasper Vrugt, Kamini Singha, Jim Yeh, Adam Pidlisecky)

The problem

Nitrate contamination has long been recognized as a major water quality issue in agricultural watersheds. Efforts to control non-point source pollution require the identification of source areas, the spatial and temporal variability of properties controlling flow and transport, and an understanding of the distributed (or isolated) nature of discharge into streams. Improved water quality monitoring and modeling programs, including development of technologies that are capable of collecting long time-course data, would be useful for scientists studying nitrate transport processes and for development of best management practices in local watersheds. At the hillslope scale, surface and bedrock topography, geologic stratification, antecedent moisture and soil layering all control water flow.

In soils, remnant structure of the original bedrock can lead to preferential flow patterns, leading to spatial concentrations of water and solutes that are not well described by Darcy?s approach to uniform flow. In areas with steep slopes, thin soils, and matrix hydraulic conductivities above the maximum rainfall intensity, water moves vertically to depth (as matrix or preferential flow), perches at the soil-bedrock or an impeding layer at depth, and then moves laterally along the lower portion of the profile. Growing evidence suggests that the most common mechanism for delivery of water from slopes into valley bottom and riparian areas is lateral subsurface flow in hillslopes, triggered by a perched water table. This storm flow is particular important because this near-stream area can change rapidly during rainfall-runoff events, and can serve as the focal point for non-point source loading of nitrogen to streams. Additionally, the collection of point measurements of nitrate concentration or groundwater fluxes to streams is time consuming and often unrepresentative of the process at larger scales, and large-scale, integrated measurements give no estimates of variability. Groundwater contributions to surface water bodies have been found to be spatially heterogeneous, and have been found to vary over several orders of magnitude within short distances and as a function of discharge.

Identifying heterogeneous streambed characteristics that control groundwater discharge and hyporheic exchange is critical to improving quantification of water quality in downgradient rivers and estuaries. Besides heterogeneity, temporal scales are also important: seasonal variations in nitrate concentrations in streams are often attributed to seasonal loading or land use. Unfortunately, few methods are available to collect data at a spatial or temporal scale appropriate for simulating groundwater contributions to stream solute transport along a river continuum through these seasonal changes. Capturing hillslope-scale heterogeneity and the dynamics of precipitation thresholds leading to subsurface stormwater generation may be difficult in field settings where limited probe data are generally available.

For quantifying transport risk, estimating saturation dynamics through time is necessary. However, the investigation of hillslope networks is technology limited, and most methods for accurately identifying and measuring subsurface networks in the field are destructive. To understand dynamics at the hillslope or catchment scale, more exhaustive measurements are required than can be measured with point-scale timedomain reflectometry or heat dissipation probes. Noninvasive geophysical techniques may provide spatially exhaustive maps about spatial and temporal heterogeneity not otherwise attainable. However, which methods to use, and what data to collect over these large spatial scales, where small-scale feature may control flow, is an important research question. We will evaluate the worth of geophysical data for forecasting and predicting flow and transport in watershed systems given a filtering framework outlined below. *The solution* We propose a framework for simultaneous inversion of hydrologic and geophysical data for determining changes in soil moisture, a controlling variable in watershed-scale nitrate transport. The idea behind this framework is to couple multiple numerical forward models?for flow, transport, and geophysics?to find locations where new data would best help constrain estimates of the state space or model parameters of interest. This could be done either deterministically or stochastically. This framework is outlined in Figure 3, and intentionally kept somewhat general.

Numerous research questions exist, including how to 1) build G*, the combined ?sensitivity? metric that

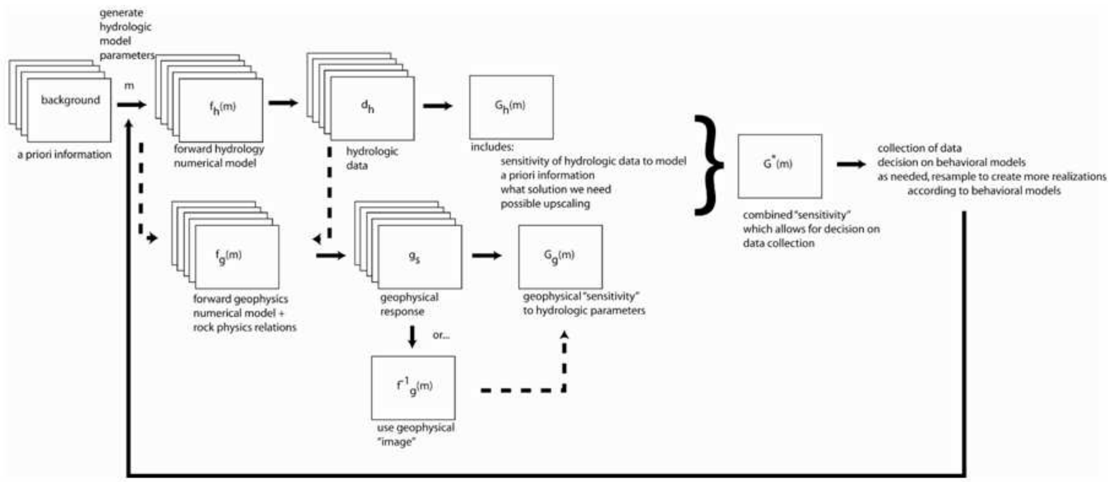

Figure 24.6: Flow chart for simultaneous inversion of hydrologic and geophysical data.

determines where to best sample new hydrologic and geophysical data, 2) determine appropriate rock physics relations, 3) quantify model structural error, 4) deal with the issue that geophysical images are not data.

Outcome of the Meeting

Hydrogeophysics is, by its nature, integrative; but, it is critical that the application of geophysics is driven by hydrologic questions and any hydrogeophysical application remains linked to the hydrologic aims. We refer to the process of integrating geophysical and other data into a hydrologic assessment as hydrogeophysical inversion. Currently, there is much disagreement regarding the differences among approaches to hydrogeophysical inversion, often stemming from a lack of common terminology. To clarify discussions among hydrologists and geophysicists, we propose the following definitions:

Independent hydrogeophysical inversion: this is the simplest and often the most practical approach, wherein hydrologic interpretations are based on hydrogeologic properties and states that are inferred from independent interpretations of geophysical surveys. In many cases, the investigation may be considered to be hydrogeophysical because it has a shallow, hydrogeophysical target. But, the geophysical inversion is identical to that used in classical geophysics.

Joint hydrogeophysical inversion: in this approach, additional information that describes the relationships among different measurement types is used to interpret instrument responses simultaneously. As with independent geophysical inversion, this includes joint inversion of multiple geophysical methods in a manner that is identical to classical geophysical methods with subsequent use of the results for hydrologic investigations. However, joint hydrogeophysical inversion can also include simultaneous or sequential interpretation of hydrologic and geophysical data.

Coupled hydrogeophysical inversion: In some cases, especially when monitoring transient hydrologic processes, a hydrologic model can be used to relate geophysical and hydrologic measurements in time and space. Coupled hydrogeophysical inversion approaches make direct use of a hydrologic process model as part of the geophysical inversion. Often, this can eliminate the need to conduct classical geophysical inversions (e.g. construction of images of geophysical property distributions). The fundamental difference between joint and coupled hydrogeophysical inversion is that the joint inversion combines multiple measurement types through correlative relationships of the inferred properties (i.e. empirical, physical, or statistical relationships between the hydraulic properties of interest and the properties that are measured or inferred with geophysical instruments); coupled inversion integrates hydrologic process models in the geophysical inversion.

One of the key conclusions drawn through our discussions is that geophysics can only be used effectively in hydrologic studies if it is integrated in entire hydrologic analysis. To explain how geophysics can be inte-

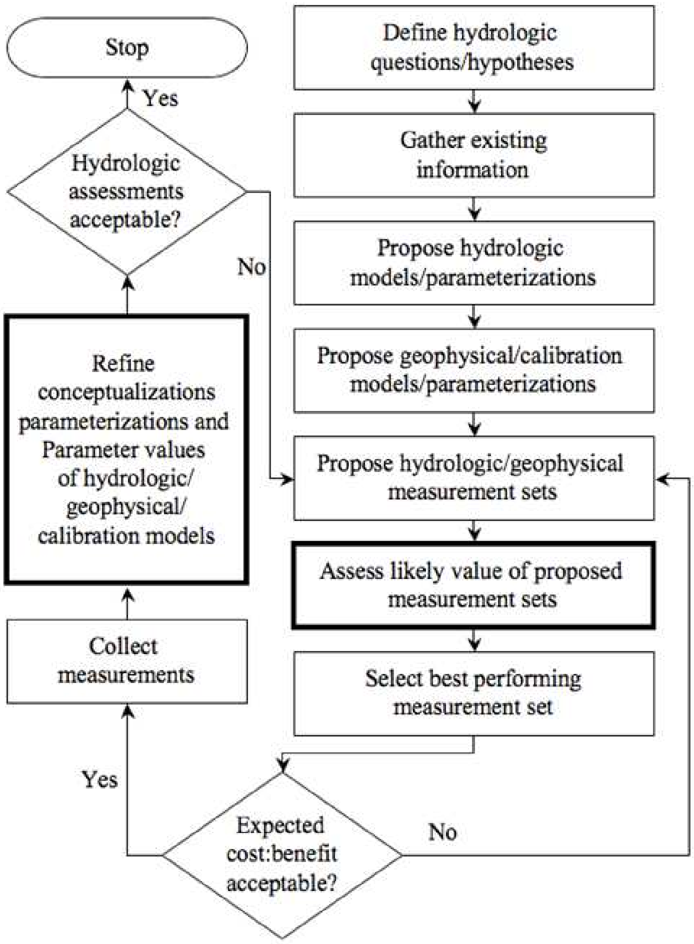

Figure 24.7: Hydrogeophysical work flow.

grated more completely, we show an idealized workflow for a hydrologic analysis that includes geophysics (Figure 7). The workflow is based on a multi-model approach to hydrologic analysis. These models are intended to capture the range of conceptualizations, parameterizations, and parameter values that represent our physical understanding of the hydrologic system and the responses of geophysical instruments. The physics captured by these models includes hydrologic processes (e.g. flow and transport), geophysical processes (e.g. electromagnetic or seismic responses to controlled or natural sources), and relationships among rock and fluid properties and measurable geophysical properties. Within this workflow, the purpose of hydrogeophysics is to provide information that allows for discrimination among these proposed models. At the conclusion of the hydrologic investigation, the ensemble of models that are plausible, based on all observations, can be used to make probabilistic predictions to support scientific analysis and/or decision-making.

There are two key steps that should include a hydrogeophysical analysis, which are highlighted on the flowchart. First, efficient hydrogeophysical characterization and monitoring requires quantitative assessment of the likely contribution of proposed measurement sets to discriminate among conceptual models and to refine the numerical or analytical model calibrations. This assessment is most effective if it is performed in the context of the specific hydrologic questions of interest and of the proposed numerical or analytical hydrologic, geophysical, and calibration models that will be used for the analysis. Specifically, when considering geophysical measurements for a hydrologic study, the geophysicist should determine whether the geophysical instrument is likely to respond to the expected hydrologic responses, whether the responses are likely to be large compared to the sources of uncertainty in interpreting the geophysical measurements, and whether the data, if collected, would reduce the bias and/or uncertainty of the hydrologic assessments of interest. Ideally, this should be considered in a quantitative framework that allows for the comparison of multiple proposed measurement sets. Second, once the geophysical data are collected, they should be used together will all other data to reject conceptual models that are not consistent with all of the data and to refine the remaining numerical or analytical representations of these conceptual models to be most consistent with all of the observations. This step requires a choice of hydrogeophysical inversion approach. Neither independent, nor joint, nor coupled hydrogeophysical inversion is universally preferred. Rather, the choice of the most appropriate approach depends on the complexity of the problem, the availability of supporting relationships, and whether the process of interest is steady-state or transient.

Through our discussion during the workshop, we identified three primary areas in which substantial progress can be made in the next five years:

1. Hydrologists are currently working to develop effective methods to generate ensembles of models that capture the range of possible hydrologic conceptualizations and parameterizations. Hydrogeophysicists can adopt some of these approaches to incorporate different conceptualizations of the responses of geophysical instruments to property distributions (geophysical forward models) in their interpretations. This is particularly important for relationships between physical and geophysical properties, which are often very poorly understood and rarely characterized at the field scale;
2. In the past, several hydrologists have had negative experiences with geophysics, in part because of the inappropriate application of geophysical methods to hydrologic problems. Hydrogeophysics would benefit greatly if more objective methods were available to guide in the design of measurement sets that consider the spatial sensitivity patterns of geophysical measurement methods, the spatial resolution of imaging methods, the magnitude and characteristics of the measurement uncertainties (noise), the effects of uncertainty in field-scale rock physics relationships, and the complementarity of different measurements types;
3. The likely value of geophysical (or other) measurements must be defined on the basis of the likely improvement that they will provide for specific hydrologic questions. We need to develop quantitative approaches to compare proposed measurement sets to consistently identify high-value geophysical measurement sets that add to existing information and improve specific hydrologic analyses.

We expect that some progress will be made through the judicious use of synthetic studies. In particular, these synthetic studies should be designed to demonstrate the limitations of proposed measurement methods or analysis approaches with the aim of moving the methods to the field. We propose to establish a central portal for the sharing of these synthetic models to allow for inter-comparison of measurements and analyses. Fundamental advances will require that synthetic studies move to field trials.

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Chapter 25

Quantum Computation with Topological Phases of Matter (08w5103)

Jul 20 - Jul 25, 2008

Organizer(s): Marcel Franz (University of British Columbia), Michael H. Freedman (Microsoft Corporation), Yong-Baek Kim (University of Toronto), Chetan Nayak (University of California, Los Angeles), Kirill Shtengel (University of California, Riverside)

Overview of the Field

Quantum computers, if realized in practice, promise exponential speed-up of some of the computational tasks that conventional classical algorithms are intrinsically incapable of handling efficiently. Perhaps even more intriguing possibility arises from being able to use quantum computers to simulate the behavior of other physical systems – an exciting idea dating back to Feynman.

Unfortunately, realizing a quantum computer in practice proves to be very difficult, chiefly due to the debilitating effects of decoherence plaguing all possible schemes which use microscopic degrees of freedom (such as nuclear or electronic spins) as basic building blocks. From this perspective, topological quantum computing offers an attractive alternative by encoding quantum information in nonlocal topological degrees of freedom that are intrinsically protected from decoherence due to local noise.

Recent Developments and Open Problems

Over the last few years there have been substantial advances in both our understanding of how to compute with topological phases, and our understanding of topological phases themselves in various physical manifestations. The important features of these phases include topological order – the ground state degeneracy that depends on the topology of the underlying 2D surface – as well as nontrivial, often fractional statistics of their excitations. The goal of this workshop was to both study the physical nature of topological phases as well as to address the most important theoretical issues connected with any attempt to practically realize a topological quantum computer. One of the main objectives of the proposed workshop was to bring together experts from different fields including condensed matter physics, quantum optics and theory of quantum information and quantum computation. The exchange of ideas between researchers working on these subjects has resulted in making new inroads into this broad, inter-disciplinary field. Specifically, the discussions focused on the following open questions:

1. Physical systems with topological order. So far, of experimentally observed systems, only Fractional Quantum Hall systems are believed to possess topological order. Numerous other possibilities have been discussed recently, ranging from atomic systems in optical lattices to Josephson junction arrays to frustrated magnetic systems. How to engineer systems supporting a topological phase remains an open question.

2. Fractional Quantum Hall Effect and related systems. Recently, new experiments purported to probe the quasiparticle statistics in the Fractional Quantum Hall systems have been reported by Goldman's group. However, their results appear to be open to interpretation. Hence a clear, unambiguous experimental evidence of fractional statistics remains to be confirmed. Experimental detection of non-Abelian anyons and related topological order remains an open problem despite several recent theoretical suggestions. How to control topological excitations, a crucial part of building a topological quantum computer, also remains to be explored.

3. Topological Algorithms and Computational Architectures Given that such topological phases do exist, and are capable of performing universal quantum computation, one must ask how to build efficient architecture and how one would actually go about performing such computations. The structure of topological phases is extremely complex and imposing the traditional qubit architecture may not be the most efficient scheme.

Presentation Highlights

The five days of the workshop were devoted to five different topics. Here, we give a brief outline of the presentations given by the participants.

Day 1: Topological phases and topological order

Paul Fendley: "Topological order from quantum loops and nets" — I define models of quantum loops and nets that have ground states with topological order. These make possible excited states comprised of deconfined anyons with non-abelian braiding. With the appropriate inner product, these quantum loop models are equivalent to net models whose topological weight involves the chromatic polynomial. A simple Hamiltonian preserving the topological order is found by exploiting quantum self-duality. For the square lattice, this Hamiltonian has only four-spin interactions.

C. Castelnovo: "Topological phases at finite temperature" — We study topological order in a toric code in three spatial dimensions, or a 3+1D Z2 gauge theory, at finite temperature. We compute exactly the topological entropy of the system, and show that it drops, for any in- finitesimal temperature, to half its value at zero temperature. The remaining half of the entropy stays constant up to a critical temperature Tc, dropping to zero above Tc. These results show that topologically ordered phases exist at finite temperatures, and we give a simple interpretation of the order in terms of fluctuating strings and membranes, and how thermally induced point defects affect these extended structures. Finally, we discuss the nature of the topological order at finite temperature, and its quantum and classical aspects.

X.-G. Wen: "Classifying FQH states through pattern of zeros" — A large class of fractional quantum Hall (FQH) states can be classified according to their pattern of zeros, which describes the way ideal ground state wave functions go to zero as various clusters of electrons are brought together. In this paper we generalize this approach to classify multilayer FQH states. Such a classification leads to the construction of a class of non-Abelian multilayer FQH states that are closely related to $\hat{g}_k$ parafermion conformal field theories, where $\hat{g}_k$ is an affine simple Lie algebra. We discuss the possibility of some of the simplest of these non-Abelian states occuring in experiments on bilayer FQH systems at $\nu = 2/3, 4/5, 4/7$, etc.

J. Slingerland: "Condensation induced transitions between topological phases" — We investigate transitions between topologically ordered phases in two spatial dimensions induced by the condensation of a bosonic quasiparticle. To this end, we formulate an extension of the theory of symmetry breaking phase transitions which applies to phases with topological excitations described by quantum groups or modular tensor categories. This enables us to deal with phases whose quasiparticles have non-integer quantum dimensions and obey braid statistics. Many examples of such phases can be constructed from two-dimensional rational conformal field theories and we find that there is a beautiful connection between quantum group symmetry breaking and certain well-known constructions in conformal field theory, notably the coset construction, the construction of orbifold models and more general conformal extensions. Besides the general framework, many representative examples are worked out in detail.

P. Bonderson: "Measurement-Only Topological Quantum Computation" — We describe measurement only topological quantum computation using both projective and interferometrical measurement of topological charge. We demonstrate how anyonic teleportation can be achieved using "forced measurement" protocols for both types of measurement. Using this, it is shown how topological charge measurements can be used to generate the braiding transformations used in topological quantum computation, and hence that the physical transportation of computational anyons is unnecessary. We give a detailed discussion of the anyonics for implementation of topological quantum computation (particularly, using the measurement-only approach) in fractional quantum Hall systems.

Day 2: p-wave superconductors and superfluids, Topological insulators

C. Kallin: "Is Sr_2RuO_4 a chiral p-wave superconductor?" — Much excitement surrounds the possibility that strontium ruthenate exhibits chiral p-wave superconducting order. Such order would be a solid state analogue of the A phase of He-3, with the potential for exotic physics relevant to quantum computing. We take a critical look at the evidence for such time-reversal symmetry breaking order. The possible superconducting order parameter symmetries and the evidence for and against chiral p-wave order are reviewed, with an emphasis on the most recent theoretical predictions and experimental observations. In particular, attempts to reconcile experimental observations and theoretical predictions for the spontaneous supercurrents expected at sample edges and domain walls of a chiral p-wave superconductor and for the polar Kerr effect, a key signature of broken time-reversal symmetry, are discussed.

V. Gurarie: "Creating stable p-wave atomic superfluids" — We study theoretically a dilute gas of identical fermions interacting via a p-wave resonance. We show that, depending on the microscopic physics, there are two distinct regimes of p-wave resonant superfluids, which we term "weak" and "strong". Although expected naively to form a BCS-BEC superfluid, a strongly-resonant p-wave superfluid is in fact unstable towards the formation of a gas of fermionic triplets. We examine this instability and estimate the lifetime of the p-wave molecules due to the collisional relaxation into triplets. We discuss consequences for the experimental achievement of p-wave superfluids in both weakly- and strongly-resonant regimes.

J. Moore: "Topological insulators: overview and relevance to quantum computing" — Spinorbit coupling in some materials leads to the formation of surface states that are topologically protected from scattering. Theory and experiments have found an important new family of such materials. Topological insulators are materials with a bulk insulating gap, exhibiting quantum-Hall-like behaviour in the absence of a magnetic field. Such systems are thought to provide an avenue for the realization of fault-tolerant quantum computing because they contain surface states that are topologically protected against scattering by time-reversal symmetry.

S.-S. Lee: "Many-body generalization of the Z2 invariant in the time reversal symmetric topological insulator" — We propose a many-body generalization of the Z2 topological invariant for the quantum spin Hall insulator, which does not rely on single-particle band structures. The invariant is derived as a topological obstruction that distinguishes topologically distinct many-body ground states on a torus. It is also expressed as a Wilson-loop of the SU(2) Berry gauge field, which is quantized due to the time-reversal symmetry.

N. Read: "Adiabatic statistics, quasiparticle spin, and Hall viscosity in quantum Hall states and $p_x + ip_y$ paired superfluids" — Many trial wavefunctions for fractional quantum Hall states in a single Landau level are given by functions called conformal blocks, taken from some conformal field theory. Also, wavefunctions for certain paired states of fermions in two dimensions, such as $p_x + ip_y$ states, reduce to such a form at long distances. Here we investigate the adiabatic transport of such many-particle trial wavefunctions using methods from two-dimensional field theory. One context for this is to calculate the statistics of widely-separated quasiholes, which has been predicted to be non-Abelian in a variety of cases. The Berry phase or matrix (holonomy) resulting from adiabatic transport around a closed loop in parameter space is the same as the effect of analytic continuation around the same loop with the particle coordinates held fixed (monodromy), provided the trial functions are orthonormal and holomorphic in the parameters so that the Berry vector potential (or connection) vanishes. We show that this is the case (up to a simple area term) for paired states (including the Moore-Read quantum Hall state), and present general conditions for it to hold for other trial states (such as the Read-Rezayi series). We argue that trial states based on a non-unitary conformal field theory do not describe a gapped topological phase, at least in many cases. By considering adiabatic variation of the aspect ratio of the torus, we calculate the Hall viscosity, a non-dissipative viscosity coefficient analogous to Hall conductivity, for paired states, Laughlin states, and more general quantum Hall states. Hall viscosity is an invariant within a topological phase, and is generally proportional to the "conformal spin density" in the ground state.

Day3: Fractionalization of charge and statistics in FQHE and other systems

W. Kang: "Experimental Study of Mesoscopic Quantum Hall Interferometers" — The fractional quantum Hall effect is presently the most promising platform for a topological quantum computer among various candidate systems. The global topological protection afforded by fractional quantum Hall effect produces fault-tolerance in a topological quantum computer. A topological quantum computer consequently becomes immune against the effects of local quantum decoherence. A fault-tolerant qubit can be constructed by taking advantage of the non-Abelian braiding statistics of elementary excitations (called anyons) which are thought to exist in certain, exotic fractional quantum Hall states. Experimental goals include detection and manipulations of the postulated non-Abelian anyons in quantum interferometers constructed from high quality semiconductor heterostructures.

S. Vishveshwara: "Correlators and Fractional Statistics in the quantum Hall bulk" — We derive single-particle and two-particle correlators of anyons in the presence of a magnetic field in the lowest Landau level. We show that the two-particle correlator exhibits signatures of fractional statistics which can distinguish anyons from their fermionic and bosonic counterparts. These signatures include the zeroes of the two-particle correlator and its exclusion behavior. We find that the single-particle correlator in finite geometries carries valuable information relevant to experiments in which quasiparticles on the edge of a quantum Hall system tunnel through its bulk.

S. Simon: "Other Quantum Hall States, Hamiltonians, and Conformal Field Theories" — We construct a family of BCS paired composite fermion wavefunctions that generalize, but remain in the same topological phase as, the Moore-Read Pfaffian state for the half-filled Landau level. It is shown that for a wide range of experimentally relevant inter-electron interactions the groundstate can be very accurately represented in this form.

B. Seradjeh: "Zero modes and fractionalization in bilayer-graphene exciton condensate" — A real-space formulation is given for the recently discussed exciton condensate in a symmetrically biased graphene bilayer. We show that in the continuum limit an oddly-quantized vortex in this condensate binds exactly one zero mode per valley index of the bilayer. In the full lattice model the zero modes are split slightly due to intervalley mixing. We support these results by an exact numerical diagonalization of the lattice Hamiltonian. We also discuss the effect of the zero modes on the charge content of these vortices and deduce some of their interesting properties.

Day 4: FQH States

M. Fisher: "Tunneling and edge transport in non-Abelian quantum Hall states" — We analyze charge-$e/4$ quasiparticle tunneling between the edges of a point contact in a non-Abelian model of the $\nu = 5/2$ quantum Hall state. We map this problem to resonant tunneling between attractive Luttinger liquids and use the time-dependent density-matrix renormalization group (DMRG) method to compute the current through the point contact in the presence of a *finite voltage difference* between the two edges. We confirm that, as the voltage is decreases, the system is broken into two pieces coupled by electron hopping. In the limits of small and large voltage, we recover the results expected from perturbation theory about the infrared and ultraviolet fixed points. We test our methods by finding the analogous non-equilibrium current through a point contact in a $\nu = 1/3$ quantum Hall state, confirming the Bethe ansatz solution of the problem.

E. Ardonne: "Non-abelian quantum Hall states: what can be learned from the thin-torus limit" — We analyze the non-abelian Read-Rezayi quantum Hall states on the torus, where it is natural to employ a mapping of the many-body problem onto a one-dimensional lattice model. On the thin torus–the Tao-Thouless (TT) limit–the interacting many-body problem is exactly solvable. The Read-Rezayi states at filling $\nu = \frac{k}{kM+2}$ are known to be exact ground states of a local repulsive $k+1$-body interaction, and in the TT limit this is manifested in that all states in the ground state manifold have exactly k particles on any $kM+2$ consecutive sites. For $M \neq 0$ the two-body correlations of these states also imply that there is no more than one particle on M adjacent sites. The fractionally charged quasiparticles and quasiholes appear as domain walls between the ground states, and we show that the number of distinct domain wall patterns gives rise to the nontrivial degeneracies, required by the non-abelian statistics of these states. In the second part of the paper we consider the quasihole degeneracies from a conformal field theory (CFT) perspective, and show that the counting of the domain wall patterns maps one to one on the CFT counting via the fusion rules. Moreover we extend the CFT analysis to topologies of higher genus.

J. Eisenstein: "Edge State Heat Transport in the Quantum Hall Regime" — Heat transport in the quantum Hall regime is investigated using micron-scale heaters and thermometers positioned along the edge of a millimeter-scale two dimensional electron system (2DES). The heaters rely on localized current injection into the 2DES, while the thermometers are based on the thermoelectric effect. In the $\nu = 1$ integer quantized Hall state, a thermoelectric signal appears at an edge thermometer only when it is "downstream", in the sense of electronic edge transport, from the heater. When the distance between the heater and the thermometer is increased, the thermoelectric signal is reduced, showing that the electrons cool as they propagate along the edge.

G. Ortiz: "Symmetries, dimensional reduction and topological quantum order" — Are systems that display Topological Quantum Order (TQO), and have a gap to excitations, hardware fault-tolerant at finite temperatures? We show that in surface code models that display low d-dimensional Gauge-Like Symmetries, such as Kitaev's and its generalizations, the expectation value of topological symmetry operators vanishes at any non-zero temperature, a phenomenon that we coined thermal fragility. The autocorrelation time for the non-local topological quantities in these systems may remain finite even in the thermodynamic limit. We provide explicit expressions for the autocorrelation functions in Kitaev's model. If temperatures far below the gap may be achieved then these autocorrelation times, albeit finite, can be made large. The physical engine behind the loss of correlations at large spatial and/or temporal distance is the proliferation of topological defects at any finite temperature as a result of a dimensional reduction. This raises an important question: How may we best quantify the degree of protection of quantum information in a topologically ordered system at finite temperature?

A. Stern: "Possible future experiments with non-abelian quantum Hall systems" — We show that non-abelian quantum Hall states can be identified by experimental measurements of the temperature dependence of either the electrochemical potential or the orbital magnetization. The predicted signals of non-abelian statistics are within experimental resolution, and can be clearly distinguished from other contributions under realistic circumstances. The proposed measurement technique also has the potential to resolve spin-ordering transitions in low density electronic systems in the Wigner crystal and strongly-interacting Luttinger liquid regimes.

Day 5: Interacting anyons etc.

S. Trebst: "Interacting anyons in topological quantum liquids: Things golden" — We show that chains of interacting Fibonacci anyons can support a wide variety of collective ground states ranging from extended critical, gapless phases to gapped phases with ground-state degeneracy and quasiparticle excitations. In particular, we generalize the Majumdar-Ghosh Hamiltonian to anyonic degrees of freedom by extending recently studied pairwise anyonic interactions to three-anyon exchanges. The energetic competition between two- and three-anyon interactions leads to a rich phase diagram that harbors multiple critical and gapped phases. For the critical phases and their higher symmetry endpoints we numerically establish descriptions in terms of two-dimensional conformal field theories. A topological symmetry protects the critical phases and determines the nature of gapped phases.

L. Fidkowski: "Infinite randomness in the Golden chain" — Topological insulators supporting non-abelian anyonic excitations are at the center of attention as candidates for topological quantum computation. In this paper, we analyze the ground-state properties of disordered non-abelian anyonic chains. The resemblance of fusion rules of non-abelian anyons and real space decimation strongly suggests that disordered chains of such anyons generically exhibit infinite-randomness phases. Concentrating on the disordered golden chain model with nearest-neighbor coupling, we show that Fibonacci anyons with the fusion rule $\tau \otimes \tau = \mathbf{1} \oplus \tau$ exhibit two infinite-randomness phases: a random-singlet phase when all bonds prefer the trivial fusion channel, and a mixed phase which occurs whenever a finite density of bonds prefers the τ fusion channel. Real space RG analysis shows that the random-singlet fixed point is unstable to the mixed fixed point. By analyzing the entanglement entropy of the mixed phase, we find its effective central charge, and find that it increases along the RG flow from the random singlet point, thus ruling out a c-theorem for the effective central charge.

J. Pachos: "Exact demonstration of non-Abelian statistics for the honeycomb lattice model" — The classification of loop symmetries in Kitaev's honeycomb lattice model provides a natural framework to study the abelian topological degeneracy. We derive a perturbative low-energy effective Hamiltonian, that is valid to all orders of the expansion and for all possible toroidal configurations. Using this form we demonstrate at what order the system's topological degeneracy is lifted by finite size effects and note that in the thermodynamic limit it is robust to all orders. Further, we demonstrate that the loop symmetries themselves correspond to the creation, propagation and annihilation of fermions. Importantly, we note that these fermions, made from pairs of vortices, can be moved with no additional energy cost.

N. Bonesteel: "Topological Quantum Computing with Read-Rezayi States" — Read-Rezayi fractional quantum Hall states are among the prime candidates for realizing non-Abelian anyons which in principle can be used for topological quantum computation. We present a prescription for efficiently finding braids which can be used to carry out a universal set of quantum gates on encoded qubits based on anyons of the Read-Rezayi states with $k > 2$, $k \neq 4$. This work extends previous results which only applied to the case $k = 3$ (Fibonacci) and clarifies why in that case gate constructions are simpler than for a generic Read-Rezayi state.

G. Moller: "Paired Composite Fermion States" — We provide numerical evidence for composite fermion pairing in quantum Hall bilayer systems at filling $\nu = 1/2 + 1/2$ for intermediate spacing between the layers. We identify the phase as $p_x + ip_y$ pairing, and construct high accuracy trial wavefunctions to describe the groundstate on the sphere. For large distances between the layers, and for finite systems, a competing "Hund's rule" state, or composite fermion liquid, prevails for certain system sizes. We argue that for larger systems, the pairing phase will persist to larger layer spacing.

Scientific Progress Made

The chief obstacle facing any practical realization of a quantum computer is decoherence; interactions with the environment tend to scramble the fragile quantum state that is needed to effect a useful computation. One strategy, pursued by most researchers in this field, is to minimize the effect of decoherence by clever engineering and use of error correcting codes. Whether or not this will ultimately lead to a usable device is an open question. In 1997 Kitaev proposed a radically different approach to solve this problem: use a quantum state encoded in global topological properties of a system that are inherently immune to the debilitating effects of decoherence. Kitaevs proposal relies on the remarkable occurrence in nature of states of matter that possess topological order. The ground state of such systems exhibits degeneracy, which however, one cannot detect by any local measurement. To do so one must place the system onto a manifold with nontrivial topology (e.g. torus) and perform a highly nonlocal measurement of some quantity. By contrast, the environment, which couples only to the local degrees of freedom, cannot distinguish between the degenerate ground states and thus cannot affect the quantum state encoded as the linear superposition of the individual ground states. Such a system then represents an ideal quantum bit ("qubit") in which all errors are corrected automatically at the physical level.

The Workshop summarized worldwide progress made to date towards the ultimate realization of a topological quantum computer. It has been concluded that this beautiful idea faces considerable but not insurmountable practical hurdles. Of all experimentally realizable systems only FQHE is known to unambiguously possess topological order. Abelian anyons have indeed been experimentally confirmed for certain filling fractions ν. However, in order to implement a universal quantum computer non-abelian anyons are needed. These are expected to occur at $\nu = 5/2$ in the Moore-Read Pfaffian state, but have not yet been experimentally observed. Even if the existence of non-abelian anyons is confirmed it is not at all clear how to create and manipulate them in a controlled fashion. In a sense the very property which makes anyons potentially useful their complete decoupling from the environment makes their manipulation difficult.

Participants discussed other emerging new physical systems that could potentially be used as a platform for topological quantum computation. These include string-net condensates in strongly correlated electron systems, exotic superconductors and superfluids, and the recently discovered topological insulators. The expectations were high especially regarding the latter due to the fact that these materials manifest their topologically non-trivial behavior even at room temperature. This is in contrast to FQHE or exotic superconductors which exhibit interesting behavior only at cryogenic temperatures and therefore expensive and complicated cooling machinery would typically be required to operate any device based on these systems. Participants were optimistic that the advances in material synthesis, experimental manipulation and detection, combined with the recent progress in quantum algorithms will lead to major breakthroughs in the coming years, culminating in a working prototype of topological quantum computer.

List of Participants

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Chapter 26

Modeling the Impact of Policy Options during Public Health Crises (08w5043)

Jul 27 - Aug 01, 2008

Organizer(s): Fred Brauer (University of British Columbia), Zhilan Feng (Purdue University), John Glasser (US Centers for Disease Control and Prevention)

Motivation for the Workshop

While many of us have been thinking about pandemic influenza lately, when we submitted our proposal three years ago, SARS was fresh in our minds. We weren't as useful to policymakers as we wanted to be during that crisis and frankly, don't believe any other modelers were either. This is not to say interesting articles weren't published, some by workshop participants, but we didn't affect the global response. We attributed our collective failure in part to few of us understanding what policymakers needed or few policymakers understanding what we had to offer. Our solution was to mix those interested in working together in a setting conducive to getting to know each other's needs and capabilities.

Five participants in this workshop were physicians, internists or pediatricians with infectious disease subspecialties. One was a health communicator, and the rest were more or less applied mathematicians. We range from population biologists – of which there were two – to at least one pure mathematician, who fortunately for us became interested in infectious diseases. Roughly a third staffed governmental or multi-governmental agencies and two-thirds were academicians. Finally, we were joined by three normaliens, students at the Ecole normale supérieure de Cachan and civil servant trainees (i.e., they have 10-year contracts with the State, which pays their salaries).

How modelers can help policymakers prepare for, and facilitate sound policy decisions during foreseeable health crises

John Glasser

"Modeling contributed little to policymaking during the last crisis because few of us understand that process and even fewer policymakers understand ours. I attended several SARS workshops, one right here. One could infer – from our presentations – we believed policymakers wanted to know what $\mathcal{R}_0$ was and if the equilibria of arbitrary models were locally, if not globally stable. As they actually needed help deciding what to do, we contributed very little to their global response.

“My own experience began well enough: Two CDC people asked me to evaluate quarantine. I made a model, estimated the biological parameters from the initial case series in Hong Kong, fit control parameters to hospital admissions, isolations, discharges and deaths during the outbreak in Singapore, and compared final sizes with proportion quarantined – isolated before they became ill – at its estimated value and zero. As these results differed by only a handful, I concluded the impact of quarantine was small. While correct, that was not the desired answer.

“In the outbreaks in Singapore and Taiwan, only 5% of probable SARS cases were quarantined. No matter how effective an intervention, if it misses the target 95% of the time, it cannot have much impact. By showing how much impact quarantine *could* have, modelers actually contributed to the problem - a) tens of thousands quarantined, at enormous social cost, b) persistent misunderstanding - versus solution. Why?

“It was difficult to tell who had been infected before they developed symptoms, especially given uncertainty about the mode of transmission. What could authorities have done instead? Because infected people were not particularly infectious until acutely ill – common knowledge now, but Dashun deduced it from only 30 days of hospital records – 1) encouraging people with prodromal symptoms to seek care, especially if they might have been exposed to someone since diagnosed, and helping 2) clinicians to diagnose and 3) infection-control personnel to isolate them effectively, would have had much greater impact.

“In the possibly nave belief that such results would have been more valuable in real time (e.g., *before* billions were spent on quarantine), we modeled a generic respiratory disease and interventions likely to be available, and Zhilan derived the reproduction number and took its partial derivatives with respect to control parameters. She is embedding such analytical results in a Mathematica™ notebook that could be used both with initial guesstimates and increasingly reliable estimates of the biological parameters. Her objective is to develop a tool that could help policymakers decide how to respond in the next crisis. We plan to revisit the SARS outbreaks and ask our EOC staff to evaluate a prototype in a simulated EID outbreak.

“I frankly don’t know how else to demonstrate what they have to offer, but other contributors to this session, if not workshop participants, surely will have other ideas.”

David Earn

Some time ago, given that vaccine distribution policies affect the threshold for elimination of diseases such as measles and polio, David wondered how he would implement them. In 1994, the UK conducted an expensive mass vaccination campaign to forestall a predicted measles epidemic due to susceptible adolescents and young adults. It is difficult to assess the benefit, especially as measles is endemic again in the UK now. Similarly, he interviewed people involved in the 2001 foot and mouth epidemic, and had difficulty determining if modeling had an impact via suggesting new or confirming the wisdom of existing ideas.

He was personally involved in the 2003 SARS outbreak in Toronto by a hospital administrator, who called and asked for help he was ill prepared to provide. He thought about why Toronto and why – once introduced – SARS spread. SARS was introduced to Toronto via travel patterns, after which it spread partly by virtue of a misdiagnosis due to co-morbidity and partly exceeding capacity of negative pressure rooms. This led him to think about the economics of surge capacity. If we knew what decisions would be required of policymakers during emergencies, we might be able to obtain the information we need to help in advance.

Fred Roberts

Fred was involved in TOPOFF3, but not as a modeler. In future exercises, modelers should design, participate and analyze. This exercise was highly controlled, without stochastic effects, flexibility in event course by virtue of choices made early on, $\cdots$, and participants identified the infectious agent long before they would have in reality (and just happened to have appropriate materials). As information was consistent, there was no chaos.

We could model how to transport people who might be infectious, food, materials, all while providing security. The most successful portable dispensary violated the rules (i.e., dispensed to a few people who went into the community and distributed). How could we determine if centralization or de-centralization would be best, who had the necessary information and how best to communicate with them? What if primary communications were disabled? Should we use the media as a back-up? Modeling could have improved this exercise.

In reality, there will be personnel as well as technical problems. Terrorists will use primary attacks as diversions and then attack the responders. In New Jersey, a "Preparedness College" is exploring these and other issues (e.g., dealing with uncertainty, communicating risk, $\cdots$). Isn't this exactly what video game designers do?

Simon Levin

Modelers could contribute by anticipating needs, detecting threats, designing stockpiles and infection-control wards, and exploring possible responses (e.g., quarantine and isolation). There are roles for detailed models of specific threats and generic ones that extract principles, for scenarios that lay out possible outcomes and for simulation trainers.

Agent-based models were useful in preparing for pandemic influenza (e.g., via MIDAS), but dimensionality must be reduced to make results more robust. We have put too much faith in untested assumptions. Bioterrorism is a game (i.e., terrorists respond to our responses), so we must adapt. Actions useful early on won't have any impact later.

Game theory is an under-exploited area, so a good way for modelers to contribute. Modelers can help to determine what information is needed, versus easily obtained, and some might be obtained in advance. Established inter-personal relations, partnerships, $\cdots$ will facilitate cooperation, but we'll be more helpful in preparing for crises than in responding.

We could help policymakers to develop better mental models. We cannot anticipate all data needed, so must be involved during crises. But effectiveness during depends on preparation. One way of establishing relationships is to help solve routine problems (e.g., design programs for new vaccines, and monitor to ensure policy goals are being met).

Spatial spread of pathogens (and policy implications, opportunities)

Julien Arino: Meta-population models: theory and an example

Julien discussed meta-population models for the spread of infectious diseases, mostly from a modeling versus theoretical point of view, showing what type of problems could be described with this tool. Then he presented a project on air traffic he is conducting with colleagues at Saint Michael's Hospital, in Toronto.

Steven Riley: Hedging against antiviral resistance during the next influenza pandemic using small stockpiles of an alternate chemotherapy

The effectiveness of single-drug interventions to reduce morbidity and mortality during the next influenza pandemic will be substantially weakened if transmissible strains emerge that are resistant to the stockpiled drugs. Steven used a multi-strain stochastic transmission model of influenza to show that the spread of antiviral drug resistance can be effectively reduced by deploying a small stockpile of a secondary drug during the early phase of local epidemics. He considered two alternative strategies for using the small secondary stockpile: early combination chemotherapy (ECC, individuals are treated with both drugs in combination while both are available); and sequential multi-drug chemotherapy (SMC, individuals are treated only with the secondary drug until exhausted and then with the primary drug). He investigated all potentially important regions of unknown parameter space and found that both ECC and SMC reduced the cumulative attack rate and the resistant attack rate unless the probability of emergence of resistance to the primary drug was so low that resistance was unlikely to be a problem or so high that resistance emerged as soon as primary drug monotherapy began. He extended his model using flight volume data between 105 large cities to investigate the robustness of these resistance-limiting strategies on a global scale. Intriguingly, so long as populations that were the main source of resistant strains employed these strategies (SMC or ECC), those same strategies were also effective for populations far from the source even when some intermediate populations failed to control resistance (by implementing monotherapy). In essence, the interconnectedness of the global network dampened the international spread of resistant strains with its many wild-type epidemics. His results demonstrate that the augmentation of existing stockpiles of oseltamivir with smaller stockpiles of a second drug would be an effective and inexpensive epidemiological hedge.

Michael Johansson: Spatio-temporal dynamics of dengue

When and where will outbreaks happen? Periodicity may be due to weather, host immunity, interaction among serotypes (e.g., replacement), or viral evolution. In Thailand, population centers are supposed to drive multi-annual periodicity, whereas it seems to be weather in Puerto Rico (e.g., temperature in rainy areas and rainfall in dry ones). What data are needed and how should we analyze them (e.g., Morlet wavelets)?

Pauline van den Driessche: Spatial heterogeneity: meta-population disease models

Pauline motivated modeling spatial phenomena and focused on mathematics for discrete spaces, meta-population SEIR models in particular. She derived some mathematical results, added biological details as needed for specific problems and considered their implications.

Mathematical epidemiology for policymakers (what they need to know to understand the literature, collaborate with modelers)

Fred Brauer

Fred gave a brief description of the MITACS-PIMS summer schools on modeling of infectious diseases in Banff (2004), Toronto (2006), and Edmonton (2008). The goals of these schools were to introduce mathematical modeling of infectious diseases to mixed groups of students from mathematical and health sciences with the hope of encouraging epidemiologists to appreciate modeling. A central part of these programs is the development and study of models by mixed groups, with some students trained in mathematics and others epidemiology. The material in the schools was quite mathematical, using calculus and qualitative properties of ordinary differential equations.

Christophe Fraser

The Imperial College course is designed for a widening array of public health practitioners. We introduce the simple models, show how they relate to more complex ones, and emphasize parameter estimation and case studies. Our goal is to make students intelligent collaborators and consumers of models. We developed the “MRC Centre for Outbreak Analysis and Modeling” to formalize ad hoc work begun with former students. PhD students and post-docs trained in biology are the best teachers because they concentrate on ‘why’ versus ‘how.’

Linda Gao

Linda described challenges of communicating to her college emergency response committee and county ER coordinator how models can help with decision-making in times of crisis.

Other crises (dengue, malaria, polio, global warming)

Jim Alexander: Residual issues in polio eradication that might be amenable to modeling

Achieving and maintaining elimination despite outbreaks of wild or vaccine-derived strains are the main issues. OPV and IPV both have roles in polio eradication.

Ellis McKenzie: Malaria models and intervention policies: history and prospects

In the century since Ross published the first mathematical model of malaria, models developed to inform research and intervention programs have met with varying degrees of success. The modeling enterprise has grown from relatively simple analytic systems to vast individual-based simulations, but basic questions remain about how biological knowledge can be incorporated and biological unknowns addressed at appropriate, useful scales. These questions will be increasingly critical as models begin to encompass operational, economic and other factors, to become multi-disciplinary tools meant to inform policy decisions and to guide investment in and implementation of interventions. Lessons from past experience, and from a recent example, can help modelers address these challenges.

Heterogeneous transmission by setting (e.g., households) or activity (e.g., age groups) and intervention targeting

Frank Ball: Vaccination and intervention strategies for epidemics among a population of households

Frank gave a brief introduction to models for epidemics among a population of households, then spoke about vaccination schemes that are implemented in advance of outbreaks, deriving optimal such schemes, and finally described some more recent work in which vaccination (and other intervention strategies) takes place in response to detected cases in households.

Christophe Fraser: Modeling household transmission for historical and future epidemics

Households play an important role in disease transmission and should be considered when designing public health responses. Christophe described some historical models, mathematical and mechanical, used to simulate epidemics in populations of households. He derived some methods for estimating household reproduction numbers in emerging infections, and showed some applications to influenza. He also introduced some inequalities that help determine the magnitude of biases in simple models that ignore household heterogeneities.

Gabriela Gomes (discussion of the utility of GripNet for influenza modeling)

Jamie Lloyd-Smith: Disease invasion dynamics in spatially heterogeneous populations

Spatial structure in human and animal populations often can be represented by subpopulations or patches with individuals moving among them. Typically there is some degree of heterogeneity among patches that may influence transmission dynamics. Jamie discussed stochastic models addressing the influence of spatial structure and heterogeneity on the invasion of infectious diseases, focusing on between-patch movement rates.

Lorenzo Pellis: SIR epidemics in socially structured populations - presence of households and workplaces

Lorenzo presented a stochastic model for the spread of an SIR disease in a fully susceptible population with a social structure characterized by the presence of households and workplaces. He recalled a previously defined threshold parameter, and defined a new household-to-household reproduction number, R_H. Among other properties, it is related to a secure vaccination coverage (i.e., proportion of households whose vaccination reduces R_H and other reproduction numbers at least to 1, if not below).

James Watmough (discussion of impact of detail included in infectious disease models on our advice to decision-makers)

Engaging policymakers (what they really want from modelers)

Jen-Hsiang Chuang: Engaging policymakers - what they really want from modelers

At the Center for Disease Control in Taiwan, we increasingly desire transmission models constructed for emerging infections such as pandemic influenza, re-emerging infections such as HIV/AIDS, tuberculosis, dengue fever and enterovirus, and vaccine-preventable diseases such as chickenpox and seasonal influenza. We want models constructed using our observations 1) to evaluate or simulate the impact of certain policies in Taiwan (such as harm reduction strategies and needle exchange programs for intravenous drug users to reduce HIV transmission), 2) to predict the impact of epidemics (such as the peak size of enterovirus epidemics and estimating the number of patients with severe complications) on the healthcare system, and 3) to simulate the impacts of different control policies for newly emerging diseases (such as school or class closure policies for enterovirus or vaccinating children against enterovirus 71 should a vaccine become available).

It is important for policymakers to understand modelers' approaches and key assumptions. Yet modelers typically publish complex and possibly irrelevant information, or simply "black boxes", without explaining their main ideas. To facilitate policymakers' understanding of modelers' approaches and findings, a set of general guidelines (e.g., a publication requirements checklist) should be formulated as a universal reference for modeling publications. This would ensure consistently high standards in the practice of infectious disease modeling and allow policymakers to make better use of modelers' findings.

In addition, policymakers may not be able to determine the quality and validity of a modeling paper after reading through it. Therefore, an evaluation methodology should be developed to aid in assessing modeling papers. Evidence-based medicine (EBM) has been adopted by major international medical journals, which applying strict criteria to determine the quality and validity of clinical research. In studies using EBM strategies, the key details are summarized in a concise yet informative abstract accompanied by expert commentary on the clinical applications of the studies. The EBM approach could be used to assess modeling papers to help policymakers determine the quality and validity of such studies.

Lastly, a registry for documenting mathematical epidemiology studies would provide a comprehensive collection accessible to all involved in public health decision-making at the click of a mouse. Thus, it is useful to set up a database that can be searched systematically to allow policymakers to find studies most relevant to their interests.

Richard Hatchett: Inexact science and the development of public health emergency preparedness policy

In February of 2007, the US Centers for Disease Control and Prevention (CDC) released its Interim Prepandemic Planning Guidance: Community Strategy for Pandemic Influenza Mitigation in the United States - Early, Targeted, Layered Use of Nonpharmaceutical Interventions, culminating a year-long policy development process that incorporated insights derived from computational models, close scrutiny of historical data, and inductive reasoning from incomplete observational data about the "microdynamics" of pandemic and seasonal influenza. Richard coordinated computational modeling of various pandemic influenza mitigation strategies by National Institute of General Medical Sciences grantees, as recently described (PNAS 2008;105:4639-44), and analyzed the efficacy of non-pharmaceutical interventions in selected U.S. cities during the 1918 influenza pandemic (PNAS 2007;104:7582-7). This analytical work was augmented by an extensive survey of the scientific literature concerning the epidemiology and population dynamics of influenza, interviews with influenza experts, and socialization of the proposed response strategy through a variety of outreach and focus group meetings. The development of the community mitigation strategy for pandemic influenza illustrates how insights about the population dynamics of a contagious pathogen may inform the development of emergency preparedness and response plans and more generally, how scientific data and hypotheses must be balanced against other considerations in the development of public policy.

Compartmental vs. network or individual-based modeling (indications for each approach)

Gerardo Chowell: Signatures of non-homogeneous mixing in disease outbreaks

Despite its simplifying assumptions, SEIR-type models continue to provide useful insights and predictive capability. However, non-homogeneous mixing models such as those for social networks are often assumed to provide better predictions of the benefits of various mitigation strategies such as isolation or vaccination. In practice, it is rarely known to what extent SEIR-type models will adequately describe a given population. Gerardo's goal was to evaluate possible retrospective signatures of non-homogeneous mixing. Each signature evaluated the goodness of fit of SEIR-type model predictions to actual epidemics. For example, the extent of agreement between the observed and predicted final outbreak sizes based on reproduction number estimates arising from fitting various portions of the epidemic curve are possible signatures. On the basis of simulated outbreaks, he concluded that such signatures could detect non-SEIR-type behavior in some but not all social structures considered.

Markus Schwehm: Integration of compartmental and individual-based models

At ExploSYS, we have implemented two models for pandemic influenza. InfluSim is a compartmental model used by several health care agencies worldwide for pandemic influenza preparedness planning. SimFlu is an individual- and network-based model with more detailed intervention options. Both models have different purposes - while the compartmental model can evaluate general interventions like treatment and social distancing, the individual-based model can evaluate containment strategies at the beginning of an outbreak. In this contribution, we will present an integrated approach. Consider a large sub-population like the employees of a company or soldiers in a military unit. The subgroup will inevitably have contact with the pandemic ongoing in the outside population. To optimally protect them from the pandemic, it is possible to execute individually targeted interventions within the subgroup. The resulting model consists of a compartmental model for the outside population and an individual- and network-based model within the subgroup.

Da-Wei Wang: Efficiently implementing programs for individual-based models

Da-Wei discussed an approach to individual-based modeling with he has attained performance via desktop computers exceeding that attained via super-computers elsewhere.

Ping Yan: Unifying statistical inference and mathematical compartment models

Among mathematical models of infectious disease, compartment models account for biological and environmental as well as clinical aspects. The number of parameters tends to be large and all may not be identifiable from the same data. Therefore, parameters are often assigned based on other studies. To be mathematically tractable, many models implicitly assume time durations between pairs of successive events in the system are exponentially distributed. Models with non-exponential distributions are more realistic, but involve systems of Volterra renewal type integro-differential equations. Not only do they introduce more parameters that make fitting models to data even more challenging, but also involve convolution terms that increase the difficulty of assessing parameters statistically. On the other hand, statistical models are designed from observations of the system. They have fewer parameters. They tend to focus on one or few specific aspects of the system instead of the whole system with the focus on fitting models to data and short term predictions. Parameters also may be detached from any biological meaning.

These two approaches are regarded by many as different paradigms rather than a continuous modeling spectrum. Ping presented some ideas of using statistical inferences to build compartment models and then estimate the parameters in a single analysis based on data from a typical outbreak. He used some past experience from the SARS outbreaks to highlight data typically collected at the beginning and during outbreaks. A key difficulty to unifying statistical inference and compartment models is the gap between what are usually observable (i.e., incubation period, clinical serial interval) in statistical inferences and what are usually not observable in compartment models, durations based on infectiousness (e.g., latent and infectious periods). To overcome this difficulty, one needs to break down the observable time intervals, such as the incubation period into the latent period and a portion of the infectious period. This involves the de-convolution of terms in the integro-differential equations.

Ping demonstrated successful application to a mumps outbreak that took place in a post-secondary institution in eastern Canada between February 2007 and 2008. The model structure and disease transmission parameters are determined from statistical inferences. Sensitivity analyses are conducted for the environment, such as (i) the initial proportion of infected individuals in the population and (ii) the average number of new susceptible people joining the "currently" susceptible population per time unit.

Evolution in response to host defenses, newly available hosts

In this session, we discussed questions relating to the challenges for public health of pathogen adaptation to host interventions. In particular, we focused on the evolution of antimicrobial resistance in response to treatment, consequences for the control of influenza and pandemic planning, and the evolutionary response of pathogens to large scale vaccination programs. We discussed what the most urgent research questions that can be approached using mathematical modeling were and what modeling approaches and techniques might be needed.

Troy Day: Evolution in response to public health interventions

Troy discussed a few of the best-available examples of pathogen evolution in response to vaccination, and highlighted some of the unanswered empirical question involved. He then considered how one might model the evolutionary consequences of interventions more generally, both for endemic diseases and for newly emerging pathogens. This latter part focused on influenza, and highlighted many of the challenges, both from a modeling standpoint, and from the standpoint of connecting such models to data.

Zhilan Feng: Effects of antiviral use on epidemics of influenza and resistance

To explore influenza medication strategies (prophylaxis, post-exposure medication and treatment at successive clinical stages) that may affect evolution of resistance (select for resistant strains or facilitate their subsequent spread), Zhilan elaborated a published transmission model. Then she derived the reproduction numbers of sensitive and resistant strains, peak and final sizes, and time to peak. These analytical results permit her to a) deduce the consequences vis--vis resistance evolution of planned medication strategies and b) explore others that might better attain policy goals (i.e., without compromising the future effectiveness of anti-viral medications).

She described the published model briefly and our elaboration in detail, highlighting features that explain why important results differ. While reproduction numbers are very complex expressions in models with multiple infectious stages, she described hers intuitively. And then she demonstrated Mathematica notebooks that illustrate these and other analytical results. Before using those tools to explore the implications vis--vis control and resistance of various medication strategies, she wishes to consult subject matter experts and policymakers to ensure she has represented the biology correctly and understands the policy issues.

Gabriela Gomes (Variant surface antigen repertoires of *Plasmodium falciparum* shaped by within-host competition and between-host transmission)

Mirjam Kretzschmar: Effects of long term vaccination and adaptation of pathogens: the example of pertussis

Mirjam described a model of the Dutch hypothesis for the resurgence of pertussis throughout the developed world, but particularly in the Netherlands, namely selection by vaccination for strains against which the vaccine is ineffective.

Rongsong Liu: Control strategies in a two-strain influenza model

Rongsong considered optimal medication strategies (fraction treated, timing of treatment given a fixed amount of drugs) in a model with drug sensitive and resistant strains.

Jamie Lloyd-Smith: Challenges in modeling pathogen adaptation

In this talk, Jamie aimed to raise general questions about how to incorporate adaptive evolution into models of pathogen transmission dynamics, such as: "How should we think about 'fitness landscapes' for pathogens in the context of transmission models? "How can we cope with the multiple scales of pathogen fitness that are relevant? "What data do we need to construct, parameterize and validate these models?"

Dashun Xu: An age-structured influenza model with a resistant strain

Dashun derived the reproduction numbers of sensitive and resistant strains in an age-structured model with prophylaxis, post-exposure medication, and treatment, and considered the impact of medication timing on control and evolution of resistance.

Adapting modeling approaches to problems

Mac Hyman

Mac related an experience in which solving a practical public health problem required increasingly complex models. But he began with a simple model and added complexity only as indicated by comparison of predictions and observations. This was refreshing in view of the extremely complex and untested, if testable individual-based models used for problems that could be addressed via simpler models.

Game theory and applications to decision-making about health

Simon Levin: Games and more

Simon argued that theories of games and human behavior will play an increasing role in disease modeling. Tightening feedback via local control can enhance cooperation (and coexistence), or foster greed and selfish behavior. Social norms are needed to reinforce collectively beneficial human behavior vis-à-vis health-care, including in emergency situations. Health-care involves games between physicians, patients, hospitals, HMOs and insurers, pharmaceutical companies, and multiple social systems. There are n-player games (e.g., anti-biotic resistance, hospital size and prevalence of nosocomial infections) and public goods games (individuals acting in their self-interest without accounting for social costs).

Eun-ha Shim: Antiviral intervention during pandemic influenza

Eunha studied the optimal level of drug use from individual and community perspectives. As these differ, she investigated the possible role of individual perception. She found that people overestimate the risk of infection, underestimate the efficacy of antiviral drugs for prophylaxis and treatment, and overestimate the risk of developing resistance. These discrepancies can be reduced by education.

Immunoepidemiology (how disparate individual immune responses affect epidemiological patterns)

Jonathan Dushoff: Immuno-epidemiology and policy

Jonathan discussed epidemiological models (e.g., dose-response, partial immunity, and cross-immunity), thresholds for disease elimination, and the relationship between acquired immunity and tendency to oscillate. In conceptual modeling, we start with assumptions, construct formal models, and analyze them, possibly deriving insights (e.g., if sub-populations are relatively isolated and have high risks of infection, disease will be harder to eliminate unless we focus on most vulnerable populations). But we must interpret them biologically. If we cannot explain conceptual results in simple terms, we should mistrust our models. Can acquired immunity lead to backward bifurcations and, if so, what are the implications for malaria endemism and eradication? It depends on whether asymptomatic cases spread more or less than symptomatic ones. Does chemotherapy (which prevents development of immunity) change this? If so, on what time-scale might a changeover occur?

Christophe Fraser: Transmission of influenza in households during the 1918 pandemic

Christophe described several household models fitted to newly unearthed data from the 1918 pandemic in Maryland. Two striking features of the best fitting model are absence of asymptomatic infections and prior immunity (22%) decreased final attack rate from 60 to the observed 25%. Estimates of the infectiousness of influenza that do not account for prior immunity are too low. However, his analyses do not account for age or under-reporting.

Jamie Lloyd-Smith: The influence of heterogeneity in host immune competence on pathogen emergence

Hosts with weakened immune systems are often posited to act as stepping stones for pathogen emergence. Such hosts have increased susceptibility to infection and altered clinical courses of disease, often showing higher viral loads or prolonged infections. Jamie presented theoretical work exploring the influence of heterogeneous host immunocompetence on the evolutionary emergence of novel pathogens. He addressed the idea that immunocompromised hosts with prolonged infections can act as incubators for viral diversity, and discuss implications of these models for pathogen surveillance and control.

Policy needs (how modelers can assist in meeting institutional obligations)

Lance Rodewald (CDC)

Lance described some of the many opportunities for modeling in our routine work (e.g., strengthening ACIP recommendations, deciding how much vaccine to stockpile, assessing the economic value of public health programs, and the impact of school laws).

Diane Simpson (CDC)

Diane explored our obligations to various constituencies. Health authorities want help projecting the time-course of crises, identifying critical triggers and gates, and determining their need for resources and extraordinary authority. They may also want recommendations for allocating pharmaceuticals or implementing non-pharmaceutical interventions (e.g., quarantine, school closures, $\cdots$). Political leaders want help understanding crises, determining their seriousness, deciding how to allocate resources, and if and when to request help or use extraordinary measures. Medical practitioners want to know how patient care will be affected and what prevention and treatment to recommend. The media want accurate and timely information and credible viewpoints (they might juxtapose to create controversy). The public wants to be kept informed about likely outbreak size, how fast it may spread and where resources are best located. They expect health authorities to use those resources proactively. Likely challenges are competing modelers and other experts, and fixation on quantitative versus qualitative predictions (i.e., policymakers don't want confidence intervals).

Richard Hatchet (NIH)

This workshop is a model for how to engage policymakers. 1) Market and frame results. Some people can enjoy symphonies on paper, but most need to hear them played. 2) Engage and sustain relationships with policymakers, who will be interested in infectious disease dynamics insofar as insights are translated into possible actions. If you reach out (i.e., convince them that modeling can provide insights), they will listen. Offer diverse solutions to the problems confronting them. 3) Consider feasibility constraints, be an engineer versus scientist. The logistics may not be fascinating intellectually, but they are essential for the formulation of sound policy. The wind is in your sails.

Lara Wolfson (WHO): Modelers and modeling in global public health - present and future

Lara described models that have been used for various purposes at the WHO and some of the trade-offs between requirements of more complex models, the accuracy of readily available data, and the cost of better data, if indeed they could be collected. She also described why we need to learn to admit errors and to represent our results as educated guesses versus truth.

List of Participants

Alexander, Jim (US Centers for Disease Control and Prevention)
Arino, Julien (University of Manitoba)
Ball, Frank (University of Nottingham)
Brauer, Fred (University of British Columbia)
Chowell, Gerardo (Arizona State University)
Chuang, Jen-Hsiang (Centers for Disease Control Taiwan)
Day, Troy (Queens University)
Dushoff, Jonathan (McMaster University)
Earn, David (McMaster University, Department of Mathematics & Statistics)
Feng, Zhilan (Purdue University)
Fraser, Christophe (Imperial College of Science, Technology & Medicine)
Galvani, Alison (Yale University)
Gao, Linda (North Central College)
Glasser, John (US Centers for Disease Control and Prevention)
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Chapter 27

Analytic Tools in Computational Complexity (08w5094)

Aug 03 - Aug 08, 2008

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

An important development in the study of computational complexity has been increased role of analytic methods. Fourier analysis has become an essential tool of the field, playing a critical role in the study of interactive proofs, the computational hardness of approximation problems, and the learnability of Boolean functions. The notion of Gowers uniformity (which was introduced by Gowers to give an analytic proof of Szemeredi's theorem on arithmetic progressions, and whose use can be viewed as "generalized Fourier analysis") has also been recently employed in the context of Probabilistically Checkable Proofs and hardness of approximation. A new paradigm in computational complexity is beginning to emerge, which involves reducing high dimensional discrete problems that arise in the study of Boolean functions to high dimensional continuous problems and then applying analytic methods to the resulting continuous problems.

Presentation Highlights

Avi Wigderson gave a tutorial on many applications of partial derivatives in complexity. Alexander Sherstov gave a tutorial on the matrix sign rank, which has found so many recent applications to communication complexity lower bounds.

In addition to these two tutorials, the workshop had a great number of excellent results presented. One of the most exciting results presented at the workshop was by Zeev Dvir, giving a simple and elegant solution to the finite-field version of Kakeya Conjecture (with an application to pseudorandomness).

However, Dvir's presentation was just one out of a large number of exciting new developments in computational complexity. The following is a summary of the presented results, grouped by topic.

PCPs

SUBHASH KHOT, **Inapproximability of NP-complete Problems, Discrete Fourier Analysis, and Geometry**

This talk is an overview of some recent results on inapproximability of NP-complete problems and their connections to discrete Fourier analysis and isoperimetric problems.

DANA MOSHKOVITZ, **Two-Query PCP with Sub-Constant Error** (based on joint work with Ran Raz)

We show that the NP-Complete language 3Sat has a PCP verifier that makes two queries to a proof of almost-linear size and achieves sub-constant probability of error $o(1)$. The verifier performs only projection tests, meaning that the answer to the first query determines at most one accepting answer to the second query.

Previously, by the parallel repetition theorem, there were PCP Theorems with two-query projection tests, but only (arbitrarily small) constant error and polynomial size. There were also PCP Theorems with sub-constant error and almost-linear size, but a constant number of queries that is larger than 2.

As a corollary, we obtain a host of new results. In particular, our theorem improves many of the hardness of approximation results that are proved using the parallel repetition theorem. A partial list includes the following:

1. 3Sat cannot be efficiently approximated to within a factor of $7/8 + o(1)$, unless $P = NP$. This holds even under almost-linear reductions. Previously, the best known NP-hardness factor was $7/8 + \epsilon$ for any constant $\epsilon > 0$, under polynomial reductions (Hastad).

2. 3Lin cannot be efficiently approximated to within a factor of $1/2 + o(1)$, unless $P = NP$. This holds even under almost-linear reductions. Previously, the best known NP-hardness factor was $1/2 + \epsilon$ for any constant epsilon¿0, under polynomial reductions (Hastad).

3. A PCP Theorem with amortized query complexity $1 + o(1)$ and amortized free bit complexity $o(1)$. Previously, the best known amortized query complexity and free bit complexity were $1 + \epsilon$ and ϵ, respectively, for any constant $\epsilon > 0$ (Samorodnitsky and Trevisan).

4. Clique cannot be efficiently approximated to within a factor of $n^{1-o(1)}$, unless $ZPP = NP$. Previously, a hardness factor of $n^{1-\epsilon}$ for any constant $\epsilon > 0$ was known, under the assumption that $P = NP$ does not hold (Hastad and Zuckerman).

One of the new ideas that we use is a new technique for doing the composition step in the (classical) proof of the PCP Theorem, without increasing the number of queries to the proof. We formalize this as a composition of new objects that we call Locally Decode/Reject Codes (LDRC). The notion of LDRC was implicit in several previous works, and we make it explicit in this work. We believe that the formulation of LDRCs and their construction are of independent interest.

RAN RAZ, **A Counterexample to Strong Parallel Repetition**

I will give a short introduction to the problem of parallel repetition of two-prover games and its applications to theoretical computer science, mathematics and physics. I will then describe a recent counterexample to the strong parallel repetition conjecture (a conjecture that would have had important applications).

The parallel repetition theorem states that for any two-prover game, with value $1-\epsilon$ (for, say, $\epsilon < 1/2$), the value of the game repeated in parallel n times is at most $(1-\epsilon^3)^{\Omega(n/s)}$, where s is the answers' length (of the original game). Several researchers asked whether this bound could be improved to $(1-\epsilon)^{\Omega(n/s)}$; this question is usually referred to as the strong parallel repetition problem. A positive answer would have had important applications. We show that the answer for this question is negative.

More precisely, we consider the *odd cycle game* of size m; a two-prover game with value $1-1/2m$. We show that the value of the odd cycle game repeated in parallel n times is at least $1-(1/m)\cdot O(\sqrt{n})$. This implies that for large enough n (say, $n \geq \Omega(m^2)$), the value of the odd cycle game repeated in parallel n times is at least $(1-1/4m^2)^{O(n)}$.

Thus:

1. For parallel repetition of general games: the bounds of $(1-\epsilon^c)^{\Omega(n/s)}$ given in [4, 2] are of the right form, up to determining the exact value of the constant $c \geq 2$.
2. For parallel repetition of XOR games, unique games and projection games: the bounds of $(1-\epsilon^2)^{\Omega(n)}$ given in [1] (for XOR games) and in [3] (for unique and projection games) are tight.
3. For parallel repetition of the odd cycle game: the bound of $1-(1/m)\cdot\tilde{\Omega}(\sqrt{n})$ given in [1] is almost tight.

A major motivation for the recent interest in the strong parallel repetition problem is that a strong parallel repetition theorem would have implied that the *unique game conjecture* is equivalent to the NP hardness of distinguishing between instances of Max-Cut that are at least $1-\epsilon^2$ satisfiable from instances that are at most $1-(2/\pi)\cdot\epsilon$ satisfiable. Our results suggest that this cannot be proved just by improving the known bounds on parallel repetition.

ANUP RAO, **Rounding Parallel Repetitions of Unique Games** (based on joint work with Boaz Barak, Moritz Hardt, Ishay Haviv, Oded Regev and David Steurer).

We show a connection between the semidefinite relaxation of a unique game and its behavior under parallel repetition. Specifically, denoting by $val(G)$ the value of a two-prover unique game G, and by $sdpval(G)$ the value of a natural semidefinite program to approximate $val(G)$, we prove that for every l, if $sdpval(G) \geq 1-\delta$, then $val(G^l) \geq 1-O(\sqrt{l\delta(\log k - \log\delta)})$. Here, G^l denotes the l-fold parallel repetition of G, and k denotes the alphabet size of the game. For the special case where G is an XOR game (i.e., $k=2$), we obtain the bound $1-O(\sqrt{l\delta})$. For games with a significant gap between the quantities $val(G)$ and $sdpval(G)$, our result implies that $val(G^l)$ may be much larger than $val(G)^l$, giving a counterexample to the strong parallel repetition conjecture.

In a recent breakthrough, Raz has shown such an example using the max-cut game on odd cycles. Our results are based on a generalization of his techniques.

RYAN O'DONNELL, **Zwick's Conjecture is implied by most of Khot's Conjectures** (based on joint work with Yi Wu)

In 1998 Zwick proved that $P = naPCP_{1,5/8}(O(\log n), 3)$ and conjectured that $naPCP_{1,5/8+\epsilon}(O(\log n), 3) = NP$ for all $\epsilon > 0$. Hastad's contemporary result $NP = naPCP_{1,3/4+\epsilon}(O(\log n), 3)$ was not improved until 2006, when Khot and Saket lowered the $3/4$ to $20/27$. We prove Zwick's $5/8$ Conjecture, assuming Khot's "d-to-1 Conjecture" for any constant d. The necessary Long Code testing analysis uses a mix of older (Hastad-type) and new (Mossel-type) ideas.

GUY KINDLER, **Can cubic tiles be sphere-like?** (based on joint work with Ryan O'Donnell, Anup Rao, and Avi Wigderson)

The unit cube tiles R^d by Z^d, in the sense that its translations by vectors from Z^d cover R^d. It is natural to ask what is the minimal surface area of a body that tiles R^d by Z^d. The volume of any such body should clearly be at least 1, and therefore its surface area must be at least that of a unit volume ball, which of order $\sqrt{d}$. The surface area of the cube, however, is of order d, and no better tiling was known. In this work we use a random construction to show that the optimal surface area is indeed of order $\sqrt{d}$, namely there exist bodies that tile R^d as a cube would, but have sphere-like surface areas.

Tiling problems were considered for well over a century, but this particular tiling problem was also recently considered in computer science because of its relations with the Unique Games conjecture and with the Parallel Repetition problem. Indeed, our current result follows from the same idea that was used recently by Raz in his counter example for the strong Parallel Repetition conjecture.

Quantum computation

ODED REGEV, **Unique Games with Entangled Provers are Easy** (based on joint work with Julia Kempe and Ben Toner)

We consider one-round games between a classical verifier and two provers who share entanglement. We show that when the constraints enforced by the verifier are "unique" constraints (i.e., permutations), the value of the game can be well approximated by a semidefinite program. Essentially the only algorithm known previously was for the special case of binary answers, as follows from the work of Tsirelson in 1980. Among other things, our result implies that the variant of the unique games conjecture where we allow the provers to share entanglement is false. Our proof is based on a novel "quantum rounding technique", showing how to take a solution to an SDP and transform it to a strategy for entangled provers.

SCOTT AARONSON, **How To Solve Longstanding Open Problems In Quantum Computing Using Only Fourier Analysis**

I'll discuss some simple-looking conjectures in Fourier analysis of Boolean functions which, if proved, would lead to breakthrough results in quantum complexity theory. These potential breakthroughs include an oracle relative to which BQP is not in the polynomial hierarchy, and the impossibility of a random oracle separation between BPP and BQP. I'll also discuss the partial progress that I and others have been able to make toward resolving these conjectures.

Communication complexity

ALEXANDER SHERSTOV, **The Sign-Rank of** AC^0 (based on joint work with Alexander Razborov)

We prove that $\Sigma_2^{cc} \not\subseteq UPP^{cc}$, thereby solving a long-standing open problem in communication complexity posed by Babai, Frankl, and Simon (1986).

In more detail, the sign-rank of a matrix $M = [M_{ij}]$ with $+/-1$ entries is defined as the least rank of a real matrix $A = [A_{ij}]$ with $M_{ij}A_{ij} > 0$ for all i, j. We prove a lower bound of $2^{\Omega(m)}$ on the sign-rank of the matrix $[f(x,y)]_{x,y}$, where $f(x,y) = \bigwedge_{i=1}^{m} \bigvee_{j=1}^{m^2} (x_{ij} \wedge y_{ij})$. This is the first exponential lower bound on the sign-rank of AC^0, and it immediately implies the separation $\Sigma_2^{cc} \not\subseteq UPP^{cc}$.

Our result additionally implies a lower bound in learning theory. Specifically, let $\phi_1, \ldots, \phi_r : \{0,1\}^n \to R$ be functions such that every DNF formula $f : \{0,1\}^n \to \{+1,-1\}$ of polynomial size has the representation $f = sign(a_1 * \phi_1 + \cdots + a_r * \phi_r)$ for some reals $a_1, \ldots, a_r$. We prove that then $r > 2^{\Omega(n^{1/3})}$, which essentially matches an upper bound of $2^{\tilde{O}(n^{1/3})}$ 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 substantially generalizes and strengthens the results of Krause and Pudlak (1997).

PAUL BEAME, **Multiparty Communication Complexity of** AC^0 (based on joint work with Dang-Trinh Huyuh-Ngoc)

We prove non-trivial lower bounds on the multiparty communication complexity of AC^0 functions in the number-on-forehead (NOF) model for up to $\Theta(\sqrt{\log n})$ players. These are the first lower bounds for any AC^0 function for $\omega(\log\log n)$ players. In particular we show that there are families of depth 3 read-once AC^0 formulas having k-player randomized multiparty NOF communication complexity $n^{\Omega(1/k)}/2^{O(k)}$. We show similar lower bounds for depth 4 read-once AC^0 formulas that have nondeterministic communication complexity $O(\log^2 n)$, yielding exponential separations between k-party nondeterministic and randomized communication complexity for AC^0 functions. As a consequence of the latter bound, we obtain a $2^{\Omega(\log^1 /2n/k^1 /2)-k}$ lower bound on the k-party NOF communication complexity of set disjointness. This is non-trivial for up to $\Theta(\log^{1/3} n)$ players which is significantly larger than the up to $\Theta(\log\log n)$ players allowed in the best previous lower bounds for multiparty set disjointness.

New directions

MADHU SUDAN, **Towards Universal Semantic Communication** (based on joint work with Brendan Juba)

Is it possible for two intelligent players to communicate meaningfully with each other, without any prior common background? What does it even mean for the two players to understand each other? In addition to being an intriguing question in its own right, we argue that this question also goes to the heart of modern communication infrastructures, where misundestandings (mismatches in protocols) between communicating players are a major source of errors. We believe that questions like this need to be answered to set the foundations for a robust theory of (meaningful) communication.

In this talk, I will describe what computational complexity has to say about such interactions. Most of the talk will focus on how some of the nebulous notions, such as intelligence and understanding, should be defined in concrete settings. We assert that in order to communicate "successfully", the communicating players should be explicit about their goals – what the communication should achieve. We show examples that illustrate that when goals are explicit the communicating players can achieve meaningful communication.

BOAZ BARAK, **Public Key Cryptography from Different Assumptions** (based on joint work with Avi Wigderson)

We construct a new public key encryption based on two assumptions:

1. One can obtain a pseudorandom generator with small locality by connecting the outputs to the inputs using any sufficiently good unbalanced expander.
2. It is hard to distinguish between a random graph that is such an expander and a random graph where a (planted) random logarithmic-sized subset S of the outputs is connected to fewer than $|S|$ inputs.

The validity and strength of the assumptions raise interesting new algorithmic and pseudorandomness questions, and we explore their relation to the current state-of-art.

Pseudorandomness and explicit combinatorial constructions

ZEEV DVIR, **The finite field Kakeya conjecture and applications to the construction of mergers and extractors** (joint work with Avi Wigderson)

A Kakeya set in F^n, where F is a finite field, is a set containing a line in every direction. The finite field Kakeya conjecture states that the size of such sets is bounded from below by $C_n * |F|^n$, where C_n depends only on the dimension n.

The interest in this problem came first from Mathematics as a finite field analog of the famous Euclidean Kakeya problem and later from Computer Science as a problem related to explicit constructions of mergers and extractors.

I will talk about the recent proof of this conjecture (Dvir 2008) and its application to the construction of mergers and extractors (Dvir & Wigderson 2008).

SHACHAR LOVETT, **Worst case to average case reductions for polynomials** (based on joint work with Tali Kaufman)

A degree-d polynomial p in n variables over a field F is equidistributed if it takes on each of its $|F|$ values close to equally often, and biased otherwise. We say that p has a low rank if it can be expressed as a bounded combination of polynomials of lower degree. Green and Tao (2007) have shown that bias imply low rank over large fields (i.e. for the case $d < |F|$). They have also conjectured that bias implies low rank over general fields. In this work we affirmatively answer their conjecture. Using this result we obtain a general worst case to average case reductions for polynomials. That is, we show that a polynomial that can be approximated by few polynomials of bounded degree, can be also exactly computed by few polynomials of bounded degree. We derive some relations between our results to the construction of pseudorandom generators.

EMANUELE VIOLA, **Hardness amplification proofs require majority** (based on joint work with Ronen Shaltiel)

Hardness amplification is a major line of research that mainly seeks to transform a given lower bound (e.g. a function that has correlation at most 99% with small circuits) into a strongly average-case one (i.e. a function that has negligible correlation with small circuits). Strongly average-case lower bounds are of central importance in complexity theory and in particular are necessary for most cryptography and pseudorandom generators.

In this work we show that standard techniques for proving hardness amplification against a class of circuits require that same class of circuits to compute the Majority function.

Our work is most significant when coupled with the celebrated "natural proofs" result by Razborov and Rudich (J. CSS '97) and Naor and Reingold (J. ACM '04), which shows that most lower-bounding techniques cannot be applied to circuits that can compute Majority. The combination of our results with theirs shows that *standard techniques for hardness amplification can only be applied to those circuit classes for which standard techniques cannot prove circuit lower bounds*. This in particular explains the lack of strong average-case lower bounds for a number of circuit classes for which we have lower bounds.

Our results also show a qualitative difference between the direct product lemma and Yao's XOR lemma, and they give tight bounds on the number of queries needed for hardness amplification.

RONEN SHALTIEL, **Unconditional weak derandomization of weak algorithms: Explicit versions of Yao's Lemma**

The (easy direction) of Yao's minmax lemma says that if there is a randomized algorithm A which solves some problem (meaning that for every input, A succeeds with high probability) then there is a deterministic algorithm B of "roughly the same complexity" that solves the problem well on average (meaning that B succeeds with high probability on a random input). This can be viewed as "weak derandomization" and the statement follows by an averaging argument: there exist a fixed value r for A's random coins such that hardwiring r into A produces the deterministic algorithm B. Note that this averaging argument does not provide an explicit way to find r.

Recently, Zimand (building on an approach by Goldreich and Wigderson) proved an explicit version of the implication for randomized decision trees which toss "few" random coins. In this work, we consider weak derandomization of various classes of randomized algorithms.

We give a different proof of Zimand's result. Our proof generalizes to any class of randomized algorithms as long as one can explicitly construct an appropriate randomness extractor. Using this approach we prove unconditional weak derandomization results for communication games, constant depth circuits and streaming algorithms. More precisely we show that:

1. Given a randomized communication protocol that tosses few random coins and assuming that this protocol is explicitly constructible (in the sense that players can compute their strategy in polynomial time). Then, there is an explicitly constructible deterministic communication protocol of comparable communication complexity that simulates the randomized protocol correctly on most inputs.

2. Given a randomized algorithm that can be implemented by a uniform family of poly-size constant depth circuits we construct a uniform family of deterministic poly-size constant depth circuits that succeed on most inputs. (A classic result by Nisan and Wigderson gives a deterministic circuit that succeeds on all inputs but has quasi-polynomial size).

Our techniques follow the approach of Goldreich and Wigderson in the sense that we also "extract randomness from the input". However, in contrast to previous papers we use seedless extractors rather than seeded ones. We use extractors for bit-fixing sources (for decision trees) 2-source extractors (for communication games and streaming algorithms) and PRG based extractors (for constant depth circuits).

LUCA TREVISAN, **Dense Subsets of Pseudorandom Sets** (based on joint work with Omer Reingold, Madhur Tulsiani, and Salil Vadhan)

A theorem of Green, Tao, and Ziegler can be stated (roughly) as follows: if R is a pseudorandom set, and D is a dense subset of R, then D may be modeled by a set M that is dense in the entire domain such that D and M are indistinguishable. (The precise statement refers to"measures" or distributions rather than sets.) The proof of this theorem is very general, and it applies to notions of pseudorandomness and indistinguishability defined in terms of any family of distinguishers with some mild closure properties. The proof proceeds via iterative partitioning and an energy increment argument, in the spirit of the proof of the weak Szemeredi regularity lemma. The "reduction" involved in the proof has exponential complexity in the distinguishing probability. We present a new proof inspired by Nisan's proof of Impagliazzo's hardcore set theorem. The reduction in our proof has polynomial complexity in the distinguishing probability and provides a new characterization of the notion of "pseudoentropy" of a distribution. We also follow the connection between the two theorems and obtain a new proof of Impagliazzo's hardcore set theorem via iterative partitioning and energy increment. While our reduction has exponential complexity in some parameters, it has the advantage that the hardcore set is efficiently recognizable.

Error-correcting codes

DAVID ZUCKERMAN, **List-Decoding Reed-Muller Codes Over Small Fields** (based on joint work with Parikshit Gopalan and Adam Klivans)

We present the first local list-decoding algorithm for the rth order Reed-Muller code $RM(r,m)$ over F_2 for $r > 1$. Given an oracle for a received word $R : F_2^m \to F_2$, our randomized local list-decoding algorithm produces a list containing all degree r polynomials within relative distance $2^{-r} - \epsilon$ from R for any $\epsilon > 0$ in time $poly(m^r, \epsilon^{-r})$. The list size could be exponential in m at radius 2^{-r}, so our bound is optimal in the local setting. Since $RM(r,m)$ has relative distance 2^{-r}, our algorithm beats the Johnson bound for $r > 1$.

In the setting where we are allowed running-time polynomial in the block-length, we show that list-decoding is possible up to even larger radii, beyond the minimum distance. We give a deterministic list-decoder that works at error rate below $J(2^{1-r})$, where $J(d)$ denotes the Johnson radius for minimum distance d. This shows that $RM(2,m)$ codes are list-decodable up to radius s for any constant $s < 1/2$ in time polynomial in the block-length.

Over small fields F_q, we present list-decoding algorithms in both the global and local settings that work up to the list-decoding radius. We conjecture that the list-decoding radius approaches the minimum distance (like over F_2), and prove this when the degree is divisible by $q - 1$.

RAGESH JAISWAL, **Uniform Direct Product Theorems** (based on joint work with Russell Impagliazzo, Valentine Kabanets, and Avi Wigderson)

Direct Product Theorems are formal statements of the intuition: "if solving one instance of a problem is hard, then solving multiple instances is even harder". For example, a Direct Product Theorem with respect to bounded size circuits computing a function is a statement of the form: "if a function f is hard to compute on average for small size circuits, then $f^k(x_1, ..., x_k) = f(x_1), ..., f(x_k)$ is even harder on average for certain smaller size circuits". The proof of the such a statement is by contradiction: we start with a circuit which computes f^k on some non-negligible fraction of the inputs and then use this circuit to construct another circuit which computes f on almost all inputs. By viewing such a constructive proof as decoding certain error-correcting code, it was independently observed by Trevisan and Impagliazzo that constructing a single circuit is not possible in general. Instead, we can only hope to construct a list of circuits such that one of them computes f on almost all inputs. This makes the list size an important parameter of the Theorem which can be minimized. We achieve optimal value of the list size which is a substantial improvement compared to previous proofs of the Theorem. In particular, this new version can be applied to uniform models of computation (e.g., randomized algorithms) whereas all previous versions applied only to nonuniform models (e.g., circuits).

Computational learning

ROCCO SERVEDIO, **Testing Fourier dimensionality and sparsity** (based on joint work with Parikshit Gopalan, Ryan O'Donnell, Amir Shpilka and Karl Wimmer)

We present a range of new results for testing properties of Boolean functions that are defined in terms of the Fourier spectrum. Broadly speaking, our results show that the property of a Boolean function having a concise Fourier representation (or any sub-property thereof) is locally testable.

We first give an efficient algorithm for testing whether the Fourier spectrum of a Boolean function is supported in a low-dimensional subspace of F_2^n (equivalently, for testing whether f is a junta over a small number of parities). We next give an efficient algorithm for testing whether a Boolean function has a sparse Fourier spectrum (small number of nonzero coefficients). In both cases we also prove lower bounds showing that any testing algorithm — even an adaptive one — must have query complexity within a polynomial factor of our algorithms, which are nonadaptive. Finally, we give an "implicit learning" algorithm that lets us test any sub-property of Fourier concision.

Our technical contributions include new structural results about sparse Boolean functions and new analysis of the pairwise independent hashing of Fourier coefficients from (Feldman et al., FOCS 2006).

ADAM KLIVANS, **Agnostically Learning Decision Trees** (based on joint work with Parikshit Gopalan and Adam Kalai)

We give a query algorithm for agnostically learning decision trees with respect to the uniform distribution on inputs. Given black-box access to an arbitrary binary function f on $\{0,1\}^n$, our algorithm finds a function that agrees with f on almost (within an ϵ fraction) as many inputs as the best fitting size-t decision tree in time $poly(n, t, 1/\epsilon)$. This is the first polynomial-time algorithm for learning decision trees in a harsh noise model. The core of our learning algorithm is a procedure to implicitly solve an ℓ_1 minimization problem in 2^n dimensions using an approximate gradient projection method.

Cryptography

SALIL VADHAN, **Why Simple Hash Functions Work: Exploiting the Entropy in a Data Stream** (based on joint work with Michael Mitzenmacher (SODA 2008) plus improvements with Kai-Min Chung (RANDOM 2008, "Tight Bounds for Hashing Block Sources")

Hashing is fundamental to many algorithms and data structures widely used in practice. For theoretical analysis of hashing, there have been two main approaches. First, one can assume that the hash function is truly random, mapping each data item independently and uniformly to the range. This idealized model is unrealistic because a truly random hash function requires an exponential number of bits to describe. Alternatively, one can provide rigorous bounds on performance when explicit families of hash functions are used, such as 2-universal or $O(1)$-wise independent families. For such families, performance guarantees are often noticeably weaker than for ideal hashing.

In practice, however, it is commonly observed that simple hash functions, including 2-universal hash functions, perform as predicted by the idealized analysis for truly random hash functions. In this paper, we try to explain this phenomenon. We demonstrate that the strong performance of universal hash functions in practice can arise naturally from a combination of the randomness of the hash function and the data. Specifically, following the large body of literature on random sources and randomness extraction, we model the data as coming from a "block source," whereby each new data item has some "entropy" given the previous ones. As long as the (Renyi) entropy per data item is sufficiently large, it turns out that the performance when choosing a hash function from a 2-universal family is essentially the same as for a truly random hash function. We describe results for several sample applications, including linear probing, balanced allocations, and Bloom filters.

Computer algebra

CHRIS UMANS, **Fast polynomial factorization and modular composition in any characteristic** (based on joint work with Kiran Kedlaya)

We give an algorithm for modular composition of degree n univariate polynomials over a finite field F_q requiring $O(n \log q)^{1+o(1)}$ bit operations. As an application, we obtain a randomized algorithm for factoring degree n polynomials over F_q requiring $O(n^{1.5} \log q + n \log^2 q)^{1+o(1)}$ bit operations, improving upon the methods of von zur Gathen & Shoup (1992) and Kaltofen & Shoup (1998). Our results also imply algorithms for irreducibility testing and computing minimal polynomials whose running times are best-possible, up to lower order terms.

The first step is to reduce modular composition to certain instances of multipoint evaluation of multivariate polynomials. We then give an algorithm that solves this problem optimally (up to lower order terms). The main idea is to lift to characteristic 0, apply a small number of rounds of multimodular reduction, and finish with a small number of multidimensional FFTs. The final evaluations are then reconstructed using the Chinese Remainder Theorem. As a bonus, we obtain a very efficient data structure supporting polynomial evaluation queries, which is of independent interest.

Our algorithm uses techniques which are commonly employed in practice, so it may be competitive for real problem sizes. This contrasts with previous asymptotically fast methods relying on fast matrix multiplication.

General complexity theory

MARIO SZEGEDY, **Long Codes and the the Dichotomy Conjecture for CSPs** (based on joint work with Gabor Kun)

The well known dichotomy conjecture states that for every family of constraints the corresponding CSP is either polynomially solvable or NP-hard. We establish a three ways connection between the conjecture, asymptotic behavior of iterated maps related to non-linear dynamical systems, and the type of Fourier analytic techniques used in the theory of Probabilistically Checkable Proofs and property testing. To demonstrate the power of our newly found connections we give an analytic proof for the Hell-Nešetřil theorem about the dichotomy for undirected graphs.

We also contribute to the theory of non-linear dynamical systems by giving a characterization of multivariate functions (maps) over a finite domain that, when iterated sufficiently many times, become arbitrarily "resilient" to changing any fixed number of inputs in an arbitrary manner.

Finally, we obtain a new characterization of algebras that avoid types 1 and 2.

MARK BRAVERMAN, **The complexity of simulating Brownian Motion**

We analyze the complexity of the Walk on Spheres algorithm for simulating Brownian Motion in a domain Omega in R^d. The algorithm, which was first proposed in the 1950s, produces samples from the hitting probability distribution of the Brownian Motion process on boundary of Omega within an error of epsilon. The algorithm is used as a building block for solving a variety of differential equations, including the Dirichlet Problem.

The WoS algorithm simulates a BM starting at a point $X_0 = x$ in a given bounded domain Ω until it gets ϵ-close to the boundary of Ω. At every step, the algorithm measures the distance d_k from its current position X_k to the boundary of Ω and jumps a distance of $d_k/2$ in a uniformly random direction from X_k to obtain X_{k+1}. The algorithm terminates when it reaches X_n that is ϵ-close to the boundary of Ω.

It is not hard to see that the algorithm requires at least $\Omega(\log 1/\epsilon)$ steps to converge. Only partial results with respect to upper bounds existed. In 1959 M. Motoo established an $O(\log 1/\epsilon)$ bound on the running time for convex domains. The results were later generalized for a wider, but still very restricted, class of planar and 3-dimensional domains by G.A. Mikhailov (1979). In our earlier work (2007), we established an upper bound of $O(\log^2 1/\epsilon)$ on the rate of convergence of WoS for arbitrary planar domains.

We introduce subharmonic energy functions to obtain very general upper bounds on the convergence of the algorithm. Special instances of the upper bounds yield the following results for bounded domains Ω:

- if Ω is a planar domain with connected exterior, the WoS converges in $O(\log 1/\epsilon)$ steps;
- if Ω is a domain in R^3 with connected exterior, the WoS converges in $O(\log^2 1/\epsilon)$ steps;
- for $d > 2$, if Ω is a domain in R^d, the WoS converges in $O((1/\epsilon)^{2-4/d})$ steps;
- for $d > 3$ if Ω is a domain in R^d with connected exterior, the WoS converges in $O((1/\epsilon)^{2-4/(d-1)})$ steps;
- for any d if Ω is a domain in R^d bounded by a smooth surface, the WoS converges in $O(\log 1/\epsilon)$ steps.

We also demonstrate that the bounds are tight, i.e. we construct a domain from each class for which the upper bound is exact. Our results give the optimal upper bound of $O(\log 1/\epsilon)$ in many cases for which only a bound polynomial in $1/\epsilon$ was previously known.

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Chapter 28

The stable trace formula, automorphic forms, and Galois representations (08w5040)

Aug 17 - Aug 22, 2008

Organizer(s): James Arthur (University of Toronto), Michael Harris (Universite de Paris 7), Eric Urban (Columbia University), Vinayak Vatsal (University of British Columbia)

Overview of the Field

The heart of Langlands' program reinterpreting much of number theory in terms of automorphic forms is his *Functoriality Conjecture*. This is a conjecture associating the automorphic representations on a pair of connected reductive groups over a number field F, say G and H, whenever there is a homomorphism of the appropriate type between the corresponding L-groups

$$h : {}^L H \to {}^L G.$$

The structure of functoriality is largely captured in terms of parametrization of automorphic representations of a given group G by homomorphisms

$$\phi : \mathcal{L}_F \to {}^L G$$

where $\mathcal{L}_F$ is the hypothetical Langlands group.

In the analogous conjectured parametrization of irreducible representations of a reductive group G over a local field K, the Langlands group is replaced by the Weil-Deligne group W_K; in this setting one can state precise conjectures in terms of known objects, and these conjectures were proved when $G = GL(n)$ during the 1990s. This represents the first step to the extension of local class field theory to the non-commutative context, whereas the Langlands functoriality conjectures for automorphic forms are to be understood as generalizations of global class field theory. In particular, the Artin conjecture on holomorphy of Artin L-functions follows from Langlands' Functoriality Conjecture applied when H is the trivial group.

The most comprehensive technique for proving the Functoriality Conjecture in the cases in which it has been established is the Arthur-Selberg trace formula. This was used by Lafforgue to prove the global Langlands conjecture for $GL(n)$ over a global field of positive characteristic, and has had a variety of striking applications to number fields, including the Jacquet-Langlands correspondence and its generalizations in higher dimensions and the Arthur-Clozel theory of cyclic base change for $GL(n)$. Each special case of functoriality has been of enormous importance in number theory.

Recent Developments and Open Problems

Until recently, applications of the trace formula were limited to the cases in which it could be stabilized. With the proof of the fundamental lemma for unitary groups by Laumon and Ngô, followed by its extension to all groups by Ngô – together with the proof that the fundamental lemma depends only on the residue field, first by Waldspurger, more recently by Cluckers, Hales, and Loeser – Arthur's stabilization of the trace formula is close to being complete, and the simple trace formula can be stabilized in a number of situations. This makes it possible to carry out the applications of the trace formula anticipated more than two decades ago by Langlands, Kottwitz, and Arthur. The previous week's summer school concentrated on the background to these applications, in connection with the Paris project to edit a series of books under the common title *Stabilization of the trace formula, Shimura varieties, and arithmetic applications*, and with Arthur's forthcoming book on functoriality for classical groups. Among the applications discussed at this workshop are

1. The functorial transfer of automorphic representations from classical groups (Sp and SO) to $GL(n)$, contained in Arthur's forthcoming book. This was the subject of Arthur's two lectures;

2. The construction and analysis of local L-packets for quasi-split classical groups (symplectic, special orthogonal, and unitary) in terms of the local Langlands parametrization for $GL(n)$. This is due in part to Arthur and in part to Moeglin, who derive the result from global methods, and was the subject of Moeglin's lectures;

3. The study of the Galois representations arising in the cohomology of Shimura varieties; this was explicitly the subject of the lectures of Morel and Shin, and was the motivation for the lectures of Labesse and Clozel, who presented chapters of the Paris book project.

Various recent results on the fundamental lemma, including Ngô's work and extensions thereof, were presented by Tuan, Chaudouard, Hales, and Waldspurger. The lectures of Haines, Fargues, and Mantovan were all concerned with properties integral models of Shimura varieties and related local moduli spaces. Applications of the Galois representations on cohomology of Shimura varieties to questions on the border between Iwasawa theory and p-adic automorphic forms were presented in the talks of Emerton and Bellaïche. Finally, Lapid spoke on work in progress with Finis and Müller on combinatorial questions related to Arthur's invariant trace formula, with a view to analytic applications.

Presentations

J. Arthur, Functorial transfer for classical groups, I, II

Let G be a quasisplit special orthogonal or symplectic group. Then G represents a twisted endoscopic datum for a general linear group GL(N). The goal is to classify the representations of G, both local and global, in terms of those of GL(N). This will allow us to extend the main theorems of GL(N), namely the classification of isobaric representations by Jacquet-Shalika. the classification of the discrete sprectrum by Moeglin-Waldspurger, and the local Langlands classification established by Harris-Taylor and Henniart, to the classical group G.

The strategy is to compare the twisted trace formula for GL(N) with the stable trace formulas of the various G, and the ordinary trace formula of G with the stable trace formulas of its endoscopic groups. This is now within reach, thanks to the recent prooof of the fundamental lemma, in all its forms, by Laumon-Ngo, Ngo, Chaudouard-Laumon, Waldspurger and Cluckers-Hales-Loeser, following earlier ideas of Goresky-Kottwitz-Macpherson, and the reduction of the Kottwitz-Langlands-Shelstad transfer conjecture to the fundamental lemma by Waldspuger. In the lectures, the speaker described in precise form the classification theorems for G that one obtains from these comparisons. He then described the relevant terms in the various trace formulas, and some of the techniques needed to carry out the comparisons.

J.-P. Labesse, Stable simple base change for unitary groups

This talk is a summary of the speaker's chapter, entitled "Changement de base CM et séries discrètes," in the first book of the Paris project. Let F be a totally real field of degree $d \geq 2$ and E a quadratic CM extension of F. Let U be a unitary group of degree n over F, corresponding to this extension. Under additional simplifying hypotheses, one can obtain optimal results relating the stable trace formula for U to the twisted trace formula for $G = GL(n)_E$. Let f be a test function for U and ϕ a matching function on G, or equivalently on L, the non-trivial component of the semidirect product of G with $\{1, \theta\}$, where θ acts on G by Galois conjugation composed with transpose inverse. If $U = U^*$ is the quasi-split inner form, f_∞ is a very cuspidal discrete series pseudocoefficient and if ϕ_∞ is a matching very cuspidal Lefschetz function, then one has the identity

$$T^L_{disc}(\phi) = ST^{U^*}_{disc}(f).$$

In other words U^* is the only twisted endoscopic group to contribute to the twisted stable trace formula for G. This can be extended to write the stable trace formula for any U satisfying these hypotheses, with f_∞ as above, as a sum of terms corresponding to twisted traces for products of general linear groups over E. Under additional simplifying hypotheses (U is quasi-split at all finite places, E/F unramified at all finite places, the test functions are spherical at all inert places), one obtains multiplicity one results for automorphic representations of U of discrete series type at infinity. If n is odd and U has signature $(n-1, 1)$ at one real place and is definite at all others, one finds under these simplifying hypotheses that a θ-stable cuspidal cohomological automorphic representation Π of G descends to a stable L-packet of U with n members, each with multiplicity one, at least when the infinitesimal character of Π_∞ is sufficiently regular.

L. Clozel, Simple endoscopic transfer for unitary groups

This talk is a summary of the final chapter, entitled "Simple endoscopic transfer for unitary groups," in the first book of the Paris project, written by the speaker together with M. Harris and J.-P. Labesse. Let F and E, but now assume n is an even integer, and consider the unitary group U of degree $n+1$ with signature $(n, 1)$ at one real place and is definite at all others, and quasi-split at finite places. The objective is to study the contribution to the stable trace formula of U of θ-stable automorphic cuspidal representations of $GL(n) \times GL(1)$ or, equivalently, of the endoscopic group $H = U(n)^* \times U(1)$ of G. Let Π be a fixed θ-stable cuspidal cohomological automorphic representation of $GL(n)_E$, and let χ be a variable θ-stable automorphic representation of $GL(1)$. Under the simplifying hypotheses above, the contribution of the pair (Π, χ) to the automorphic spectrum of U is either an n-tuple of distinct automorphic representations of discrete series type or a singleton. If it is an n-tuple, Kottwitz' results on the zeta functions of Shimura varieties of PEL type imply that the corresponding Galois representation is weakly associated to the original Π. The main theorem is that, under a weak regularity hypothesis on Π_∞, then χ can be chosen so that one obtains an n-tuple. This depends on the calculation of the sign of a normalized intertwining operator, acting on Eisenstein series on $GL(n+1)_E$ attached to the Levi factor $GL(n) \times GL(1)$ but involving θ, and on the explicit determination of the signs in Shelstad's transfer of discrete series packets from H to G.

M. Emerton, p-adically completed cohomology

This evening lecture was an informal introduction to the speaker's approach to the study of p-adic variation of automorphic forms. The p-adically completed cohomology can be defined purely topologically for any tower of locally symmetric spaces. In the case of classical modular forms, p-adically completed cohomology plays a crucial role in the speaker's work on the Fontaine-Mazur conjecture for 2-dimensional Galois representations. Study of this cohomology for other groups is intimately connected with the mysterious properties of torsion in cohomology of locally symmetric spaces, and is only in its first stages. The speaker presented a number of recent results and conjectures on the topic, some contained in his joint work with F. Calegari.

J. Bellaïche, Endoscopic tempered points on unitary eigenvarieties

Although only p-adic deformations of endoscopic *non-tempered* automorphic representations (or A-packets) of unitary groups are related to the deepest cases of Bloch-Kato conjectures, their *tempered* counterpart are interesting on their own, and much simpler to study. In this talk, the speaker considered an automorphic *tempered* endoscopic A-packet (that is, an L-packet) for a unitary groups in n variables, compact at infinity, together with a refinement assumed to be anti-ordinary. These data correspond to a point on the eigenvariety of the unitary groups. The main result is that this point is smooth if and only if, the packet is of type $(1, \dots, 1)$; in other words if the attached Galois representation is a sum of n characters. This lead to the proof of non-vanishing results for some Galois cohomology groups of p-adic Galois representations, which do not seem to be easily provable otherwise.

C. Moeglin, Local Arthur packets

In this talk, the speaker explained how to use the transfer of character identities via endoscopy and twisted endoscopy, due to Arthur, to compute stable Arthur packets of representations for a classical group. The most important result is the fact that multiplicity one in packets of discrete series implies multiplicity one in general packets. The speaker then explained some qualitative results about the Langlands parameters of any representation in an Arthur packet. Roughly speaking, the speaker proved the idea of Clozel that in such a packet, any given representation is "more tempered"' (giving a precise meaning to such an assertion) than the representations in the Langlands packet associated and contained in it. The talk concluded by giving some applications, mostly conjectural, to the determination of the residual (non cuspidal) spectrum for adelic classical groups.

E. Lapid, On some aspects of Arthur's non-invariant trace formula (joint work with T. Finis and W. Müller)

The speaker discussed some analytic and combinatorial aspects pertaining to the non-invariant trace formula (i.e. Arthur's early work). A natural question is to understand the class of test function for which the trace formula identity extends. In the spectral side, the problem is to explicate the limits which appear in Arthur's fine spectral expansion in terms of first order derivatives of co-rank one intertwining operators. The solution is analogous to a volume formula for polytopes due to P. McMullen and R. Schneider. This volume formula should also play a role in the geometric side. However, as of now, the authors only understand the geometric side completely in the case of $GL(2)$. (This entails rewriting the non-elliptic terms in the trace formula.)

E. Mantovan, Integral models for toroidal compactifications of Shimura varieties

This talk was a report on joint work-in-progress with Moonen dealing with the construction of integral models for toroidal compactifications of Shimura varieties of PEL type at unramified primes. In the cases of good reduction, such a theory already exists due to the work of Faltings and Chai and more recently to Lan and Rozensztajn. The present project focuses on the cases of bad reductions at primes which divide the level.

The main goal is to extend known results on integral models of Shimura varieties to their compactifications. In particular, the lecture focused on the construction of integral models whose vanishing cycles sheaves can be controlled in terms of those of the corresponding local models constructed by Rapoport and Zink. These results (which for Shimura varieties of PEL type are due to Harris and Taylor in some special cases, and in general to the speaker) provides descriptions of the cohomology of the Shimura varieties in terms of that of their local models and of other simpler varieties, called Igusa varieties. Such formulas provide some insight on the Galois representations arising in the cohomology of the Shimura varieties. E.g., they are used, in the work of Harris and Taylor and more recently of Shin, to establish some instances of Langlands correspondences.

Following Pink's work on arithmetic compactifications of Shimura varieties, the authors consider a natural stratification of the boundary of toroidal compactifications where each stratum is itself a Shimura variety of mixed type, lying above a pure Shimura variety. For Shimura varieties of PEL type and unramified primes, they prove the existence of integral models of smooth toroidal compactifications whose vanishing cycle sheaves, when restricted along the boundary strata, agree with the pullback of the vanishing cycle sheaves of the corresponding underlying pure Shimura varieties (and thus can be controlled in terms of their local models).

In the case of PEL Shimura varieties, the boundary strata have a moduli interpretation as classifying spaces for rigidified 1-motives with additional structures, lying above the corresponding moduli spaces for abelian varieties. The existence of integral models of toroidal compactifications is thus addressed by investigating an appropriate notion of level structure on a 1-motive and its induced structure on the associated abelian variety.

L. Fargues, The p-adic geometry of moduli spaces of abelian varieties and p-divisible groups

In [1], Gerd Faltings has shown the existence of a link between Lubin-Tate and Drinfeld towers (see [3] too). Using the link between Drinfeld's Ω space and the Bruhat-Tits building of $PGL_{n/\mathbf{Q_p}}$ one can use this to define an Hecke equivariant "parametrization" by the geometric realization of this Bruhat-Tits building of the Berkovich space associated to the Lubin-Tate tower with infinite level. This parametrization has been studied in detail in [4].

The Lubin-Tate tower can be seen as tubes (or p-adic Milnor fibers) over some "supersingular" points in the reduction mod p of some particular type of Shimura varieties (unitary type with signature $(1, n-1) \times (0, n) \times \cdots \times (0, n)$ at a split prime p). In fact one can extend the results of [4] to define and study an Hecke equivariant parametrization of the p-adic Berkovich analytic space associated to this Shimura variety with infinite level at p by compactifications of the preceding buildings. In this parametrization the boundary stratification of the compactified building corresponds to the Newton stratification of the Shimura variety. For $n = 2$ one recovers Lubin's theory of the canonical subgroup. For general n this should be helpful to construct a theory of p-adic automorphic forms on those Shimura varieties generalizing Katz theory for modular curves (for $n = 2$ the structure of the Bruhat-Tits tree being "simple" one can compute everything, but in general the structure of the building is more complicated).

The speaker proposed a new way to stratify and define fundamental domains for the action of p-adic Hecke correspondences on more general moduli spaces (Rapoport-Zink spaces or general PEL type Shimura varieties). In [2] the author has defined Harder-Narasimhan type filtrations for finite flat group schemes over unequal characteristic complete valuation rings. Stuhler and Grayson have developed reduction theory for the action of arithmetic groups on archimedean symmetric spaces using Harder-Narasimhan filtrations for hermitian vector bundles in the sense of Arakelov geometry. A theory for finite flat group schemes is used to define a reduction theory for p-divisible groups (like reduction theory for quadratic forms) and to define fundamental domains for the action of Hecke correspondences on some Rapoport-Zink spaces and Shimura varieties. Those fundamental domains are interesting from the point of view of the associated period mapping. When one starts from a $\overline{\mathbf{Q}}$-point in our Shimura variety the associated point in the fundamental domain is a point in the Hecke orbit where the Faltings height of the associated abelian variety is minimized in its p-isogeny class.

T. Haines, Test functions for some Shimura varieties with bad reduction

This talk reviewed some aspects of Shimura varieties with parahoric level structure at p, and outlined an approach to study Shimura varieties with $\Gamma_1(p)$-level structure at p by relating that situation to the Iwahori-level case. The general expectation is that the test functions appearing in the twisted orbital integrals in the "point counting" formula can always be taken to lie in the center of an appropriate local Hecke algebra. In the parahoric case, this is known in several cases (joint work with Ngo B.C.) and in the $\Gamma_1(p)$-case this is the subject of work in progress with M. Rapoport. The main result so far is limited to the family of unitary Shimura varieties known as the "Drinfeld case", and states that there the test function is a sum of functions indexed by certain characters χ on the Iwahori, and each such function is in the center of the Hecke algebra of $\Gamma_1(p)$-bi-invariant functions on $GL(n)$ which transform under the Iwahori by χ^{-1}. Furthermore, the test function can be identified explicitly via Hecke algebra isomorphisms in terms of functions in the centers of the Iwahori-Hecke algebras attached to the semistandard Levi subgroups of $GL(n)$ (which are indexed also by the various χ).

S.W. Shin, Construction of Galois representations

Let Π be any cuspidal automorphic representation of $GL(n)$ over a CM field F. If Π is conjugate self-dual and cohomological, it is part of the global Langlands conjecture that there exists an n-dimensional ℓ-adic representation $R(\Pi)$ of the full Galois group for F which corresponds to Π via the local Langlands correspondence (established by Harris-Taylor and Henniart) at every finite place. If Π is square-integrable at a finite place, this result is proved by work of Clozel, Kottwitz, Harris-Taylor and Taylor-Yoshida. Their result is based on the study of unitary Shimura varieties and base change for unitary groups in the case of trivial endoscopy.

In his talk the speaker reported on the recent proof that $R(\Pi)$ as above exists, without assuming Π is square-integrable at a finite place. When n is odd, this result was worked out by Morel and Shin, using the stable base change for unitary groups after Labesse. When n is even, the problem is harder and more interesting. Harris observed that one might use the endoscopy for $U(n)$ coming from $U(n-1) \times U(1)$, generalizing the method of Blasius of Rogawski for $n = 3$. Clozel, Harris and Labesse worked out endoscopy and base change results for unitary groups in this setting; combined with the results of Kottwitz and Morel, they in particular obtain n-dimensional ℓ-adic representations that correspond to Π at almost all places. On the other hand, one has to compute the Galois action on the cohomology of Shimura varieties at all places, including places of bad reduction. Following the strategy of Harris-Taylor, in view of their deep result on the cohomology of the Lubin-Tate deformation spaces, the problem quickly reduces to the representation-theoretic understanding of the cohomology of Igusa varieties. This can be done by a counting point formula for Igusa varieties and its stabilization, combined with the trace formula techniques. The speaker tried to explain how all these can be put together into a somewhat different construction of a representation $R(\Pi)$ with the desired local properties at all places prime to ℓ.

LECTURES ON THE FUNDAMENTAL LEMMA

Ngo Dac Tuan, Introduction to B.C. Ngô's proof

This purpose of this talk is to sketch the proof of the fundamental lemma due to Ngô Bao Chu. Conjectured by Langlands and Shelstad, the fundamental lemma constitutes an essential step in the stabilization of the elliptic part of the Arthur-Selberg trace formula. Roughly speaking, it claims an local identity between the κ-orbital integral of a reductive group and the stable orbital integral of its endoscopic group associated to κ.

The approach of Ngô is geometric. By studying the perverse cohomology of the Hitchin fibration over a projective smooth curve over a finite field, he proves not only the fundamental lemma but also a geometric stabilization theorem. The important ingredients of his proof are, in the first place, a product formula connecting the Hitchin fibration and the affine Springer fibers, whose properties are well known; in the second place, the so-called strong support theorem.

P.-H. Chaudouard, On the truncated Hitchin fibration and the weighted fundamental lemma (Joint work with Gérard Laumon)

Ngô Bao Châu recently proved the fundamental lemma of Langands and Shelstad in full generality. In fact, Ngô proved a Lie algebra version of the fundamental lemma for local fields of equal characteristics. But it is known that this implies the fundamental lemma for groups and for local fields of characteristic 0 (works of Hales, Waldspurger ...). Ngô's method is geometric as was the proof of the unitary case by Laumon and Ngô. It consists in a cohomological study of elliptic part of the Hitchin fibration.

The framework is the following : C is a connected projective curve over a finite field and D is an effective divisor on C. For the group $GL(n)$, the whole space is the algebraic stack of pairs $(\mathcal{V}, \theta)$ where $\mathcal{V}$ is a vector bundle and θ is an endomorphism $\mathcal{V} \to \mathcal{V}(D)$. The base of the fibration is the space of all characteristic polynomials and the Hitchin morphism is the "characteristic polynomial" morphism. There is a generalization of these definitions for any reductive group.

Over the elliptic open set (for $GL(n)$ this is the open set of generically irreducible characteristic polynomials), the Hitchin morphism is proper. Moreover the number of rational points in each fiber is essentially a global orbital integral which appears in the Arthur-Selberg trace formula. These two facts are no longer true outside the elliptic set. However, if one wants a geometric interpretation of the other geometric terms of the trace formula (i.e. the weighted orbital integrals), one needs to go “outside” the elliptic set.

In this talk which is based on a joint work of the speaker with Gérard Laumon, a truncated version of the Hitchin fibration was introduced. Roughly speaking this is essentially a “good” open substack of the Hitchin fibration. But as in the elliptic case, it has two basic properties : the restriction of the Hitchin morphism to the truncated Hitchin fibration is proper and the number of rational points in each fiber is a global weighted orbital integral introduced by Arthur.

Extending Ngô’s arguments, one can deduce the weighted version of the fundamental lemma conjectured by Arthur. Thanks to Waldspurger’s works, this gives the weighted fundamental lemma or local fields of characteristic 0.

T. Hales, The transfer principle for the fundamental lemma

The purpose of this talk is to explain how the identities of various fundamental lemmas fall within the scope of the transfer principle, a general result of Cluckers and Loeser that allows one to transfer theorems about identities of p-adic integrals from one collection of fields to others. In particular, once the fundamental lemma has been established for one collection of fields (for example, fields of positive characteristic), it is also valid for others (fields of characteristic zero). The main result has been obtained independently by Waldspurger.

Most of this talk is a report on the work of Cluckers and Loeser on motivic integration for constructible functions. A subassignment is a collection of sets indexed by fields of characteristic zero, such that the set attached to K is a subset of $K((t))^m \times K^n \times \mathbf{Z}^r$ for some m, n, r (not depending on K). A definable subassignment is one for which there exists a formula in the three-sorted language of Denef-Pas which determines the subset for each K. Definable subassignments gives the objects of a category, whose morphisms are functions whose graphs are also definable subassignments. For each definable subassignment a ring $C(X)$ of constructible functions is given, that gives the ring of integrands for a field-independent integration. The cell-decomposition theorem of Denef-Pas gives a integration on $IC(X) \subset C(X)$. There is a specialization theorem that relates integration on $IC(X)$ with integration on non-archimedean local fields.

All of the data of the fundamental lemma can be expressed in terms of the the ring $IC(X)$. This gives a field-independent formulation of the fundamental lemma. The general transfer principle for $IC(X)$ implies that the fundamental lemma can be transferred from fields of positive characteristic to fields of characteristic zero. The details have been written in an article by the same title for the Lie algebra version of the fundamental lemma, in both the weighted and unweighted cases.

Outcome of the Meeting

The conclusion of the conference is that, thanks to the breakthrough on the fundamental lemma, the Langlands program for endoscopy, including Arthur’s multiplicity conjectures and Kottwitz’ related conjectures on the zeta functions of Shimura varieties, is well on its way to completion, at least for classical groups. Open questions fall into two large categories. The first class consists of applying the results of Langlands’ program to questions in number theory. The lectures of Emerton and Bellaïche described two active research projects concerned with such applications. Other talks of this sort would have been scheduled had it been decided to devote more time to lectures.

Langlands’ program is still in its infancy, and nearly everything remains to be done, even though endoscopy may soon be complete. The second class of open questions has to do with functoriality “beyond endoscopy.” That will have to wait for a future meeting.

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Chapter 29

Numerical Methods for Nonlinear Hyperbolic PDE and their Applications (08w5024)

Aug 31 - Sep 05, 2008

Organizer(s): Ian Mitchell (University of British Columbia), Stanley Osher (University of California, Los Angeles), Chi-Wang Shu (Brown University), Hongkai Zhao (University of California, Irvine)

Nonlinear partial differential equations (PDEs) of hyperbolic type have wide and important uses in science and engineering. To name just a few examples, consider hyperbolic conservation laws in fluid dynamics; Hamilton-Jacobi equations in optimal control, geometric optics and computer vision; or Boltzmann and kinetic equations in gas dynamics and nanotechnology. Due to the nonlinearity and hyperbolic nature, singularities develop in solutions. Some notion of weak solution and/or extra physical conditions—such as the viscosity solution or the entropy condition—must be defined in order to prove mathematically both existence and uniqueness of a meaningful solution. Closed form analytic solution is unlikely in all but the most simple cases; consequently, numerical approximations are crucial in practice. Developing efficient and robust numerical algorithms for these PDEs is a challenging task due to their nonlinearity and the potential for singularities in the solution.

A few of the common difficulties faced in the numerical analysis and computational approximation process include:

- Causality and entropy conditions of the underlining PDE must be correctly enforced in numerical schemes for stability and convergence to the weak solution.
- Possible singularities in the solution must be handled without introducing oscillations or instabilities. At the same time, high order accuracy away from singularities is highly desirable.
- Discretization of steady state problems leads to large systems of nonlinear equations, so efficient solvers must be found.
- Many practical problems feature multiple scales in time and space.
- Proving or even demonstrating convergence of numerical methods, especially high order nonlinear methods, remains a challenging task.

Recently, there have been many new developments in numerical methods as well as emerging new applications for nonlinear hyperbolic PDEs. As just two examples, discontinuous Galerkin (DG) methods have shown promising progress in dealing with various kinds of nonlinear hyperbolic PDEs, and fast sweeping methods (FSM) have demonstrated efficient iterative solution of static hyperbolic problems on unstructured meshes.

The goal of the workshop was to bring together experts as well as junior researchers who are approaching nonlinear hyperbolic PDEs from different perspectives, including numerical analysis, algorithms and applications. The participants shared a common interest in nonlinear hyperbolic differential equations, but brought a wider range of expertise than would have been available at shorter and more focused venues (such as conference mini-symposia).

The workshop was a success, featuring talks ranging from theoretical numerical analysis to algorithm development, from high level overviews to detailed descriptions of both solved and open problems, and with applications from biology to fluid dynamics to traffic estimation to tomography. Informal discussion topics were even more varied, ranging from the surprise weather—snow in August!—to ongoing disagreements over the relative merits of sweeping and marching schemes for stationary Hamilton-Jacobi equations. The comfortable environment of BIRS, friendly atmosphere and interesting talks/discussions made this workshop very enjoyable.

Overview of the Field

Hyperbolic PDEs

The prototypical *hyperbolic PDE* is the linear one-way wave equation:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = u_t + au_x = 0, \tag{29.1}$$

where a is a constant (the wave speed), t is the time variable, x is the spatial variable, and $u = u(t, x)$ is the dependent, unknown solution. An *initial value problem* (IVP) involves solving (29.1) over $x \in \mathbb{R}$ subject to initial conditions

$$u(0, x) = u_0(x), \tag{29.2}$$

where $u_0(x)$ is given. An *initial-boundary value problem* (IBVP) generally involves solving (29.1) over $x \in \Omega \subset \mathbb{R}$ subject to both initial conditions (29.2) (where $u_0(x)$ need be defined only for $x \in \Omega$) and boundary conditions

$$u(t, x) = u_\Omega(t, x) \qquad \text{for } x \in \partial\Omega$$

where $u_\Omega(t, x)$ is given. More generally, a linear system of PDEs

$$u_t + Au_x + Bu = F(t, x) \tag{29.3}$$

for $x \in \mathbb{R}^n$ is hyperbolic if the matrix A is diagonalizable and has real eigenvalues. For example, the classical second order linear wave equation

$$u_{tt} - a^2 u_{xx} = 0$$

can be rewritten in the form (29.3), where the eigenvalues of A are $\pm a \in \mathbb{R}$.

A key property of hyperbolic PDEs is the existence of characteristics along which information about the solution propagates at finite speed. In the case of (29.1), the characteristic is defined by $x = x_0 + at$, and from this characteristic we can determine an analytic solution to the IVP (29.1)–(29.2) as $u(t, x) = u_0(x - at)$. Other hyperbolic PDEs give rise to multiple and more complicated characteristics, and more complex relationships between the characteristics and the solution; however, the existence of characteristics and their relationship to the solution are properties often exploited by numerical approximation schemes. In contrast, neither elliptic PDEs, such as Laplace's equation for steady state potential, nor parabolic PDEs, such as the heat equation, have such finite speed characteristics.

The PDEs given above are all examples of linear hyperbolic PDEs. These PDEs have been subject to intensive and successful scrutiny over centuries, we have long standing conditions under which they are well-posed, and depending on the complexity of the initial and boundary conditions we can in many cases develop analytic solutions.

Unfortunately, there are many important hyperbolic PDEs which are nonlinear. Examples of long-standing nonlinear hyperbolic PDEs include the (inviscid) Burgers' equation

$$u_t + \left(\frac{u^2}{2}\right)_x = 0,$$

the Euler equations of gas dynamics

$$\begin{aligned} \rho_t + \nabla \cdot (\rho u) &= 0, \\ (\rho u)_t + \nabla \cdot (u \times \rho u) + \nabla p &= 0, \\ E_t + \nabla \cdot (u(E + p)) &= 0, \end{aligned}$$

and the Hamilton-Jacobi-Bellman (HJ) equation of optimal control

$$u_t + \min_{a \in \mathcal{A}} f(x, a) \cdot \nabla u = 0.$$

Nonlinear PDEs such as these are often much more challenging to analyze than their linear cousins. Not only are conditions under which they are well-posed not always available, but they may in fact fail to have classical solutions; for example, the solution to Burgers' equation with a smooth sinusoidal initial condition will develop a discontinuity (a *shock*) after finite time, at which point the derivatives in the PDE no longer exist. Suitable definitions of weak solutions have been developed [2]—the entropy condition for conservation laws, or viscosity solutions for Hamilton-Jacobi equations are two examples—but analytic solutions to particular problems are only rarely available. Consequently, we must turn to numerical approximations.

Before a brief background on those numerical methods, we will also note that many PDEs which are not technically hyperbolic are still approached with hyperbolic techniques because their solutions are strongly influenced by characteristics and wave-like behaviors. Examples include convection dominated diffusion problems, the Navier-Stokes equations for fluid simulation, degenerate parabolic equations (a generalization of HJ PDEs), and the steady state versions of these equations (which are technically nonlinear elliptical). Many of the discussions below apply also to these relatives of nonlinear hyperbolic PDEs, and they were also featured in several of the workshop's talks.

Numerical Methods

Hyperbolic PDEs arise in many practical engineering and scientific problems, but except for isolated cases they can only rarely be solved analytically. Consequently, numerical algorithms for approximating their solution have been studied since the earliest days of computing. A first key challenge is that the solution $u(t, x)$ is a continuous function over a continuous space, mapping from an uncountably infinite domain into an uncountably infinite range, and it must be reduced to an finite dimensional system to be represented in the finite, discrete memory of a computer. A second key challenge is that the PDE is a potentially nonlinear differential equation, which must somehow be converted to an explicit algebraic equation which the arithmetic unit of the computer can evaluate.

Both challenges are solved by some form of *discretization*, although the term can refer to any of several very different processes depending on the context. Even though a PDE is uniquely defined and well behaved analytically, there are many possible ways of discretizing and considerations such as consistency, accuracy and stability must be taken into account to chose the correct ones. For example, the continuous domain of x and t is typically (but not always) discretized by creating a *grid* containing *nodes* (zero dimensional points in the domain), *edges* (one dimensional lines), *faces* (surfaces of codimension one in domains of dimension three or higher) and *cells* (the full dimensional spaces between the faces). Grids come in many flavors—orthogonal, structured, semi-structured, unstructured, and/or adaptive—and may treat the time dimension t the same as or differently than the spatial dimension(s) x. Particular types of numerical approximation schemes are often closely tied to certain features of the class of grids for which they are designed.

Modern approximation methods can be broadly classified into the categories of:

- *Finite difference methods* (FD) [5]. In FD the solution $u(t, x)$ is represented by values of u at the nodes in the grid. The PDE is discretized into an algebraic form that can be solved on a computer by taking finite differences of these solution values over a small number of neighboring nodes (the *stencil*) to represent the derivatives. The discretization of the PDE is often split, either discretizing first in space and then in time (the *method of lines*) or the other way around.

- *Finite element methods* (FE) [3]. In FE the solution $u(t, x)$ is represented as a linear combination of a collection of basis functions, where each basis function has only finite (and typically very local) support on the grid. The PDE is discretized via a conversion to a variational form which eventually gives rise to equations which can be solved for the coefficients in the linear combination of basis functions. FE is a type of *Galerkin* method.

- *Finite volume methods* (FV) [4]. In FV the solution $u(t, x)$ is represented by storing for each cell in the grid the average value of the solution over that cell. The behavior of the PDE is approximated by solving *Riemann problems* along each cell boundary. Riemann problems are essentially analytic solutions of the PDE for piecewise constant (or piecewise polynomial for higher order accurate schemes) initial conditions, which can be used as local approximations if the discretization of space and time are sufficiently fine.

- *Spectral methods* [1]. In spectral methods there is no discretization of the domain (eg: no grid). The solution $u(t, x)$ is represented as a linear combination of a collection of basis functions which do not have local support; for example, the Fourier Transform of $u(t, x)$. A main advantage of the spectral method is high order accuracy when the underlying solution is smooth and the domain is regular.

Regardless of its type, the typical goal when designing a numerical approximation scheme is *convergence*: that the error in the approximation will approach zero as some measure of the discretization approaches zero. For example, in a FD scheme the error is measured by comparing the approximation at a node with the true value of the solution at that node, and overall error is taken as the maximum, root mean square or average error over all of the nodes in the grid. A FD scheme is convergent if this error will go to zero as the distance between nodes (and time step, if time is discretized separately) is taken to zero.

Depending on the scheme, the error may go to zero faster or slower as a function of the discretization parameter. The *order of accuracy* of a scheme measures that rate; for example, if dividing the node spacing by two in a FD scheme causes the error to fall by eight then the scheme is called third order accurate. By definition, any scheme with greater than zero order accuracy is convergent, but we typically seek schemes of second or higher order when possible.

Direct proof of convergence is often challenging. For linear PDEs, the Lax-Richtmyer Equivalence theorem states that a consistent scheme for a well-posed IVP is convergent if and only if it is stable [5]. Informally, *consistency* is the property that the discretization of the PDE approaches the true PDE as the discretization parameter is taken to zero, while *stability* is the property that the approximation does not blow up; there are fairly standard approaches for demonstrating both on the types of schemes mentioned above.

Unfortunately, the Lax-Richtmyer Equivalence theorem does not apply to nonlinear PDEs. In some cases a similar theorem is available; for example, for HJ PDE schemes it has been shown that consistency, stability and a form of monotonicity ensure convergence, but it has also been shown that monotone schemes cannot be better than first order accurate. In other cases, such as the Navier-Stokes equations, there are no proofs of convergence.

When no theory is available, then convergence is demonstrated empirically by examining the behavior of the error as the discretization is refined on an example with known solution. Such empirical study is also necessary when using schemes with theoretical convergence on real problems, since convergence is a limiting property and does not ensure sufficient accuracy to solve the problem for any particular finite discretization size. Broader concepts of error are also available to empirical studies, such as the correct location of a shock being more important than its precise height, or vice-versa. In fact, even quantitative measures of error may be abandoned in favor of qualitative measures, such as the “eye-ball” norm (in other words, does the behavior look realistic) quoted so often in physically-based computer animation.

The emphasis in the preceding paragraphs on accuracy and convergence should not be taken to imply that they are the only important aspects of numerical method design. Other aspects that are often considered include:

- Efficient algorithms. Compare two schemes run on the same grid. If one produces an approximation that is twice as accurate but takes eight times longer to run, then it is often possible to get better results by applying the other, faster scheme on a finer grid.
- Efficient implementations. Numerical algorithms for PDEs require a lot of memory. In order to achieve their peak processing capacity, modern processors have a deep cache hierarchy between main memory and the CPU. Careful consideration of how memory is accessed can result in significantly faster programs.
- Generality. The more general the algorithm, the broader the class of PDEs which can make use of any implementations. On the other hand, specialized algorithms can often take advantage of special properties of the PDE in order to improve accuracy and/or efficiency. Furthermore, when developing methods for use in a particular application field, it is often vital that the assumptions, vocabulary and formulations used in that field are adopted so that practitioners in the field will feel comfortable with the scheme or software.
- Ease of use and modification. Some researchers write short new demonstration code for each publication, while others are using huge legacy codes developed over decades. Some frequently discard their code, some release their code publicly, and some sell their code, either directly as executables, or indirectly through consulting services. Different goals and audiences lead to different algorithm and implementation choices.

The choice of participants for this meeting was driven by the goal of bringing together a variety of viewpoints on and expertise in the development of numerical methods for nonlinear hyperbolic PDEs, their relatives, and their applications.

Recent Developments and Open Problems

Examples of recent successes for nonlinear hyperbolic problems include *essentially non-oscillatory* (ENO) and *weighted ENO* (WENO) FD schemes for approximating the derivatives (and more generally interpolation) of solutions which may not be differentiable or even continuous. Among FE methods, various *discontinuous Galerkin* discretizations have been proposed. Among truly hyperbolic problems the progression of time provides a known directionality to characteristics, of which explicit time integrators can take advantage; however, for stationary HJ PDEs the characteristic direction is not known in advance and a number of *fast marching* and *fast sweeping* schemes have been proposed to try to efficiently determine these directions under a variety of assumptions about the PDE.

That said, there remain many unsolved issues. Error estimation and convergence analysis are not available for high order nonlinear methods, such as ENO/WENO schemes. The appropriate adaptation of fast schemes to non-convex stationary HJ PDEs is still unclear because the understanding of the proper characteristics for the viscosity solution is quite formal; consequently, there is little guidance in constructing monotone upwind solution schemes. The Schrodinger and nonlinear Boltzmann transport equations are examples of other important physical models whose approximations pose challenges due to their high dimensionality and strong nonlinearity.

Presentation Highlights

As usual, many speakers chose to give talks slightly or entirely different from what they had initially proposed when the preliminary program was developed. The organizers were cognizant of the weather forecasts and rather chilly conditions (for August)—the free afternoon was shifted from Wednesday to Tuesday in order to take advantage of a dry day. We were also fortunate to have two last-minute speakers volunteer to fill gaps in the program: Raymond Spiteri and Christian Claudel.

The BIRS provided workshop web space was used to set up a web page where many of the talks are posted. The talks of the speakers whose names are followed by a "*" in the list below are available at this site. Speakers are listed alphabetically; a listing in order of their presentations is given on the web site.

- Remi Abgrall* in talk entitled "Non-oscillatory Very High Order Residual Distribution Schemes for Steady Hyperbolic Conservation Laws: Preliminary Results" presented a systematic construction for numerical approximations of steady hyperbolic problems which is both high order and has a very compact stencil, with demonstration on compressible flows.

- Christian Claudel gave a brief talk describing how the conservation-law form Lighthill-Whitham-Richards model of traffic flow can be transformed into a Hamilton-Jacobi PDE, which can then be solved using numerical methods from viability theory. The advantage of the transformation and numerical methods is that "boundary" conditions interior to the domain are easily accommodated, such as what would be generated by emerging new cell phone technology.

- Pierre Degond* in a talk entitled "Fluid models for Complex Systems" discussed two models of individual and collective behavior among animal populations: First, a continuum model derived from a widely used discrete particle model due to T. Vicsek, and second, a new model proposed on the basis of biological experiments on fish behavior called the persistent turning walker.

- Roberto Ferretti* in a talk entitled "Stability of Large Time-Step Schemes and the relationship between Semi-Lagrangian and Lagrange-Galerkin Techniques" compared the two broad classes of large time-step schemes. While the former has a cleaner and more general stability analysis, its cannot be implemented in exact form. The theoretical analysis of the latter is not complete, but its implementation is much simpler. Roberto showed that by using a suitable basis, SL schemes can be regarded as LG schemes and therefore stability of SL schemes can be demonstrated in a wider range of situations.

- Irene Gamba* in a talk entitled "Spectral-Lagrangian Solvers for Non-linear, Non-conservative Boltzmann Transport Equations" presented a deterministic spectral solver for rather general collision kernels of the BTE. Computation of the nonlinear Boltzmann collision integral and conservation issues caused by spectral methods are resolved by framing the conservation properties in the form of a constrained minimization problem easily solved by a Lagrange multiplier method. An implementation was benchmarked on several examples, including a space inhomogeneous BVP where it was successful at capturing a discontinuous behavior of the solution.

- Shi Jin in a talk entitled "Eulerian Gaussian Beam Methods for the Schrodinger Equation in the Semi-classical Regime" gave the first of two talks about Eulerian Gaussian beam methods.

- Chiu-Yen Kao* in a talk entitled ""Cell Cycle Control at the First Restriction Point and its Effect on Tissue Growth" discussed analysis, simulation and control of a continuum model of cell growth, reproduction and death.

- Randall J. LeVeque* in a talk entitled "Quadrilateral Grids and Finite Volume Methods on the Sphere" explained recent work on FV methods adapted to the sphere and other non-rectangular domains. To fit non-rectangular shapes, these logically rectangular grids must use nonsmooth and non-orthogonal mappings; however, second order accuracy is possible.

- Jian-Guo Liu in a talk entitled "All Speed Asymptotic Preserving Schemes for Fluid and Plasma" described schemes that avoid stiffness and numerical dissipation at low speeds while still being effective at shock capturing for Mach numbers on the order of one.

- Yingjie Liu* in a talk entitled "Hierarchical Reconstruction for Discontinuous Galerkin Method on Triangular Meshes with a WENO-type Linear Reconstruction" explained how to build a WENO-type linear reconstruction at each hierarchical stage in which the weights are nearly mesh independent and relatively simple. The resulting reconstruction reduces abrupt stencil shifts and better resolves contacts. Interestingly, this nonlinear hierarchical reconstruction method avoids large drops in CFL number as the order increases, and despite multiple reconstructions does not lead to excessive smearing.

- H. Pino Martin* in a talk entitled "Numerical Challenges for Direct and Large-Eddy Simulations of Highly Compressible Turbulence" discussed the challenges of generating high fidelity simulations of complex flows in real engineering problems, such as reusable launch vehicles and scramjet engines. Shock capturing methods such as WENO have been successfully adapted to generate direct numerical simulation (DNS) of these flows on massively parallel platforms. A database of such DNS results has been released for download by the community. Converged DNS data is now being used to construct robust and more efficient Large-Eddy Simulations (LES) through shock-confining filters.

- Ian M. Mitchell* in a talk entitled “The Flexible, Extensible & Efficient Toolbox of Level Set Methods and The Ellipsoidal Particle Level Set Method” described two separate projects. The toolbox of level set methods implements many schemes for time-dependent Hamilton-Jacobi equations and dynamic implicit surfaces in an easy-to-use and publicly available set of Matlab routines. The ellipsoidal particle level set method is an attempt to adapt the original particle level set method—which efficiently reduced volume conservation errors in dynamic implicit surface simulations—to handle flows in which characteristics cross.

- Jianliang Qian* in a talk entitled “Eulerian Gaussian Beams for Schrödinger Equations in the High Frequency Regime” gave a second talk on Gaussian beam methods. While traditional Gaussian beam schemes use Lagrangian ray tracing, the new Eulerian framework provides for a uniform distribution of phases and amplitudes in the phase space. Another major advantage is that solutions for different IC can be determined at reduced cost by modifying the summation formula. Numerical experiments show that this approach yields accurate semi-classical solutions even at caustics.

- Susana Serna in a talk entitled “A Characteristic-based Nonconvex Entropy-Fix Upwind Scheme for the Ideal Magnetohydrodynamic Equations” discussed a characteristic based upwind scheme that uses a spectral decomposition in local wavefields derived from an analysis of the wave structure of ideal MHD equations. The new scheme is able to detect local regions containing nonconvex singularities and to handle an entropy correction by prescribing a local viscosity that ensures convergence to the entropy solution. Tests of a high order accurate version of the scheme on one and two dimensional MHD problems were also described.

- Raymond Spiteri gave a talk analyzing the commonly used combination of ENO/WENO spatial discretization schemes and Strong Stability Preserving (SSP) temporal discretization schemes. SSP schemes are temporal discretizations with higher orders of accuracy that are guaranteed to be stable when combined with a spatial discretization that is itself stable when used with the first order accurate forward Euler temporal discretization in a method of lines approach. However, it is common if rarely stated knowledge that some ENO/WENO spatial discretizations are not be stable when used with forward Euler, so the stability analysis for SSP schemes is not applicable. Despite this fact, many ENO/WENO/SSP combinations are empirically stable and in practice very effective; this talk presented a rigorous stability analysis of several common combinations.

- Chi-Wang Shu* in a talk entitled “High Order Shock Capturing Schemes—An Overview” gave a survey of high order schemes for hyperbolic problems, with an emphasis on describing and comparing WENO FD, WENO FV, and DG FE schemes. Recent developments included well-balanced high order schemes, a high order conservative Lagrangian type scheme for the compressible Euler equations, and superconvergence and time evolution of DG FE solutions for hyperbolic equations.

- Tao Tang in a talk entitled “Moving Grid Methods and Multi-Mesh Methods” started by describing an adaptive, moving grid strategy that automatically adjusts the FE to resolve relevant scales in a multiscale simulation. The efficiency of the strategy is improved through a decoupling that reduces an important matrix to block tridiagonal form. The scheme is demonstrated on dendritic growth simulations, which also make use of multiple meshes to improve the efficiency of approximating different variables in the coupled system.

- Alexander Vladimirsky in a talk entitled “Causal Numerical Methods for Hyperbolic Problems” described how “causal methods” for Eulerian frameworks (including fast marching methods) maintain the advantages of easy resolution control, high accuracy and low complexity treatment of crossing characteristics, but can still take advantage of Lagrangian characteristic information to decouple the resulting nonlinear systems of equations and achieve efficient solutions. This class of methods was demonstrated with specific schemes for viscosity solutions of static Hamilton-Jacobi equations and multi-valued solutions of general first order PDEs.

- Yong-Tao Zhang in a talk entitled "Uniformly Accurate Discontinuous Galerkin Fast Sweeping Methods" presented recent work on using DG schemes for the local solvers in fast sweeping methods to achieve higher orders of accuracy. A key challenge—enforcing causality in the compact DG solver—is addressed by constructing causality indicators which are initialized by an approximation from a first order accurate sweeping method, and then corrected as the second order accurate DG scheme iterates. Second order accuracy is achieved in numerical examples.

- Hongkai Zhao in a talk entitled "Contraction Property of the Fast Sweeping Method" demonstrated some contraction properties that arise when upwind local solvers are combined with fast sweeping Gauss-Seidel iterations for stationary Hamilton-Jacobi equations. These properties have useful implications on the numerical error of not only the solution itself, but also its gradient, which is important in many applications of Hamilton-Jacobi equations.

Outcomes

A fair number of attendees came from a community of researchers who have been studying numerical algorithms for nonlinear hyperbolic PDEs for many years, and hence they know one another well. Among this group, there have been many comments about the benefits of a relatively lengthy and isolated opportunity to discuss problems in depth without the distractions of a large conference or the narrow bandwidth of remote collaboration. A concrete example of the benefits is an idea for improving fast sweeping methods which arose from discussions between Yongtao Zhang, Chi-Wang Shu and Hongkai Zhao and which will soon lead to a paper submission.

Among the other attendees—both researchers in related fields and students—there was much exchange of ideas about what schemes might prove useful in application areas, what properties and features are most important in those fields, and what implementation and ancillary features (such as visualization or code reuse) are becoming available in new languages and platforms. For example, H. Pino Martin (from Mechanical & Aerospace Engineering at Princeton) thought that some of the recently developed methods could be useful in her work on large-eddy simulations of highly compressible turbulence, and suggested that we collect the talks on the BIRS website so that she and other attendees could more easily follow-up on potential ideas and collaborations.

The benefits of workshops of this nature are also challenging to judge after only a few months. As an example of the long term benefits, there was an example posed around 2005 by Alexander Vladimirsky which was supposed to disprove claims that fast sweeping methods would converge in a finite number of iterations. In a BIRS workshop in December 2006, Ian Mitchell implemented several versions of the example and demonstrated that (to floating point precision) the number of iterations was finite, and actually decreased as the grid resolution increased, which lead to many discussions. In this year's workshop, Hongkai Zhao analyzed and rigorously explained the phenomenon.

On behalf of the attendees, the organizers would like to thank BIRS and the Banff Center staff for an outstanding opportunity to pursue the challenges of numerical methods for nonlinear hyperbolic PDEs and their applications.

List of Participants

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Degond, Pierre (Universite Paul Sabatier)
Ferretti, Roberto (Universita degli Studi di Roma Tre)
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Kao, Chiuyen (Ohio State University)
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Zhang, Yongtao (University of Notre Dame)
Zhao, Hongkai (University of California, Irvine)

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Chapter 30

Understanding the New Statistics: Expanding Core Statistical Theory (08w5071)

Sep 14 - Sep 19, 2008

Organizer(s): Rudolf Beran (University of California, Davis), Iain Johnstone (Stanford University), Ivan Mizera (University of Alberta), Sara van de Geer (Eidgenössische Technische Hochschule Zürich)

Overview of the Field, and Recent Developments

As proposed, the focus of the workshop was core statistical theory—something that in past might have been called "mathematical statistics", were not this name so closely associated with the 1960's vision of statistics before the computer revolution changed the discipline. The emphasis was on "the new statistics", relevant theory for the data-analytic circumstances. (The note [1], authored by one of the organizers, brings more detailed historical analysis and discussion of recent aspects.)

Several participants of the workshop recognized somewhat polemical nature of the term "new statistics", which quickly became a sort of recurrent mantra in the discussions. However, "new" does not imply negation of "old" here. The viewpoint of one of the former editors of JASA, that the theoretical underpinnings of statistical science "hold firm as ever", was not really challenged at the meeting. While the past have seen a lot of crystallization of ideas one one hand and fierce ideological disputes on another, the present is characterized not any of these prevailing over others, but by a totally different, in mathematical parlance orthogonal angle of view.

Such a perception shift was caused in the first place by the burgeoning development of "statistical sciences", that is, disciplines that rely on statistical theory to express their specific ideas, like econometrics, genomics, signal processing, or machine learning. These days, statisticians can be found at various places, not necessarily mathematical or statistical departments; for instance, among Nobel laureates in economics. The turmoil in statistical sciences led to a tremendous reevaluation of the "core of statistics" as defined in [3]: the subset of statistical activity that is focused inward, on the subject itself, rather than outward, towards the needs of statistics in particular scientific domains. The character of this reappraisal did not have that much character of confirmation or refutation, but more that of assessing relevance and usability. Although nothing is definitive in this respect—the supposedly barren fields of yesterday may turn fertile irrigated by the demands of applications—statisticians witnessed that some of the items on their buffet tables were in strong demand, and some of them remained unnoticed. As emphasized in the talks of several participants, the past differences in tastes (say, regarding the use or abuse of inverse probability in statistical deliberations) are felt to be much less divisive now; there are issues now that are more important than sectarian quarrels.

To acquire some feeling about the current situation, the workshop brought together a number of leading-edge researchers in mathematical statistics (a considerable number of them affiliated with computer science rather than classical statistical departments), together with key people from the statistical sciences and other communities practicing data analysis—to assess, in certain selected areas (hopes to seize such an important and complex problematic in its totality would be indeed futile), “what is hot and what is not”. The results were partly expected, partly surprising. The areas of concentration were the following.

Presentation Highlights

The New Asymptotics and Random Matrices

One of the possible approaches capable of formalizing some phenomena occurring in “large p, small n”, is the asymptotic theory of random matrices, the theme of the opening talk of the workshop, Null Distributions for Largest Eigenvalues in Multivariate Analysis, presented by Iain Johnstone, Stanford. The theme was eigenvalues of Wishart matrices: while these play a central role in classical multivariate analysis, a new impetus to approximate distribution results has come from methods that imagine the number of variables as large. Johnstone focused on the largest eigenvalue in particular, and briefly reviewed null distribution approximations in terms of the Tracy-Widom laws. The second part of Johnstone’s talk described the work in progress on concentration inequalities for the largest eigenvalue in the ”two Wishart” case, such as canonical correlations.

Noureddine El Karoui (Berkeley) in Spectral Properties of Kernel Matrices with High-Dimensional Input Data addressed kernel matrices, a special form of matrices used in various areas of machine learning and statistics. For instance, they are sometime used to perform non-linear versions of principal component analysis (PCA).

There has been little work so far investigating their spectral properties when the dimension of the data (p) is of the same order of magnitude as the number of observations (n). El Karoui discussed some results concerning this asymptotic setting, assuming standard and less standard models used in random matrix theory for the data. In particular, it can be shown that for these models, kernel random matrices behave essentially like linear operator—a sharp difference with the low dimensional setting where p is held fixed—where they approximate the spectra of certain integral operators. El Karoui discussed also the proof, highlighting some potential geometric limitations of standard random matrix models for statistical applications, and also some robustness (and lack thereof) results against these geometric features for classical random matrix results.

Random matrix theory then became one of the recurring themes in the other days. Art B. Owen (Stanford, jointly with Patrick Perry) presented a talk entitled Cross-Validation for the Truncated SVD and the Non-Negative Matrix Factorization. Owen and Perry study sample reuse methods like the bootstrap and cross-validation, methods which are widely used in statistics and machine learning. These methods provide measures of accuracy with some face value validity that is not dependent on strong model assumptions. They depend on repeating or omitting cases, while keeping all the variables in those cases. But for many data sets, it is not obvious whether the rows are cases and columns are variables, or vice versa.

For example, with movie ratings organized by movie and customer, both movie and customer IDs can be thought of as variables. Owen and Perry looked at bootstrap and cross-validation methods that treat rows and columns of the matrix symmetrically. They got the same answer on X as on X'. While McCullagh has proved that no exact bootstrap exists in a certain framework of this type (crossed random effects), they showed that a method based on resampling both rows and columns of the data matrix tracks the true error, for some simple statistics applied to large data matrices. They also looked at a method of cross-validation that leaves out blocks of the data matrix, generalizing a proposal due to Gabriel that is used in the crop science literature. They found empirically that this approach provides a good way to choose the number of terms in a truncated SVD model or a non-negative matrix factorization and applied some recent results in random matrix theory to the truncated SVD case.

The connection to the asymptotics of random matrices was imminent also in the topic of the talk of Marc Hallin (Universiteé Libre de Bruxelles) who spoke about The General Dynamic Factor Model developed by Forni et al. (2000) for the analysis of large panels of time series data. Although developed in an econometric context, this method is likely to apply in all fields where a very large number of interrelated time series or signals are observed simultaneously. Hallin considered the problem of identifying the number q of factors driving the panel. The proposed criterion was based on the fact that q is also the number of diverging eigenvalues of the spectral density matrix of the observations as the cross-sectional dimension n goes to infinity. Hallin gave sufficient conditions for consistency of the criterion for large n and T (where T is the series length), showed how the method can be implemented, and presented simulations and empirics illustrating its excellent finite sample performance. The application to real data brought some new contribution in the debate on the number of factors driving the US economy.

The New Asymptotics and Sparse Representations

Sara van de Geer (ETH Zürich, jointly with Peter Bühlmann and Lukas Meier) in her talk on High-Dimensional Additive Modeling considered a high-dimensional additive regression model of the form

$$y = f_1(x) + \cdots + f_p(x) + \epsilon,$$

where the f_j are unknown smooth functions of the covariable x, and where p is large, possibly larger than the number of observations n. She proposed to use penalized least squares to estimate the f_j. The first question to address is then: how to choose the penalty? For this purpose, she first considered the penalized least squares problem in general terms, with splines and the lasso as special cases; then she discussed the trade-off between theoretically 'ideal' but computationally less ideal penalties. With these insights, it is possible to consider 3 possible penalties for the high-dimensional additive model, having in mind the "sparse" situation, where most of the f_j are actually zero. She presented results amounting to oracle type of inequalities in this setting, a simulation study, and an application to real data.

Sparsity was then the theme of several ensuing talks. Marten Wegkamp (Florida State) in Generalized Support Vector Machines in Sparse Settings considered the problem of binary classification where one can, for a particular cost, choose not to classify an observation, and presented a simple oracle inequality for the excess risk of structural risk minimizers, using a generalized hinge loss and a lasso type penalty. He showed that it is possible to obtain fast rates, regardless of the behavior of the conditional class probabilities, if the Bayes discriminant function can be well approximated by a sparse representation.

Florentina Bunea (Florida State) in Honest Inference in Sparse High-Dimensional Models studied the topic of ℓ_1 regularized or lasso type estimation, the topic that has received considerable attention over the past decade. Recent theoretical advances have been mainly concerned with the risk of the estimators and corresponding sparsity oracle inequalities. In her talk, Bunea investigated the quality of the ℓ_1 (and the closely related $\ell_1 + \ell_2$) penalized estimators from a different perspective, shifting the emphasis to correct, non-asymptotic, model identification. She illustrated the merits and limitations of these methods in high dimensional generalized regression and mixture models and discussed an important consequence of this analysis: if the "true" model is identifiable, good estimation/prediction properties of the parameter estimates are not necessarily needed for correct model identification.

An small sensation of the first day was Benedikt M. Pötscher (Vienna), who in his talk, Confidence Sets Based on Sparse Estimators Are Necessarily Large, pointed out some deficiencies in some of the recent sparsity results, deficiencies that can be seen as special cases of some classical and well-known, but perhaps somewhat forgotten phenomena. In particular, he showed that the confidence sets based on sparse estimators are large compared to more standard confidence sets, which demonstrates that the sparsity of an estimator comes at a substantial price in terms of the quality of the estimator. His results were set in a general parametric or semiparametric framework.

A different approach to sparse representation was presented by Lawrence Brown (University of Pennsylvania, jointly with Eitan Greenstein). In Non-parametric Empirical Bayes and Compound Bayes Estimation of Independent Normal Means, Brown considered the classical problem of estimating a vector $\mu = (\mu_1, \ldots, \mu_n)$, based on independent observations $Y_i \sim N(\mu, \sigma^2)$, where μ_i themselves are independent realizations from a completely unknown distribution G_n. Brown proposed an easily computed estimator $\tilde{\mu}$ and studied the ratio of its expected risk $E_{G_n} E_\mu(\|\tilde{\mu} - \mu\|)$ to that of the Bayes procedure. He showed that under very mild conditions, this ratio approaches 1 as $n \to \infty$, and considered also a related compound decision theoretic formulation, where this estimator is asymptotically optimal relative to the best possible estimator given the values of the order statistics $\mu_{(*),n} = (\mu_{(1)}, \ldots, \mu_{(n)})$. In the discussion of this proposal, Brown reminded the audience that there has been much contemporary interest in estimators that are valid in sparse settings; settings such as those for which $p_n \to 0$ and $G_n(\{u\}) = p_n$ if $u = 0, = 1 - p_n$ if $u = u_n$. The conditions on the sequences G_n or $\{\mu_{(*),n}\}$ for asymptotic optimality of $\tilde{\mu}$ are only mildly restrictive, and include a broad range of problems involving sparsity. In particular, the proposed estimator is asymptotically optimal in moderately "sparse" settings - ones such as those described just above in which $np_n \to \infty$ and $n(1 - p_n) \to \infty$ $0 < \liminf u_n, \limsup u_n < \infty$. He also reported a simulation study to demonstrate the performance of our estimator, showing that in moderately sparse settings his estimator performs very well in comparison with current procedures tailored for sparse situation, and adapts also well to non-sparse situations, and concluded his talk by a very interesting application to baseball data.

Kjell Doksum (University of Wisconsin, jointly with Shijie Tang and Kam Tsui) focused On Nonparametric Variable Selection, in the setting of regression experiments involving a response variable Y and a large number d of predictor variables (X's) many of which may be of no value for the prediction of Y and thus need to be removed before predicting Y from the X's. His talk considered procedures that select variables by using importance scores that measure the strength of the relationship between predictor variables and a response. In the first of these procedures, scores are obtained by randomly drawing subregions (tubes) of the covariate space that constrain all but one predictor and in each subregion computing a signal to noise ratio (efficacy) based on a nonparametric univariate regression of Y on the unconstrained variable. The regions are adapted to boost weak variables iteratively by searching (hunting) for the regions where the efficacy is maximized. The efficacy can be viewed as an approximation to a one-to-one function of the probability of identifying features. By using importance scores based on averages of maximized efficacies, we develop a variable selection algorithm called EARTH (Efficacy adaptive regression tube hunting). The second importance score method (RFVS) is based on using Random Forest importance values to select variables. Computer simulations show that EARTH and RFVS are successful variable selection methods when compared to other procedures in nonparametric situations with a large number of irrelevant predictor variables. Moreover, when each is combined with the model selection and prediction procedure MARS, the tree-based prediction procedure GUIDE, or the Random Forest prediction method, the combinations lead to improved prediction accuracy for certain models with many irrelevant variables. Doksum gave conditions under which a version of the EARTH algorithm selects the correct model with probability tending to one as the sample size tends to infinity, even if d tends to infinity as n tends to infinity, and concluded his talk with the analysis of a real data set.

In a similar vein, Hannes Leeb (Yale) proposed methodology for Evaluating and Selecting Models for Prediction Out-Of-Sample. The problem he studied, in the framework of the regression with random design, was that of selecting a model that performs well for out-of-sample prediction, focusing on a statistically challenging scenario where the number of potentially important explanatory variables can be infinite, where no regularity conditions are imposed on unknown parameters, where the number of explanatory variables in a "good" model can be of the same order as sample size, and where the number of candidate models can be of larger order than sample size.

The Role of Geometry

The geometric line of the workshop started by the talk of Peter Kim (Guelph, jointly with Peter Bubenik, Gunnar Carlsson, and Zhiming Luo) entitled Geometric and Topological Methods for High-Dimensional Data Analysis. Kim examined the estimation of a signal embedded in white noise on a compact manifold, where a sharp asymptotic minimax bound can be determined under the sup-norm risk over Hölder classes of functions, generalizing similar results available for spheres in various dimensions. The estimation allows for the development of a statistical Morse theory using the level sets of the estimated function and together with the sup-norm bound allows the bounding of the Hausdorff distance in a persistence diagram in computational algebraic topology.

Mikhail Belkin (Ohio State) in his talk Spectral and Geometric Methods in Learning discussed some of the methods from a variety of spectral and geometry-based methods that became popular for various tasks of machine learning (such as dimensionality reduction, clustering and semi-supervised learning) and recent theoretical results on their convergence. A particularly interesting part of his talk was a proposal how spectral methods can be used to estimate parameters in the mixtures of Gaussian distributions.

The correspondence with information-theoretical aspects through convex geometry embedded in the duality theory of convex optimization was the theme of two talks. Michael Jordan (Berkeley, jointly with XuanLong Nguyen and Martin Wainwright), in On Surrogate Loss Functions and f-Divergences) looked at binary classification, where the goal is to estimate a discriminant function γ from observations of covariate vectors and corresponding binary labels. He considered an elaboration of this problem in which the covariates are not available directly, but are transformed by a dimensionality-reducing quantizer Q, and presented conditions on loss functions such that empirical risk minimization yields Bayes consistency when both the discriminant function and the quantizer are estimated. These conditions were stated in terms of a general correspondence between loss functions and a class of functionals known as Ali-Silvey or f-divergence functionals. Whereas this correspondence was established by Blackwell (1951) for the 0-1 loss, Jordan presented an extension of the correspondence to the broader class of surrogate loss functions that play a key role in the general theory of Bayes consistency for binary classification. The result makes it possible to pick out the (strict) subset of surrogate loss functions that yield Bayes consistency for joint estimation of the discriminant function and the quantizer.

Ivan Mizera (University of Alberta, jointly with Roger Koenker) in Quasi-Concave Density Estimation: Duality in Action explored the duality aspects in maximum likelihood estimation of a log-concave probability density formulated as a convex optimization problem. It was shown that an equivalent dual formulation is a constrained maximum Shannon entropy problem. Mizera considered also closely related maximum Renyi entropy estimators that impose weaker concavity restrictions on the fitted density, notably a minimum Hellinger discrepancy estimator that constrains the reciprocal of the square-root of the density to be concave; a limiting form of these estimators constrains solutions to the class of quasi-concave densities.

Algorithmic Inspirations

Speakers in this area mostly addressed various aspects of regularization as recently used in statistical methods. Saharon Rosset (Tel Aviv, jointly with G. Swirzscz, N. Srebro, J. Zhu) in ℓ_1 Regularization in Infinite Dimensional Feature Spaces discussed the problem of fitting L1 regularized prediction models in infinite (possibly non-countable) dimensional feature spaces. The main contributions were: (a) Deriving a generalization of L1 regularization based on measures which can be applied in non-countable feature spaces; (b) Proving that the sparsity property of L1 regularization is maintained in infinite dimensions; (c) Devising a path-following algorithm that can generate the set of regularized solutions in “nice” feature spaces; and (d) Presenting an example of penalized spline models where this path following algorithm is computationally feasible, and gives encouraging empirical results.

Roger Koenker (University of Illinois) in Computational Pathways for Regularized Quantile Regression recalled that in the beginning was the weighted median of Boscovich and Laplace; much later, Edgeworth (1888) nearly discovered the simplex algorithm, and Frisch (1956) almost proposed the interior point (log-barrier) method for linear programming; finally, modern variants of these methods, aided by recent developments in sparse linear algebra, are highly effective in many statistical applications. However, in regression settings with large, dense designs these methods perform quite poorly. Fortunately, old-fashioned simplex-type parametric programming methods come to the rescue for some problems of this type. Koenker reported on some computational experience in such situations, and make some more speculative remarks on implications for the choice of the ubiquitous regularization parameter. A common feature of the foregoing approaches to computation is that they all seek the path to enlightenment via some form of regularization.

The algorithmic inspiration of Giles Hooker (Cornell) for his Inference from Black Boxes came from the fields of machine learning or data mining, which produced a multitude of tools for “algorithmic learning”. Such tools are frequently ad hoc in nature, justified by some heuristics and can be challenging to analyze mathematically. Moreover, these routines produce prediction prediction functions that are typically algebraically complex and difficult to interpret.Nonetheless, there has been considerable interest in tools to “x-ray the black box”. Many of these tools can be understood in terms of the functional ANOVA decomposition. This decomposition represents a high dimensional function in terms of an additive expansion of lower dimensional components and allows us to quantify measures like variable importance and the average effect of certain variables. In his talk, Hooker examined the practical and theoretical challenges in turning such diagnostic procedures into formalized statistical tests. Specifically, he examined bootstrap inference about the functional ANOVA relationships in the underlying structure of the data. His aim was to be generic in the sense of providing tools that are universally applicable, regardless of the learning algorithm employed.

A yet another application of regularization methods, Inpendence and Conditional Independence with

Reproducing Kernels, was presented by Kenji Fukumizu (Institute of Statistical Mathematics). He proposed new nonparametric methodology for dependence of random variables, with application to dimension reduction for regression. The methodology uses the framework of reproducing kernel Hilbert spaces (RKHS) defined by positive definite kernels. In this methodology, a random variable is mapped to a RKHS, thus random variables on the RKHS are considered. Fukumizu showed that the basic statistics such as mean and covariance of the variables on the RKHS can capture all the information on the underlying probabilities, and provide a method of characterizing independence and conditional independence. The framework of RKHS enables to derive a practical and efficient way of computing estimators defined on RKHS. Using the characterization of conditional independence, Fukumizu introduced a method of dimension reduction or feature extraction of the covariates is introduced for regression problems, and derived a practical algorithm to extract an effective linear feature. The method is of wide applicability; it does not require any strong assumptions on the type of variables or the probability of variables, which are often imposed by other methods of dimension reduction. Consistency of the estimator was proved under weak condition, and some experimental results show the method is practically competitive.

Rudolf Beran (Davis) in Penalized Fits of Multivariate Responses to Covariates considered a complete k-way layout of d-dimensional mean vectors, in which each mean vector is an unknown function of k real-valued covariates whose values are known, and the covariates may be either ordinal or nominal. There is at least one observation with error on each of the unknown mean vectors; the problem is to estimate the mean vectors efficiently, without making any assumption about the function that relates them to the known covariates. Both theory and practice have made it clear that the unconstrained least squares estimator of the mean vectors is unsatisfactory unless the data provides substantial replication. In his talk, Beran defined a candidate class of penalized least squares (PLS) estimators suitable for the problem. A separate quadratic penalty term is devised for each of the main effects and interactions in the MANOVA decomposition of the mean vectors. The construction of the penalty terms draws on vague notions about the unknown function that links the means to the covariates. Before being summed, each penalty term is weighted by right multiplication with a $d \times d$ symmetric positive semidefinite matrix. The candidate PLS estimators thereby accomplish, as special cases, both MANOVA submodel selection and dimensionality reduction. The matrix penalty weights were chosen to minimize estimated quadratic risk over the candidate class of PLS estimators; it was shown that, as the number of cells in the complete k-way layout tends to infinity, the candidate PLS estimator with smallest estimated risk converges, in loss or risk, to the candidate estimator with smallest actual loss or risk. The asymptotics make no assumptions about the unknown d-dimensional mean vectors in the k-way layout and require no replication. The talk was concluded by a case study on multivariate response data illustrating how the proposed adaptive estimator works.

A different, but very appealing inspiration by algorithmic methods was presented by Marloes Maathuis (ETH Zürich, jointly with Markus Kalisch and Peter Bühlmann), who studied Variable Importance Based on Intervention Calculus. It is assumed that we have observational data, generated from an unknown underlying directed acyclic graph (DAG) model, and it is well-known that a DAG is not identifiable from observational data, but it is possible to consistently estimate an equivalence class of DAGs. Moreover, for any given DAG, causal effects can be estimated using intervention calculus. In her talk, Maathuis combined these two parts. For each DAG in the estimated equivalence class, she used intervention calculus to determine the causal effects of the covariates on the response. This yields a collection of possible causal effects for each covariate. Maathuis showed that the distinct values in this set can be consistently estimated by an algorithm that uses only local information of the graph. This local approach is computationally fast and also has advantages from an estimation point of view. Maathuis proposed to use summary measures of the set of possible causal effects to determine variable importance; in particular, to use the minimum absolute value of this set, since that is a conservative bound on the size of the causal effect.

Old as a Backbone of the New Statistics

Two of the talks happened to be aimed at a reflection about foundations. Bertrand Clarke (University of British Columbia) proposed Coordinating Theory, motivated by the impact of new data types and the compartmentalization of subfields of statistics. His theory intends to interrelate the disparate principles and practices of Statistics within one framework in, as he argued, “a good time to crystallize what unites us in statistics.” The key features are predictive optimality and a unified variance bias treatment; the approach includes Bayes, Frequentist and other perspectives, including subsidiary criteria, such as robustness and efficiency. An an application of this framework, Clarke presented a comparison of three predictors in the context of a complex data set, formalizing one meaning of complexity for data. His computations verify that taking model uncertainty into account explicitly can lead to better predictions. According to his words, "if a Coordinating Theory could be found, it would serve the same role in statistics as Newton's Laws did for physics or evolution does for biology."

A View From a Limited Perspective was a title of the talk of Laurie Davies (University of Duisburg–Essen). It touched on various topics—the location-scale problem, approximation of a data set, topologies, likelihood, stability, regularization, the analysis of variance, sparsity, nonparametric regression, smoothness, shape, the role of asymptotics, optimality, theorems and procedures—on which this Davies has some experience, and also his unique personal perspective.

Another two presentations were devoted to random effects, a theme where "old statistics" has still much to say. Peter McCullagh (University of Chicago) in Random Effects and Estimating Equations, addressed the consequences for random-effects models of the sampling scheme or recruitment strategy used to enroll units. This issue does not usually arise in typical agricultural or horticultural field trials or laboratory experiments, but it does arise in clinical trials and in social-science areas such as marketing studies. McCullagh suggested a point-process model as a way to generate units in an automatic random manner, thereby avoiding the notion of units altogether.

Debashis Paul (Davis, jointly with Jie Peng and Prabir Burman) in Statistical Modeling Through Nonlinear Mixed Effects Dynamics focused on a class of models where the observations are longitudinal data measured for several subjects, and the trajectories are modeled as random and noisy realizations of a smooth process described by a first order nonlinear differential equation. Paul proposed a procedure based on numerically solving an ODE for the associated initial value problem to estimate the underlying dynamics from the observed data, studied the corresponding model selection problem, proposed an inferential framework for this class of problems, and provided illustrations of the method with simulated and real data examples.

Wolfgang Polonik (Davis, jointly with David Mason) in Asymptotic Normality of Plug-In Level Set Estimates spoke about level sets, regions where a target function f exceeds a given threshold value c. Such sets play a vital role in various fields of applications, such as anomaly detection, astronomical sky surveys, flow cytometry, and image segmentation. Other statistical applications of level sets include classification and visualization of multivariate densities. Algorithms have been devised for fast computation of level set estimates in large dimension, and consistency as well as optimal and 'fast' rates of convergence have been derived. While these results are interesting from a theoretical and computational point of view, they are not too helpful for statistical inference. Polonik addressed the problem of inference for level sets by focusing on a plug-in estimator (based on a kernel density estimator) of a density level set. As a distance measure, he considered the set-theoretic difference between the estimate and the target set, presented conditions under which such plug-in level set estimates are asymptotically normal, and discussed potential applications of such results to binary classification.

David Mason (University of Delaware, jointly with Julia Dony, Uwe Einmahl and Jan Swanepoel) discussed in Recent Results on Uniform in Bandwidth Consistency of Kernel-Type Function Estimators a general method based on empirical process techniques to prove uniform in bandwidth consistency of kernel-type function estimators. Examples include the kernel density and distribution function estimators, the Nadaraya-Watson regression function estimator, the conditional empirical process and conditional U-statistic. The results are useful to establish uniform consistency of data-driven bandwidth kernel-type function estimators.

Aurore Delaigle (University of Bristol) spoke about Design-Adaptive Local Polynomial Estimator for the Errors-in-Variables Problem, focusing on local polynomial estimators, a very popular techniques of nonparametric regression estimation that received great attention in the literature. Their simplest version, the local constant estimator, can be easily extended to the errors-in-variables context by exploiting its similarity with the deconvolution kernel density estimator. The generalization of the higher order versions of the estimator, however, is not straightforward and has remained an open problem for the last 15 years. In her talk, Delaigle showed how to construct local polynomial estimators of any order in the errors-in-variables context, discussed their asymptotic properties and illustrated their finite sample performance on numerical data examples.

Finally, Vladimir Vovk (Royal Holloway) in Predictive Regression: In Defence of the Old Statistics addressed the following problem: given the past data $(x_1, y_1), ..., (x_N, y_N)$ and a new vector x_{N+1} of explanatory variables, predict the new response variable y_{N+1}. The classical, and much criticized, assumption is the Gauss linear model: nothing is assumed about the explanatory vectors x_n, and the response y_n is modelled as a linear function of x_n plus an IID Gaussian noise. In the theoretical "new statistics" the Gauss linear model is usually replaced by the IID model: the observations (x_n, y_n) are independent and identically distributed.

This greatly weakens the restriction on the distribution of responses given the explanatory vectors, but imposes restrictions on the distribution of explanatory vectors: for example, now they cannot be chosen by a free agent, and the prediction procedure cannot be used for control. The two models are not comparable: either has important advantages over the other. Vovk stated and discussed two relatively recent results. 1. Under the Gauss linear model and when used in the on-line mode, the classical prediction intervals based on Student's t-distribution fail to contain y_n independently for different n. Therefore, the chosen significance level translates into the frequency of error. 2. There exists an algorithm, Ridge Regression Confidence Machine, that satisfies analogous properties under the iid model: the probability of error is equal to the chosen significance level, and errors are made independently for different observations.

Object-oriented Data Analysis

Another recurring theme of the workshop was delineated by the one of the opening talks. Steve Marron (University of North Carolina) spoke about High Dimension Low Sample Size Mathematical Statistics by Steve Marron, the rapidly proliferating, but less mathematically analyzed theme—perhaps because the usual asymptotics are no longer relevant. He deems that a more appropriate HDLSS asymptotic theory, based on fixed sample size, with increasing dimension, is perhaps surprisingly relevant and useful. Results so far fall into two classes. The first is the discovery that, modulo rotation, random HDLSS data have a rigid deterministic structure, which reveals a number of useful statistical insights. The second is a class of results studying commonly used estimators, such as principal component direction vectors, are either consistent or strongly inconsistent (i.e. the angle between to the direction being estimated tends to 90 degrees), depending on the strength of the signal in the data.

Jim Ramsay (McGill), in Parameter Cascading for High Dimensional Models, spoke about high dimensional models that often involve three or more classes of parameters. Nuisance parameters are required to fit the data, are large in number, their number tends to depend on how much data is available, often define localized effects on the fit, and their values are seldom of direct interest. Structural parameters are the conventional kind; a small fixed number and their values are of interpretive importance. Above these are the complexity parameters that define the overall complexity of the solution. Ramsay defined a general framework for parameter estimation that synthesizes a variety of common approaches and brings some important new advantages. The parameter cascade approach involves defining nuisance parameters as functions of structural parameters, and in turn defines structural parameters as functions of complexity parameters. The method is much easier to program and tends to be much more computationally stable than classic marginalization approaches, and is an attractive alternative to MCMC.

Christopher Genovese (Carnegie-Mellon, jointly with Marco Pacifico Perone, Isabella Verdinelli, and Larry Wasserman), spoke about Finding Filaments, one-dimensional curves embedded in a point process or random field. He considered the problem of reliably detecting and estimating filaments, the problem arising in a wide range of applications. Statistical techniques exist for for finding one (or a few) filaments, but these methods do not handle noisy data sets with many filaments. Other methods can be found in the astronomy literature, but they do not have rigorous statistical guarantees. Genovese discussed two methods and their underlying theory. The first method locates filaments by finding regions where certain paths constructed from the data are highly concentrated. Concentration here refers to a formal density of paths. Genovese defined this density and constructed a consistent estimator of it. The second method combines nonparametric regression with vector quantization to partition the space into a collection of smooth curves. Genovese illustrated the procedure and assessed its theoretical performance. The two methods come from different theoretical directions and give different insights into the problem.

Martin Bilodeau (Université de Montréal) spoke about Discovering Dependencies in Multivariate Data and in Stationary Sequences. The Möbius transformation of probability cells in a multi-way contingency table is used to partition the Pearson chi-square test of mutual independence into A-dependence statistics. Bilodeau proposed a similar partition for a universal and consistent test of serial independence in a stationary sequence of a categorical variable, which can be adapted whether using estimated or theoretical marginal probabilities. With the aim of detecting a dependence of high order in a long sequence, A-dependence terms of the partition measuring increasing lagged dependences can be combined in a Box-Pierce type test of serial independence. Bilodeau presented a real data analysis of a nucleotides sequence using the Box-Pierce type test. A non parametric test of the mutual independence between many numerical random vectors is also proposed. This test is based on a characterization of mutual independence defined from probabilities of half-spaces in a combinatorial formula of Möbius. The critical values of the proposed test are computed with the bootstrap which is shown to be consistent. Another similar test, with the same asymptotic properties, for the serial independence of a multivariate stationary sequence is also proposed.

The workshop was concluded by the talk The Joy of Text by Andrey Feuerverger (Toronto), who introduced some new classes of statistical problems associated with computationally intensive statistical analysis of textual documents intended for a variety of purposes. These include the dating (or calendaring) of undated textual documents by comparing their contents with those of dated documents, and the sorting of a collection of documents into chronological order by means of comparing word sequences in the documents.

Scientific Progress Made

As mentioned at the beginning, the lessons learned at the meeting were partly expected, partly surprising. Several of the talks (Pötscher, McCullagh, Vovk, among others) underlined the continuity, the potential of the established statistical thinking if well understood and appropriately used. For instance, Benedikt Pötscher in his talk characterized himself as "a messenger from the past"; nevertheless, the impact of his talk concerned very recent themes. Summarizing this point, "old statistics" is not passé, only some of its too specialized disputes; and "new statistics" does not necessarily means "right" or "better".

As expected, several areas of recent research confirmed themselves as particularly active and fertile directions: random matrices, sparse representation, geometric theory, regularization, algorithms. They may be in different stages of development and evolution; assessing those may be somewhat delicate and it is probably best to refer to the list of contributions for an ultimate prespective. Nevertheless, what may be said that each of these offers a promise of substantial research contributions in the years to come.

Of course, the progress in statistical sciences is by no means expected only in the just named areas. There are vast areas of very active research that were inevitably omitted at the meeting at this size; glimpses to other of them have been given by several talks. If one has to summarize here, the common prevailing focus would be less on rounding the angles and complementing the existing methodologies— not on "filling the gaps in the literature", but rather on creating them; the economic law of diminishing returns seems to be fully applicable also here, and first insights and often approximate solutions are typically more appreciated as later improvements and refinements.

Another recurring theme is an emphasis on complexity, both of the data and methods of their analysis, and the subsequent management of this complexity by conceptual and algorithmic means. While the past methodologies amounted to fitting of and inferences about several numbers, slowly moving to lines and curves, the present practice of "object oriented data analysis" goes far beyond the "classical nonparametric perspectives": the fitted concepts are collection of curves, algebraic structures like graphs and trees, and parameter cascades.

An important outcome of the meeting was the renewed recognition of the vital need of theoretical reflection. As mentioned already in the proposal, the rapidly growing needs of the statistical sciences provide raw material for future core research in statistics and motivates the development of trustworthy, user-friendly statistical methodology. However, as Sara van de Geer pertinently remarked, there may be way too many data analytic proposals out there; one desperately needs some insights. In this context, it is worth to repeat that statistics indeed fluctuates between import and export mode: importing raw data-analytic ideas inspired by the technology and problems of the moment and exporting refined data-analytic procedures, whose characteristics are understood theoretically and experimentally, to the community of quantitative scientists. The phrase "core of statistics" refers precisely to the intellectual basis for the export mode.

Finally, a positive feeling which was also to some extent felt in the community is that of the renewed awareness of common roots and inclinations. It turns out that the schism indicated at the beginning of this decade by [2] was perhaps slightly overstated, driven perhaps rather by a desire to be polemic with certain surviving tendencies at that time; it seems that the atmosphere in the data-analytic community at the end of this decade is much more about collaboration and unification; the divisive aspects seem to be less pronounced.

Outcome of the Meeting

Writing at this point that "the workshop has been a success" would be hardly a surprising twist in the context of BIRS final reports. While the feelings of the participants are probably on the high side, influenced also by the excellent weather we were lucky to enjoy, the full appreciation of the impact of the the workshop, its objectives and contents will be clear only with some time.

Nonetheless, there is one important objective that might have already been achieved, as stressed in the Tuesday evening round-table discussion by one of the organizers, Iain Johnstone. He recalled a recent workshop funded by NSF's Division of Mathematical Sciences at which speakers representing a variety of domains of statistical application emphasised the role of statistical theory in identifying, articulating and developing intersections in concepts and methods across the many areas in which statistical thinking is used. In this particular context, it is clear that the fact that a BIRS workshop like this—*planned and approved well before the NSF workshop was conceived*—not only happens, but convincingly demonstrates that cultivating statistical theory is a vital necessity for the healthy life of the statistical discipline, and that it is theory that often propels the applications—this fact alone may mean that the objectives of the meeting were met.

The workshop was attended by 41 confirmed (and present) participants, whose list is attached as appendix to this report. About 8–10 were in the "early pre-tenured" stage of their career (graduate students, postdocs, fresh assistant professors). We would like to extend our thanks to BIRS and its scientific director, Nassif Ghoussoub, for the opportunity to organize the workshop, and to all BIRS staff, especially to Alitha D'Ottavio and Brenda Williams, for help.

List of Participants

Belkin, Mikhail (Ohio State University)
Beran, Rudolf (University of California, Davis)
Bilodeau, Martin (Universite de Montreal)
Brown, Lawrence (Larry) (University of Pennsylvania)
Bunea, Florentina (Florida State University)
Chen, Gemai (University of Calgary)
Chenouri, Shojaeddin (University of Waterloo)
Clarke, Bertrand (University of British Columbia)
Davies, Laurie (University of Duisburg-Essen)
Delaigle, Aurore (University of Bristol)
Doksum, Kjell (University of Wisconsin)
El Karoui, Noureddine (University of California Berkeley)
Farahmand, Amir massoud (University of Alberta)
Feuerverger, Andrey (University of Toronto)
Fukumizu, Kenji (Institute of Statistical Mathematics)
Genovese, Christopher (Carnegie Mellon University)
Hallin, Marc (Universite Libre de Bruxelles)
Hlubinka, Daniel (Charles University)
Hooker, Giles (Cornell University)
Johnstone, Iain (Stanford University)
Jordan, Michael (University of California Berkeley)
Kim, Peter (University of Guelph)
Koenker, Roger (University of Illinois at Urbana-Champaign)
Kovac, Arne (University of Bristol)
Leeb, Hannes (Yale University)
Maathuis, Marloes (Eidgenössische Technische Hochschule Zürich)

Marron, J. S. (Steve) (University of North Carolina Chapel Hill)
Mason, David M. (University of Delaware)
McCullagh, Peter (University of Chicago)
Mizera, Ivan (University of Alberta)
Owen, Art B. (Stanford University)
Paul, Debashis (University of California Davis)
Poetscher, Benedikt M. (University of Vienna)
Polonik, Wolfgang (University of California Davis)
Rajaratnam, Bala (Stanford University)
Ramsay, Jim (McGill University)
Rosset, Saharon (Tel Aviv University)
van de Geer, Sara (Eidgenössische Technische Hochschule Zürich)
Vovk, Vladimir (Royal Holloway, University of London)
Wegkamp, Marten (Florida State University)
Zlatev, Boyko (University of Alberta)

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Chapter 31

Number Theory and Physics at the Crossroads (08w5077)

Sep 21 - Sep 26, 2008

Organizer(s): Charles Doran (University of Washington), Sergei Gukov (University of California, Santa Barbara), Helena Verrill (Louisiana State University), Noriko Yui (Queens University), Don Zagier (Max-Planck-Institut fuer Mathematik)

The fourth of this series of workshops in the interface of number theory and physics met at BIRS in the week of September 21 for five days. The workshop was a huge success. Altogether thirty-nine mathematicians and physicists converged at the BIRS for the five day's scientific endeavor. There were 22 one hour talks, and lots of time was allotted for informal discussions.

Lectures by mathematicians were designed to familarize physicists on modular forms, quasimodular forms, modularity of Galois representations, zeta-functions and L-series, among others. Vice versa, lectures by physicists were intended toward educating mathematicians about some aspects of mirror symmetry, conformal field theory, quantum field theory, black holes in connection with number theory.

Topics of lectures ranged from various aspects of modular forms, differential equations, conformal field theory, black holes, wall-crossings, topological strings and Gromov–Witten invariants, holomorphic anomaly equations, mirror symmetry, among others. More detailed descriptions of scientific activities will be reported on in Section 4.

Though number theorists and string theorists have been working on modular forms, quasimodular forms, Jacobi forms and more generally automorphic forms in their respective fields, there have been very little interactions between the two sets of researchers, although with some exceptions. In other words, both camps have been living in parallel universes. This workshop brought together researchers in number theory, algebraic geometry, and physics (string theory) whose common interests are centered around modular forms. We witnessed very active and intensive interactions of both camps from early mornings to late nights. We all felt that all things modular have came together at BIRS from both sides: number theory and physics (in particular, string theory). At the end of the workshop, all participants felt that both camps have finally crossed boundaries and established relatively comfortable rapport.

There was a strong desire to have this kind of workshops more frequently at BIRS. However, the deadline to submit a follow-up workshop in 2010 was September 29, 2008! and the organizers felt that we needed more time to access the impact of the 2008 workshop and then plan for the next one. Consequently, we are planning to submit a follow-up proposal for the year 2011. The organizers will be Victor Batyrev, Chuck Doran, Sergei Gukov, Noriko Yui and Don Zagier.

Contents

3. Summary of scientific and other objectives
4. Summary of scientific activities
5. References
6. Titles and abstracts at the workshop
7. Participants

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Originally, Helena Verrill (Louisiana State University, USA) was listed as an organizer. However, she declined to serve as an organizer due to her maternity duties.

2. Press Release: Number Theory and Physics at the Crossroads

In the recent years, the world has seen explosive interactions between Number Theory, Arithmetic and Algebraic Geometry, and Theoretical Physics (in particular, String Theory). To name a few, the classical modular forms, quasi-modular forms, and Jacobi forms appear in many areas of Physics, e.g., in mirror symmetry, topological quantum field theory, Gromov-Witten invariants, Calabi-Yau manifolds and in block holes. Also modularity questions of Calabi-Yau varieties and other higher dimensional varieties in connection with Langlands Program are getting considerable attention and feedbacks from physics. Zeta-functions and L-series enter scenes at various places in physics. Via renormalization, Feynman integrals are related to multiple zeta-values, and purportedly to motives. Calculations of the energy and charge degeneracies of black holes lead surprisingly to Jacobi forms and Siegel modular forms.

There have been strong desires among mathematicians and physicists for more workshops directed to the areas of number theory and physics at the crossroads. This workshop responded to that demand and brought together many leading researchers working in the interface of number theory, arithmetic/algebraic geometry and theoretical physics to BIRS.

The newly launched international research journal, "Communications in Number Theory and Physics" (http://www.intlpress.com/CNTP) published by International Press, will provide a venue for dissemination of results at this crossroads well into the future. Participants are encouraged to submit their written up talks and further new results to the journal.

3. Summary of scientific and other objectives

Physical duality symmetries relate special limits of the various consistent string theories (Types I, II, Heterotic string and their cousins, including F-theory) one to another. By comparing the mathematical descriptions of these theories, one reveals often quite deep and unexpected mathematical conjectures. The best known string duality to mathematicians, Type IIA/IIB duality also called *mirror symmetry*, has inspired many new developments in algebraic and arithmetic geometry, number theory, toric geometry, Riemann surface theory, and infinite dimensional Lie algebras. Other string dualities such as Heterotic/Type II duality and F-Theory/Heterotic string duality have also, more recently, led to series of mathematical conjectures, many involving elliptic curves, K3 surfaces, and modular forms.

In recent years, we have witnessed that modular forms, quasi-modular forms and automorphic forms play central roles in many areas of physics, e.g., quantum field theory, conformal field theory, mirror symmetry, and 4D gauge theory. Most prominently, generating functions counting the number of curves on Calabi–Yau manifolds (e.g., Gromov–Witten invariants), elliptic genera/partition functions of conformal field theory, and generating functions in 4D gauge theory are all characterized by some kinds of modular forms (classical modular forms, quasi-modular forms, Jacobi forms, Siegel modular forms. etc.)

This has led to a realization that we ought to assess with vigor the role of number theory, in particular that of modular forms, in physics in general. Indeed, there have been at least three efforts along this line in Canada, in terms of a series of workshops devoted to this goal. One of the first in this series was the Fields workshop on "Calabi–Yau Varieties and Mirror Symmetry", 2001; its follow-up five-day workshop was held at BIRS in 2003. The most recent one was the five-day workshop on "Modular Forms and String Duality" at BIRS in 2006. The Proceedings of these three past workshops have been published (see references). This brings the workshop on "Number Theory and Physics at the Crossroads" as the fourth in this series.

It brought together mathematicians and physicists working on problems inspired by string theory. Many researchers in string theory and number theory, working on the same or related problems from different angles came together at BIRS. This synthesis proved powerful and beneficial to both parties involved; simply put, the workshop was a huge success. There was an overwhelming consensus from researchers working at the crossroads of number theory and physics to organize this kind of workshop more frequently. In particular, many researchers are extremely eager to have another five-day workshop at BIRS in two or three years time.

A new research journal "Communications in Number Theory and Physics" (published by International Press of Boston) has been launched, specifically devoted to subject areas at the crossroads of number theory and physics. The editors-in-chief of this new journal are Robert Dijkgraaf, David Kazdhan, Maxim Kontsevich, and Shing-Tung Yau. The journal has entered its second year, and has proved to be a spectacular success! Some members of the editorial board took part in the workshop.

One of the principal goals of this workshop is to look at various modular forms, zeta-functions, L-series, Galois representations, arising from Calabi–Yau manifolds, conformal field theory, quantum field theory, and 4D gauge theory. The subject area of interest might be classified into not clearly disjoint sets of the following subjects:

(a) Modular, quasimodular, Siegel, and Jacobi modular forms, and their applications.
(b) Topological string theory, mirror symmetry and modular forms.
(c) Modularity of Galois representations, and arithmetic questions.
(d) Conformal field theory and modular forms.
(e) Holomorphic anomaly equations.
(f) Differential equations.
(g) Wall-crossing formula.
(h) Other topics in the interface of number theory and physics.

4. Summary of scientific activities

The workshop's kick-off talk was delivered by Sergei Gukov giving scientific directions to the entire workshop.

S. Gukov illustrated by a number of examples analogies and cross currents between number theory and physics. For instance, counting certain invariants in number theory (.e.g., zeta-functions, L-series concocted by counting number of rational points), and some counting invariants in physics (e.g. Z-functions, partition functions in quantum field theory formed by counting Gromov-Witten invariants, or BPS states, elliptic genera in conformal field theory) share common modular properties.

(a) Modular, quasimodular, Siegel, and Jacobi modular forms, and their applications

D. Zagier gave an introduction of mock modular forms, a new type of modular object whose theory was developed by S. Zwegers and which has potential applications to the theory of black holes.

A. Dabholkar explained a recent application of Siegel modular forms in counting the microstates of black holes. For instance, the Igusa cusp Siegel form of genus 2 appeared in a description of the partition function of dyonic black holes in $N = 4$ compactifications.

A. Clingher discussed a family of lattice polarized K3 surfaces polarized by the rank 17 lattice $H_2 \oplus E_8 \oplus E_7$. He explained how to classify these K3 surfaces in terms of Siegel modular forms.

(b) Topological string theory, mirror symmetry and modular forms

V. Bouchard discussed modular properties of generating functions of open orbifold Gromov–Witten invariants. The solutions to loop equations in matrix model theory yield B-model amplitudes, and they are quasimodular forms of weight 0 for $SL_2(\mathbf{Z})$ in case of genus 1.

E. Scheideggar reported on his proof of the Yau–Zaslow conjecture for all curves on K3 surfaces.

(c) Modularity, and arithmetic questions

D. Ramakrishnan discussed the audacity of hope focusing on a specific question, *the geometric realization problem*: Let π be a $\mathbf{Q}$-rational. even self-dual regular cusp form o $GL_n(\mathbf{Q})$ of weight $m > 0$. Then does there exist a Calabi–Yau variety $X/\mathbf{Q}$ of dimension m and a motive M such that $\pi \leftrightarrow M \subset H^m(X)$ with $M^{m,0} \neq 0$?

R. Schimmrigk gave a physicist's understanding of modularity of Calabi–Yau threefolds over $\mathbf{Q}$ and D-branes.

(d) Conformal field theory and modualr forms

T. Gannon's talk was concerned with rational conformal field theory (RCFT) or rational vertex operator algebras (RVOA). The main point was that characters associated to RVOA are vector-valued modular forms for $SL_2(\mathbf{Z})$ or $\Gamma(2)$. Moonshine modules are explained as such examples.

C. Keller discussed a generalization of recursion relations between n-point functions to those of the $N = 2$ supersymmetry case. The recursion relations yielded generalized Eisenstein series, which were then used to construct modular covariant differential operators on the space of weak Jacobi forms. His talk was video-taped.

J. Manschot reported on the relation between supersymmetric black holes of $N = 2$ supergravity and modular forms. In particular, it was shown that microscopic counting function of some class of black holes is expressed in terms of Jacobi forms.

(e) Holomorphic anomaly equations

S. Hosono reported on his recent work on the BCOV rings over the moduli space of Calabi–Yau threefolds, which are regarded as generalizations of the ring of almost holomorphc modular forms and quasimodular forms for elliptic curves.

A. Klemm reported that modularity and the gap conditions make the holomorphic anomaly equation completely integrable for non-compact Calabi–Yau manifolds. As an application of this result, he laid out an algorithm for computing higher genus closed string amplitudes in terms of almost holomorphic modular forms.

(f) Differential equations

Candelas discussed special geometry of Calabi–Yau threefolds over $\mathbf{C}$ and $\mathbf{F}_p$, mostly focusing on one-parameter family of quintic mirror Calabi–Yau threefolds.

Lewis discussed an algorithm based on the Griffiths–Dwork for computing Picard–Fuchs differential equations for families of singular varieties, e.g., families of lattice polarized K3 surfaces.

Yamazaki reported on a new algorithm for constructing all rational solutions to the KdV hierarchy, which was based on the study of degenerate fibers of the Mumford systems in terms of Jacobian variety.

Zudilin used analytic method to study Picard–Fuchs differential equations of order m for periods of (1-parameter) families of Calabi–Yau manifolds ($m = 2, 3, 4, 5$). All differential equations were of hypergeometric type and found some new algebraic transformations among hypergeometric series satisfying certain linear differential equations of order $m \leq 5$.

(g) Wall-crossing formula

A. Neiztke and D. Gaiotto explained the wall-crossing formula due to Kontsevich and Soibelmann from geometric and physical points of view.

(h) Miscellaneous topics

P. Gunnells gave a lively talk on Weyl group Dirichlet series in several complex variables. He presented an idea of construction of Weyl group Dirichlet series.

D. Kazhdan discussed Satake isomorphism for Kac–Moody groups.

M. Kerr considered two different constructions of motivic cohomology classes on families of toric hypersurfaces and on Kuga varieties. As an application, he discussed how algebraic K-theory can be used in local mirror symmetry.

F. Rodriguez–Villegas described a tight connection between the geometry of character varieties of Riemann surfaces and the Macdonald polynomials arising from combinatorics.

5. References

Books and Lecture Notes

[B1] **The 1,2,3 of Modular Forms**, by J.H. Bruinier, G. van der Geer, G. Harder and D. Zagier, Lectures at a Summer School in Nordfjordeid, Norway, Universitext, Springer-Verlag, 2008.

[B2] **Calabi–Yau Varieties and Mirror Symmetry**, edited by N. Yui and J. Lewis, Fields Institute Communications Vol. **38**, Proceedings of the Fields Institute Workshop on Calabi–Yau Varieties and Mirror Symmetry 2001, AMS/FIC, 2003.

[B3] **Mirror Symmetry V**, edited by N. Yui, S.-T. Yau and J. Lewis, AMS/IP Stud. in Advanced Math. bf 38, Proceedings of the BIRS Workshop on Calabi–Yau Varieties and Mirror Symmetry 2003, AMS/IP, 2006.

[B4] **Modular Forms and String Duality**, edited by N. Yui, H. Verrill and C. Doran, Fields Institute Communications Vol. **54** Proceedings of the BIRS Workshop on Modular Forms and String Duality 2006, AMS/FIC, 2008.

[CNTP] **Communications in Number Theory and Physics**, International Press of Boston, launched in 2007. http://www.intlpress.com/CNTP

The recent book [B1] about elliptic modular forms, Hilbert modular forms and Siegel modular forms would become standard introduction to modular forms of one, two and more variables.

The most recent references on topics in the interface of number theory and physics are [B2,B3, B4]. All three books are proceedings of the workshops on number theory and physics held at the Fields Institute (2001), and subsequently att BIRS (2003) and (2006), edited by Noriko Yui et al. These references have served as the cornerstone for the rapidly developing topics discussed at the workshop.

The newly launched international research journal [CNTP] has been devoted to topics in the interface of number theory and physics.

Articles

The recent articles relevant to the talks presented at this workshop may be found on arXiv.

6. Titles and Abstracts of Talks at the Workshop

SEPTEMBER 22, 2008

9:00–9:20 **S. Gukov**: *Overview of the workshop*

9:30–10:30 **F. Rodriguez-Villegas**: *Mixed Hodge polynomials of character varieties of Riemann surfaces*

Ever since Weil we know that counting points of varieties over finite fields yields topological information about them. In this talk I will describe such a calculation for the varieties of the title (parameterizing representations of the fundamental group of a Riemann surface into GL_n).

I will first discuss the main ingredients of the calculation, which involves an array of techniques from combinatorics and representation theory of finite groups of Lie type. In the process we discover an unexpected relation to certain quiver varieties. I will describe some conjectures that the outcome of the calculation naturally gave rise to. These predict the full mixed Hodge polynomials of the varieties and give a geometric backbone to the connection between the character and quiver varieties.

Besides their intrinsic interest the varieties in question are closely related to the moduli spaces of Higgs bundles on the surface. Somewhat surprisingly we discover a tight connection between the geometry of these character varieties and the Macdonald polynomials of combinatorics.

This is joint work with T. Hausel and E. Letellier

11:00–12:00 **A. Neitzke** : *Wall-Crossing and Hyperkahler Geometry, Part I*

We will describe recent work on the physical and geometric interpretation of the Kontsevich-Soibelman wall-crossing formula (WCF). We argue that the WCF (in the "non-gravitational" case) expresses the continuity of a certain hyperkahler metric, which arises physically as the moduli space of gauge theory on R^3xS^1, and can be constructed by solving a certain infinite-dimensional Riemann-Hilbert problem. In the first talk we describe our physical setup, the hyperkahler metric and its relation to the WCF. In the second talk we describe a close connection between this construction and the "$tt*$ geometry" of Cecotti and Vafa, and explain some specific examples which arise from D-brane constructions; in these examples the relevant hyperkahler spaces are moduli spaces of ramified Higgs bundles.

This talk has two parts. Part I will be given by A. Neitzke, and Part II by G. Daiotto.

14:30–15:30pm **D. Gaiotto**: *Wall-Crossing and Hyperkahler Geometry, Part II*

16:00–17:00 **T. Gannon**:*Vector-valued modular forms and Moonshine*

The bulk of my talk will review the theory of vector-valued modular forms for subgroups of the modular group, being developed by Peter Bantay and myself. I'll explain applications to conformal field theory and to moonshine. In particular, I'll explain how the 4-point conformal blocks on a sphere, and the 1- and 2-point conformal blocks on a torus, for any rational conformal field theory, fit into this framework, and how this therefore suggests a far-reaching extension of Monstrous Moonshine.

19:00–20:30 **D. Zagier** : *Part I: Mock modular forms*

19:00–20:30 **A. Dabholkar** : *Part II: Modular forms and black holes*

A recent application of Siegel modular forms for counting the microstates of black holes is discussed. The partition function of dyonic black holes in N=4 string compactifications is naturally given in terms of inverse of certain Siegel modular forms of Sp(2, Z) and its congruence subgroup. Fourier coefficients of these partition functions give the black hole degeneracies. In particular it is shown how the contour dependence in extracting the Fourier coefficients and its relation to the moduli dependence of the black hole degeneracies. Possible connections with mock modular forms are outlined.

SEPTEMBER 23, 2008

9:30–10:30 **V. Bouchard**: *Topological open strings on orbifolds*

Using the new recursive approach to the B-model inspired by matrix models, we study modular properties of topological open string amplitudes on mirrors of toric Calabi-Yau threefolds. As an application, we "modular transform" the large radius amplitudes to the orbifold point. Through mirror symmetry, the resulting amplitudes compute a new type of invariants: open string Gromov-Witten invariants of orbifolds.

11:00–12:00 **E. Scheideggar**: *Noether–Lefshetz Theory and the Yau–Zaslow Conjecture*

The Yau–Zaslow conjecture determines the reduced genus Gromov–Witten invariants of K3 surfaces in terms of the Dedekind η-function. Classical intersections of curves in the moduli space of K3 surfaces with Noether–Lefschetz divisors are related to 3–fold Gromov–Witten theory via the K3 invariants. The classical intersections of these curves and divisors are determined in terms of vector-valued modular forms. The 3–fold invariants are calculated using mirror symmetry. Via a detailed study of the STU model (determining special curves in the moduli space of K3 surfaces), we prove the Yau-Zaslow conjecture for all curve classes on K3 surfaces.

14:30–15:30 **C. Keller**: *Conformal field theory and modular differential operators for weak Jacobi forms*

For bosonic conformal field theories, there are recursion relations between n-point functions first introduced by Zhu. Applying these relations, one can obtain in a natural way modular covariant differential operators acting on modular forms.

These recursion relations can be generalized to the $N = 2$ supersymmetric case. In this case the object of interest is the elliptic genus, which is a weak Jacobi form of weight 0. The recursion relations motivate the introduction of generalized versions of the Eisenstein series. These generalized Eisenstein series can then be used to construct modular covariant differential operators on the space of weak Jacobi forms.

16:00–17:00 **T. Yamazaki**: *Degenerate fibers of the Mumford system and rational solutions to the KdV hierarchy*

This is a joint work with P. Vanhaecke and R. Inoue. We study the structure of a degenerate fiber of the Mumford system in term of the (compactified) Jacobian variety. As an application, we obtain a new algorithm to construct all rational solutions to the KdV hierarchy.

19:00–20:00 **D. Kazhdan**: *Satake isomorphism for Kac–Moody groups*

20:00–21:00 **M. Kerr**: *The Abel-Jacobi map on the Eisenstein symbol*

In this talk we consider two different constructions of motivic cohomology classes on families of toric hypersurfaces and on Kuga varieties. Under suitable modularity conditions on the former we say how the constructions ”coincide”, obtaining a complete explanation of a phenomenon observed by Villegas, Stienstra, and Bertin in the context of Mahler measure. (This is where the AJ computation on the Kuga varieties, done using our formula with J. Lewis and S. Mueller-Stach, will be summarized.) We will use this to elducidate the consequences of a conjecture of Hosono and the role played by algebraic K-theory in local mirror symmetry. The material I will cover in my talk is mostly joint work with Charles Doran.

SEPTEMBER 24, 2008

9:30–10:30 **D. Ramakrishnan**: *Modular forms and Calabi-Yau varieties*

This talk will furnish an explanation, with a few key (positive) examples, of the following question which evolved in the speaker's joint work with Kapil Paranjape: Given a regular cusp form f on $GL(n)$ with rational coefficients and (motivic) weight w, is there a Calabi-Yau variety X over the rationals of dimension w, and equipped with an involution not fixing $H^{w,0}(X)$, such that the (rank n) motive $M(f)$ of f occurs in $H^w(X)$? Moreover, can one choose X to be a ”bare-bone envelope” of $M(f)$, i.e., whose cohomology contains only Artin-Tate motives besides that of F? The simplest cases to consider are the classical holomorphic newforms for $SL(2, Z)$ of weight $2k$ and rational coefficients, such as the Delta function. Time permitting, the talk will also briefly explore the compatibility of our question with Langlands's principle of functoriality, especially the product structure. The focus of this lecture will be in the converse direction to the usual, deep association of modular forms to Calabi-Yau (and more general)

11:00–12:00 **S. Hosono**: *BCOV ring and anomaly equations*

I will introduce a certain differential ring, which I call BCOV ring, defined over the moduli space of Calabi-Yau hypersurfaces. Then, I will write the holomorphic anomaly equation due to Bershadsky-Cecocci-Ooguri-Vafa (BCOV) as an differential equation in this BCOV ring in general.

As an application, I will focus on the modular anomaly equation for $\frac{1}{2}$K3, which is written in the ring of quasi-modular forms. I will show that the BCOV holomorphic anomaly equation in this case is equivalent to the modular anomaly equation.

19:00–20:00 **P. Candelas**: *Special geometry for CY manifolds over* $\mathbf{C}$ *and* $\mathbf{F}_p$

20:00–21:00 **J. Manschot**: *Partitition functions for supersymmetric black holes*

In this talk, I will review the connection between supersymmetric black holes of $N = 2$ supergravity and modular forms. It is shown that the microscopic counting of a specific class of black holes is captured by a (generalized) Jacobi form, or equivalently a vector-valued modular form. This reproduces the entropy as suggested by supergravity. In the second part of the talk, I will discuss negative weight Poincare series, and the calculation of the dimension of the space of the relevant vector-valued modular forms.

SEPTEMBER 25, 2008

9:30–10:30 **A. Clingher** : *Lattice Polarized K3 Surfaces and Siegel Modular Form*

This talk will discuss a special family of complex algebraic K3 surfaces polarized by the rank-seventeen lattice $H + E_8 + E_7$. In terms of Hodge theory, these surfaces are naturally related to principally polarized abelian surfaces. I will outline the geometry of the correspondence as well as present an explicit classification of these special K3 surfaces in terms of Siegel modular forms. This is joint work with Charles Doran.

11:00–12:00 **A. Klemm**: *Integrability of the holomorphic anomaly equation*

We show that modularity and the gap condition makes the holomorphic anomaly equation completely integrable for non-compact Calabi-Yau manifolds. This leads to a very efficient formalism to solve the topological string on these geometries in terms of almost holomorphic modular forms. The formalism provides in particular holomorphic expansions everywhere in moduli space including large radius points, the conifold loci, Seiberg-Witten points and the orbifold points. It can be also viewed as a very efficient method to solve higher genus closed string amplitudes in the $\frac{1}{N^2}$ expansion of matrix models with more then one cut.

14:30–15:30 **R. Schimmrigk**: *Motivic L-functions in string theory and D-branes*

Motivic L-functions have been useful to understand the geometry of string compactifications in terms of the theory on the worldsheet. In this talk this application of L-functions is extended in two ways. The first extension relates L-functions to D-branes, providing a second physical interpretation of this object. The second extension uses L-function to establish relations between bosonic flat string theory and supersymmetric compactified strings.

16:00–17:00 **W. Zudilin**: *Algebraic transformations of Calabi–Yau differential equations*

My talk will be based on joint work with Heng Huat Chan, Gert Almkvist and Duco van Straten.

In our study of Picard–Fuchs differential operators of Calabi–Yau type we discover some curious relations of hypergeometric series

$$ {}_mF_{m-1}\left(\begin{matrix} a_1, & a_2, & \dots, & a_m \\ & b_2, & \dots, & b_m \end{matrix} \,\middle|\, z\right) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n \cdots (a_m)_n}{(b_2)_n \cdots (b_m)_n} \frac{z^n}{n!} $$

satisfying linear differential equations

$$ \left(\theta \prod_{j=2}^{m} (\theta + b_j - 1) - z \prod_{j=1}^{m} (\theta + a_j)\right) y = 0, \qquad \text{where} \quad \theta = z\frac{\mathrm{d}}{\mathrm{d}z}, $$

of order $m = 2$, 3, 4 and 5. In the 'classical' situation (when $m = 2$ or 3), most of the corresponding identities come from modular parametrizations of the series; on this way we can give, for example, algebraic expressions for the generating series of the Apéry numbers, Domb's numbers and many others, in hypergeometric forms. Different methods (analytic transformations of the differential equations and study of their monodromy) allow us to prove all other identities we have discovered. A particular example of our findings for hypergeometric differential equations of order 4 and 5 may be interpreted as a higher analogue of Clausen's formula

$$ {}_2F_1\left(\begin{matrix} a, b \\ a + b + \frac{1}{2} \end{matrix} \,\middle|\, z\right)^2 = {}_3F_2\left(\begin{matrix} 2a, 2b, a + b \\ a + b + \frac{1}{2}, 2a + 2b \end{matrix} \,\middle|\, z\right). $$

19:00–20:00 **J. Lewis**:*Normal Forms and Picard-Fuchs Equations for Families of K3 Surfaces over Modular Varieties*

We will start with an overview of the Griffiths-Dwork algorithm for using residues to compute Picard-Fuchs equations for families of Calabi-Yau varieties. This algorithm applies to generically smooth families of hypersurfaces in projective space, and has been generalized to families of ample quasi-smooth varieties in simplicial projective toric varieties. We will discuss both difficulties and successes in applying the algorithm to families of singular varieties. The specific families of lattice-polarized K3 surfaces studied are those supported on modular curves, Humbert surfaces, and Shimura curves under the geometric correspondence described in the talk by A. Clingher. This is joint work with A. Clingher, C. Doran, and U. Whitcher.

20:00–21:00 **P. Gunnells**: *Weyl group multiple Dirichlet series*

Weyl group multiple Dirichlet series are Dirichlet series in several complex variables whose coefficients are constructed from n-th order Gauss sums, with groups of functional equations isomorphic to Weyl groups.

Such series in more than one variable first appeared in the work of Siegel, who constructed a series attached to the A2 root system by taking the Mellin transform of a half-integral weight Eisenstein series. Ultimately all such series are expected to be Whitaker coefficients of Eisenstein series on metaplectic groups, although this has only been proved in certain cases.

Unlike the usual Dirichlet series, multiple Dirichlet series do not in general have an Euler product. Instead, they satisfy a ”twisted multiplicativity”: the coefficients of an n-th order series are multiplicative up to certain products of n-th order power residue symbols. Nevertheless, description of these series boils down to specification of their p-parts.

In this talk we describe a construction of Weyl group multiple Dirichlet series that is uniform for all root systems and for all n. We construct the p-parts using a deformation of the Weyl character formula. The resulting p-parts are fascinating combinatorial objects that resemble characters of representations of simple complex Lie algebras, but with each weight multiplied by a product of n-th order Gauss sums.

SEPTEMBER 26, 2008

9:00–12:00 *Informal discussions*

7. Participants We had in total 39 participants for the workshop, out of which 14 were either graduate students or postdoctoral fellows. We had two last minutes cancellations (Xenia de la Ossa (Oxford, UK), and Kentaro Hori (Toronto, Canada)).

Batyrev, Victor (University of Tubingen)
Bouchard, Vincent (Harvard University)
Candelas, Philip (University of Oxford)
Clingher, Adrian (University of Missouri-St.Louis)
Dabholkar, Atish (Center National de la Research Scientifique)
Dimofte, Tudor (Caltech)
Doran, Charles (University of Washington)
Eager, Richard (University of California at Santa Barbara)
Gaiotto, Davide (Institute for Advanced Study, Princeton)
Gannon, Terry (University of Alberta)
Gukov, Sergei (University of California, Santa Barbara)
Gunnells, Paul (University of Massachusetts Amherst)
Hosono, Shinobu (The University of Tokyo)
Kazhdan, David (Hebrew University)
Keller, Christoph (Eidgenössische Technische Hochschule Zürich)
Kerr, Matt (University of Durham)
Klemm, Albrecht (University of Bonn)
Konishi, Yukiko (Kyoto University)
Lewis, Jacob (University of Washington)
Livne, Ron (Hebrew University)
Manschot, Jan (University of Amsterdam)
Marion, Samantha (University of Alberta)
McKay, John (Concordia University)
Miller, Robert (University of Washington)
Minabe, Satoshi (Institut des Hautes Etude Scientifiques)
Neitzke, Andy (Institute for Advanced Study, Princeton)
Novoseltsev, Andrey (University of Alberta)
Ramakrishnan, Dinakar (Caltech)
Rodriguez Villegas, Fernando (University of Texas at Austin)
Samol, Kira (University of Mainz)
Scheidegger, Emanuel (University of Augsburg)
Schimmrigk, Rolf (Indiana University South Bend)
Walcher, Johannes (CERN)
Yamazaki, Takao (Tohoku University)

Yang, Yifan (National Chiao Tung University)
Yeats, Karen (Boston University)
Yui, Noriko (Queens University)
Zagier, Don (Max-Planck-Institut fuer Mathematik)
Zudilin, Wadim (Steklov Mathematical Institute)

Chapter 32

Random Matrices, Inverse Spectral Methods and Asymptotics (08w5017)

Oct 05 - Oct 10, 2008

Organizer(s): Estelle Basor (American Institute of Mathematics), Marco Bertola (Concordia University), Betrand Eynard (SPhT CEA Saclay), John Harnad (Concordia University and Centre de Recherche Mathematique), Alexander Its (Indiana University - Purdue University at Indianapolis), Ken McLaughlin (University of Arizona)

Participants at the workshop ranged over a number of different fields, ranging from theoretical physics and random matrix theory through algebro-geometry and integrable systems, to asymptotic analysis in the complex domain. We will start with an overview of a few of the fields represented at the workshop.

Overview of the Field

The workshop's two main highlights were Random Matrices and Spectral Methods: in fact the methods that are employed in the treatment of both subjects have many areas of overlap. The mathematics that has been developed for Random Matrix Theory in the past two decades is astonishingly rich and includes variational techniques, inverse spectral methods as applied to nonlinear integrable differential and difference systems, new asymptotic techniques, such as the nonlinear steepest descent method, free probability and large deviations methods. The results obtained have found new applications in a stunningly wide range of areas of both mathematics and theoretical physics such as, for example, approximation theory, orthogonal polynomials and their asymptotics, number theory, combinatorics, dynamical systems of integrable type, representation theory of finite and infinite groups, growth phenomena, quantum gravity, conformal field theory, supersymmetric Yang-Mills theory and string theory. The principal goal of Random Matrix Theory (RMT) is the description of the statistical properties of the eigenvalues or singular values of ensembles of matrices with random entries subject to some chosen distribution, in particular when the size of the matrix becomes very large. The prototypical example consists in the study of the ensemble of $N \times N$ Hermitean matrices M with a probability measure invariant under conjugation by unitary matrices. The simplest such class (and the most studied) consists of statistical models where the probability measure can be written as

$$\mathrm{d}\mu(M) := \frac{1}{Z_N} \mathrm{e}^{-\Lambda \mathrm{Tr} V(M)} \mathrm{d}M \tag{32.1}$$

with $V(x)$ –a scalar function– called the **potential** and Λ a (large) parameter. The normalizing factor $Z_N = Z_N[V, \Lambda]$ is called the *partition function* and plays crucial role in the combinatorial part of the theory for its connections to enumerations of ribbon graphs (see the talks of Pierce and Ercolani).

When studying the statistics of the eigenvalues, Mehta and Gaudin [8, 7] showed that all the information can be extracted from the knowledge of the associated orthogonal polynomials

$$\int_{\mathbb{R}} p_n(x)p_m(x)\mathrm{e}^{-\Lambda V(x)}\mathrm{d}x = h_n\delta_{nm}\ ,\ \ h_n>0,\ \ p_n(x)=x^n+\dots \tag{32.2}$$

and the associated **kernel**

$$K_N(x,x') := \mathrm{e}^{-\frac{\Lambda}{2}(V(x)+V(x'))}\frac{1}{h_{N-1}}\frac{p_N(x)p_{N-1}(x')-p_{N-1}(x)p_N(x')}{x-x'} \tag{32.3}$$

out of which all correlation functions $\mathbb{P}_N(\lambda_1,\dots,\lambda_k)$ for k eigenvalues from the spectrum of M can be computed in terms of determinants [7].

$$\mathbb{P}_N(\lambda_1,\dots,\lambda_k) = \det\left(K_N(\lambda_i,\lambda_j)\right)_{1\le i,j\le k}\ , \tag{32.4}$$

The first breaktrhough came when it was recognized [6] that the above orthgonal polynomials can be characterized in terms of a **Riemann–Hilbert problem**; the second one came with the application of the **nonlinear steepest descent** method [1, 3, 4] to this Riemann–Hilbert problem, since it led to results about the universal properties of the kernel in various scaling regimes.

The statistical distributions that occur in this regime of large sizes display some features which are very ”robust” in the sense that they appear rather independently of the distribution chosen for the matrix entries. This phenomenon goes under the general heading of “universality” and it is not conceptually dissimilar from the more commonly known central limit theorem. An example of these results is that the largest eigenvalue distribution has been shown to possess a limiting distribution (the Tracy-Widom distribution), expressible in closed form in terms of the Hastings-McLeod solution of the Painlevé II equation [10]. This was first established in the case of the Gaussian unitary ensemble of random matrices (i.e. $V(x)=x^2$), but was later extended to even quartic potentials [1] and real analytic potentials [2], using [3]. The form of the asymptotic result is:

$$\lim_{N\to\infty}\mathbf{Prob}\left(\lambda_{\max} < \beta + cN^{-2/3}s\right) = F_{TW}(s) \tag{32.5}$$

where the constant c depends on the external field V, and $F_{TW}(s)$ is the famous Tracy-Widom distribution, independent of the specific form of V.

Inverse spectral theory

RMT can be thought of as an application of the study of spectra of large operators in the “forward” direction; its converse application is what underlyies the area of “inverse spectral methods”.

The simplest example is the Korteweg–de Vries equation (and its associated hierarchy), determining the evolution in ”time” of the potential $u(x,t)$ in the Schrödinger equation

$$\mathcal{L} := -\partial_x^2 + u(x,t) \tag{32.6}$$

in such a way that the spectrum of $\mathcal{L}$ as an operator on $L^2(\mathbb{R},\mathrm{d}x)$ is independent of time. The evolution of $u(x,t)$ is nonlinear according to the celebrated KdV equation

$$u_t + u_{xxx} + u\,u_x = 0 \tag{32.7}$$

which describes propagation of (nonlinear) waves in shallow water (in a uni-dimensional approximation); the support of the spectrum of the associated *Lax operator* $\mathcal{L}$ is preserved, but some data in the so–called *scattering data* evolve according to a linear equation and in a simple way.

Therefore, while the original evolution of u is nonlinear, the *scattering data evolution* is “trivial” and all the nonlinearity is hidden in the map that associates to each potential $u(x,t)$ (where t figures as a parameter) the spectral data, and viceversa.

In particular, the “viceversa” direction, namely the **inverse spectral transform** can be achieved in terms of the solution of an integral equation (Gel’fand-Levitan-Marchenko), which can also be recast into an appropriate 2×2 Riemann–Hilbert problem.

We see here where the point of contacts of RMT and ISM lie; the techniques deployed to analyze the relevant Riemann–Hilbert problems in asymptotic regimes are identical on a "philosophical" level, with details of implementation that are understandably of a quite different nature.

The evolution of the KdV equation is just the first example of many other nonlinear evolution equations. The second fundamental example is the semi-classical analysis of the focusing nonlinear Schrödinger equation:

$$i\epsilon\psi_t + \frac{\epsilon^2}{2}\psi_{xx} + |\psi|^2\psi = 0, \qquad \psi(x,0) = A_0(x)e^{iS_0(x)/\epsilon}. \tag{32.8}$$

The formal WKB guess, $\psi(x,t) \sim A(x,t)e^{iS(x,t)/\epsilon}$, leads to a coupled system of pdes for A and S that are *elliptic* rather than hyperbolic. Thus, although the NLS initial value problem is well-posed in standard Sobolev spaces, the singular limit $\epsilon \to 0$, raises the fundamental analytical question: how does the NLS initial value problem regularize an ill-posed singular limit?

The Connection to Orthogonal Polynomials and Hankel determinants

The partition function of matrix models

$$Z_N[V] := \int \mathrm{d}M \mathrm{e}^{-\Lambda \mathrm{Tr} V(M)} \tag{32.9}$$

is intimately connected to the theory of orthogonal polynomials, as we briefly recall below. Here, $\mathrm{d}M$ stands for the standard Lebesgue measure on the vector space of Hermitean matrices of size $N \times N$. The parameter Λ that appears in these formulas is a convenience *scaling parameter*: in the study of the model for large sizes N of the matrices, one concurrently sends Λ to infinity in such a way that N/Λ remains bounded. For simplicity we take V -the *potential*- to be a polynomial

$$V(x) = \sum_{j=1}^{\nu} \frac{t_j}{j} x^j . \tag{32.10}$$

Consider the measure

$$w_\Lambda(x)dx := \exp\left[-\Lambda V(x)\right]dx. \tag{32.11}$$

Let us define $\{p_j(x;\ N,\ \mathbf{t})\}_{j=0}^{\infty}$ to be the sequence of polynomials orthogonal with respect to the measure $w_\Lambda(x)dx$. That is, $\{p_j(x;\ N,\ \mathbf{t})\}_{j=0}^{\infty}$ satisfies

$$\int_{-\infty}^{\infty} p_j p_k w_N dx = \begin{cases} 0 & j \neq k \\ 1 & j = k \end{cases} , \tag{32.12}$$

and $p_j(x;\ N,\ \mathbf{t}) = \gamma_j^{(N)} x^j + \cdots$, $\gamma_k^{(N)} > 0$. (The leading coefficient $\gamma_k^{(n)}$ is of course dependent on the parameters $t_1, \ldots, t_\nu$, however we suppress this dependence for notational convenience.) The fact of the matter is that $Z_N(\mathbf{t})$ may also be defined via

$$Z_N(\mathbf{t}) = N! \prod_{\ell=0}^{N-1} \left(\gamma_\ell^{(N)}\right)^{-2} . \tag{32.13}$$

Z_N is also defined via

$$Z_N(t_1, \ldots, t_\nu) = N! \begin{vmatrix} c_0 & c_1 & \cdots & c_{N-1} \\ c_1 & c_2 & \cdots & c_N \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ c_{N-1} & c_N & \cdots & c_{2N-2} \end{vmatrix} , \tag{32.14}$$

where $c_j = \int_{\mathbb{R}} x^j w_N(x)dx$ are the moments of the measure $w_N(x)dx$, and the determinant above is called a Hankel determinant (see, for example, Szegö's classic text [9]). The asymptotic expansion (32.17) constitutes a version of the strong Szegö limit theorem for Hankel determinants. The strong Szegö limit theorem concerns the asymptotic behavior of Toeplitz determinants associated to a given measure on the interval $(0, 2\pi)$ (see [9] for more information).

Amongst the main achievements of the past decade or so are;

• the development and deployment of the nonlinear steepest descent method and Riemann–Hilbert method for the study of asymptotic properties in RMT and orthogonal polynomials;

• The discovery that the Tracy-Widom probability distributions originally arising in random matrix theory are also present in the asymptotic statistical behavior of longest increasing subsequence problems in combinatorics, as well as in the limiting statistics of random tiling problems, random growth processes, interacting particle systems and queueing theory;

• the discovery and proof of the universality classes of the sine, Airy and Bessel kernels;

• the connection between matrix integrals and the enumeration of graphs on surfaces;

• the relation of partition functions and spacing distributions to tau functions in integrable systems and isomonodromic deformations;

• the surprising coincidence of the distributions in the Gaussian Unitary Ensemble and the nontrivial zeroes of the Riemann zeta function;

• the spectral duality in multi–matrix models;

• the connection between large N limits, dispersionless hierarchies, critical limits and minimal CFT (Conformal Field Theory).

Combinatorics, Quantum gravity, Liouville CFT

In the context of combinatorics, Matrix integrals were introduced in 1974 (t'Hooft) and in the 80's (in the work of Brezin Itzykson Parisi Zuber, David, Ambjorn, Kazakov, for instance (note this is by no means a complete list)) as a tool for counting discrete surfaces, and led to a domain of physics called 2D quantum gravity, or CFT coupled to Liouville gravity, which is, at its core, the combinatorics of maps of given genus. CFT and Liouville theory are still very active topics in physics, and many new results have been obtained recentely about boundary operators (Zamolochikov). The fact is (following t'Hooft and later Brezin Itzykson Parisi Zuber) that the formal large N expansion of matrix integrals is the generating function for the enumeration of maps of a given genus. Thus, 2D gravity and CFT consist in computing the large N expansion of formal matrix integrals, and several progress have been made. It was understood in 1995 (Ambjorn, Chekhov, Kristjansen, Makeenko) how to extract in principle the large N expansion from the loop equation method, and the link with algebraic geometry was progressively uncovered (Kazakov Marshakov, Chekhov, Mironov, Dijkgraaf, Eynard, Bertola, Kostov, and so many others), and some recent progress 2004 (Eynard, Chekhov, Orantin), where some simple explicit formulae for this expansion in terms of algebraic geometric symplectic invariants of the spectral curve were found. On the more mathematical side of things, in 2003 Ercolani and McLaughlin proved that in some region of the parameter space, the large N expansion of the formal matrix integral is convergent and coincides with the actual (not formal) matrix integral.

Recent Developments and Open Problems

Recent developments include

• The discovery that random tri-diagonal matrices can produce any member of the so-called general β ensembles.

• The proof of existence of a limiting density of states near the "Wigner semicircle" for banded random matrices using super-symmetric techniques by Disertori, Pinson, and Spencer.

• The application of techniques, originally developed for the analysis of integrable systems, to orthogonal polynomials, approximation theory, and random matrix theory.

• The discovery that probability distributions originally arising in random matrix theory are also present in the asymptotic statistical behavior of longest increasing subsequence problems in combinatorics, as well as in the limiting statistics of random tiling problems, random growth processes, interacting particle systems and queueing theory.

• The emergence of these distributions as universal distribution functions, appearing repeatedly in unexpected areas, ranging from spacing between cars when parallel parked, to waiting times in actively controlled transportation (bus) systems.

• The insight that determinantal particle processes form a strong link between random matrices and representation theory

• The recent flood of conjectures involving the Riemann zeta function and integrals arising in random matrix theory.

• The establishment of universality for local eigenvalue spacings for symmetry classes other than GUE.

Open areas of research include:

• analysis of nonintersecting brownian motion;

• higher order critical phenomena in random matrices;

• statistics of eigenvalues of sample covariance matrices with non-null covariance matrix random matrices with external source (beyond the Gaussian case);

• coupled random matrix theory;

• asymptotics of multiple orthogonal polynomials

• random tiling problems with boundary

• asymptotics for β ensembles

Very recent and at times tenuous connections can be found in the following areas:

• mathematical physics and the Schramm-Loewner Evolution equations

• statistical physics and the Razumov–Stroganov conjecture

• topological string theory, random matrices and QCD

Presentation Highlights

The fifteen hour-long contributions can be grouped in the following areas:

1. Riemann–Hilbert methods applied to nonlinear partial/ordinary differential equations (Buckingham, DiFranco, Jenkins, Miller, Niles);
2. Orthogonal polynomials in the plane (Balogh, Putinar);
3. applications to graphical enumerations (Ercolani, Pierce, Prats Ferrer);
4. multiple orthogonality and applicaton to multi-matrix models (Gekhtman, Lee, Szmigielski);
5. fermionic methods for computation of multiple integrals (Harnad, Wang);
6. Probabilistic methods on non-invariant ensemble (Soshnikov).

Due to Visa problems we regret the absence of Irina Nenciu, who had to forfeit at the last minute.

(1) Riemann–Hilbert methods

The talks were divided into applications of RH methods to classical ODEs of Painlevé type (Buckingham, diFranco, Niles) and the dispersionless asymptotics for the Nonlinear Schroedinger equation (Jenkins and Miller).

The Painlevé functions, or transcendents, are solutions of certain nonlinear differential equations; in applications to random matrix theory and two–dimensional statistical models it is sometimes necessary to compute integrals of the transcendent. For example, in computing the asymptotics of the Tracy–Widom distribution mentioned above (32.5) the behavior has been obtained in the original work, up to an overall constant, whose value was conjectured but not proved. Such constant is precisely related to one such integral of a Painlevé transcendent and its determination is an important technical achievement. In other instances of such integrals, their value is not known, not even conjecturally. The talks by Buckingham and diFranco brought to the attention of the audience some new methods to obtain these values by clever manipulations of the associated linear problem, thus providing an important general mindset in approaching such problems.

The methods rely upon the nonlinear steepest descent approach, the same that can be used in the study of the dispersionless asymptotics of the nonlinear Schroedinger equation; here, Miller's talk showed some applications to experimental physics and what a theoretical approach can predict.

(2) Orthogonal polynomials in the plane These are holomorphic polynomials which are orthogonal with respect to a measure on the complex plane typically supported on subsets of positive Lebesgue measure. There are two main lines of research. On one side are Bergmann polynomials, namely polynomials which are orthogonal w.r.t the Lebesgue measure restricted to some (possibly multiply connected) domain $\mathcal{D}$;

$$\int_{\mathcal{D}} p_n(z)\overline{p_m(z)}\mathrm{d}^2 z = \delta_{nm} \tag{32.15}$$

Important questions are related to the characterization of the asymptotic distribution of the roots of these polynomials and how this may depend on the geometry of $\mathcal{D}$ and how to effectively reconstruct the shape of $\mathcal{D}$ from the knowledge of a finite number of the moments of the measure. An **archipelago** is the term used by Putinar and collaborators to denote (in a picturesque form) a domain consisting of several connected components. A typical example is the domain consisting of several disjoint disks. For such an archipelago, the talk of Putinar showed that –depending on the geometry– the zeroes distribute along one–dimensional arcs, which may be outside of $\mathcal{D}$ (but always in its convex hull) and how the shape of $\mathcal{D}$ can be reconstructed (in approximate form) from the knowledge of the moments or –which is equivalent– the orthogonal polynomials.

Of a similar tone was Balogh's talk, which reported on recent progress in establishing the validity of certain outstanding conjectures regarding the distribution of zeroes of OPs and relationships with the harmonic measure of domains. Here the setting is different inasmuch as the polynomials are orthogonal w.r.t. to a *weight* on $\mathbb{C}$, namely a positive function with sufficient decay at infinity. In contrast to the above setting of the archipelago, there is no intrinsic geometrical input from the start. However, for weights of the form

$$w(z,\overline{z}) = \mathrm{e}^{-\Lambda(|z|^2 + h(z,\overline{z}))}\ , \quad h(z,\overline{z}) = \text{ harmonic}$$

it is conjectured that the roots of the polynomials as $n \to \infty, \Lambda \to \infty, n/\Lambda = \mathcal{O}(1)$ distribute on arcs that constitute the so–called *mother body* of a domain related to the choice of function $h(z,\overline{z})$. Balogh's talk reported on recent progress made in verifying such conjecture for the particular choice of $h(z,\overline{z}) = \beta \ln|z-a|$, where the asymptotic domain is related to the Youkowsky airfoil. This is an important result because it proves to be the first rigorous such proof of the conjecture, using Riemann–Hilbert methods.

(3) Application to graphical enumerations

The connection between the partition function of matrix models and enumeration of graphs on Riemann–surfaces was in fact one of the first breaktrhough that showed the breadth of applicability of matrix models [5].

For example, a partition function of the form

$$Z_N = \int \mathrm{d}M \mathrm{e}^{-N\mathrm{Tr}(M^2 + t_4 M^4)} \tag{32.16}$$

admits an asymptotic expansion

$$\log\left(\hat{Z}_N\right) = N^2 e_0(t_4) + e_1(t_4) + \frac{1}{N^2} e_2(t_4) + \cdots\ , \tag{32.17}$$

where $\hat{Z}_N = Z_N/Z_N(0)$. The coefficients in the Taylor expansions of the functions $e_g(t_4)$ count the number of graphs with only four–valent vertices that can be drawn on a Riemann surface of genus g. This can be generalized to arbitrary valence by adding corresponding terms $t_j M^j$ in the exponen of (32.16).

The expression is also a solution of the Toda hierarchy, namely of certain nonlinead PDEs: the information from this latter can be used to deduce combinatorical identities for the coefficients of the expansion (32.17) and Ercolani's talk reported on recent progress in this direction.

In Pierce's talk a generalization was presented whereby the matrix integral in (32.16) is replaced by integration over real–symmetric or symplectic matrices. The resulting partition functions solve a different hierachy of PDEs that goes under the name of "Pfaffian lattice equations". A universality between all three ensembles of random matrices can be established; as a consequence the leading orders of the free energy for large matrices agree (up to a rescaling of the parameters). Also, Pierce showed an explicit formula for the two point function F_{nm} which represents the number of connected ribbon graphs with two vertices of degrees n and m on a sphere, basing the derivation on the Faber polynomials (and its Grunsky coefficients) defined on the spectral curve of the dispersionless Toda lattice hierarchy.

With different methods and scope, Prats Ferrer's talk showed the method of the "loop equations" in the computation of the above-mentioned combinatorial generating functions in very general models involving not one, but several matrices coupled in chains, and the limit where this chain becomes a continuum.

(4) Multiple orthogonality and application to multi–matrix models

Multi–matrix models are a (relatively) new frontier of random matrices; applications are to refined enumerations of *colored* ribbon graphs and new universality results. A new model where the interaction between the matrices is of determinantal form has been introduced by Bertola, Gekthman and Szmigielski. Szmigielski showed the origin of the model in the connection with the inverse spectral problem for the "cubic string", namely the boundary value problem for the ODE

$$\Phi'''(\xi) = -zm(\xi)\Phi(\xi) \tag{32.18}$$

where z is the eigenvalue parameter and the problem is that of reconstructing $m(\xi)$ from the knowledge of the eigenvalues (with suitable boudary values) of the above equation. This appeared in the study of deGasperis–Procesi *peakons*, namely nonsmooth soliton solutions of the homonymous nonlinear wave equation. Gekhtman showed how the problem is connected to matrix models and a new class of biorthogonal polynomials, satisfying

$$\int_{\mathbb{R}_+}\int_{\mathbb{R}_+} p_n(x)q_m(y)\frac{\alpha(x)\mathrm{d}x\beta(y)\mathrm{d}y}{x+y} = \delta_{nm} \tag{32.19}$$

for arbitrary positive measures $\alpha(x)\mathrm{d}x, \beta(y)\mathrm{d}y$ on the positive axis. Their main properties are very close to corresponding ones in the classical theory of orthogonal polynomials; simplicity of the roots, interlacing properties and total positivity of the moment matrix. A characterization of Cauchy BOPs in terms of a 3 by 3 matrix Riemann- Hilbert problem was detailed.

The Dyson model describes the random walk of particles on the line subjected to mutual repulsion; consequently the walks are self-avoiding. Lee's talk recalled how the model can be phrased as a two–matrix model with exponential interaction and how the gap probabilities can be interpreted in terms of isomonodromic theory à la Jimbo-Miwa-Ueno. Once more, the connection is established through the reduction of the model to suitable biorthogonal polynomials. This important contribution shows that the gap probability solve a nonlinear PDE with the Painlevé property.

(5) Fermionic methods The talks of Harnad and Wang showed the use of Fermionic methods in the investigation of matrix integrals. One considers a matrix integral of the type illustrated above (and more general ones) as *expectation values* of (possibly formal) operators on the Fermi–Fock space, namely the exterior space modeled on some abstract (but sometimes quite concrete) separable Hilbert space. Similar methods are used by Okounkov in dealing with the statistical properties of "melting chrystals" or random stepped surfaces. Harnad's talk showed the wide encompassing results that can be demonstrated by an appropriate choice of the operator whose expectation value is being computed; depending on the choice of operator, a very large class of matrix models and multi-matrix model can be recast in this framework. This yields, as an immediate consequence, a method to show that partition functions are Kadomtsev–Petviashvili tau functions (or generalizations thereof) and hence one may derive hierarchies of partial differential equations. In this vein, Wang's talk illustrated this very general statement in the particular case of the Wishart ensemble, which was not immediately captured in the general setting of Harnad's talk.

(6) Probabilistic methods Soshnikov was the sole representative of probability theory and its applications to random matrices; his talk discussed the Wigner ensemble. This is a random matrix ensemble which is not invariant under the adjoint action of the unitary group. Wigner matrices are random matrices whose entries are independently (and possibly identically) distributed; only in the case of iid *normal* (i.e. Gaussian) variables the ensemble has the unitary symmetry, and in this case it is amenable to the "usual" Hermitean model as discussed above. As soon as the distribution is not normal, new challenges arise since it is not possible to write a closed form for the induced probability distribution on the spectrum. New methods of free probability and large deviation techniques must be deployed.

Scientific outcome

The group of participant was very focused and homogeneous in interests, which facilitated the cross-interaction between the participants. True to the empirical theorem of the six degrees of separation, all participants were separated at most by three steps in collaborative distance and had known each other from previously. Several had ongoing collaborations (Bertola-Gekhtman-Szmigielsky, Buckingham-McLaughlin-Miller, diFranco-Miller, Ercolani-Pierce, McLaughlin-Jenkins, Bertola-Harnad, Balogh-Bertola-Lee-McLaughlin-Prats Ferrer).

Given the proximity of interest, it is not surprising that new projects were started during the workshop, like the collaboration between Harnad and Wang on fermionic interpretation of matrix models with external source, the project (in advanced stage of completion by now) between Buckingham, Lee and Pierce on the Riemann–Hilbert approach of the self-avoiding random walkers with few outliers and the very active discussions on the algebro-geometric approach vs analytic one in studying the "loop equations" in the context of random matrix models, between Prats Ferrer, McLaughlin and Ercolani.

As often happens during workshops, papers may not be written in full but the seeds of fruitful collaborations are sown.

The organizers are extremely thankful to the support staff at BIRS for facilitating an extremely successful, pleasant, and smooth-running workshop.

List of Participants

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Chapter 33

Topological Methods for Aperiodic Tilings (08w5044)

Oct 12 - Oct 17, 2008

Organizer(s): Lorenzo Sadun (University of Texas at Austin), Ian Putnam (University of Victoria)

Overview of the Field

The study of aperiodic tilings began with the work of Hao Wang in the 1950's. It was energized by examples given by Raphael Robinson in the 1960's and, more famously, Roger Penrose in the 1970's. See [Se, GS] for overviews of the subject. Penrose's example was striking because it admitted rotational symmetries which are impossible in periodic tilings. Perhaps the most significant development was in the early 1980's, when physical materials, now called quasi-crystals, were discovered which possessed the same rotational symmetries forbidden in periodic structures and yet displayed a high degree or regularity [SBGC]. The field since then has been characterized by an interesting mix of a wide variety of mathematical and physical subjects. Among the former are discrete geometry, harmonic analysis, ergodic theory, operator algebras and topology. This workshop was designed to highlight recent progress in the areas of topology and ergodic theory [Sa1].

Ergodic theory and dynamical systems are natural tools for the study of aperiodic patterns. Rather than study a single aperiodic pattern, dynamical systems prefers to study a collection of such objects which are globally invariant under translations (and perhaps other rigid motions of the underlying space as well). In fact, many of the examples are exactly that: a class of objects with very similar properties. At the same time, it is very natural to construct a class from a single pattern by looking at all other patterns which have exactly the same collection of local data. More specifically, given an aperiodic pattern P, look at all P' such that the intersection of P' with any bounded region appears somewhere in P. Finally, this approach of looking at a collection of patterns grew naturally in physical models for quasi-crystals.

The key step in this approach is establishing some kind of finiteness condition of the collection. Looking at such systems from a probabilistic point of view, this means finding a finite measure which is invariant under the translation action. In most examples, this measure not only exists, but is unique.

From a topological point of view, the aim is to find some natural topology in which the action is continuous and the collection is compact. Compactness is the analyst's analogue of finite. Such topologies were easily developed - they are natural extensions of topologies on shift spaces which are standard in symbolic dynamics.

To elaborate a little, suppose one considers point sets in a Euclidean space which are uniformly dense (for some fixed positive radius R, the R-balls around all points cover the space) and uniformly discrete (for some fixed radius r, the r-balls around the points are pairwise disjoint). Such a set is called a Delone set, but here we require the same two constants to be good for all elements of the collection. A neighbourhood base for the topology is as follows. For a fixed point set P, open set U in the underlying space and positive constant ϵ, look at all other points sets P' such that $P' \cap U$ is within ϵ of the restriction of $P \cap U$. (This is not quite correct because of what is happening near the boundary of U, but it will suffice for the moment.)

This topology first appeared as a tool, since it makes the collections of interest compact and hence many standard results of dynamics may apply. Later, it was observed by a number of people that the local structure of the space could be described quite explicitly, as follows. A collection of tilings is said to have *finite local complexity* if, for fixed $R > 0$, the number of different patterns which occur inside an R-ball as one considers all patterns in the collection, modulo translation, is finite. (This can be generalized by replacing the group of translations by other subgroups of the isometry group of the underlying space.) This is often satisfied and it implies that, locally, the space is the cartesian product of a Euclidean space and a totally disconnected space. This result was improved to a global version by Sadun and Williams [SW]: the space is a fibre bundle over the a torus (with the same dimension as the space being tiled) with totally disconnected fibres.

Anderson and Putnam [AP] considered tilings obtained by the so-called substitution method. These possess a type of self-similarity present in both the Robinson and Penrose examples. They observed that a good deal could also be said about the global structure of the space of tilings. This was done by presenting the space as an inverse limit of simpler spaces which, in most examples, are branched manifolds. In particular, it meant that the cohomology of the space was a computable invariant. This idea was extended by Bellissard, Benedetti and Gambaudo [BBG] and also by Gähler and Sadun [Sa2] to more general tiling spaces. In another direction, Forrest, Hunton and Kellendonk [FHK] took a different approach to provide an effective method for computing the cohomology of those tilings which arise from the so-called projection method.

The computation of the cohomology of tiling spaces was motivated by another important factor. Bellissard gave a construction of a C^*-algebra from a tiling [Be1, KeP1, BHZ]. This C^*-algebra is a model for electron motion in a quasicrystal. In this framework, the K-theory of this C^*-algebra carries important information about the physics. Due to a result of Connes, this K-theory is the same as the K-theory of the tiling space itself. Cohomology and K-theory are closely related, especially for low-dimensional spaces.

Recent Developments and Open Problems

There have been a number of interesting developments over the past few years. The over-riding theme has been to understand exactly what the cohomology of the tiling space is measuring. There seems to be a sense that it is a quantitative measure of aperiodicity, but this has not been formulated in a precise way.

In this direction, Kellendonk and Putnam [KeP2] were able to give a more geometric interpretation of cohomology by using the notion of pattern equivariant differential forms. Given a point pattern P in Euclidean space (or a tiling), a function on the space is called P-equivariant if there is $R > 0$ such that the value of f at x only depends on the pattern P within a ball of radius R around x. More precisely, if $(P - x) \cap B(0, R) = (P - y) \cap B(0, R)$ then $f(x) = f(y)$. The collection of P-equivariant differential forms with the usual exterior differential is a chain complex and its cohomology is isomorphic to the Cech cohomology of the hull with real coefficients. On the other hand, the differential forms have more geometric content than the Cech cocycles. In particular, it is possible to average these over the space in a meaningful way and this produces a map from the cohomology to the exterior algebra of Euclidean space. The complete data contained in this combination of cohomology and this map is not fully understood. In particular, the first cohomology group seemed to play a distinguished role which is also not clear.

Continuing further in this line, Clark and Sadun [CS] gave a description of how elements of the first cohomology of the tiling space could be seen to parameterize deformations of the tilings. This provides a nice framework for dealing with various subtle issues in comparing the various ways in which two tiling spaces may be regarded as equivalent. It also raises a number of questions, both about deformations and also about various variants of the cohomology.

Barge and Diamond [BD] have given a complete classification of tiling spaces in one dimension. Much of this analysis is devoted to understanding ‘asymptotic composants’: pairs of path connected subspaces (which must be homeomorphic to the real line) which are asymptotic in some precise sense. It is too much to hope that such a treatment will extend completely to higher dimensions, but it is natural to ask what aspects will or if there is a certain class of tiling spaces for which a parallel development will work.

There has been a great deal of progress in recent years on tilings which fail to have finite local complexity with respect to translations. The first type of tiling where this condition fails is in tilings that have tiles appearing in infinitely many orientations. The most famous example is the pinwheel tiling. As mentioned above, this can be regarded as having finite local complexity by replacing the translation group of the Euclidean space by the full isometry group. However, there are a number of other examples of substitution tilings where the tiles, which are polygons, fail to meet vertex to vertex after substitution. This produces the possibility of continuous 'sheers'. Although the condition of FLC fails, Frank and Sadun [FS] have given a concrete description of the tiling space as an inverse limit of CW complexes where the sheer is represented by added dimensions in the cells. The construction works very well on specific examples, but a general theory of all such tilings is still elusive.

Presentation Highlights

Simultaneous with our half workshop was another on self-similar groups. Since there were common themes, especially around the concept of self-similarity, there were several introductory talks given to both groups simultaneously. Volodia Nekrashevych explained self-similar groups to the tilings workshop, and Lorenzo Sadun explained non-periodic tilings to the group theorists. These provided an interesting insight into some different fields for both groups. Some of these connections are still developing. For example, Putnam is continuing discussions in an informal way with Nekrashevych.

Our goal for the workshop was *not* to have everybody present a technical talk on his or her latest result, but rather to have an opportunity for everybody to learn about the big ideas that are driving the field. We polled the participants about what they wanted to learn, and then drafted speakers to talk about these subjects. We also allotted big time slots for the most popular subjects, so that questions could be asked and answered in depth.

Pierre Arnoux and his collaborators have been studying aperiodic substitution tilings for a number of years. Their examples are quite concrete and are strongly motivated by problems in number theory and symbolic dynamics. Put briefly, the usual continued fraction expansion can best be viewed as starting from a number (usually irrational) and 1. Here, the starting is an N-tuple instead of a pair and the goal is to develop a multi-continued fraction algorithm and to understand its geometric nature. This produces tilings in a very natural way, but unlike most from the tilings community, the tiles are fractals (such as the Rauzy fractal), rather than polygons. Arnoux gave an excellent introduction to the subject which highlighted the motivation and that ran for three hours (with a short break).

On the other hand, Arnoux and his collaborators were not at all familiar with the idea of using careful analysis of the topological structures of the space of tilings and invariants like cohomology in their study. In response, Lorenzo Sadun gave a tutorial on tiling cohomology.

Marcy Barge gave another long lecture on the state of the art in one-dimension tilings, and also discussed ideas (and partial results) for extending these results to higher dimensions. In particular, the lecture explained possible extensions of the idea of asymptotic composants to higher dimensions and showed some important motivating examples.

One area which the organizers developed quite deliberately was the use of tools from non-commutative geometry. A great deal of impetus in the subject, including the use of cohomology as an invariant, came from the work first of Bellissard and later Kellendonk on the C^*-algebras associated to aperiodic structures. Connes' program of non-commutative geometry is advancing quite rapidly and providing new tools and techniques to study such algebras, adapted from notions of classical geometry. In particular, John Pearson, a recent Ph.D. student of Bellissard, gave a long lecture on his thesis, in which he constructs spectral triples (a non-commutative analogue of a manifold together with a Dirac operator) from a Cantor set with an ultrametric. This is only the first step toward providing something along these lines for tiling spaces, but already the analysis is subtle and a surprising amount of structure may be detected. Since the meeting, there has been considerable progress in this direction by Bellissard, Julien and Savinien.

Another lecture was presented by Hervé Oyono-Oyono on his solution (joint with Benameur) of the gap labeling problem of Bellissard. This problem was open for quite sometime before being solved simultaneously by three groups: Bellissard-Benedetti-Gambaudo, Benameur-Oyono and Kaminker-Putnam. All three proofs rely on Connes' index theorem for foliated spaces. But the Benameur-Oyono proof has more the flavour of non-commutative geometry by using cyclic cohomology.

There were several talks about tilings that lack finite local complexity, either because of rotational properties or because of shears. Jean Bellissard began this theme by explaining how such tilings are very natural in physics, and sketching how the K-theory and C*-algebras associated with such tilings relate to the physical properties of the tilings. Natalie Frank described a family of substitutions that have two realizations: either as a discontinuous substitution on a tiling with finite complexity, or as a continuous substitution on a tiling with shears. She posed interesting, and still unresolved, questions on how these tilings may be related. In an informal evening session, John Hunton presented the computation of the cohomology of the pinwheel tiling, something recently accomplished using higher-dimensional extensions of the techniques that Marcy Barge had discussed earlier.

Until recently, it was believed that the cohomology groups of tiling spaces were always torsion-free. A theorem to that effect had even been announced. Frank Gähler proved this wrong, and found that a number of well-known tilings have torsion in their cohomologies. (This also occurs in tilings with rotational properties, such as the pinwheel.) He explained the computational techniques that led to this discovery.

Although the meeting was built around sharing big ideas of general interest, we also wished to give junior researchers the chance to present some of their results. On Thursday we had mostly shorter talks, and split into parallel sessions in the afternoon. Gähler's and Frank's talks have already been described. Samuel Petite described progress in understanding the topology of tilings of hyperbolic space. Jean Savinien, a student of Jean Bellissard, described a new method for the computations of cohomology of tilings and its relations to K-theory based on ideas of Pimsner. Hervé Oyono-Oyono also related discussed the C^*-algebras associated to various tilings of hyperbolic space constructed by Penrose, including a description of their K-theory groups. It was interesting to contrast this work with earlier work in the Euclidean case. Antoine Julien, a student of Kellendonk's talked about his thesis work which relates cohomology with the complexity of the projection method tilings. This application of cohomology is a rather expected one, but suggests that many other possibilities exist along such lines.

Ian Putnam closed off the presentations with a description of a variant on K-theory for Smale spaces. Smale spaces are dynamical systems where the neighborhood of each point is the product of a (uniformly) contracting space and a uniformly expanding space. Substitution tilings spaces are always Smale spaces, but the concept is far more general. It is an open question how, for tiling spaces, this new invariant relates to the usual K-theory.

Scientific Progress Made

The biggest effects of the conference involve cross-pollination between diverse research groups and will take time to bear fruit. However, there were a number of concrete advances made at the conference.

Barge, Hunton and Sadun completed work on a large project extending ideas of Barge and Diamond from one dimension to higher dimensions. This included the computation of the pinwheel cohomology, a problem that had resisted repeated efforts for many years.

Recently, Giordano, Matui, Putnam and Skau have given a classification of minimal actions of the groups $\mathbb{Z}^d, d \geq 1$ on a Cantor set. This involves constructing a sequence of finite equivalence relations on the space whose union is an approximation to the orbit relation. But there are many technical issues involved that need to be satisfied before reaching the desired conclusion. Such dynamical systems are very closely realted to aperiodic tilings. Initially, many examples of aperiodic tilings were known to be suspensions of such systems, but Sadun and Williams actually proved that under mild hypotheses, any the hull of any tiling of d-dimensional Euclidean space is the d-fold suspension of an action of $\mathbb{Z}^d$ on a totally disconnected space. Bellissard and his collaborators had begun to consider the kind of finite approximations in the Giordano-Matui-Putnam-Skau construction in this seeting of tilings. They had a number of discussions with Giordano on this subject. Specific properties of these approximations may have implications in the setting of non-commutative geometry. The first results of these investigations have recently appeared (as a preprint). On the other hand, the lack of concrete computable examples if the Giordano-Matui-Putnam-Skau construction has been a problem. So there was a good deal of interest from these people in the kind of tilings and actions studied by Arnoux and Siegel, where the arithmetic data seems to provide quite explicit methods.

Outcome of the Meeting

The meeting has had the effect of generating a number of new connections between previously diverse groups: the topology of tilings people (Barge, Sadun, Putnam), arithmetic tilings (Arnoux, Siegel), dynamical systems (Giordano) and operator algebraists (Bellissard, Oyono-Oyono, Petit) and even the self-similar group theorists from the other meeting (Nekrashevych). These connections have continued to develop at other meetings since: Strobl, Austria and Leicester, U.K. in 2009 and at a large program in Luminy in 2010.

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Chapter 34

Self-Similarity and Branching in Group Theory (08w5066)

Oct 12 - Oct 17, 2008

Organizer(s): Rostislav Grigorchuk (Texas A & M University), Benjamin Steinberg (Carleton University), Zoran Sunic (Texas A & M University)

Overview of the Field and Workshop Objectives

The idea of self-similarity is one of the most basic and fruitful ideas in mathematics of all times. In the last few decades it established itself as the central notion in areas such as fractal geometry, dynamical systems, and statistical physics. Recently, self-similarity started playing a role in algebra as well, first of all in group theory.

Regular rooted trees are well known self-similar objects (the subtree of the regular rooted tree hanging below any vertex looks exactly like the whole tree). The self-similarity of the tree induces the self-similarity of its group of automorphisms and this is the context in which we talk about self-similar groups. Of particular interest are the finitely generated examples, which can be constructed by using finite automata. Groups of this type are extremely interesting and usually difficult to study as there are no general means to handle all situations. The difficulty of study is more than fairly compensated by the beauty of these examples and the wealth of areas and problems where they can be applied.

One of the earliest examples of a self-similar group, is the famous Grigorchuk 2-group, introduced in [4]. This group was the first example of a group of intermediate growth, solving the celebrated Milnor problem. It was also the first example of an amenable group that is not elementary amenable.

The idea of branching entered Algebra via the so-called branch groups that were introduced by Grigorchuk at St. Andrews Group Theory Conference in Bath 1997. Branch groups are groups that have actions of ‘branch type’ on spherically homogeneous rooted trees. The phrase “of branch type” means that the dynamics of the action (related to the subnormal subgroup structure) mimics the structure of the tree. Spherically homogenous trees appear naturally in this context, both because they are the universal models for homogeneous ultra-metric spaces and because a group is residually finite if and only if it has a faithful action on a spherically homogeneous tree.

The importance of the choice of the ‘branch type’ action is reflected in the fact that it is the naturally opposite to the so-called diagonal type. While any residually finite group can act faithfully on a rooted homogeneous tree in a diagonal fashion, the actions of branch type are more restrictive and come with some structural implications. The Grigorchuk 2-group is the prototypical example of a finitely generated branch group.

Actions of branch type give rise to many examples of just-infinite groups (thus answering a question implicitly raised in [3] on existence of exotic examples of just infinite groups) and to a number of examples of ‘small groups’ (or atomic groups) in the sense of S. Pride [7]. Branch groups also played a role in the construction of groups with non-uniform exponential growth, answering a question of Gromov [9].

The ideas of self-similarity and branching interact extremely well in group theory. There is a large intersection between these two classes of groups and this workshop was devoted to some important features and examples of this interaction.

The subject of self-similarity and branching in group theory is quite young and the number of different directions, open questions, and applications is growing rather quickly.

Of particular importance, is the relationship of self-similar groups to Julia sets and fractals from holomorphic dynamics via iterated monodromy groups, introduced by Nekrashevych [5]. This led to the solution of the longstanding ‘Twisted Rabbit Problem’ by Bartholdi and Nekrashevych [2].

In addition to the standard objectives of a mathematical workshop, this meeting was intended to serve as a forum for

- Formal exchange of information and ideas through formal presentations.

We strongly emphasized the secondary (but nevertheless absolutely crucial) aspects of such a meeting as a forum for

- Informal exchange of information and ideas through informal conversations, chance meetings, learning by “osmosis”, and so on.

- Furthering of the existing collaborative efforts between the participants, as well as development of new professional relations.

To accomplish these objectives the number of formal plenary presentations were kept to 3–4 per day in order to save time for the following activities:

- Meetings in smaller groups focused on specific aspects and goals, such as profinite aspects, holomorphic dynamics and iterated monodromy groups, amenability and probabilistic aspects, algebraic and algorithmic aspects, including connections to automata. All participants were included in such activities according to their own inclination. The goal of these focused teams was to make progress toward resolving some of the more challenging problems in the area, at least at the level of establishing lasting and directed collaborative efforts, based on sound working ideas and strategies.

- Demonstration of GAP packages for working with self-similar groups, developed by graduate students D. Savchuk and Y. Muntyan at Texas A & M University. The work on the packages was supported by an NSF grant of R. Grigorchuk and Z. Sunic and the packages are freely accessible to anyone interested in using them.

- Problem session at the beginning and end of the Workshop.

Press Release

The Banff International Research Station hosted top researchers in its workshop on ”Self-Similarity and Branching in Group Theory”, October 12 – October 17, 2008. The importance of self-similarity and branching phenomena in group theory has recently come to the forefront. Self-similar groups are the algebraic counterparts to fractals. Fractals quite often arise as Julia sets of certain rational functions, say polynomials. For instance, the Basilica of Saint Mark fractal is the Julia set of the polynomial $z^2 + 1$. The famous Sierpinski gasket is also the Julia set of a rational function. To each such rational function, there is associated a self-similar group, which encodes algebraically the Julia set and the dynamics of the rational function on the Julia set.

The study of self-similar groups has led to new insights and a better understanding of fractals and their related dynamics. A longstanding-problem concerning the rabbit fractal and the airplane fractal was solved via the method of self-similar groups. Self-similar groups also have interactions with Computer Science, since much of their structure can be encoded by finite state machines. These machines can be used in turn to produce the fractals.

Basic notions

Definition of a self-similar group

For an alphabet X on k letters, the set of all finite words X^* over X has the structure of a rooted regular k-ary tree in which the empty word is the root and each vertex u has k children ux, $x \in X$. Denote the group of automorphisms of the tree X^* by $Aut(X^*)$.

For a tree automorphism $g \in Aut(X^*)$ and a vertex $u \in X^*$, define the **section** of g at u to be the unique tree automorphism g_u such that the equality

$$g(uw) = g(u)g_u(w)$$

holds for all words $w \in X^*$.

A group of tree automoprhisms $G \leq Aut(X^*)$ is **self-similar** if all sections of all elements in G are elements in G.

Geometric definition of a branch group

Let T be a spherically homogeneous tree. For a group of tree automorphisms $G \leq Aut(T)$ define the rigid stabilizer at the vertex $u \in T$ by

$$RiSt_G(u) = \{g \in G \mid Supp(g) \in T_u\},$$

where T_u is the subtree of T hanging below the vertex u. The rigid stabilizer of the n-th level L_n in T is defined by

$$RiSt_G(L_n) = \langle RiSt_G(u) \mid u \in L_n\rangle = \prod_{u \in L_n} RiSt_G(u)$$

A group G is **geometrically branch group** is it is a spherically transitive subgroup of $Aut(T)$, for some spherically homogeneous tree T, such that all rigid level stabilizers $RiSt_G(L_n)$ have finite index in G.

Algebraic definition of a branch group

A group G is **algebraically branch group** if there exists a sequence of integers $\overline{k} = \{k_n\}_{n=0}^{\infty}$ and two decreasing sequences of subgroups $\{R_n\}_{n=0}^{\infty}$ and $\{V_n\}_{n=0}^{\infty}$ of G such that

(1) $G = R_0 = V_0$

(2) $k_n \geq 2$, for all $n > 0$, $k_0 = 1$

(3) for all n,

$$R_n = V_n^{(1)} \times V_n^{(2)} \times \cdots \times V_n^{(k_0 k_1 k_2 \ldots k_n)}, \tag{34.1}$$

where each $V_n^{(j)}$ is an isomorphic copy of V_n,

(4) for all n, the product decomposition (34.1) of R_{n+1} is a refinement of the corresponding decomposition of R_n in the sense that the j-th factor $V_n^{(j)}$ of R_n, $j = 1, \ldots, k_0 k_1 \ldots k_n$ contains the j-th block of k_{n+1} consecutive factors

$$V_{n+1}^{((j-1)k_{n+1}+1)} \times \cdots \times V_{n+1}^{(jk_{n+1})}$$

of R_{n+1},

(5) for all n, the groups R_n are normal in G and

$$\bigcap_{n=0}^{\infty} R_n = 1,$$

(6) for all n, the conjugation action of G on R_n permutes transitively the factors in (34.1), and

(7) for all n, the index $[G : R_n]$ is finite.

Open Problems

A number of open problems about self-similar groups and branch groups were raised.

1. Are all contracting self-similar groups amenable? Contracting groups do not have free subgroups (Nekrashevych [6]).

2. Are all automaton groups of polynomial growth amenable? Groups of bounded growth (Bartholdi, Kaimanovich, Nekrasheyvch [1]) and linear growth (Amir, Angel, Virag) are amenable. Groups of polynomial growth do not have free subgroups (Sidki [8]).

3. Is there a residually finite non-amenable group without free subgroups?

4. Is the word problem decidable for finitely generated self-similar groups? How about the uniform problem where the groups are given by functional recursion?

5. Can one decide whether an initial automaton has finite order?

6. Can one decide whether an initial automaton is spherically transitive? (This can be done for n-adic transformations).

7. Can one decide whether an automaton group is infinite?

8. Can one decide whether an automaton group is spherically transitive? (This is decidable for groups of n-adic transformations).

9. Is the word problem for automaton groups PSPACE complete? (It is easy to see that the problem is in PSPACE).

10. Are the products of closed subgroups in the Grigorchuk group closed?

11. Is solvability of equations decidable for the Grigorchuk group?

12. Do contracting groups have decidable conjugacy problem?

13. Do automaton groups have decidable conjugacy problem?

14. Does every hyperbolic group have a faithful self-similar action?

15. Construct self-similar actions of free pro-p groups.

16. What are the kernels of the natural action of fiitely generated algebraically branch groups on rooted trees. In particular, does the center always have finite index in the kernel?

17. Are there finitely generated nonamenable branch groups without free subgroups?

18. Is every maximal subgroup of a finitely generated branch group necessarily of finite index?

19. Do there exist finitely presented branch groups?

20. Is the conjugacy problem decidable in all finitely generated branch groups in which the word problem is decidable?

21. Are all finitely generated hereditarily just infinite groups linear? Do there exist finitely generated, hereditarily just infinite, torsion groups?

Abstracts

Speaker: **Miklos Abert** (University of Chicago)
Title: *On weak containment of measure preserving actions*
Abstract: We study asymptotic properties of chains of subgroups in residually finite groups using the dynamics of boundary representations and the structure of periodic invariant measures on Bernoulli actions. This allows us to analyze when the Schreier graphs coming from a chain of subgroups can approximate another action of the group. For chains with property tau, we exhibit a strong rigidity result, while for amenable groups, we prove that every chain approximates every action. As a byproduct, we show that covering towers of regular graphs admit a new kind of spectral restriction which is related to the independence ratio. This leads us to solve a problem of Lubotzky and Zuk. In another direction, we relate the cost of a boundary representation to the growth of rank and the first L^2 Betti number of the group. This allows us to relate the 'fixed price problem' of Gaboriau to the 'rank vs Heegaard genus' conjecture in 3-manifold theory and show that they contradict each other.

Speaker: **Gideon Amir** (University of Toronto)
Title: *Amenability of automata groups with linear growth automorphisms*
Abstract: We prove using random walks that automata of linear growth generate amenable groups, generalizing previous work of Bartholdi, Kaimanovich and Nekrashevych. This is joint work with O. Angel and B. Virag.

Speaker: **Yair Glasner** (Ben Gurion)
Title: *A zero-one law for finitely generated subgroups of* $SL(2, Q_p)$.
Abstract: Let $G = SL(2, Q_p)$. Let $k > 2$ and consider the space $Hom(F_k, G)$ where F_k is the free group on k generators. This space can be thought of as the space of all marked k-generated subgroups of G, i.e., subgroups with a given set of k generators.

There is a natural action of the group $Aut(F_k)$ on $Hom(F_k, G)$ by pre-composition. I will prove that this action is ergodic on the subset of dense subgroups. This means that every measurable property either holds or fails to hold for almost all k-generated subgroups of G together.

Speaker: **Volodymyr Nekrashevych** (Texas A&M)
Title: *Self-similar groups, limit spaces and tilings*
Abstract: We explore the connections between automata, groups, limit spaces of self-similar actions, and tilings. In particular, we show how a group acting "nicely" on a tree gives rise to a self-covering of a topological groupoid, and how the group can be reconstructed from the groupoid and its covering. The connection is via finite-state automata. These define decomposition rules, or self-similar tilings, on leaves of the solenoid associated with the covering.

Speaker: **Olga Kharlampovich** (McGill)
Title: *Undecidability of Markov Properties*
Abstract: A group-theoretic property P is said to be a Markov property if it is preserved under isomorphism and if it satisfies:

1. There is a finitely presented group which has property P.
2. There is a finitely presented group which cannot be embedded in any finitely presented group with property P.

Adyan and Rabin showed that any Markov property cannot be decided from a finite presentation. We give a survey of how this is proved.

Speaker: **Alexei Miasnikov** (McGill)
Title: *The conjugacy problem for the Grigorchuk group has polynomial time complexity*
Abstract: We discuss algorithmic complexity of the conjugacy problem in the original Grigorchuk group. Recently this group was proposed as a possible platform for cryptographic schemes (see [4, 15, 14]), where

the algorithmic security of the schemes is based on the computational hardness of certain variations of the word and conjugacy problems. We show that the conjugacy problem in the Grigorchuk group can be solved in polynomial time. To prove it we replace the standard length by a new, weighted length, called the *norm*, and show that the standard splitting of elements from $St(1)$ has very nice metric properties relative to the norm.

Speaker: **Mark Sapir** (Vanderbilt)
Title: *Residual finiteness of* 1*-related groups*
Abstract: We prove that with probability tending to 1, a 1-relator group with at least 3 generators and the relator of length n is residually finite, virtually residually (finite p)-group for all sufficiently large p, and coherent. The proof uses both combinatorial group theory, non-trivial results about Brownian motions, and non-trivial algebraic geometry (and Galois theory). This is a joint work with A. Borisov and I. Kozakova.

Speaker: **Dmytro Savchuk** (Texas A&M)
Title: *GAP package AutomGrp for computations in self-similar groups and semigroups: functionality, examples and applications*
Abstract: Self-similar groups and semigroups are very interesting from the computational point of view because computations related to these groups are often cumbersome to be performed by hand. Many algorithms related to these groups were implemented in AutomGrp package developed by the authors (available at http://www.gap-system.org/Packages/automgrp.html). We describe the functionality of the package, give some examples and provide several applications. This is joint with Yevgen Muntyan

Speaker: **Benjamin Steinberg** (Carleton)
Title: *The Ribes-Zalesskii Product Theorem and rational subsets of groups*
Abstract: Motivated by a conjecture of Rhodes on finite semigroups and automata, Ribes and Zalesskii proved that a product of finitely many finitely generated subgroups of a free group is closed in the profinite topology. We discuss a proof of this result due to the speaker and Auinger, as well as generalizations to other groups by various authors. Applications are given to computing membership in rational subsets of groups. In particular, for a torsion group, like the Grigorchuk group, every rational subset is a finite union

$$\bigcup gH_1 \cdots H_n$$

of translates of products of finitely generated subgroups and so such a separability result would give decidability of membership in rational subsets.

Speaker: **Zoran Šunić** (Texas A&M)
Title: *Branching in group theory*
Abstract: We provide an introduction to the notion of a branch group. We cover the definition, motivation, examples, and some basic properties. In addition, we mention some applications that are based on the branch structure of the given branch groups.

Speaker: **Yaroslav Vorobets** (Texas A&M)
Title: *Automata generating free groups and free products of cyclic groups*
Abstract: An invertible finite automaton canonically defines a finitely generated group of automorphisms of a regular rooted tree. We will describe a class of finite automata that define free nonabelian groups. Freeness is established via the dual automaton approach, which provides a new techniques to solve the word problem for automaton groups.

The GAP package AutomGrp

One of the highlights of the meeting was a tutorial by Savchuk on his program with Muntyan implementing self-similar groups in GAP. We include here some screenshots from the tutorial.

Automaton groups and semigroups can be defined in "AutomGrp" are as follows.

Automaton groups:

```
gap> GrigorchukGroup :=
     AutomatonGroup("a=(1,1)(1,2),b=(a,c),c=(a,d),d=(1,b)");
< a, b, c, d >

gap> Basilica := AutomatonGroup( "u=(v,1)(1,2), v=(u,1)" );
< u, v >
```

Automaton semigroups:

```
gap> SG := AutomatonSemigroup( "f0=(f0,f0)(1,2), f1=(f1,f0)[2,2]" );
< f0, f1 >
```

Self-similar groups:

```
gap> WRG := SelfSimilarGroup("x=(1,y)(1,2),y=(z^-1,1)(1,2),z=(1,x*y)");
< x, y, z >
```

The package computes basic properties of groups/semigroups generated by automata.

```
gap> IsSphericallyTransitive(GrigorchukGroup);
true

gap> IsAbelian(GrigorchukGroup);
false

gap> IsFractal(GrigorchukGroup);
true

gap> IsAmenable(GrigorchukGroup);
true
```

Basic operations: sections

```
gap> Section(p*q*p^2, [1,2,2,1,2,1]);
p^2*q^2

gap> Decompose(p*q^2);
(p*q^2, q*p^2)(1,2)

gap> Decompose(p*q^2,3);
(p*q^2, q*p^2, p^2*q, q^2*p, p*q*p, q*p*q, p^3, q^3)(1,8,3,5)(2,7,4,6)
```

Finding relations in groups and semigroups.
The following command finds all relations in Grigorchuk group up to length 16

```
gap> FindGroupRelations(GrigorchukGroup,8);
a^2
b^2
c^2
d^2
b*c*d
d*a*d*a*d*a*d*a
c*a*c*a*c*a*c*a*c*a*c*a*c*a*c*a
[ a^2, b^2, c^2, d^2, b*c*d, d*a*d*a*d*a*d*a, c*a*c*a*c*a*c*a*c*a*c*a*c*a*c*a]
```

Or all relations in $\langle ac, ada\rangle$ up to length 10

```
gap> FindGroupRelations([a*c,a*d*a], ["p", "q"], 5);
q^2
q*p*q*p^-1*q*p*q*p^-1
p^-8
[ q^2, q*p*q*p^-1*q*p*q*p^-1, p^-8 ]
```

Find all elements in Grigorchuk group of order 16 up to length 5

```
gap> FindElements(GrigorchukGroup,Order,16,5);
[ a*b, b*a, c*a*d, d*a*c, a*b*a*d, a*c*a*d, a*d*a*b, a*d*a*c, b*a*d*a,
  c*a*d*a, d*a*b*a, d*a*c*a, a*c*a*d*a, a*d*a*c*a, b*a*b*a*c, b*a*c*a*c,
  c*a*b*a*b, c*a*c*a*b ]
```

Order of an element
In Basilica group the element $u^{35}v^{-12}u^2v^{-3}$ has infinite order

```
gap> Basilica := AutomatonGroup( "u=(v,1)(1,2), v=(u,1)" );
< u, v >
gap> Order( u^35*v^-12*u^2*v^-3 );
infinity
```

Contracting groups. We can check that `WRG` is contracting and compute the nucleus.

```
gap> IsContracting( WRG );
true
gap> GroupNucleus( WRG );
[ 1, y*z^-1*x*y, z^-1*y^-1*x^-1*y*z^-1, z^-1*y^-1*x^-1, y^-1*x^-1*z*y^-1,
  z*y^-1*x*y*z, x*y*z ]
```

Outcome of the Meeting

The meeting successfully served its main purpose of providing a forum for exchange of recent results and new ideas, as well as establishing new collaborative efforts aimed at solving problems that were already known or were introduced during the meeting. In addition, the idea of having a presentation of the freely available GAP package of Muntyan and Savchuk for working with self-similar groups proved to be very well received, as many participants realized the ease with which this package could be used and its efficiency at performing calculations (leaving the user to only worry about the more creative side of his/her research). Also, all participants responded positively to the idea to have representatives of the two Workshops that were present at Banff at the same time give introductory presentations to the participants of the other Workshop.

Rostislav Grigorchuk and Yair Glasner made progress on the question whether all maximal subgroups in finitely generated branch groups have finite index extending their observation that maximal subgroups in branch groups are themselves branch groups.

Volodymyr Nekrashevych defined a notion of a self-similar groupoid (of a self-covering bimodule), which generalizes self-similar groups, self-coverings of topological spaces (such as post-critically finite rational functions restricted to their Julia sets) and adjacency groupoids of self-similar aperiodic tilings.

Zoran Šunić proved results on distance transitivity of the Hanoi Towers group $H^{(k)}$. In addition, he showed that every normal subgroup N in a distance 2-transitive group of tree automoprhisms acts transitively on every subtree T_u such that there exists $n \in N$ that fixes u and acts nontrivially on the children of u. In particular, every normal subgroup that stabilizes level n but does not stabilize level $n+1$ acts transitively on all subtrees hanging at level n.

Graduate students present at the meeting obtained several ideas for questions they could try to work on and include in their dissertations. For instance, Mccune will try to determine which right-angled Artin groups can be realized as automaton groups, Savchuk will try to determine if the construction of free products of cyclic groups of order 2 suggested by Šunić is correct, and Benli became interested in L-presentations of branch groups.

List of Participants

Abert, Miklos (University of Chicago, Department of Mathematics)
Amir, Gideon (University of Toronto)
Benli, Mustafa G. (Texas A&M University)
Bumagin, Inna (Carleton University)
Glasner, Yair (Ben Gurion University of the Negev)
Grigorchuk, Rostislav (Texas A&M University)
Kharlampovich, Olga (McGill University)
Mccune, David (University of Lincoln at Nebraska)
Miasnikov, Alexei (McGill University)
Morris, Dave (University of Lethbridge)
Nekrashevych, Volodymyr (Texas A&M University)
Sapir, Mark (Vanderbilt University)
Savchuk, Dmytro (Texas A&M University)
Steinberg, Benjamin (Carleton University)
Sunic, Zoran (Texas A&M University)
Vorobets, Yaroslav (Texas A&M University)
Vorobets, Mariya (Texas A&M University)

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Chapter 35

Mathematical Theory of Resonances (08w5092)

Oct 19 - Oct 24, 2008

Organizer(s): Tanya Christiansen (University of Missouri), Richard Froese (University of British Columbia), Maciej Zworski (University of California at Berkeley)

Research

The conference gathered a diverse group of experts working on different aspects of mathematical theory of resonances.

Certain topics were subject to particularly lively discussions:

- Lower bounds on resonances using several complex variable methods; C Guillarmou and F Naud started the investigation of these methods (used by T Christiansen and P Hislop) in the context of geometric scattering.
- D Jakobson and F Naud started a collaboration on lower bounds for resonances for Schottky quotients which resulted in the preprint

  `http://www.math.mcgill.ca/jakobson/papers/resonance-lowbd.pdf`

  (with the BIRS conference acknowledged).
- N Burq's talk led to some discoveries about the work of H Christianson and the discussions resulted in an ongoing collaboration.
- D Bindel provided M Zworski with new codes for computing resonances relevant to the latter's collaboration with experimental physicists (H Manoharan's group at Stanford).
- S Nonnenmacher and M Zworski made progress in the ongoing project on resonances for chaotic scattering with topologically one dimensional trapped sets.
- W Müller and A Vasy discussed resonances for locally symmetric spaces.
- D Borthwick, T Christiansen, P Hislop, and P Perry made progress on a project involving the distribution of resonances for perturbations of infinite volume hyperbolic manifolds.

Titles and abstracts

I. Alexandrova Title: The Structure of the Scattering Amplitude for Schrodinger Operators with a Strong Magnetic Field

Abstract: We study the microlocal structure of the semi-classical scattering amplitude for Schrodinger operators with a strong magnetic field at non-trapping energies. We prove that, up to any order, the scattering amplitude can be approximated by a semi-classical pseudodifferential-operator-valued Fourier integral operator.

D. Bindel Title: Numerical methods for resonance calculations

Abstract: In this talk, I revisit the problem of computing resonances for one-dimensional Schroedinger-type operators in two ways: using perfectly matched absorbing layers (a variant on complex scaling) and by converting the problem to a nonlinear eigenvalue problem. For each formulation, I describe both the numerical methods and error estimates for the computation.

If time permits, I will also talk about an application of resonances in micro-mechanical components from next-generation cell phone designs, and say how we used perfectly matched layers to compute resonances in this problem.

D. Borthwick Title: The Poisson formula for resonances on manifolds hyperbolic near infinity.

Abstract: We present some very developments on the distribution of resonances for conformally compact manifolds which are hyperbolic near infinity. These include (1) the optimal upper bound on the resonance (or scattering pole) counting function, (2) the Poisson formula for the regularized wave trace, (3) optimal lower bounds for resonances, and (4) Weyl asymptotics for the relative scattering phase defined by a compact perturbation.

V. Bruneau Title: Regularized determinant and semi-classical resonances

Abstract: Based on a joint work with J.M. Bouclet I will show that the resonances can be view as zeroes of some regularized determinants. It works for long range perturbations of the Laplacian. Some "Breit-Wigner" approximation of regularized spectral shift function can be deduced.

Nicolas Burq Title: Probabilistic Sobolev embeddings and behaviour of solutions to wave equations

Colin Guillarmou Title: Resonances in hyperbolic geometry

Peter Hislop Title: Resonances for Schrödinger operators with compactly supported potentials

Abstract: The resonance counting function for Schrödinger operators $H_V = -\Delta + V$ on $L^2(\mathbb{R}^d)$, for $d \geq 1$, with compactly-supported, real- or complex-valued potentials V is known to be bounded above by $C_V(r^d + 1)$. The main result is that for a dense G_δ-set of such potentials, the resonance counting functions have the maximal order of growth d. For the even dimensional case, it is shown that the resonance counting functions have maximal order of growth on each sheet Λ_m, $m \in \mathbb{Z}\backslash\{0\}$, of the logarithmic Riemann surface. This results is obtained by constructing a certain plurisubharmonic function from the determinant of a modified S-matrix and proving that the order of growth of the counting function can be recovered from a suitable estimate on this function. An example is constructed in each even dimension of a potential having a resonance counting function bounded below by $C_m r^d$ on each sheet.

M. Hitrik Title: Non-elliptic quadratic forms and operators with double characteristics

Abstract: This is a report on a work in progress together with Karel Pravda-Starov. For a class of non-selfadjoint pseudodifferential operators with double characteristics, we study semiclassical resolvent bounds and estimates for low lying eigenvalues. Specifically, assuming that the quadratic approximations along the characteristics enjoy an ellipticity property along a suitable symplectic subspace of the phase space, we establish semiclassical hypoelliptic a priori estimates with a loss of a full power of the semiclassical parameter. We also compute the (discrete) spectrum of the associated quadratic operators and describe the large time behavior for the corresponding heat semigroups.

D. Jakobson Title: Estimates from below for the spectral function and for the remainder in Weyl's law on negatively-curved surfaces

Abstract: We obtain asymptotic lower bounds for the spectral function of the Laplacian on compact manifolds. In the negatively curved case, thermodynamic formalism for hyperbolic flows is applied to improve the estimates. Our results can be considered pointwise versions (on a general manifold) of lower bounds (due to Hardy and Landau) for the error term in the Gauss circle problem. We next discuss lower bounds for the remainder in Weyl's law on negatively-curved surfaces. Our approach works in variable negative curvature, and is based on wave trace asymptotics for long times, thermodynamic formalism for hyperbolic flows, and small-scale microlocalization. This is joint work with I. Polterovich and J. Toth.

A. Martinez Title: Resonances for non-analytic potentials (joint work with T. Ramond and J. Sjöstrand)

Abstract: We consider semiclassical Schrödinger operators on $\mathbb{R}^n$, with C^∞ potentials decaying polynomially at infinity. The usual theories of resonances do not apply in such a non-analytic framework. Under some additional conditions, we show that resonances are invariantly defined up to any power of their imaginary part. The theory is based on resolvent estimates for families of approximating distorted operators with potentials that are holomorphic in narrow complex sectors around $\mathbb{R}^n$.

Marco Merkli Title: Time-dependent Resonance Theory for Open Quantum Systems

Abstract: We consider interacting quantum systems of the type S+R, where S is a system of interest and R is a reservoir. While S has finitely many degrees of freedom, R is a spatially infinitely extended dissipative system. The central problem in the theory of open quantum systems is to describe the reduced dynamics of S, which is induced by the interaction with R. I present a theory of quantum resonances which allows for a detailed description of the dynamics of the reduced denisty matrix of S, valid for all times and for a small, fixed interaction strength between S and R. In the present setting, resonances come about by perturbation of embedded eigenvalues of the generator of dynamics, and they are described by analytic spectral deformation. I illustrate the theory with applications to quantum computing. In this situation, S is a chain of N spins 1/2, representing an N-qubit quantum register. I will give decoherence rates and show how they behave as functions of the complexity N. This is joint work with G.P. Berman and I.M. Sigal.

L. Michel Title: Semiclassical analysis of a random walk on a manifold

W. Müller Title: Distribution of resonances on locally symmetric spaces of finite volume

S. Nakamura Title: Time-dependent scattering theory for Schrödinger operators on scattering manifold (joint work with K. Ito)

Abstract: We propose a time-dependent approach to the scattering theory for Schrödinger operators on manifolds with asymptotically conic structure. We use a simple comparison system and the 2-space scattering theory of Kato to define wave operators and the scattering matrix.

S. Nonnenmacher Title: Quantum resonances in presence of a fractal trapped set (collab. with M.Zworski)

Abstract: We investigate the resonance spectrum close to the real axis, for a certain type of semiclassical Schrodinger operators. The smooth potential (or curved part of the metric) is taken of compact support, while the metric is Euclidean near infinity. Furthermore, we assume that, near a certain positive energy, the dynamics generated by the corresponding classical Hamiltonian admits a hyperbolic trapped set, which is generally "fractal". We show that, provided this trapped set is "thin enough", resonances near this energy cannot be "too close" to the real axis. More precisely, we show that the corresponding quantum decay rates are uniformly bounded from below by the topological pressure, a quantity characterizing the classical flow on the trapped set. This generalizes similar results by Ikawa for Euclidean obstacle scattering. We also prove a resolvent estimate analogous with the case of a single trapped orbit. Finally, we partially describe the phase space structure of the "resonant eigenstates": they are microlocalized along the unstable manifold of the trapped set.

P. Perry Title: Scattering Theory for Complex Manifolds with CR-Boundary

Abstract: This talk concerns joint work with Peter Hislop and Siu-Hung Tang. A pseudoconvex domain in $\mathbb{C}^n$ such as the complex unit ball is a model of a complex manifold with CR-boundary. When equipped with a Kahler metric of Bergmann type, the interior becomes a complete Riemannian manifold and one can study scattering theory for the Laplacian. We'll show that certain poles of the scattering operator determine CR-covariant differential operators analogous to the GJMS operators that occur as poles of the scattering operator for the conformally compact Einstein manifolds studied by Graham and Zworski; we'll also give a geometric condition under which this construction works for complex manifolds with strictly pseudoconvex boundary. A key ingredient in the construction is a global approximate solution of the complex Monge-Ampere equation.

Vesselin Petkov Title: Analytic continuation of the resolvent of the Laplacian and the dynamical zeta function for open billiards

A. Vasy Title: High energy estimates on the analytic continuation of the resolvent and wave propagation on the De Sitter-Schwarzschild space

Abstract: In this joint work with Richard Melrose and Antonio Sa Barreto we construct a high energy parametrix for the analytic continuation of the resolvent of the Laplacian on asymptotically hyperbolic spaces which are close to hyperbolic space; this parametrix is valid uniformly in a strip beyond the real axis. We use this and cutoff resolvent estimates of Bony and Haefner to obtain resolvent estimates on weighted spaces for the spatial "Laplacian" on De Sitter-Schwarzschild space (which, near infinity, is close to the hyperbolic Laplacian). This is then used to derive the asymptotics of solutions of the wave equation. Some similar results on wave asymptotics were obtained by Dafermos and Rodinianski.

Georgi Vodev Title: Distribution of the resonances for the ellasticity system with dissipative boundary conditions

J. Weir Title: A non-self-adjoint differential operator with purely real spectrum

Abstract: There are few examples of non-self-adjoint operators whose spectra are purely real, other than those which are similar to self-adjoint operators. We consider a highly non-self-adjoint differential operator arising in fluid mechanics which depends upon a small parameter ϵ. This operator is not similar to any self-adjoint operator, yet we identify a self-adjoint Sturm-Liouville operator which has the same spectrum, thus proving that the spectrum is real. By studying this self-adjoint operator, we then determine the asymptotic distribution of the eigenvalues and the behaviour of the spectrum as $\epsilon \to 0$.

Participants

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Bindel, David (Courant Institute of Math. Sciences (New York University)
Borthwick, David (Emory University)
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Christiansen, Tanya (University of Missouri)
Christianson, Hans (Massachusetts Institute of Technology)
Datchev, Kiril (University of California, Berkeley)
Froese, Richard (University of British Columbia)
Guillarmou, Colin (Université de Nice)
Hislop, Peterm (University of Kentucky)
Hitrik, Michael (University of California, Los Angeles)
Jakobson, Dmitry (McGill University)
Martinez, André (Università di Bologna)
Merkli, Marco (Memorial University)
Michel, Laurent (Université de Nice)
Müller, Werner (Universität Bonn)
Nakamura, Shu (University of Tokyo)
Naud, Frederic (Université d'Avignon)
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Chapter 36

Interactions Between Noncommutative Algebra and Algebraic Geometry (08w5072)

Oct 26 - Oct 31, 2008

Organizer(s): Colin Ingalls (University of New Brunswick), Michael Artin (Massachusetts Institute of Technology), Lance Small (University of California, San Diego), James Zhang (University of Washington)

Overview of the Field

The root of noncommutative algebra goes back to 1843 when Hamilton discovered the quaternions. The subject of abstract algebra has been developed since the early twentieth century by Wedderburn, Artin, Brauer, Noether, and later by Amitsur, Jacobson, Kaplansky, Goldie, Herstein and many others. New research topics in noncommutative algebra and its interplay with other fields such as Lie theory, geometry and physics has emerged in recent years. The structure of noncommutative algebras has been understood by the use of algebraic, combinatorial, geometric and homological means.

Noncommutative algebraic geometry is an interdisciplinary subject that arises from the interaction between noncommutative algebra and algebraic geometry. Originated by Artin, Schelter, Tate and Van den Bergh [6, 9, 10], noncommutative projective geometry has grown from the basic principle that the global techniques of classical projective algebraic geometry furnish powerful methods and intuition for the study of noncommutative graded algebras. Specifically, the category of graded modules modulo those of finite length over a noetherian connected graded algebra form an appropriate analogue for the category of coherent sheaves on a projective variety [12]. This technique has been particularly successful in understanding important classes of noncommutative algebras.

Over the last fifteen years, noncommutative projective curves have been ”understood” by Artin and Stafford [7, 8] in terms of graded algebras of Gelfand-Kirillov dimension two and by Reiten and Van den Bergh [40] in terms of proper categories of global dimension two. More recently, noncommutative projective surfaces have been studied extensively by many researchers. The birational theory of noncommutative projective surfaces was extended in the work of Chan and his coauthors [23, 24, 25, 27, 26] using ideas of Mori’s minimal model program. The moduli of Azumaya algebras on surfaces have been studied by Artin and de Jong [5]. Various explicit and interesting examples of noncommutative surfaces have been examined. Regular algebras of global dimension three were classified by Artin, Schelter, Tate and Van den Bergh in 1980’s [6, 9, 10].

There have been many recent developments in the classification of regular algebras of global dimension four (or their associated quantum projective three spaces) in papers by Lu, Palmieri, Shelton, Stephenson Vancliff, Wu and Zhang [44, 45, 35, 53] and others.

Many new techniques have been introduced and used in noncommutative algebra and noncommutative algebraic geometry. Also applications of noncommutative algebraic geometry have been found. Stacks, derived categories, tilting and dualizing complexes are currently standard tools in the subject. The purpose of this workshop was to discuss various aspects of the interaction between noncommutative algebra and algebraic geometry, including the latest developments in noncommutative algebraic geometry and their applications.

Recent Developments and Open Problems

Recent Developments

An active research topic in the subject, with many participants, remains the classification of noncommutative surfaces (both in the setting of orders and of highly noncommutative algebras) and higher dimensional noncommutative analogues of projective space. This has again lead to interesting new concepts like naïve blow-ups [33], double Ore extensions [59] and their generalizations. It has also lead to various generalizations of Koszul duality for non-quadratic algebras [17]. Some of the best-understood noncommutative surfaces are the del Pezzo surfaces introduced by Van den Bergh in his work on noncommutative blow-ups [55]. They have resurfaced in recent work of Auroux, Katzarkov and Orlov on homological mirror symmetry [13]. New constructions of such surfaces have recently appeared in work of Etingof and Ginzburg [28] and these are, in turn, related to graded Calabi-Yau algebras.

Developments in noncommutative algebraic geometry provide new ideas and even new research directions to commutative algebra, noncommutative algebra and algebraic geometry. Many basic concepts, including rigid dualizing complexes, strongly noetherian rings, twisted homogeneous coordinate rings, point varieties and **Z**-algebras, that first appeared in noncommutative algebraic geometry, are now routinely used in other contexts. For example, rigid dualizing complexes have been used to give a completely new approach to Grothendieck duality in the commutative case [58], as well as in the study of Noetherian noncommutative Hopf algebras [20]. In another direction, **Z**-algebra techniques are fundamental to the work on graded twisted Weyl algebras [47] and Cherednik algebras [31, 32]. As an illustration of the applications to the other areas, we mention three different papers. The first is the work of Van den Bergh on noncommutative crepant resolutions [56] that establishes a noncommutative model for resolution of singularities and avoids the technical issue of blowing up in commutative algebraic geometry. Noncommutative crepant resolutions have been used in both commutative algebra and algebraic geometry. The second is the paper by Ben-Zvi and Nevins [16] which used the techniques of noncommutative algebraic geometry to provide a bridge between KP soliton equations and Calogero-Moser many-body systems. The ramifications of this work and related moduli questions remains an active area of research. A recent work of Okounkov on random surfaces [39] gave an surprising application of noncommutative algebraic geometry to the study of difference equations and probability, which could further relate this new subject to a broader aspect of mathematics.

Noncommutativity has proved to be stacky. Recently, algebraic stacks were used by Lieblich to study finite dimensional division algebras over fields of transcendence degree two [34], by Chan to study noncommutative projective schemes, and by Reichstein to study essential dimension [21]. The theory of algebraic stacks (and possible generalizations) provides a powerful idea/method for a large class of noncommutative rings and schemes with big centers, including noncommutative Calabi-Yau algebras. Examples show that the stacky structure can be realized by using appropriate categories, which agrees with the basic principle of noncommutative algebraic geometry. Further research on algebraic stacks would be beneficial to the subject.

Ideas from representation theory play an important role in the recent developments. Derived Categories are used more and more, and there are many examples of commutative and noncommutative varieties who share their derived category with representations of a noncommutative finite dimensional algebra (in a slightly more general setting, the finite dimensional algebras should be replaced by finite dimensional DG-algebras or finite dimensional A_∞-algebras). Invariants defined by using derived categories such as Rouquier's dimension, thick subcategories, t-structures, and rigid dualizing complexes would have significant impacts to the study of noncommutative algebra and geometry.

Another important advance has been in the study of combinatorial aspects of noncommutative algebra. Bell recently proved that an affine prime Goldie algebra of quadratic growth is either primitive or satisfies a polynomial identity [14], answering a famous question of Small in the affirmative. Smoktunowicz has proved a ”gap” theorem stating that there is no connected graded affine domain with Gelfand-Kirillov dimension between 2 and 3 in [52]. Centralizers of elements in algebras of low Gelfand-Kirillov dimension have been studied in detail [15, 51].

Open Questions

Here is a partial list of open questions in the field.

1. Artin's conjecture and classification of noncommutative projective surfaces.

In 1992 Artin conjectured that every division algebra of transcendence degree two that comes from a noncommutative projective surface is either finite over its center, q-ruled, or q-rational (including the Sklyanin division ring) which correspond to all known noncommutative projective surfaces up to birational equivalence [4]. Artin proved that these division algebras are non-isomorphic by showing that their prime divisors are different [4]. This conjecture is very natural after the landmark work of Artin and Stafford [7, 8] that classified all noncommutative projective curves (or noncommutative graded domains of Gelfand-Kirillov dimension two). As mentioned above a great deal of research has been motivated by Artin's conjecture: the work of Chan, Hacking, Ingalls, Kulkarni, and Nyman [24, 25, 23, 27, 26], the manuscript by Artin and de Jong [5], and the series of papers by Keeler, Rogalski, Stafford and Sierra [33, 41, 3, 4, 46], and Van den Bergh's theory of monoidal transformations [55]. Artin's conjecture is the first step towards the classification of noncommutative projective surfaces. At this point Artin's conjecture is still one of the main open questions in noncommutative algebraic geometry and the classification of noncommutative projective surfaces seems a long way off.

2. Classification of quantum $\mathbf{P}^n$.

This is another major open question in the field. A subquestion is the classification of (Artin-Schelter) regular algebras of global dimension large than three. Since the classification of regular algebras of global dimension three in 1980s, many researchers have been interested in regular algebras of global dimension four. For example, a recent paper by Cassidy-Vancliff introduced the notion of a graded skew Clifford algebra [22] aiming at constructing more regular algebras with finite point modules. Lu, Palmieri, Wu and Zhang used A_∞-algebra methods to attack this problem [35]. One special class of regular algebras is so-call Sklyanin algebras [48, 49] that have been understood by Odesskii, Feigin, Smith, Stafford, Tate and Van den Bergh [37, 38, 50, 54]. The general classification has not been finished, even for global dimension four.

3. Geometric aspect of quantum groups.

Quantum groups (or noncommutative and noncocommutative Hopf algebras) have been studied extensively for more than twenty years and their algebraic and representation-theoretic aspects are understood to a large degree. However, the geometric aspect of quantum groups is less well-understood. Using cohomology, the geometry of the Koszul dual of some special quantum groups were studied by Ginzburg and Kumar in [30]and by Friedlander and Suslin in [29]. A more direct approach to the question has not been established. Ideas and techniques in noncommutative algebraic geometry should be useful in this study. Another interesting open question about quantum groups and Hopf algebras is Brown's conjecture: Every noetherian affine Hopf algebra has finite injective dimension [18, 19]. A partial answer is given in the PI case [57].

4. Ideals theory of Iwasawa algebras.

Noncommutative Iwasawa algebras have repeatedly been used in Iwasawa theory, which is probably the best general technique in arithmetic geometry for studying the mysterious relations between exact arithmetic formulae and special values of L-functions. The Iwasawa algebras Γ_G and their companion Ω_G form an interesting class of noncommutative complete semilocal noetherian algebras. For simplicity we assume that the compact p-adic analytic group G is uniform. In this case both Γ_G and Ω_G are local and have various nice homological properties – see the survey paper by Ardakov and Brown [1]. The structure of Iwasawa algebras and modules over them have been studied extensively by several authors from an algebraic point of view and one of the main questions in this research direction is the Ardakov-Brown Question [1]: Let G be almost simple and uniform. Are there prime ideals of Ω_G other than zero and the maximal ideal? This was verified only for G being congruence subgroups of $SL_2(\mathbf{Z}_p)$ [2, 3]. New techniques are needed for handling the higher dimensional cases.

5. Dimension theory in noncommutative algebra and noncommutative algebraic geometry.

One difficult issue in noncommutative algebra/geometry is to find an effective dimension theory. Some generalizations of commutative dimension theory such as Krull dimension do not give the correct numbers in the noncommutative case, while others are not easy to compute. Gelfand-Kirillov dimension is a commonly used dimension function and is relatively easy to compute in many cases. One open question about Gelfand-Kirillov dimension is: under what reasonable hypotheses, is it an integer? The recent works of Bell [14] and Chan [27] are dependent on a good behavior of a dimension function.

Presentation Highlights

Speaker: **Jason Bell** (Simon-Fraser University)
Title: *Centralizers in finitely generated algebras and in division algebras*
Abstract: We look at the problem of describing centralizers in algebras and in division algebras. Our main result is that if A is a finitely generated complex noetherian algebra of GKdimension strictly less than 4 then the centralizer of a non-scalar element satisfies a polynomial identity. We also look at the connection between transcendence degree of subfields and the size of centralizers in division algebras and formulate a few conjectures.

Speaker: **Daniel Chan** (University of New South Wales)
Title: *A non-commutative Mori contraction*
Abstract: One of M. Artin's conjectures can be loosely stated as: a noncommutative surface is, up to birational equivalence, either ruled or finite over its centre. This suggests that it would be nice to have a criterion for a noncommutative surface to be ruled. In the commutative case, there is a criterion based on Mori theory. Given a K-negative extremal ray C in the cone of curves with self-intersection zero, the surface is ruled. In this talk, we discuss the possibility of a noncommutative version of this result. We show that given a noncommutative smooth projective surface (appropriately defined) which contains an object like the ray C above, there is a non-commutative "Mori contraction" to a curve. This is a report on joint work with Adam Nyman.

Speaker: **Michele D'Adderio** (University of California at San Diego)
Title: *On isoperimetric profiles of algebras*
Abstract: Isoperimetric profile in algebras was first introduced by Gromov. In this talk we show the behavior of the isoperimetric profile under various ring theoretic constructions and its relation with amenability. We show that the isoperimetric profile is a finer invariant than the lower transcendence degree, and we use it to answer a question of J.J. Zhang.

Speaker: **Birge Huisgen-Zimmermann** (University of California at Santa Barbara)
Title: *Generic representations of quivers with relations*
Abstract: The irreducible components of varieties parametrizing the finite dimensional representations of a finite dimensional algebra A are explored, in terms of both their geometry and the structure of the modules they encode; expected close connections between the two aspects are rendered more explicit. In particular, we establish the existence and uniqueness (not up to isomorphism, but in a strong sense to be specified) of generic modules, that is, of modules which display all categorically defined generic properties of the modules parametrized by a given irreducible component. Our approach to existence is largely constructive, by way of minimal projective presentations. We follow with an investigation of the properties of such generic modules with regard to quiver and relations of A. The sharpest specific results on all fronts are obtained for truncated path algebras, that is, path algebras of quivers modulo ideals generated by all paths of a fixed length.

Speaker: **Osamu Iyama** (Nagoya University)
Title: *Cluster tilting in 2-Calabi-Yau categories*

Abstract: Cluster tilting theory reveals combinatorial structure of 2-Calabi-Yau triangulated categories, and is applied to categorify Fomin-Zelevinsky cluster algebras by many authors (Buan, Marsh, Reineke, Reiten Todorov, Caldero, Chapoton, Schiffler, Keller,...).In my talk, we will introduce cluster tilting theory in 2-Calabi-Yau triangulated category. In particular, a combinatorial description of the change of endomorphism algebras of cluster tilting objects via mutation process is given in terms of Fomin-Zelevinsky quiver mutation rule and Derksen-Weyman-Zelevinsky quiver with potential mutation rule.

Speaker: **Ulrich Kraehmer** (University of Glasgow)
Title: *On the Hochschild (co)homology of quantum homogeneous spaces*
Abstract: In this talk I will speak about a generalisation of a result by Brown and Zhang establishing Poincare duality in Hochschild (co)homology for a class of algebras that can be considered as noncommutative analogues of affine homogeneous spaces.

Speaker: **Max Lieblich** (Princeton University)
Title: *The period-index problem for surfaces over finite fields*
Abstract: I will discuss the period-index problem for Brauer groups of fields of transcendence degree 2 over finite fields, and how stacky techniques relate this problem to the geometry of moduli spaces of vector bundles and to the Hasse principle for geometrically rational varieties over global fields.

Speaker: **Valery Lunts** (Indiana University)
Title: *Categorical resolution of singularities*
Abstract: This is my work in progress. I want to propose the notion of a categorical resolution of singularities, compare it with the usual resolutions in algebraic geometry and discuss some examples and conjectures.

Speaker: **Susan Montgomery** (University of Southern California)
Title: *Recent progress in "Invariant Theory" for Hopf algebras*
Abstract: Let H be a finite dimensional Hopf algebra acting on an algebra A over a field k. Recently a number of questions about the relationship between A, its subalgebra of invariants A^H, and the semi-direct product $A\#H$, open since the 1970's and 1980's, have been solved. For example: (1) if H is semisimple, then the Jacobson radical is always H-stable (this is work of Linchenko); (2) if H is semisimple and A is H-semiprime, then any H-stable left or right ideal of A intersects A^H non-trivially. I will survey some of these results and discuss their proofs.

Speaker: **Zinovy Reichstein** (University of British Columbia)
Title: *Essential dimension and algebraic stacks*
Abstract: The essential dimension of an algebraic object (e.g., of an algebra, a quadratic form, or an algebraic variety) is the minimal number of independent parameters required to define the underlying structure. This numerical invariant has been studied by a variety of algebraic, geometric and cohomological techniques. In this talk, based on joint work with P. Brosnan and A. Vistoli, I will discuss a new approach based on the notion of essential dimension for an algebraic stack.

Speaker: **Daniel Rogalski** (University of California at San Diego)
Title: *Subalgebras of the Sklyanin Algebra*
Abstract: We study subalgebras of the 3-dimensional Sklyanin algebra S, particularly those generated in degree 3. We classify such algebras which are also maximal orders. Geometrically, each such algebra 4 behaves like a blowup of the Sklaynin projective plane along a divisor of degree at most 7 on the elliptic curve.

Speaker: **David Saltman** (University of Texas at Austin)
Title: *Quaternion algebras and their maximal subfields*
Abstract: Using the generic splitting field of Amitsur, we know that two division algebras with the same splitting fields are quite close: powers of each other in the Brauer group. However, if you restrict to finite dimensional splitting fields, or even maximal subfields, the situation is much different. Over global fields, two division algebras of degree greater than 2 can have the same finite dimensional splitting fields and not be

powers of each other. However, two quaternion algebras over a global field with the same maximal subfields are isomorphic. Several people asked whether this is true in general. We will show that if youassume the center field F has zero unramified Brauer group, and D/F, D'/F are quaternion algebras with the same maximal subfields, then $D \cong D'$. We will also discuss a generalization to higher cohomology due to Skip Garibaldi.

Speaker: **Brad Shelton** (University of Oregon)

Title: *Noncommutative Koszul Algebras from Combinatorics and Topology*

Abstract: We consider a construction given by Gelfand, Retakh, Serconek and Wilson, that builds noncommutative graded quadratic algebras from finite layered graphs. A mistake in the literature suggests that all such algebras are Koszul. We give some results on the Koszul property of these algebras when the associated graph is related to a regular CW-complex.

Speaker: **Susan Sierra** (University of Washington)

Title: **The classification of birationally commutative surfaces**

Abstract: We give a complete classification of birationally commutative projective surfaces (connected $\mathbf{N}$-graded noetherian domains of GKdimension 3 that are birational to a commutative surface in Artin's sense), and show that all such algebras fall into four families determined by geometric data. We relate the geometry of the underlying data and the algebraic properties of the algebras, and discuss potential generalizations to higher dimensions. This extends results of Rogalski and Stafford in the case that the algebra is generated in degree 1.

Speaker: **Agata Smoktunowicz** (University of Edinburgh)

Title: GKdimension of factor algebras of Golod-Shafarevich algebras

Abstract: It is known that Golod-Shafarevich algebras have exponential growth. In this talk it is shown that also all non-nilpotent factor rings of generic Golod-Shafarevich algebras over fields of infinite transcendence degree have exponential growth, provided that the number of defining relations of degree less then n grows exponentially with n. This answers a question stated by Efim Zelmanov in the paper "Some open problems in the theory of infinite dimensional algebras".

Speaker: **Toby Stafford** (University of Manchester)

Title: *Applications of noncommutative geometry to Cherednik algebras*

Abstract: This talk will report on joint work with Victor Ginzburg and Iain Gordon. We establish a link between two geometric approaches to the representation theory of rational Cherednik algebras of type A: one based on noncommutative geometry; the other involving quantum hamiltonian reduction of an algebra of differential operators. This link is achieved by showing that the process of hamiltonian reduction intertwines a naturally defined geometric twist functor on D-modules with the shift functor for the Cherednik algebra. If I have time I will also apply this to the structure of characteristic cycles of modules over the Cherednik algebra.

Speaker: **Hokuto Uehara** (Tokyo Metropolitan University)

Title: *Tilting generators via ample line bundles*

Abstract: We construct tilting generators by ample line bundles under some assumptions.

Speaker: **Quanshui Wu** (Fudan University)

Title: *Non-commutative Castelnuovo-Mumford Regularity and AS regular Algebras*

Abstract: Let A be a connected graded k-algebra generated in degree 1, with a balanced dualizing complex. I will talk about the Castelnuovo-Mumford regularity and the Ext regularity and prove that these regularities coincide for all finitely generated A-modules if and only if that A is a Koszul AS-regular algebra. By using Castelnuovo-Mumford regularity, we also prove that any Koszul standard AS-Gorenstein algebra is AS-regular.

Scientific Progress Made

The meeting allowed people working in noncommutative algebraic geometry and related fields to become up to date with current progress in the field. There were also many discussions between participants yielding new research projects. This meeting had many younger speakers and participants with new connections to noncommutative algebraic geometry. There has been much recent progress in the area and the meeting was an important part of such progress.

Outcome of the Meeting

This workshop brought together 38 researchers (including three Ph.D. students) from various countries in different areas of noncommutative ring theory, algebraic geometry, representation theory and the interdisciplinary subject noncommutative algebraic geometry. There were many interesting talks and engaging discussions during the workshop. The collaborations between participants were fruitful which led some joint research projects and some of which resulted joint publications. Since this workshop, there have been a few workshops in the same topics around the world:

University of Manchester, Manchester, UK from August 3-7, 2009. RIMS, Kyoto University, Kyoto, Japan from August 24-28, 2009, Oberwolfach, Germany, May 9-15, 2010 (planed). More researchers in the related subjects have become interested in noncommutative algebraic geometry. This workshop definitely created new mathematics in noncommutative algebraic geometry and will further expand the subject.

List of Participants

Bell, Jason (Simon Fraser University)
Chan, Daniel (Univesity of New South Wales)
Chan, Kenneth (University of New South Wales)
D'Adderio, Michele (University of California - San Diego)
Goodearl, Kenneth (University of California, Santa Barbara)
Green, Ed (Virginia Tech)
Huisgen-Zimmermann, Birge (University of California, Santa Barbara)
Ingalls, Colin (University of New Brunswick)
Ishii, Akira (Hiroshima University)
Iyama, Osamu (Nagoya University)
Kawamata, Yujiro (The University of Tokyo)
Kirkman, Ellen (Wake Forest University)
KrŁhmer, Ulrich (University of Glasgow)
Kulkarni, Rajesh (Michigan State University)
Letzter, Edward (Temple University)
Lieblich, Max (Princeton University)
Lorenz, Martin (Temple University)
Lu, Di-Ming (Zhejiang University)
Lunts, Valery (Indiana University)
Montgomery, Susan (University of Southern California)
Mori, Izuru (Shizuoka University)
Nyman, Adam (University of Montana)
Reichstein, Zinovy (University of British Columbia)
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Shelton, Brad (University of Oregon)
Sierra, Susan (University of Washington)
Small, Lance (University of California, San Diego)
Smoktunowicz, Agata (University of Edinburgh)
Stafford, Toby (University of Michigan)

Todorov, Gordana (Northeastern University)
Uehara, Hokuto (Tokyo Metropolitan University)
Vancliff, Michaela (University of Texas at Arlington)
Vonessen, Nikolaus (University of Montana)
Wu, Quanshui (Fudan University)
Yekutieli, Amnon (Ben Gurion University)
Zhang, James (University of Washington)
Zhang, Jun (University of Washington)

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Chapter 37

WIN – Women in Numbers (08w5112)

Nov 03 - Nov 07, 2008

Organizer(s): Kristin Lauter (Microsoft Research), Rachel Pries (Colorado State University), Renate Scheidler (University of Calgary)

This workshop was a unique effort to combine strong broad impact with a top level technical research program. In order to help raise the profile of active female researchers in number theory and increase their participation in research activities in the field, this event brought together female senior and junior researchers in the field for collaboration. Emphasis was placed on on-site collaboration on open research problems as well as student training. Collaborative group projects introducing students to areas of active research were a key component of this workshop.

We would like to thank the following organizations for their support of this workshop: BIRS, NSA, Fields Institute, PIMS, Microsoft Research, and University of Calgary.

Rationale and Goals

There has been a recent surge of activity in number theory, with major results in the areas of algebraic, arithmetic and analytic number theory. This progress has impacted female number theorists in contradictory ways. Although the number of female number theorists has grown over the past fifteen years, women remain virtually invisible at high profile conferences and largely excluded from elite international workshops in number theory (data supporting this fact can be provided upon request). Moreover, there are not many tenured female number theorists at top research universities. This void — at conferences and at key institutions — has profound negative consequences on the recruitment and training of future female mathematicians. This workshop was meant to address these issues. The goals of the workshop were:

1. To train female graduate students in number theory and related fields;
2. To highlight research activities of women in number theory;
3. To increase the participation of women in research activities in number theory;
4. To build a research network of potential collaborators in number theory;
5. To enable female faculty at small colleges to help advising graduate students.

Participant testimonials, comments from (male and female) colleagues, and other feedback suggest that significant progress was made toward goals 1, 2, 4 and 5. In particular, the conference gave greater exposure to the research programs of active female researchers in number theory. Through collaborative projects, students participated in new research in the field, and faculty at small colleges were exposed to supervision activities. Some of the group projects will lead to new results and publications, and the conference organizers are currently exploring venues for publication of a conference proceedings volume. Work has begun on a

WiKi website that will serve as the basis for the **WIN Network**, a network for female researchers in number theory. It is the sincere hope of the workshop organizers that progress was also achieved toward goal 3 above, but only time will tell.

Participants and Format

In lieu of the goals of this workshop, participation was limited to women. The participants were 41 female number theorists – 15 senior and mid-level faculty, 16 junior faculty and postdocs, and 10 graduate students. About half of the participants, mostly faculty, were invited by the conference organizers. The remaining slots were intended for junior faculty, postdocs, and graduate students.

To that end, the organizers held an open competition involving a formal application procedure and a rigorous selection process. This was advertised in the *Association of Women in Mathematics* newsletter. Additionally, Math Departments of all PhD-granting institutions in Canada and many in the United States were contacted. 56 applicants submitted a CV and a research statement (for PDFs and junior faculty) or a list of courses taken (for grad students). After a careful and thorough review of these documents, the organizing committee selected what were deemed to be the strongest applicants for participation in the workshop.

Based on the participants' research interests and expertise, the organizers then divided the participants up into 8 research groups of 4-6 members each; usually 2 senior members (group leaders) and 2-4 junior members. Research topics ranged from algebraic, analytic and algorithmic number theory to cryptography. In consultation with their group members, group leaders chose a project topic for collaborative research during and following the conference. They provided materials and references for background reading ahead of time. The group leaders also gave talks during first three days of the meeting to introduce all participants to their respective group projects. During the last two days of the workshop, junior participants presented the progress made on the group projects. These presentations usually involved more than one presenter. As a result, essentially all workshop participants were able to give a talk, or a portion of one.

Each group also submitted a short written progress report on their project. These reports, along with the project title and the names of the group members, are included below. Collaboration on the research projects is on-going via electronic communication. Some of these projects will lead to new results and publications. The organizers also expect to publish a conference proceedings volume in the future.

Lectures (organized by project group):
A1 Speaker: Stephanie Treneer, Western Washington University
Title: Modular Forms I
Speaker: Ling Long, Iowa State University
Title: Modular Forms II

A2 Speaker: Chantal David, Concordia University
Title: Frobenius Distribution and L-functions
Speaker: Alina Cojocaru, University of Illinois at Chicago
Title: Koblitz's Conjecture on Average

B Speaker: Audrey Terras, University of California at San Diego
Title: Zeta Functions of Graphs Icharacteristic p I
Speaker: Winnie Li, Pennsylvania State University
Title: Zeta Functions of Graphs II

C Speaker: Kirsten Eisentraeger, Pennsylvania State University
Title: Computation of pairings on hyperelliptic curves I
Speaker: Edlyn Teske, University of Waterloo
Title: Computation of pairings on hyperelliptic curves II

D Speaker: Katherine Stevenson, California State University Northridge
Title: Towers of Galois covers in characteristic p I

Speaker: Rachel Pries, Colorado State University
Title: Towers of Galois covers in characteristic p II

E Speaker: Renate Scheidler, University of Calgary
Title: Class groups of function fields I
Speaker: Yoonjin Lee, Ehwa Womans University
Title: Class groups of function fields II

F Speaker: Helen Grundman, Bryn Mawr College
Title: Computations on Hilbert Modular Surfaces I
Speaker: Kristin Lauter, Microsoft Research
Title: Computations on Hilbert Modular Surfaces II

G Speaker: Mirela Ciperiani, Columbia University
Title: Galois representations I

Research Projects and Project Groups

Project A1: Modular forms – Zeros of a Class of Eisenstein Series

Participants: Sharon Garthwaite, Ling Long, Holly Swisher, Stephanie Treneer

The study of modular forms has been a central focus of number theory for more than one century. Modular forms are highly symmetric holomorphic functions defined on the Poincaré upper half plane, and the classical example of such a function is the Eisenstein series. In fact, Eisenstein series can be viewed as the building blocks of modular forms. To understand the properties of Eisenstein series is of fundamental importance to the study of modular forms and has many significant applications.

Work by R. A. Rankin, F.K.C. Rankin and H.P.F. Swinnerton-Dyer reveals that the zeros of the classical Eisenstein series $E_{2k}(z)$ for the full modular group $SL_2(\mathbb{Z})$ are all located on a particular arc of the unit circle. Equivalently, the j-values of these zeros are real and lie in the range $[0, 1728]$, where j is the classical modular j-function. Despite the efforts these and many other mathematicians, Eisenstein series still remain an intriguing source of mysteries. For example, Nozaki recently proved that the (real) zeros of classical Eisenstein series $E_{2k}(z)$ interlace with the zeros of $E_{2k+12}(z)$.

In this project, we study a class of odd weight Eisenstein series $E_{2k+1,\chi}(z)$ for the principal level 2 subgroup $\Gamma(2)$ with a character χ. It is well-known that the modular curve $X_{\Gamma(2)} = (\mathfrak{H}/\Gamma(2))^*$ for $\Gamma(2)$ is a Riemann surface of genus zero, and that the field of meromorphic functions on $X_{\Gamma(2)}$ is generated by $\lambda(z)$, the classical λ function. The Eisenstein series $E_{2k+1,\chi}(z)$ in consideration have previously been used to obtain some nice formulae of Milnor involving the number of representations of natural numbers as sums of squares or sums of triangular numbers.

For our first investigation of this topic, we obtain a generating function $cn(u)$ of $E_{2k+1,\chi}(z)$, where $cn(u)$ is a Jacobi elliptic function and satisfies a non-linear differential equation. By using the inherited recursions, we are able to compute the polynomials $f_{2k+1}(\lambda)$ which encode the λ-values of the zeros of $E_{2k+1,\chi}(z)$. Numerical data suggests that the $f_{2k+1}(\lambda)$ have real λ-values which are within $(-\infty, 0)$, and these zeros of $f_{2k-1}(\lambda)$ interlace with the zeros of $f_{2k+1}(\lambda)$; this is parallel to the results in the classical case.

On the theoretical side, we extend the approach of Rankin and Swinnerton-Dyer to show that at least 58 percent of the zeros of $f_{2k+1}(\lambda)$ are real and are within $(-\infty, 0)$. We also obtain formulas which relate the λ-values of the zeros of Eisenstein series on $\Gamma(2)$ to special values of certain L-series.

Project A2: Distributions of Traces of Cyclic Trigonal Curves over Finite Fields

Participants: Alina Bucur, Alina Cojocaru, Chantal David, Brooke Feigon, Matilde Lalín

The number of points of a hyperelliptic curve with affine model $y^2 = F(x)$ over the finite field $\mathbb{F}_q$ with q elements can be expressed as $q + S(F)$, where $S(F)$ denotes the character sum $\sum_{x\in\mathbb{F}_q} \chi(F(x))$. (Here F

is a square-free monic polynomial of degree d and q is odd.) The character sum also expresses the trace of the Frobenius for this curve of genus $g = \left[\frac{d-1}{2}\right]$.

In their seminal work [12] Katz and Sarnak showed that for fixed genus g and $q \to \infty$, $S(F)/\sqrt{q}$ is distributed as the trace of a random $2g \times 2g$ unitary symplectic matrix. On the other hand, Kurlberg and Rudnick [11] showed that for fixed q and $g \to \infty$ the limiting distribution of $S(F)$ is that of a sum of q independent trinomial random variables taking the values ± 1 with probabilities $q/(2q+2)$ and the value 0 with probability $1/(q+1)$.

The natural question to ask is what happens when one works with higher degree curves, which means that one needs to study higher order characters. For instance, over a field with $q \equiv 1 \bmod 3$, cyclic trigonal curves

$$y^3 = F(x), \tag{37.1}$$

with $F \in \mathbb{F}_q[t]$ a monic cube free polynomial of degree d, correspond to cubic extensions, and thus to cubic characters. The number of affine points of the curve over $\mathbb{F}_q$ is given by $q + S_3(F) + \overline{S_3(F)}$, where $S_3(F) = \sum_{x \in \mathbb{F}_q} \chi_3(F(x))$ and χ_3 is a fixed cubic character of $\mathbb{F}_q$. The cyclic automorphism of the curve commutes with the Frobenius automorphism and splits the first cohomology group into two eigenspaces. The trace of the Frobenius on these subspaces is given by $S_3(F)$ and $\overline{S_3(F)}$, respectively.

One could restrict the investigation to curves for which the affine model (reftriell) is smooth, which corresponds to considering only square-free polynomials F. The genus of such a curve is $g = d - 2$. In this case, the limiting distribution of the character sum $S_3(F)$ as $g \to \infty$ is that of a sum of q i.i.d. random variables taking the values 0 with probability $1/(q+1)$ and $1, \rho, \bar{\rho}$ with probabilities $q/(3q+3)$. Here ρ denotes a primitive third root of unity.

Geometrically speaking the difference between this case and the case of hyperelliptic curves considered by Kurlberg and Rudnick is that, while the moduli space of hyperelliptic curves of fixed genus g is irreducible, this is no longer the case for higher degree curves. In the trigonal case, since F is cube-free it can be written as $F = F_1 F_2^2$ where both F_1 and F_2 are square-free monic polynomials. The Riemann-Hurwitz formula tells us that the genus of (37.1) is $g = \deg F_1 + \deg F_2 - 2$. The moduli space $\mathcal{H}_{3,g}$ of cyclic trigonal curves of fixed genus g splits into irreducible subspaces indexed by pairs (d_1, d_2) with $d_1 + d_2 = g + 2$. (See [2] for further details.) We propose to investigate the limiting distribution of the character sum $S_3(F)$ in these irreducible components as either d_1 or d_2 grows, as well as over the whole moduli space $\mathcal{H}_{3,g}$ as $g \to \infty$.

Project B: Zeta functions of Graphs

Participants: Shabnam Akhtari, Habiba Kadiri, Winnie Li, Elisabeth Malmskog, Michelle Manes, Audrey Terras

Part I. The Analytic Part. We derived an analog of Weil's explicit formula for Dedekind zeta functions and plan to use it to study basic facts about the distribution of poles of the Ihara zeta function, for example. The result may also be viewed as a generalization to irregular graphs of the Selberg trace formula for a regular tree. We plan to plug in various kernels similar to those that work for the Selberg trace formula in the regular case.

Part II. Ramified Covers and Divisibility of Ihara Zetas. We investigated some examples of ramified covers in which there is divisibility of the zeta functions up to linear factors, and we plan to study connections with results for zeta functions of curves over finite fields. Here is a longer description.

The Ihara zeta function of a graph was defined by Yatsutaka Ihara in the 1960s. It was modeled on other zeta functions in its form, an infinite product over primes in the graph, and has some analogous properties, for example convergence to a rational function. Emile Artin defined the zeta function of a curve over a finite field in his 1921 thesis. Serre proved that the Artin zeta function of a covered curve divides that of the covering curve as long as the covering is defined over the base field of the zeta function.

Audrey Terras and Harold Stark have outlined a notion of unramified coverings of connected graphs, and have found that if G and H are connected graphs such that there exists an unramified covering map $H \to G$, then the reciprocal of the Ihara zeta function of G divides the reciprocal of the Ihara zeta function of H. In an attempt to extend the theory of Ihara zeta functions and draw further parallels with Artin's zeta function, we sought a notion of ramified coverings of graphs for which some divisibility relations between Ihara zeta functions could be found.

In 2007, Matthew Baker and Serguei Norine outlined a definition of covering maps of graphs and ramification in these coverings, and proved a graph theoretic analogue of the Riemann-Hurwitz formula for curves using their definitions. Adapting this notion of ramification, we found an ”almost” divisibility relationship between the Ihara zeta functions of some simple ramified covers of graphs.

In particular we found a formula for the zeta function of a complete graph on k vertices, and of a graph consisting of n copies of a complete graph on k vertices all sharing a single vertex. We considered the latter as a ramified cover of the complete graph. All terms except a cubic of the zeta function of the complete graph divide the zeta function of the covering graph. If $k = 3$ we have true divisibility, as the cubic term has a particularly simple form which divides the zeta function of the covering graph.

Project C: Elliptic Curve Cryptography

Participants: Jennifer Balakrishnan, Juliana Belding, Sarah Chisholm, Kirsten Eisenträger, Katherine Stange, Edlyn Teske

Since 2000, there has been much interest in the explicit computation of pairings on elliptic curves, as these can be used in tripartite key exchange, ID-based encryption and other cryptographic protocols. More recently, there has been heightened interest in computation of pairings on hyperelliptic curves. While hyperelliptic curves require more involved computations, they provide security comparable to that of elliptic curves while working with a smaller finite field. For example, a genus two hyperelliptic curve requires a field of only half the bit size for the same security level.

The focus of our group at WIN 2008 was to bring everyone up to speed on the current state of pairings on hyperelliptic curves. Our starting point was the 2007 survey paper by Galbraith, Hess and Vercauteren on this topic [8]. We spent the week surveying the current literature, learning the computational issues, and brainstorming questions we could explore.

We focused on the Tate pairing, as it is more efficient than the Weil pairing and more universally applicable than the eta or ate pairings, for example. We also focused on curves of genus two, as these are of primary interest for cryptographic and computational reasons. Let r be a prime dividing the order of the Jacobian of the curve C over $\mathbb{F}_q$ and let k be the smallest integer such that r divides $q^k - 1$, known as the *embedding degree* of C. Then the Tate pairing $e_r(D_1, D_2)$ maps a pair of points of the r-torsion subgroup of Jac$(C)(\mathbb{F}_{q^k})$ to an element of $\mathbb{F}_{q^k}$. The curve C and field $\mathbb{F}_q$ are carefully chosen to balance the difficulty of the discrete logarithm problem (DLP) in the r-torsion subgroup of Jac$(C)(\mathbb{F}_{q^k})$ with the difficulty of the DLP in $\mathbb{F}_q^*$. Such curves are called *pairing-friendly* (for a precise definition, see [7]).

The input to the pairing is two divisors, the first defining a function f_{D_1} on Jac(C) and the second encoding the points where the function is evaluated: $e(D_1, D_2) = f_{D_1}(D_2)$. Miller's algorithm for computing the Weil pairing has been adapted to the Tate pairing, and computes the pairing recursively [13].

The main approach to speeding up the computation of pairings is straightforward: reduce the number of computations, specifically expensive ones like field inversions. The techniques to do this, however, are varied and often apply to only special cases. During our work together, we encountered two situations which lead to some interesting questions (both open to our knowledge).

- In the case of even embedding degree k, it is “traditional” to exploit the degree two subfield, essentially replacing field inversion by conjugation. For this reason, much of the work on computation of pairings restricts to this case. As the case of odd embedding degree is neglected in the literature, it is natural to ask:

  > What computational improvements can be made in the case of $k \equiv 0 \bmod 3$ by using arithmetic in a degree 3 sub-field? Similarly, what about $k = 5$?

  These are not vacuous questions, as there exist supersingular curves with such embedding degrees. Currently, the main source for pairing-friendly genus two hyperelliptic curves is *supersingular* curves, which have embedding degree divisible by 2, 3 or 5 (see [5]).

- For many pairing-based algorithms, the technique of *denominator elimination* reduces field inversions by using an evaluation point which lies in a subfield of $\mathbb{F}_{q^k}$. Furthermore, we may often use *degenerate* divisors (divisors which involve a single non-infinite point of C) as the evaluation point. For example, in the elliptic curve case, all divisors are degenerate and the technique in [3] is to transform the divisor to one lying in a trace-zero subgroup of $E(\mathbb{F}_{q^k})$.

  However, in the genus two case, this technique transforms a degenerate divisor into a non-degenerate one. As we must now evaluate f_{D_1} at two points, this offsets the computational gain from denominator elimination. The paper [14] proposes two work-arounds in this situation; however, we would like to address the issue itself: can one find degenerate divisors lying over a subfield?

> What is the intersection of the set of degenerate divisors and the trace-zero subgroup of $Jac(C)(\mathbb{F}_{q^k})$? If it is non-empty, how can we efficiently compute elements of it (to use as evaluation points)?

Our current plan is to examine the two questions outlined above (and any related implementation questions which may arise) and incorporate our findings into a survey paper on the state of hyperelliptic pairings, thus updating the 2007 survey paper, [8].

Project D: Galois Covers of Curves in Characteristic p

Participants: Linda Gruendken, Laura Hall-Seelig, Bo-Hae Im, Ekin Ozman, Rachel Pries, Katherine Stevenson

In this group, we discussed known results and open questions about fundamental groups of curves in characteristic p and completed a project about this topic.

New phenomena in characteristic p: This project is about phenomena that occur for curves in characteristic p but not in characteristic 0. Here are some of the basic properties of complex curves that are false for k-curves if k is an algebraically closed field of characteristic $p > 0$.

A. If $\mathcal{X}$ is a complex curve and $\emptyset \neq \mathcal{B} \subset \mathcal{X}$ is a finite set, then the fundamental group $\pi_1(\mathcal{X} - \mathcal{B})$ is a free group of rank $2g_{\mathcal{X}} + |\mathcal{B}| - 1$. There exists a G-Galois cover $\varphi : \mathcal{Y} \to \mathcal{X}$ branched only at $\mathcal{B}$ if and only if G can be generated by $2g_{\mathcal{X}} + |\mathcal{B}| - 1$ elements. Given $\mathcal{X}$, $\mathcal{B}$, and G, the number of G-Galois covers $\varphi : \mathcal{Y} \to \mathcal{X}$ which are branched only at $\mathcal{B}$ is finite. These statements are false in characteristic p. For any affine k-curve $X - B$, the algebraic fundamental group $\pi_1(X - B)$ is infinitely profinitely generated.

B. The inertia groups of a cover $\varphi : \mathcal{Y} \to \mathcal{X}$ of complex curves are cyclic. By the Riemann-Hurwitz formula, the genus of $\mathcal{Y}$ is determined by $|G|$, $g_{\mathcal{X}}$, $|\mathcal{B}|$ and the orders of the inertia groups. In particular, there are no nontrivial Galois covers of $\mathbb{A}^1_{\mathbb{C}}$ since the complex plane is simply connected.

   The situation is more complicated for covers of k-curves due to the presence of *wild ramification* which occurs when p divides the order of an inertia group. The inertia groups of a wildly ramified cover are usually not cyclic. Furthermore, the inertia group I carries extra information, including a filtration of I called the ramification filtration, [18, IV]. The genus of Y now depends on this filtration.

C. If $\mathcal{X}$ is a complex curve of genus g, then there are p^{2g} points of order p on its Jacobian $J_{\mathcal{X}}$. This property is false for the Jacobian J_X of a k-curve X of genus g. In characteristic p, the number of points of order p in $J_X(k)$ equals p^f for some integer f such that $0 \leq f \leq g$. Here f is called the *p-rank* of X. The p-rank equals the maximum rank of an elementary abelian p-group which occurs as the Galois group of an unramified cover of X.

D. A cover of complex curves can only be deformed by changing the base curve $\mathcal{X}$ or the branch locus $\mathcal{B}$. In contrast, a wildly ramified cover of k-curves can almost always be deformed without varying X or B.

One can illustrate these phenomena for the group $G = \mathbb{Z}/p$. Let $h(x) \in k[x]$ have degree σ where $p \nmid \sigma$. Consider the $\mathbb{Z}/p$-Galois cover $\phi : Y \to \mathbb{P}^1_k$ branched only at ∞ given by the Artin-Schreier equation $y^p - y = h(x)$. The p-rank of Y is $f = 0$. The ramification filtration ends at index σ. The genus of Y equals $(\sigma - 1)(p - 1)/2$ and thus can be arbitrarily large. There are non-trivial families of such covers given by deforming $h(x)$. Similar results are true for G-Galois covers of a fixed affine k-curve as long as p divides $|G|$ but their proofs require advanced techniques when G is not an abelian p-group.

Open questions Let X be a smooth projective connected k-curve defined over an algebraically closed field k of characteristic $p > 0$. Let B be a non-empty finite set of points of X. Raynaud and Harbater made a crucial contribution to Galois theory [16] [10] by proving Abhyankar's Conjecture [1] which classifies the finite quotients of the algebraic fundamental group $\pi_1(X - B)$, i.e., the finite groups which occur as Galois groups for covers of X ramified only above B.

At this time, there is still no affine k-curve whose fundamental group is known. The structure of the fundamental group depends on towers of covers of curves and on the geometry of the curves in these towers. The goal of understanding fundamental groups provides a strong motivation to answer new questions about towers of covers of k-curves. Towards this goal, it is necessary to determine which inertia groups and ramification filtrations actually occur for wildly ramified covers of k-curves.

Given X, B, G, only in special cases is it known which inertia groups and ramification filtrations occur for G-Galois covers $\phi : Y \to X$ branched at B. One result is that, for any finite quotient G of $\pi_1(X - B)$ with p dividing $|G|$, then there exists a G-Galois cover $\phi : Y \to X$ branched only at B such that the genus of Y is arbitrarily large, [15]. An open problem, for a non-abelian p-group G, is to determine the smallest genus that can occur for a G-Galois cover of X branched only at B.

A crux case is to understand Galois covers of the affine line, and specifically those with small genus. By Abhyankar's Conjecture, there exists a G-Galois cover of the affine line if and only if G is quasi-p, which means that G is generated by p-groups. There are many quasi-p groups, including all simple groups with order divisible by p.

An example of a quasi-p group is $G = (\mathbb{Z}/\ell)^a \rtimes \mathbb{Z}/p$ where ℓ and p are distinct primes and a is the order of ℓ modulo p. As a group project, we calculated the minimal genus that can occur for a Galois cover of the affine line in characteristic p with this group G. We proved that there are only finitely many curves of this minimal genus which are Galois covers of the affine line with group G. The proof involved studying the action of an automorphism of order p on the ℓ-torsion of the Jacobian of an Artin-Schreier curve.

Project E: Class Groups of Function Fields

Participants: Lisa Berger, Jing Long Hoelscher, Yoonjin Lee, Jennifer Paulhus, Renate Scheidler

Let $C/\mathbb{F}_q$ denote a hyperelliptic curve of genus g over the finite field $\mathbb{F}_q$, q a prime power. For a prime ℓ consider the ℓ-rank of $\mathrm{Jac}(C)$. Over $\bar{\mathbb{F}}_q$ this rank is $2g$, and it is obtained over a finite extension $\mathbb{F}_{q^n}/\mathbb{F}_q$. In [4] Bauer et. al. provide an algorithm to determine an upper bound on n and give conditions for which their bound is exact. The authors then prove a theorem which determines a minimum base field extension that guarantees that the ℓ-rank of $\mathrm{Jac}(C)$ over $\mathbb{F}_{q^n}$ exceeds its ℓ-rank over $\mathbb{F}_q$. Our project focused on extending the theoretical results and improving the algorithm.

Consider the injection $\rho : Gal(\mathbb{F}_{q^n}/\mathbb{F}_q) \hookrightarrow GL_{2g}(\mathbb{Z}/\ell\mathbb{Z})$, and let π denote the Frobenius element restricted to $\mathbb{F}_{q^n}$, the generator of $Gal(\mathbb{F}_{q^n}/\mathbb{F}_q)$. For a fixed basis let A_π denote the matrix representation of $\rho(\pi)$ in $GL_{2g}(\mathbb{Z}/\ell\mathbb{Z})$. Since the homomorphism is injective, we have $\mathrm{ord}(A_\pi) = \mathrm{ord}(\pi) = n$. One would like to compute n by computing the order of A_π in $GL_{2g}(\mathbb{Z}/\ell\mathbb{Z})$, but this image is not known. Setting $t = q^{-s}$, the zeta function of a variety $X/\mathbb{F}_q$ may be expressed as the rational function

$$\zeta(X, s) = Z(X, t) = \frac{L(t)}{(1-t)(1-qt)} .$$

In [4] Bauer et. al. compute the L-polynomial $L(t)$ of $C/\mathbb{F}_q$ to determine the characteristic polynomial of the Frobenius element: $F(t) = t^{2g}L(t^{-1}) \pmod{\ell}$. Then, considering each possible elementary divisor decomposition and associated matrix, they determine an upper bound on the order of A_π, and hence on n. As a first step toward improving the algorithm we proved a linear algebra result which allows us to obtain the same bound on the order of the Frobenius element by computing the order of the companion matrix of its characteristic polynomial. This proves the first proposition below, a revision of Theorem 5.2 from [4]. We then considered the question of the minimum field extension of $\mathbb{F}_{q^n}/\mathbb{F}_q$ necessary to guarantee an increase in the ℓ-rank. In our project we modified this result, eliminating one of the assumptions in Theorem 5.6 of [4], proving the second proposition.

Proposition 1

Let $L(t)$ denote the L-polynomial of $C/\mathbb{F}_q$, set $F(t) \equiv t^{2g}L(t^{-1}) \bmod \ell$, so $F(t) \in \mathbb{F}_\ell[t]$. Let A_F denote the companion matrix of $F(t)$. Then $b = ord(A_F)$ is an upper bound on n and is equal to n if $F(t)$ is square free. Furthermore, let $F = P_1^{m_1} \cdots P_s^{m_s}$ be the factorization of F into distinct monic irreducibles in $\mathbb{F}_\ell[t]$, and let A_{P_i} denote the companion matrix of P_i, then $b = lcm_{1\le i\le s}\{\ell^{m_{0,i}} ord(A_{P_i})\}$, where $m_{0,i} = \lceil \log_\ell m_i \rceil$.

Proposition 2

Let $L(t)$ be the L-polynomial of $C/\mathbb{F}_q$, and set $F(t) \equiv t^{2g}L(t^{-1}) \bmod \ell$, $F(t) \in \mathbb{F}_\ell[t]$. Suppose $F(t)$ has an irreducible factor $P(t) \in \mathbb{F}_\ell[t]$. Let A_p be the companion matrix of P and $n = ord(A_p)$. Suppose $P^k(t)$ is the elementary divisor of π_{q,n_l} with the smallest power of $P(t)$. Then the ℓ-rank of Jac(C) over $\mathbb{F}_q^{n\ell^m}$ exceeds its ℓ-rank over any proper subfield by at least $\deg(P)$, where $m = \lceil \log_\ell k \rceil$.

Corollary

Let $F(t) = P_1^{m_1}(t) \cdots P_s^{m_s}(t)$ be the prime decomposition of the characteristic polynomial $F(t)$, and let $P_i^{m_{ij}}$ be the elementary divisors, where $1 \le i \le s, 1 \le j \le r_i, m_{i1} \le \cdots \le m_{ir_i}$ and $\sum_j m_{ij} = m_i$. Suppose $\ell^{\lceil \log_\ell m_{11} \rceil} ord(A_{P_1}) = \min_i\{\ell^{\lceil \log_\ell m_{i1} \rceil} ord(A_{P_i})\}$, denoted by γ. Then the ℓ-rank of $Jac(\mathbb{F}_{q^\gamma})$ is at least $\deg P_1$, and the ℓ-rank of $Jac(E)$ for any subfield $E \subset \mathbb{F}_{q^\gamma}$ is zero.

Project F: Hilbert Modular Surfaces

Participants: Helen Grundman, Jennifer Johnson-Leung, Kristin Lauter, Adriana Salerno, Bianca Viray, Erica Wittenborn

Explicit class field theory of imaginary quadratic fields is intimately connected with the geometry of elliptic curves with complex multiplication. One posits that the same should hold for explicit class field theory of quartic CM fields and abelian surfaces with complex multiplication. Unsurprisingly, the case of curves turns out to be much simpler than that of surfaces, and progress in this direction has been elusive. The goal of this project is to explore more deeply the relationship between certain class invariants of quartic CM fields studied by Goren and Lauter in [9] and the intersection numbers of special cycles on Hilbert modular surfaces conjectured by Brunier and Yang [5] by focusing on specific examples.

Igusa defined three Siegel modular functions which generate the space of modular functions on the Siegel upper half space of degree four. The class invariants that we are interested in were introduced by deShalit and Goren [6] and are closely related to the Igusa polynomials. Although these polynomials are non-canonical, one choice of j_1, j_2, j_3 is given as a quotient of Siegel modular forms where the denominator is a power of χ_{10}. This modular form has a specific geometric interpretation. For a CM abelian surface, A, we have that $\chi_{10}(A) = 0$ if and only if, A is a product of elliptic curves with the product polarization. Hence, $p \mid \chi_{10}(A)$ if and only if the reduction of A modulo p is a product of elliptic curves with the product polarization [9]. The class invariants introduced by deShalit and Goren also have the property that the primes in the denominator are exactly the primes dividing $\chi_{10}(A)$ where A has CM by K.

Our first example is the quartic CM field $K = \mathbb{Q}(i\sqrt{61 - 6\sqrt{61}})$ of discriminant 61. This field has several nice properties; in particular, $K/\mathbb{Q}$ is Galois and has class number 1. Van Wamelen has computed the Igusa class polynomials for all isomorphism classes of smooth genus two curves over $\mathbb{Q}$ whose Jacobians have complex multiplication [19]. For our example, 3, 5, and 41 divide $\chi_{10}(A)$, so we know from [9] that there exist embeddings with certain properties

$$\mathcal{O}_K \hookrightarrow \mathrm{M}_2(B_{p,\infty})$$

where $p = 3$, 5, and 41, and $B_{p,\infty}$ is the unique quaternion algebra ramified at p and ∞. The first aim of our project is to construct these embeddings.

The second aim of our project involves the intersection numbers of Hirzebruch-Zagier divisors on Hilbert modular surfaces. To make the connection to these intersection numbers, we first note that there is a strong relationship between Hilbert and Siegel modular forms. Indeed, the Siegel modular form χ_{10} yields a divisor on the Hilbert modular surface that is a sum of Hirzebruch-Zagier divisors, $\sum T_m$ where $m = \frac{d_F - x^2}{4}$ is a positive integer. So, taking $d_F = 61$, we see that the possibilities for m are 3, 9, 13, 15.

Brunier and Yang [5] give a conjectural formula for the arithmetic intersection numbers of the divisors T_M with the CM points associated to K on the Hilbert modular surface for any quartic CM field K. We calculate that, for $\sum T_m$ with the m as above, the conjectural intersection formula at the primes 3, 5, and 41 matches the power to which those primes divide χ_{10}, and attempt to find the corresponding embeddings.

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Chapter 38

Combinatorial Design Theory (08w5098)

Nov 09 - Nov 14, 2008

Organizer(s): Peter Dukes (University of Victoria), Esther Lamken (University of California), Richard Wilson (California Institute of Technology)

Overview

Combinatorial design theory is the study of arranging elements of a finite set into patterns (subsets, words, arrays) according to specified rules. Probably the main object under consideration is a balanced incomplete block design, or BIBD. Specifically, a (v, k, λ)-BIBD is a pair $(V, \mathcal{B})$, where V is a set of v elements and $\mathcal{B}$ is a collection of subsets, or blocks, of V such that

- every block contains exactly k points; and
- every pair of distinct elements is contained in exactly λ blocks.

Variations on this definition are commonly considered, and the term 'design' includes these similar contexts.

Design theory is a field of combinatorics with close ties to several other areas of mathematics including group theory, the theory of finite fields, the theory of finite geometries, number theory, combinatorial matrix theory, and graph theory, and with a wide range of applications in areas such as information theory, statistics, computer science, biology, and engineering. Like most areas of combinatorics, design theory has grown up with computer science and it has experienced a tremendous amount of growth in the last 30 years. The field has developed subfields and groups depending on the main techniques used: combinatorial, algebraic, and algorithmic/computational. There are also groups primarily involved with applications such as in coding theory, cryptography, and computer science. As design theory has grown, researchers have become increasingly specialized and focussed in subfields. In recent years, design theory has also become quite interdisciplinary with researchers found in both mathematics and computer science departments as well as occasionally in engineering or applied mathematics groups and in industrial groups. The primary objective of this workshop was to gather together researchers of all levels from different groups and from several different areas of design theory in one place with the goal of exchanging ideas and techniques from different areas.

In a time when the internet and electronic mail dominate our research communication, people forget how much the casual conversations and comments at workshops and conferences add to our research. The excitement generated at our BIRS workshop in November reminded us all how much we have to gain from spending time together and far away from our usual distractions and responsibilities. We were successful at gathering a diverse group of researchers from all levels and from several different areas of design theory. The talks spanned the field of design theory and included applications in computer science and information theory. One of the younger participants, a post-doctoral fellow, commented at the start of his talk that he'd never before had the opportunity to hear talks in so many different areas of design theory and he was really enjoying it. Each participant was given the opportunity to speak and present new research. For the new researchers and some of our foreign visitors, the talks served as an introduction to their research and interests. Many of the senior researchers used this opportunity to present the state of the art on a problem followed by a number of open problems. There were also two focused discussion sessions on open problems and conjectures - one on decompositions of graphs and the other on one-factorizations. The heart of this workshop was very much the open problems from the talks and the two discussion sessions. It was these problems that sparked the continued discussions into the evenings, on the hikes, and occasionally late into the night. Most people left for home excited about new work and projects.

Presentation Highlights and Open Problems

Graph decompositions

Decompositions of graphs were the focus of one of our discussion sessions as well as some of the talks. A large number of combinatorial design problems can be described in terms of decompositions of graphs (sometimes endowed with an edge-coloring) into prespecified subgraphs. In [18] in 1975, Rick Wilson proved necessary and sufficient conditions on n for the existence of a G-decomposition of K_n where G is a simple digraph on k vertices and K_n denotes the complete directed graph on n vertices. He also described applications and connections in design theory. It soon became clear that there were nice applications of a more colorful version of his theorem.

Consider finite edge-r-colored directed graphs where edge-r-colored means that each edge has a color chosen from a set of r colors. Let $K_n^{(r)}$ be the complete directed graph on n vertices with exactly r directed edges, one of each color, between any ordered pair of vertices. A family $\mathcal{F}$ of subgraphs of a graph K will be called a decomposition of K if every edge $e \in E(K)$ belongs to exactly one member of $\mathcal{F}$. Given a family $\mathcal{G}$ of edge-r-colored digraphs, a $\mathcal{G}$-decomposition of K is a decomposition $\mathcal{F}$ such that every graph $F \in \mathcal{F}$ is isomorphic to some graph $G \in \mathcal{G}$. In 2000, Esther Lamken and Rick Wilson established a very general result for the more colorful case, [12]. They proved necessary and sufficient conditions on n for $\mathcal{G}$-decompositions of $K_n^{(r)}$ where $\mathcal{G}$ is a family of simple edge-r-colored digraphs. They provided new proofs for the asymptotic existence of resolvable designs, near resolvable designs, group divisible designs, and grid designs and proved the asymptotic existence of skew Room-d-cubes and the asymptotic existence of $(v, k, 1)$-BIBDs with any group of order $k-1$ as an automorphism group. More recently, edge-r-colored decompositions and the main result from [12] have been used to establish existence results for Steiner systems that admit automorphisms with large cycles [19], designs with mutually orthogonal resolutions [10], resolvable graph designs [5], group divisible designs with block sizes in any given set K [16], and $\{k\}$-frames of type g^u [16].

The first talk in this area was by Amanda Malloch on joint work with Peter Dukes on the asymptotic existence of equireplicate G-decompositions. These are graph decompositions in which every point appears as a vertex of exactly the same number of G-blocks. Although BIBDs trivially enjoy this property, where G is regarded as the complete graph K_k, graphs G which are not regular require additional necessary conditions to admit equireplicate G-decompositions. Extending this work to a family of graphs, or to edge-colored graphs, remain interesting open problems. Several of Wilson's techniques were revisited in this talk, providing a good introduction to the first discussion session.

To start off that discussion session, Rick Wilson recalled a problem of interest to many of us: finding a proof of 'Gustavsson's Theorem'. Gustavsson's result, [9], says the following: Let H be a graph with h edges. There exists $N = N(H)$ and $\epsilon = \epsilon(H)$ such that for all $n > N$ if G is a graph on n vertices and m edges with $\delta(G) \geq n(1-\epsilon)$, $gcd(H)|gcd(G)$, and $h|m$, then G has an H-decomposition. This result appeared in a 1991 thesis from Stockholm University; it has not been published in a refereed journal and the author has long since left the academic world. Thus far, no one who has looked at the thesis has been convinced that it contains a detailed proof of this main result. Unfortunately, the result, which has nice applications, has made its way into the literature. It is important that either a detailed and complete proof be found or a flaw exposed in the thesis. As a result of our discussions, several of us discussed perhaps organizing a focused small research group to try and settle the problem. In the meantime, Peter Dukes has volunteered to put the thesis in .pdf form so that it is available to everyone. All of us hope that this added attention will lead to a solution to the problem of 'Gustavsson's Theorem'.

The talk by Rick Wilson was motivated by applications of edge-r-colored graphs where the graphs in $\mathcal{G}$ are no longer simple; one came from a problem on perfect cycle systems [15] and the second from nested balanced designs [17]. Rick Wilson described joint work with Anna Draganova and Yukiyasu Mutoh on the most general result for decompositions. They prove necessary and sufficient conditions for n for $\mathcal{G}$-decompositions of $K_n^{(r)}$ where $\mathcal{G}$ is a family of edge-r-colored digraphs. As of the end of the workshop, there were no examples of applications which required this full generality. One of the open questions was to find such applications. At the end of Rick's talk on the last day, Charlie Colbourn asked him if it was possible to determine necessary and sufficient conditions for the existence of a PBD with block sizes in a finite set K where the proportion of blocks of given sizes is specified. Rick has now been able to settle this problem by using a special case of the work in [12]. Perhaps generalizing this work will give us an application that requires the full generality of the new work by Draganova, Mutoh, and Wilson.

The above topics consider general graphs G and therefore results are limited to asymptotic existence. Some of the other talks dealt with concrete graph decompositions and their connections to design theory. Alex Rosa described the state of the art for decompositions of the complete 3-uniform hypergraph into Hamiltonian cycles. The problem of decomposing the complete k-uniform hypergraph into Hamiltonian cycles remains open. Curt Lindner discussed his favorite open problem on embedding partial odd cycle systems. Recently, Darryn Bryant and Daniel Horsley were able to settle Curt's conjecture on the best possible embedding for partial Steiner triple systems, [1]. The problem of finding the best possible embedding for partial odd cycle systems for cycle length greater than or equal to 5 is completely open. Curt discussed his work on the case for 5-cycles and pointed out it was unlikely to be close to the density bound.

Applications

There are numerous applications of combinatorial design theory. At the workshop, new applications were discussed in computer science, codes, networks, and information theory.

A (k, v)-hash function is a function from a domain of size k to a range of size v. An $(N; k, v)$-hash family is a set of N (k, v)-hash functions. A perfect hash family PHF$(N; k, v, t)$ (of strength t) is an $(N; k, v)$-hash family with the property that for every t-subset of the domain, at least one of the N functions maps the subset onto t distinct elements of the range. Hash functions have long been of interest in computer science and cryptography. In a recent development, Charlie Colbourn and Alan Ling have discovered that perfect hash families provide one of the best explicit constructions for covering arrays. Covering arrays are of interest in the design of experiments and in areas such as software/hardware testing and circuit testing. Charlie Colbourn described their work showing that forbidding certain sets of configurations in classical constructions for orthogonal arrays produces new perfect, separating, and distributing hash families. For fixed parameters, each forbidden configuration leads to solving a set of linear equations, and therefore, computational techniques can be used. Charlie listed several new results for the existence of covering arrays. A great deal of work remains to be done in this area to find good covering arrays. As we left BIRS, Charlie and Alan were discussing joint work with Aiden Bruen using some of his techniques from finite geometry and coding theory for constructing covering arrays and hash families. Aiden's talk was on connections between designs and codes and he described some new geometric ways of looking at the generator matrices of codes.

There are close connections between design theory and coding theory. For example, techniques from design theory are useful in constructing families of codes. Two of the talks mentioned connections between designs and optimal codes. Alan Ling described new work on constructing perfect-deletion-correcting codes that are optimal. He discussed constructions for q-ary 2-deletion- correcting codes of length 4 and q-ary 3-deletion-correcting codes of length 5 that are both perfect and optimal. As Alan noted, there are a number of open questions in this area for finding optimal codes.

Esther Lamken also mentioned that one of the motivations for constructing designs with orthogonal resolutions is some very new connections, due to Etzion [7], between these designs and optimal doubly constant weight codes.

Quantum information theory is presently making use of mutually unbiased bases, an application discussed in Hadi Kharaghani's presentation. A Hadamard matrix H is a matrix with entries in $\{\pm 1\}$ such that distinct rows are orthogonal. For $m \times m$ Hadamard matrices, one has $HH^\top = mI$. Two Hadamard matrices H, K of order $m = n^2$ are called unbiased if $HK^t = nL$, where L is another Hadamard matrix of order m. From a set of mutually unbiased Hadamard matrices, one can deduce the existence of mutually unbiased bases in $\mathbb{R}^m$. This application of design theory was very nicely received, with several interesting questions and discussions following the talk.

Existence of designs with various conditions

The central problem in design theory is determining the existence of designs. Determining the full spectrum for a class of designs usually requires a combination of techniques, combinatorial, algebraic/geometric, and computational. Existence problems and questions were described in several of the talks.

One of the most powerful techniques for determining the existence of combinatorial designs is the idea of PBD-closure, introduced by Rick Wilson in the early 1970's, [20]. The main idea is to break up blocks of a pairwise balanced design, using small examples of designs to create larger ones. Often, properties are inherited in the resultant design from the ingredients. PBD-closure underlies many existence results including the asymptotic results mentioned above on edge-colored graph decompositions. One of the highlights for constructions at the workshop was a novel – though possibly bizarre – application of PBD-closure by Peter Dukes [4] to the existence of adesigns. An adesign is a set system $(V, \mathcal{A})$, where V is a set of v points and $\mathcal{A}$ is a collection of blocks of size k, having the condition that all unordered pairs of points have a different frequency. Peter showed that by making use of 'padding by BIBDs' he can use PBD-closure to construct adesigns.

Difference sets afford another pervasive method for construction of combinatorial designs. In his talk, Qing Xiang included an update on some conjectures on difference sets. Let G be an additively written group of order v. A k-subset D of G is a (v, k, λ)-difference set of order $n = k - \lambda$ if every nonzero element of G has exactly λ representations as a difference $d - d'$ of distinct elements from D. In the early 1980s, Lander conjectured the following, [13]. Let G be an abelian group of order v and D a (v, k, λ)-difference set in G. If p is a prime dividing both v and $k - \lambda$, then the Sylow p-subgroup of G is not cyclic. This conjecture implies another well known conjecture due to Ryser that a cyclic (v, k, λ)-difference set can only exist if v and $k - \lambda$ are co-prime. Qing noted that Lander's conjecture is now known to be true when $k - \lambda = p^\ell$ where $p > 3$; this is due to work by Leung, Ma, and Schmidt [14]. Qing also described new work on the existence of skew Hadamard difference sets. Due to the speaker's unique expertise in this area, the talk was a very helpful survey for participants at the workshop. Much discussion was generated following the talk.

Broadly, several of the other talks fall into the category of constructive design theory.

Jeff Dinitz described joint work with Alan Ling and Adam Wolfe on N_2 resovable latin squares where they completely settled the existence of these designs. An N_2 resolvable latin square is a latin square with no 2×2 subsquares that also has an orthogonal mate. They used several different types of techniques to show that they could establish the existence of N_2 resolvable latin squares for all orders n with $n \neq 2, 4, 6, 8$.

Don Kreher also described joint work with Melissa Keranen, William Kocay, and Ben Li on problems for the existence of partial Steiner triple systems; they investigated resolvable, cyclic, and arbitrary regular Steiner triple systems. Don also relayed an interesting problem for triple systems. He asked whether it is possible to decompose the triples on 13 points not covered by a projective plane into nine Steiner triple systems. Alex Rosa extended the question to i projective planes and $11 - 2i$ Steiner triple systems, while Peter Dukes and Charlie Colbourn discussed preliminary approaches to the computation.

In 1989, Ron Graham asked if the 1-block intersection graphs of Steiner triple systems are Hamiltonian. This question has led to an investigation of the more general problem of ordering the blocks of designs to meet specified properties. Other ways of ordering the blocks of designs include Gray codes and universal cycles. Megan Dewar described her thesis work investigating the existence of Gray codes and universal cycles for twofold triple systems and cyclic BIBDs. She presented several new results and noted a number of open problems in this area. Her thesis has been submitted to the Canadian Mathematics Society for publication as a monograph. It represents the definitive survey on these problems.

Esther Lamken gave a survey on the state of the art for designs with sets of d mutually orthogonal resolutions. Techniques in this area include combinatorial recursions combined with direct constructions as well as using edge-r-colored decompositions of graphs. The majority of the known existence results are for balanced incomplete block designs. There are a large number of open questions in this area particularly for t-designs $(t \geq 3)$ and for all designs with d mutually orthogonal designs and $d \geq 3$. Her survey will include a list of open problems in this area, [11]. At the end of her talk and during the discussion sessions, Alex Rosa added several nice open problems in this area such as the generalized Room square problem. Many of these problems were investigated over 30 years ago without success. Jeff Dinitz and Esther Lamken have already started to investigate one of the problems Alex mentioned: finding a doubly resolvable analogue to Baranyai's theorem or a generalized Room square. One of the most intriguing open questions in this area came up again in the discussion session on 1-factorizations.

What is the upper bound for the size d of a largest set of mutually orthogonal resolutions? The current known upper bounds all come from very straightforward counting arguments. In many cases, there are constructions to show that these upper bounds can be met. However, in the case of 1-factorizations or orthogonal resolutions for $(v, 2, 1)$-BIBDs (also known as Room d-cubes), the simple counting upper bound gives us $d \leq v - 3$. Despite a great deal of work, no one has ever succeeded in constructing more than $\frac{v-2}{2}$ mutually orthogonal resolutions for a $(v, 2, 1)$-BIBD. The best construction in this area is due to Dinitz from 1980, [2]. In the early 1970's, Gross, Mullin, and Wallis conjectured that the bound for d for Room d-cubes of order $v - 1$ was $\frac{v-2}{2}$, [8]. However, in the 1980's Luc Teirlinck pointed out a connection between these designs and some nice structures in finite geometry. His work led him to believe that the bound should really be the counting bound of $v - 3$ for v sufficiently large. Settling these conjectures is one of the most interesting problems in this area.

The discussion session on 1-factorizations was started by Jeff Dinitz. He described new work on perfect 1-factorizations and in particular on perfect Room squares. A perfect Room square is one where both the row and column 1-factorizations are perfect; so it contains a pair of orthogonal perfect 1-factorizations. Jeff showed us the first new perfect Room square constructed in the last 20 years - a perfect Room square on 52 elements. This design was constructed by Adam Wolfe and was done with a considerable amount of computational work, [21]. He gave us a list of the known perfect Room squares and noted that the full existence problem remains open.

Existence and structural results for t-designs

Whereas classical design theory is generally concerned with arrangements of objects subject to pairwise constraints, t-designs extend this notion to t-wise constraints. A t-(v, k, λ) design is a pair $(V, \mathcal{B})$ where V is a set of v points and $\mathcal{B}$ is a family of k-subsets, called blocks, of V such that each distinct t-subset of V occurs in precisely λ blocks.

Masa Jimbo described new work on constructing cyclic Steiner quadruple systems. A Steiner quadruple system SQS(v) is a 3-$(v, 4, 1)$ design. If an SQS(v) admits a cycle of length v as an automorphism, it is said to be cyclic. He presented new recursive constructions and produced a number of new designs using computational techniques. In fact, the constructed designs enjoy the property that all units in the ring $\mathbb{Z}_v^\times$ act by multiplication as automorphisms. Along with the cyclic structure, these SQS have a very rich automorphism group.

Another existence result for t-designs was presented by Niranjan Balachandran. In his talk, and in informal discussions following, Niranjan discussed a large λ theorem for candelabra systems. These are especially useful in recursive constructions, where various holes can be filled with known small designs.

To complement the above existence results, there was also discussion of structure in t-designs. Two talks stand out along these lines.

Şule Yazıcı discussed defining sets in her talk. A set of blocks that is a subset of a unique t-(v, k, λ) design $D = (V, \mathcal{B})$ is a defining set of that designs. A defining set is minimal if it does not properly contain a defining set of D. Şule described several new algorithms and computational work on finding defining sets for t-designs.

Peter Dukes spoke on extensions of his doctoral thesis [3], where convexity is used to obtain additional structure on t-designs. Specifically, the approach considers the $\binom{v}{t} \times \binom{v}{k}$ zero-one inclusion matrix W_t of t-subsets versus k-subsets of a v-set V. The convex cone generated by columns of W_t is shown to be useful in ruling out various configurations in t-designs. Roughly speaking, this illustrates structure which does not even depend on using 'integral' weights for blocks. This is one nice example where our workshop touched upon techniques from pure mathematics.

Outcome

The workshop was very successful for a number of reasons. It goes without saying that each attendee benefited from the presence of others, perhaps working in important related areas but with limited opportunity for collaboration. Indeed, design theory is spread quite thinly across the world. It is also a fairly specialized field of research. Consequently, the workshop offered us a rare opportunity for detailed in-person collaboration.

Despite having limited numbers, the consensus from our participants is that we struck a good balance bringing together a variety of researchers from a variety of locations. Although pairs of researchers occasionally meet, a workshop of this kind is especially helpful for larger collaborations. For example, Peter Dukes, Esther Lamken and Alan Ling discussed possible approaches to the construction of resolvable group divisible designs. As indicated previously, several participants expressed interest in investigating 'Gustavsson's Theorem'. Whether motivated by applications or theory, we left the workshop feeling that this problem of decomposing of 'almost complete' graphs is one of the next major directions in design theory. We are hopeful that the workshop's varied slate of topics, methods and applications can help initiate research on this (and the other open problems we identified).

Another benefit was the inclusion of a few young researchers, including Niranjan Balachandran, Megan Dewar and Amanda Malloch. They were given a chance to present in an informal atmosphere, yet at the same time in a focused setting populated by area experts. Obviously, this rare combination can serve as an important boost in one's career development. For instance, Amanda Malloch received positive and helpful feedback on her Master's thesis work from Rick Wilson, on whose articles the thesis is based. Charlie Colbourn pointed out potential applications of the work.

A nice additional surprise was the mention of work of various other young researchers not in attendance. This included reference to the research of Robert Bailey, Mariusz Meska, and Adam Wolfe, among others. More generally, the workshop indirectly affected (or felt the effects of) the research of many who were not present.

Perhaps most importantly, we are confident that in time this workshop will continue to have important reverberations in design theory, as new collaborations are fostered and new ideas mature.

List of Participants

Balachandran, Niranjan (California Institute of Technology)
Bruen, Aiden (University of Calgary)
Colbourn, Charles (Arizona State University)
Dewar, Megan (Government of Canada)
Dinitz, Jeff (University of Vermont)
Dukes, Peter (University of Victoria)
Jimbo, Masakazu (Nagoya University)
Kharaghani, Hadi (University of Lethbridge)
Kreher, Donald (Michigan Technological University)
Lamken, Esther (University of California)
Lindner, Curt (Auburn University)
Ling, Alan (University of Vermont)
Malloch, Amanda (University of Victoria)
Mendelsohn, Eric (University of Toronto)
Rosa, Alexander (McMaster University)
Wilson, Richard (California Institute of Technology)
Xiang, Qing (University of Delaware)
Yazici, Emine (Koc University)

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Chapter 39

Black Holes: Theoretical, Mathematical and Computational aspects (08w5033)

Nov 09 - Nov 14, 2008

Organizer(s): Valeri Frolov (University of Alberta), Sang Pyo Kim (Asia Pacific Center for Theoretical Physics (APCTP)), Don Page (University of Alberta), Misao Sasaki (Kyoto University), Gordon Semenoff (University of British Columbia)

Introduction

During the workshop there were discussed several important subjects concerning physical and mathematical aspects of the black hole theory. They include the following topics

- Higher dimensional gravity and black holes
- Geometrical properties of higher dimensional isolated black holes
- Black holes in Randall-Sundrum models
- Black-hole–black-string transitions
- Mini black creation in the high energy collider experiments
- Generation of new solutions of higher dimensional Einstein-Maxwell equations
- Viscosity bound and AdS/CFT correspondence
- Primordial black hole formation after inflation
- Black holes in tidal environments
- New exact solutions of the higher dimensional gravity

This report contains a brief summary of the problems discussed at the workshop. It is focused on the recent developments reported at the talks, and the questions which attract main attention in the discussions.

Introduction: Black Holes and Extra Dimensions

Spacetime in physics is modeled by a differential manifold with a non-degenerate metric with the signature $(-,+,+,+)$ on it. The metric, describing the gravitational field, is a solution of the Einstein equations or their modifications. The metric specifies an interval between two close events. It also defines local null cones which determine the causal structure of the spacetime. A black hole is a spacetime region from where no information carrying signals can escape to infinity. Existence of a black hole indicates that the global causal structure of the spacetime manifold is non-trivial. The theory of black holes in the four dimensional case has been developed and main features of the 4D black holes are well understood now. The astrophysical observations gives very strong evidences of the existence of stellar mass and massive black holes. Rapid increase of the of accuracy of the observations poses new interesting problems concerning black holes, their interaction, and behavior of the matter in their vicinity. Several talks at the workshop discuss some of these problems.

The subject of black holes is now attracting a lot of attention also in the connection with the hypothesis of the existence of extra dimensions. The idea that the spacetime can have more than four dimensions is very old. Kaluza and Klein used this idea about 80 years ago in their attempts to unify electromagnetism with gravity. The modern superstring theory is consistent (free of conformal anomalies) only if the spacetime has a fixed number (10) of dimensions. It is assumed that extra dimensions are compactified. The natural size of compactification in the string theory is of order of the Planckian scale. In recently proposed models with large extra-dimensions it is also assumed that the spacetime has more than 3 spatial dimensions. New feature is that the size of the extra dimensions (up to 0.1mm) can be much larger than the Planckian size, 10^{-33}cm. In order to escape contradictions with observations it is usually assumed that the matter and fields (except the gravitational one) are confined to a four-dimensional brane representing our world, while the gravity can propagate in the bulk. In so called ADD models [1, 2] these extra dimensions are flat. In the Randall-Sundrum type of models [3, 4] the bulk 5D spacetime is curved and it has anti-deSitter asymptotics. Black holes in the string theory and in the models with larger extra dimensions play an important role serving as probes of extra dimension. Study of higher dimensional black holes is a very important problem of the modern theoretical and mathematical physics. Several talks and a lot of discussions during the workshop were devoted to these problems.

Geometrical properties of higher dimensional isolated black holes

An isolated stationary black hole in 4-dimensional asymptotically flat spacetime is uniquely specified by two parameters, its mass and angular momentum. The corresponding Kerr metric possesses a number of properties, which was called by Chandrasekhar ‘miraculous’. In particular the Kerr metric allows the separation of variables in the geodesic Hamilton-Jacobi equation and a massless field equations. These properties look ‘miraculous’ since the spacetime symmetries of the Kerr metric are not sufficient to explain them. It was shown by Carter [3] that these properties of the Kerr metric are directly connected with the existence of ‘hidden symmetries’ generated by the so-called Killing and Killing-Yano tensors. Separability of massless field equations (including the gravitational perturbations) in the Kerr metric plays a key role in study of properties of rotating black holes, including the proof of their stability and the calculation of Hawking radiation.

Recently higher dimensional analogues of the Kerr black holes attracted a lot of attention. The most general solution of the higher dimensional Einstein equations describing higher dimensional rotating black holes was obtained in 2006 by Chen, Lu and Pope [6]. During the past 2 years an important break-though in study of the properties of these solutions has been made(see e.g. [7] and references therein).

Namely, it was demonstrated that the most general higher dimensional black hole solution has many properties which are similar to the properties of the 4 dimensional Kerr metric. It was shown that the main role in the explanation of these properties is played by hidden symmetries. Besides the evident spacetime symmetries, connected with integrals of motion of the first order in momentum, higher-dimensional Kerr-NUT-(A)dS metrics possess also the hidden symmetries, connected with the conserved quantities of higher than first order in momentum. The main object in this study is a non-degenerate, rank 2, closed, conformal Killing-Yano tensor, which was called a principal conformal Killing-Yano (PCKY) tensor. It is possible to show that an external product of two closed conformal Killing-Yano tensors (CCKYT) is again a CCKYT, so

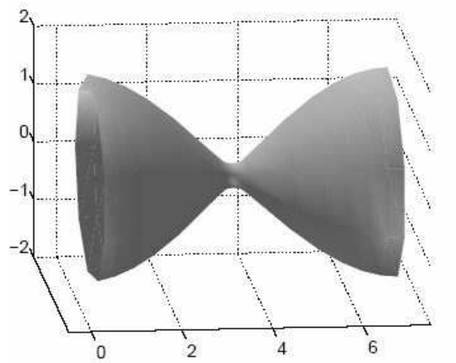

Figure 39.1: Non-uniform string (From Kol's talk at HDG, Bremen,2008)

that these objects form an algebra. Using this property it is possible to construct a tower of CCKYTs, which in its turn, generates a tower of Killing tensors. Moreover the PCKY tensor generates also a tower of the Killing vectors.

As a result, a spacetime which admits the PCKY tensor possesses the following properties: (1) Geodesics equations are completely integrable; (2) The Hamilton-Jacobi, Klein-Gordon, and Dirac equations are separable; (3) Stationary string equations are completely integrable; (4) the equations for the parallel transport of frames along geodesics in these spacetimes are integrable and can be reduced to a set of the first order ODE which allow a separation of variables. Moreover it was demonstrated that the most general solution of the Einstein equations with the cosmological constant which possesses the PCKY tensor is the Kerr-NUT-(A)dS metric. These results were presented during the workshop by scientists from the University of Alberta. Discussion of these results focused on the possibility to extend these results to the case of Einstein-Maxwell equations and a possibility of the decoupling and the variable separation in the Maxwell equations and the equations for the gravitational perturbations in the background of the spacetimes which allow the PCKY tensor. Another open problem, which was discussed during the workshop is: How the hidden symmetries become real. This question is connected with the study of the degeneracies of the PCKY tensor. Some interesting results in this direction were obtained recently.

Black holes in Randall-Sundrum models

The problem of existence of black holes in Randall-Sundrum models [3, 4] has been discussed in several publications, but it still attracts a lot of attention. The reason is that the obtained analytical results are based on some non-confirmed assumptions. In such a situation an important role is played by the numerical simulations. The problem can be formulated as a set of 2D non-linear elliptic equations with singular boundary conditions (regularity of a solution at the Anti-deSitter infinity). Namely the latter boundary condition creates a lot of problems in, both the analytical and numerical, approaches. In the talk by Hirotaka Yoshino there were given arguments, based on an accurate 4th order simulations, in favor of a conjecture of non-existence of the (large) black hole solutions in the Randall-Sundrum type II models. This talk generated a lot of discussions. Many arguments 'pro' and 'contra' of this conclusion were proposed. The discussion of the black hole problem in the Randall-Sundrum models continued during all 5 days of the workshop. This is certainly an interesting direction for the future study, which was singled out during the workshop.

Black-hole–black-string transitions

In the ADD models with large extra dimensions, the periodicity conditions are imposed on the extra dimensions. Under these conditions the black hole problem gets 'new dimensions'. Namely, besides 'standard' black holes with the spherical topology of the horizon S^{4+k} (k is the number of extra dimensions) there exist

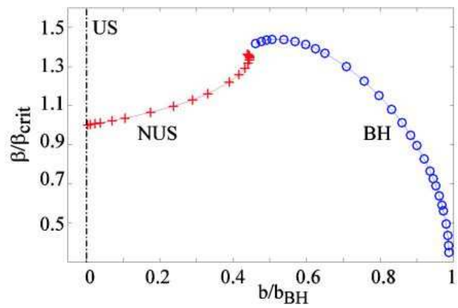

Figure 39.2: Phase diagram for a BH-BS system (From Kudo-Wiseman, 2004)

solutions of the Einstein equations, called black strings, with the topology of the horizon $S^2 \times T^k$. Thus there exist 2 different 'phases'. One can expect that when the dimensionless ratio $\alpha = r_0/L$ of the black hole size, r_0, to the size L of extra dimensions, changes there is a phase transition between black hole and black string phases. During this phase transition the Euclidean topology of the solution changes. Such transitions have been investigated for 15 years, after Gregory and LaFlamme [8] demonstrated the existence of classical instability in the solutions of the Einstein equations with compactified extra dimensions, which develops at the special critical values of the control (order) parameter α. Figure 39.2 schematically shows a non-uniform string which arises when the order parameter approaches its critical value. Figure 2 show the the tension parameter as a function of the order parameter.

During the workshop there were presented new results concerning such 'caged' black holes for the case of charged and rotation higher dimensional black holes (mainly in the talk by Kunz [9]). The discussions of this subject during workshop mainly focused on the open problem on the nature and detailed description of the BH-BS phase transitions.

Mini black creation in the high energy collider experiments

One of the main features of the popular now models with large extra dimensions is a prediction that gravity becomes strong at small distances. This conclusion implied that for the particle collision with the energy of the order of TeV the gravitational channel would be as important as the electroweak channel of the interaction. Under these conditions two qualitatively new effects are possible: (1) bulk emission of the gravitons, and (2) mini black hole production. These effects have been widely discussed in the connection with the expected new data at the Large Hadronic Collider (LHC) (see e.g. [10] and references therein).

At the workshop there was given a detailed review of the possible expected experimental consequences of the models with large extra dimensions for high energy particle collision at LHC. The talks cover the detailed description of the (higher dimensional) Hawking radiation produced by TeV scale black holes. Another problem, discussed during the workshop, is a numerical simulation of collision of two ultrarelativistic particles with a formation of a larger black hole. In these calculations the initial small black holes are used to model colliding particles. For this approach, the numerical problem becomes similar to the problem of black hole merge which has been recently under study in connection to the astrophysical applications and the LIGO project. Using similar developed tools new results were obtained for the collision of the ultrarelativistic black holes up to the gamma-factor of order of 2. In particular, the cross section of the larger black hole formation was calculated. Unfortunately, this gamma factor is much smaller than the realistic gamma factor in the collider experiments, which for the energy 7TeV is about 7,500. Discussions during the workshop were focused on the possibility to increase the value of the gamma factor, for example by combining the numerical and analytical approaches.

Generation of new solutions of higher dimensional Einstein-Maxwell equations

Solving the higher dimensional Einstein equations is a challenge because of their complexity. Nevertheless recently new physically interesting solutions were obtained by applying a method the solution generating transformations. By using the methods similar to the Belinsky-Zakharov back-scattering approach in 4D gravity, black hole solutions with the topology different from S^n were obtained (black rings, black saturns, etc.). At the workshop there was discussed a new solution generating technique in the higher dimensional gravity (Robert Mann [11]). This method allows one to obtain a charged version of the black-ring type solutions. These results looks very promising and generate a lot of discussion during the workshop.

Viscosity bound and AdS/CFT correspondence

The anti-de Sitter (AdS) – conformal field theory (CFT) correspondence has yielded striking insights into the dynamics of strongly coupled gauge fields [12]. Recently using this conjecture it was established a universal restrictions on the ratio of the viscosity and entropy density for all gauge fields in the strong coupling limit. The nature of this universality is now widely discussed. This subject was also under discussion of the workshop. Main results reported at the workshop (by Robert Myers) is the demonstration of the modifications of this inequality for a class of the 4D CFTs with the Gauss-Bonnet 5D bulk theory.

Primordial black hole formation after inflation

The subject of cosmological primordial black holes has a long history. Such black holes might be produced at the early stages of the evolution of the universe from the initial inhomogeneities of the matter. The analysis performed by Carr [13, 14] demonstrated that corresponding gravitational perturbations must be quite large, so that in the radiation dominated universe the probability of creation of PBHs is very small. During the workshop there was a discussion (generated by the talk of Misao Sasaki) of different models of behavior of the matter after the inflation in which the effect of the PBH production would be important. This subject is very important since possible observation of such primordial black holes might give an important direct information about the properties of the universe at the stage just after the inflation.

Black holes in tidal environments

Black holes interacting with surrounding objects are distorted. In particular, the black hole deformation is of interest for the problem of a black-hole–black-hole or black-hole–neutron-star coalescence. In the astrophysical set-up this distortion is small. A natural approach to describe the distortion is to use a perturbation analysis. Two problems make such an analysis complicated: non-linearity of gravity and gauge invariance reflecting the general covariance of the problem. During the workshop there was discussed a new approach to this problem developed by Eric Poisson [26] and his collaborators. A part of this discussion focused on the following problem: Is it possible to extract the information concerning the black hole distortion from the recently performed numerical calculations of the black-hole–black-hole merger.

New exact solutions of the higher dimensional gravity

There exists an interesting class of solutions of the higher dimensional vacuum Einstein equations which possesses the property that its all polynomial type invariants constructed from the Riemann tensor and its covariant derivatives vanish. In such spaces local quantum effects of the vacuum polarization vanish. This class of solutions, for example, includes physically interesting solutions, called gyratons, which describe the gravitational field created by the spinning radiation pulse. These solutions, originally obtained in the asymptotically flat spacetime, were later generalized to the spacetime with AdS asymptotics. These solutions have all the polynomial curvature invariants identical to the similar invariants in the AdS spacetime. Possible further generalizations describing the gyraton motion in a more general constant curvature spacetimes were discussed at the workshop (Andrey Zelnikov). An interesting problem is to describe the most general solutions of these type.

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Chapter 40

Symmetries of Graphs and Networks (08w5047)

Nov 23 - Nov 28, 2008

Organizer(s): Brian Alspach (University of Newcastle), Edward Dobson (Mississippi State University), Joy Morris (University of Lethbridge)

Introduction

Symmetries in graphs and networks are closely related to the fields of group theory (more specifically, permutation group theory) and graph theory. We measure symmetry using group actions, and focus our attention on vertex-transitive graphs: graphs whose automorphism group acts transitively on the set of vertices.

Although networks with high levels of symmetry do not appear often among randomly-chosen networks, they are often used in practical applications. Networks modelled on vertex-transitive graphs have been shown to be very "good" in their balance of cost (measured by the degree of each vertex in the network) against performance (how easy they are to disconnect, and the efficiency of algorithms run on them). Their symmetry often makes them relatively easy to study and understand, and has the huge advantage that "local" algorithms work globally, since the vertex-transitivity implies that all vertices hold equivalent roles within the global network. Vertex-transitive graphs also provide a beautiful context in which to study many of the general problems of graph theory; beautiful not only because of the symmetric pictures, but because of the interactions with group theory, and permutation group theory in particular. Many problems that are difficult to solve in the general context of graphs may prove tractable in this context, given our understanding of symmetry.

As the field of graph theory has emerged over the past 70 years or so (since the appearance of König's seminal book in 1936), symmetric graphs have thus become a very important area of study, and are often looked at closely by computer scientists and other network designers. Despite this, the number of mathematicians who study these graphs is quite small, and major gatherings have rarely (if ever) included symmetric graphs as a central focus. The field is growing rapidly; there were a relative trickle of papers on vertex-transitive graphs prior to 1980, but over 1500 have been published since that year, of which over 1200 have come out since 1990, and over 500 since 2000, yet there are still few "experts."

The goal of our workshop was to bring together these experts, both to share recent developments and techniques among themselves, and to provide a forum where younger, up-and-coming researchers can meet and learn from these established authorities. With just 20 invited participants, we had to be very selective in our choices of experts, younger researchers, and topics on which to focus, but the workshop was a great success. We invited 9 "overview" talks by experts, on topics within their expertise. These served to introduce the other participants to the latest results on major problems, and methods that have been or might be successful. They also included open problems that were suitable for working on during the free time included in the workshop schedule. We also included 7 talks that focussed on the particulars of recent work on more specific problems.

Although there are many regular graph theory conferences, it is rare for them to have a more specific focus. The last major events that focussed exclusively on graph symmetry were the NATO-sponsored Summer Workshop and fall conference on Symmetry in Graphs, held in Montreal in 1996. Vertex-transitive graphs have also been important components of the "Graph Theory of Brian Alspach" conference held in Vancouver in 2003, and of the Slovenian International Conferences on Graph Theory held in Bled in 2003 and in 2007, but in each case it was one of a number of important components, meaning that major researchers in the field did not attend one or both, and the schedules were too full of talks to allow for much informal interaction. The SIAM Discrete Math conferences, most recently the one in Victoria in 2006, also often include a significant selection of talks on graph symmetry, but again these are only components of very busy conferences. Many important developments have been made in the field since 1996, so there was much to be discussed at this workshop.

The Main Topics

Although there are many interesting open problems about vertex-transitive graphs, the workshop focussed on 3 broad topics:

1. automorphisms
2. Hamilton paths and cycles
3. approaches and methods

Here we provide a moderately detailed overview of the current state of each of these, as they were discussed at the workshop. Several talks during the workshop were devoted to providing more detailed background on each of these topics, to the participants.

It should be noted that due to both the limited size and the desire to focus the scope of this workshop, we made a deliberate decision to avoid some topics that have generated great interest. These include graph colourings (and the "fixing number" of graphs), graph embeddings and "maps," and infinite graph theory.

Within the class of vertex-transitive graphs, there is an important subclass: the Cayley graphs. These come up again and again in the study of vertex-transitive graphs, so we will provide a definition here. While the usual definition of a Cayley graph is constructive, beginning with a group, given the context we provide a different (equivalent) definition here. A Cayley graph, then, is a graph whose automorphism group contains a subgroup that acts not just transitively, but regularly, on the vertices of the graph. (That is, given any two vertices u and v of the graph, there is a *unique* automorphism in the subgroup that takes u to v.) If H is the regular subgroup, then we refer to the graph as a Cayley graph on the group H.

Automorphisms

Finding automorphisms

Finding the full automorphism group of a graph is a notoriously difficult problem. Even the problem of testing whether a given graph has any nontrivial automorphisms, belongs to the class NP. While it is known that almost all graphs have no nontrivial automorphisms (a result that is sometimes paraphrased as "symmetry is unusual"), it would be reasonable to suppose that restricting our attention to the class of vertex-transitive graphs might provide a great deal more information, so making this problem more tractable.

A GRR, or *graphical regular representation* of a group G is a Cayley graph Γ on G, for which the left-regular representation of G, $G_L = \mathrm{Aut}(\Gamma)$. That is, such a graph has as few automorphisms as possible, while still being vertex-transitive. Considerable work went into the study of all groups that have a GRR, and the classification was completed by Godsil in 1978 [33], and showed that with two exceptional infinite families and 13 other small exceptions, every group has a GRR. There is a conjecture (by Imrich, Lovász, Babai, and Godsil, in 1982) [8], that for any group H that does admit a GRR, almost all Cayley graphs on H are GRRs. If true, this conjecture suggests that even when there is known to be a great deal of symmetry, extra symmetry is unusual. Several results on significant families support the conjecture. Further, Dobson [21] has produced some results on significant families of groups, showing that for almost every Cayley graph Γ on such a group G, if Γ is not a GRR, then $G \lhd \mathrm{Aut}\Gamma$.

While these results do not explicitly determine automorphisms of graphs, they do suggest (roughly speaking) that the probability of a graph having a particular automorphism group decreases as the order of the group increases. We turn now to the problem of directly determining automorphism groups.

A 1901 result by Burnside [10] about permutation groups of degree p where p is prime, showed that if G is any subgroup of S_p that contains the regular representation of $\mathbb{Z}_p$, then either $G \leq \mathrm{AGL}(1,p)$, or G is doubly-transitive. Since the only connected graph on p vertices whose automorphism group is doubly-transitive is K_p (with automorphism group S_p), this result makes it fairly easy to determine the full automorphism group of any vertex-transitive graph that has a prime number of vertices. This was explicitly done by Alspach in 1973 [1]. While several generalisations of Burnside's result have been proven for permutation groups whose degree is a prime power [25, 18, 20], these results are harder to state and leave "exceptional" cases that have to be dealt with separately, if one's goal is to determine the full automorphism group of all vertex-transitive graphs on some prime power number of vertices.

Using these and other methods, the full automorphism group of the following vertex-transitive graphs have been determined (where p and q are distinct primes):

- all vertex-transitive graphs of order p [1] (see above);
- all vertex-transitive graphs of order p^2 [36, 25];
- all vertex-transitive graphs of order pq [19];
- all Cayley graphs on $\mathbb{Z}_p \times \mathbb{Z}_{p^2}$ [22];
- all Cayley graphs on $\mathbb{Z}_p^3$ (the elementary abelian group of order p^3) [23];
- all Cayley graphs on $\mathbb{Z}_n$ [38, 39, 26] (the result [47] gives a polynomial-time algorithm for determining the full automorphism group).

Some of these results are very recent, and Ted Dobson presented an overview of this topic at the workshop, mentioning methods and suggesting some open problems that could be within reach.

Semiregular Elements

A semiregular element of a permutation group, is an element all of whose cycles have the same length, in its disjoint cycle representation. The existence of a semiregular element in a permutation group is equivalent to the existence of a fixed-point-free element of prime order.

Semiregular automorphisms of vertex-transitive graphs play an important role in recursive reductions that help us understand the structure of large families of vertex-transitive graphs (see Subsubsection 40 on Normal Quotients, below). They have also been used in finding Hamilton paths and cycles (see Subsubsection 40, below), and in the enumeration of all vertex-transitive graphs on up to 26 vertices [45]. They are thus of sufficient importance to warrant special attention amongst all automorphisms of vertex-transitive graphs.

Marušič asked in 1981 [43] whether or not there is a vertex-transitive digraph that has no semiregular automorphism. To date, none has been found. Group theoretic arguments can prove that any transitive permutation group has a fixed-point-free element of prime power order, but there are transitive permutation groups that have no fixed-point-free elements of prime order (and thus, no semiregular automorphisms). Such groups are called "elusive." No known example of an elusive permutation group is "2-closed;" that is, can occur as the automorphism group of an edge-coloured (di)graph, where automorphisms must preserve the colours. In 1997, Klin [35] generalised Marušič's question, asking if every transitive finite 2-closed permutation group has a semiregular element.

Early results on this problem proved Klin's conjecture when the number of vertices is a prime power, or has the form mp where p is prime and $m < p$ [43]. Marušič's question was also answered (in the negative) in the cases of cubic vertex-transitive graphs, and vertex-transitive digraphs of order $2p^2$ [44].

By determining limitations on the classes of groups that can be elusive, recent results by Giudici [28], in some cases collaborating with Xu [31], have the following general consequences:

- every vertex-primitive graph has a semiregular automorphism;
- every vertex-quasiprimitive graph (so the automorphism group acts transitively on the vertices, and all nontrivial normal subgroups are transitive) has a semiregular automorphism;
- every vertex-transitive bipartite graph where the only system of imprimitivity is the bipartition, has a semiregular automorphism;
- all minimal normal subgroups of a counterexample to Klin's conjecture must have at least three orbits;
- every 2-arc-transitive graph has a semiregular automorphism; and
- every arc-transitive graph of prime valency has a semiregular automorphism.

Michael Giudici spoke about this problem at the workshop, explaining the methods and suggesting directions for future work. This is a very active research area, and his talk also mentioned a number of results on this problem by other researchers that have appeared in the past year, including:

- Every quartic vertex-transitive graph has a semiregular automorphism [24].
- Every vertex-transitive graph of valency $p + 1$ that admits a transitive group whose order is divisible only by 2 and p (where p is an odd prime) has a semiregular automorphism [24].
- There are no elusive 2-closed groups of square-free degree [24].
- Every arc-transitive graph with valency pq (where p and q are prime) whose automorphism group has a minimal normal subgroup with at least 3 vertex orbits, has a semiregular automorphism [56].
- If G is a transitive permutation group all of whose Sylow subgroups are cyclic, then G contains a semiregular element [37].

Recent research has also considered the possible order of a semiregular automorphism. It was shown first that all cubic vertex-transitive graphs have a semiregular automorphism of order greater than 2 [11], and more recently, that there is a function f that grows unboundedly with n, such that the automorphism group of a connected vertex-transitive cubic graph on n vertices has a semiregular subgroup of order at least $f(n)$ [40].

Isomorphic Factorisations

In the past 12 years, results have determined that there are self-complementary vertex-transitive graphs of order n if and only if each p-part of n is congruent to $1 \pmod 4$ [46], and that a self-complementary Cayley graph on the cyclic group of order n exists if and only if each prime divisor of n is congruent to $1 \pmod 4$ [27, 4]. More recently, in 2001 Li and Praeger [41] found a purely permutation group-theoretic criterion that determines whether or not a given group is a transitive subgroup of the automorphism group of some self-complementary vertex-transitive graph. This enabled them to find self-complementary vertex-transitive graphs that are not Cayley graphs, though the smallest known example has 45^2 vertices.

Li and Praeger then generalised the concept of self-complementary vertex-transitive graphs, to homogeneous factorisations of the complete graph. These are factorisations of the complete graph into isomorphic subgraphs (on the same vertex set) that admit a common vertex-transitive action. Using the theorem that every transitive permutation group has a fixed-point-free element of prime-power order, enables us to reduce any homogeneous factorisation to one that has prime index. This leads us to the study of homogeneous factorisations of prime index. Li and Praeger's permutation group-theoretic criterion that determines whether or not a given group is a transitive subgroup of the automorphism group of some vertex-transitive graph, has a direct generalisation to the prime-index case. Working with others, Li and Praeger were able to determine which types of primitive group actions on the vertices of K_n can induce a homogeneous factorisation of prime index [34].

The concept of homogeneous factorisations of complete graphs have been further generalised, to homogeneous factorisations of arbitrary vertex-transitive graphs. Interestingly, the Petersen graph never occurs as a factor in a homogeneous factorisation, but the disjoint union of 11 Petersen graphs does.

Cai Heng Li gave an overview talk on the status of all of these problems, and discussed the related problems in permutation group theory. Again, a lot of progress has been made on this topic in the past 5 years, so there was a great deal of new material to be presented.

His talk also touched on symmetrical factorisations of arc-transitive graphs: factorisations for which the restriction of the an arc-transitive subgroup of the automorphism group to each factor, acts arc-transitively on the factor. Much less is known about these.

Hamilton Paths and Cycles

Paths and Cycles

Although the problem of finding Hamilton paths and cycles in vertex-transitive graphs has been much-studied since it was first raised as a question by Lovász in 1969 [42], it remains frustratingly obdurate. There are only 4 known connected vertex-transitive graphs (on at least 3 vertices) that do not have a Hamilton cycle, and none of them are Cayley graphs. Thomassen (in 1991) [53] and Babai (in 1979) [7] have made contradicting conjectures as to whether the number of connected vertex-transitive graphs without a Hamilton cycle is finite or infinite.

The families of vertex-transitive graphs for which Hamilton cycles or paths are known to exist are still quite restricted; the most significant result is that all Cayley graphs of p-groups have Hamilton cycles; this was proven by Witte in 1986 [54]. Much of the work of finding Hamilton paths and cycles has focussed on cubic vertex-transitive graphs, for two reasons: a paucity of edges intuitively makes it harder to find paths or cycles, and the vertex-transitive graphs that do not have Hamilton cycles are all cubic. Many people have minor results on cycles in families of Cayley graphs, and Marušič has generalised many results to families of vertex-transitive graphs.

Dragan Marušič gave an overview talk about this problem, in which he suggested that given the amount of effort that has been put into solving this problem with relatively small progress, it seems that a new approach is called for. He presented two approaches that have been used recently with some success.

First he presented an approach used by Glover, Kutnar and Marušič (for example in [32]), on cubic Cayley graphs. Under this strategy, they embed the graph onto an orientable surface, and find a tree of faces in the embedding that spans all of the vertices. Then tracing the border of the tree of faces, gives a Hamilton cycle. Naturally, it is not always easy to find a tree of faces that spans all of the vertices, and sometimes a smaller tree produces a smaller path or cycle that later needs to be adjusted to produce a Hamilton path or cycle. In his talk, Marušič discussed some of the deep results that have been drawn upon to deal with such issues.

Another strategy that has been used very successfully to find Hamilton paths and cycles in vertex-transitive graphs, is to reduce the problem to a quotient graph (where an appropriate quotient exists, as for example when there is a semiregular automorphism that is not regular), find a Hamilton cycle in the quotient, and "lift" this back to the original graph, adjusting if necessary to produce a single cycle rather than a union of cycles. Although this approach has been around since at least 1948 [51], it continues to be effective. It was discussed at the workshop in the context of some individual recent results, as well as in the overview talk.

The other approach presented by Marušič has been used in recent work by himself, Du, and Kutnar, that is very close to proving that every connected vertex-transitive graph of order pq (other than the Petersen graph) has a Hamilton cycle. This uses a 1972 result by Chvátal [13] that guarantees a Hamilton cycle if a condition on the degrees of the vertices of a graph is satisfied. The strategy consists of taking a quotient of the graph with respect to a semiregular automorphism of order p, using the Chvátal theorem to find a Hamilton cycle in the quotient graph, and lifting this cycle to a Hamilton cycle in the original graph.

Hamilton Connectivity and Laceability

A graph is Hamilton-connected if there is a Hamilton path between any pair of terminal vertices. Similarly, a bipartite graph is Hamilton-laceable if there is a Hamilton path between any pair of terminal vertices in distinct parts. We say that a family of graphs is H^*-connected if the bipartite graphs in the family are Hamilton-laceable, while the other graphs are Hamilton-connected.

While these properties are interesting in their own right, proving that the cubic graphs in some family are H^*-connected and using induction to prove that all graphs in the family are H^*-connected, may actually in some cases be the easiest way of establishing the weaker result that all graphs in the family have a Hamilton path. The stronger hypothesis may make the induction step easier.

In 1980, Chen and Quimpo [12] proved that the family of connected Cayley graphs of valency at least 3 on abelian groups is H^*-connected. It was some time before further results emerged. In 2001, Alspach and Qin [5] proved that the family of connected Cayley graphs of valency at least 3 on Hamilton groups is H^*-connected. Quite recently, Alspach and Dean [3] proved that the family of connected Cayley graphs of valency at least 3 on generalised dihedral groups whose orders are a multiple of 4 is H^*-connected.

Alspach gave a talk in which he sketched the proofs of these results, each of which is inductive. Few other results about H^*-connectedness are known. In 1995, Wong [55] proved that the family of butterfly graphs is H^*-connected.

Some other recent results relate to Cayley graphs on symmetric groups:

- Every connected Cayley graph on S_n whose connection set consists of transpositions, is Hamilton-laceable [6].

- For $2 \leq k \leq n$, D_k denotes all permutations in S_n that move k successive elements and fix the other $n-k$ elements. Every Cayley graph on S_n with connection set D_k, $4 \leq k \leq n$, is Hamilton-connected [5].

Clearly, this problem remains wide open.

Approaches and Methods

Computer Use

Marston Conder gave a presentation in which he demonstrated the use of computational tools (as in GAP and Magma [9]) in his research. He pointed out the usefulness of computer-generated information in revealing patterns that can lead to new discoveries and insights.

He gave examples of the use of different algorithms to produce families of vertex-transitive graphs, and showed how clever choice of the algorithm can significantly speed up the computation, or allow us to generate much more information within a reasonable time-frame. This approach has enabled him, for example, to find all arc-transitive 3-valent graphs of small order, extending the Foster census up to 2048 vertices [15]. He also discussed how his computer-assisted determination of all orientable regular maps and hypermaps of genus 2 to 101 [14] had provided enough data that he could discern patterns never seen before, and then (in collaboration with a number of co-authors, cf. [16, 17]) use combinatorial group theory and other techniques to prove many new results about the genus spectrum of various classes of maps.

Normal Quotients

If a graph Γ is edge-transitive and connected, G is a group that acts transitively on the edges, and $\mathcal{P}$ is a partition of the vertices of Γ that is preserved under the action of G, then we can form a quotient graph $\Gamma_{\mathcal{P}}$, whose vertices are the sets in the partition, with an edge between two sets if and only if there is an edge between some pair of vertices, one of which lies in each of the two sets. Notice that the edge-transitivity and connectedness of Γ forces $\Gamma_{\mathcal{P}}$ to be connected, and G to be edge-transitive on $\Gamma_{\mathcal{P}}$. Further, no edges of Γ can lie within a block of the partition. If G is actually arc-transitive on Γ, then it will also be arc-transitive on $\Gamma_{\mathcal{P}}$. If the partition $\mathcal{P}$ is maximal, then G acts primitively on the vertices of $\Gamma_{\mathcal{P}}$.

This reduction enables us to analyse the structure of various families of edge-transitive graphs. If it happens that, for all graphs Γ in the family, all such quotients $\Gamma_{\mathcal{P}}$ remain in the family, then there is a strong relationship between typical graphs and vertex-primitive graphs in the family. We then consider the vertex-primitive graphs in the family to be the “basic” graphs in the family. Using the O’Nan-Scott Theorem that characterises the structure of primitive permutation groups, may enable us to come to some understanding of these basic graphs. Then since an arbitrary graph in the family has as a quotient some basic graph, whatever understanding we gain of the basic graphs may enable us to make deductions about the structure of all graphs in the family.

A small modification of this strategy works in the case of distance-transitive graphs [50]. If a group G acts vertex-primitively and distance-transitively on a graph Γ, then either Γ comes from a known list, or G

is of affine type or almost simple type (two of the varieties of primitive permutation groups as characterised in the O'Nan-Scott Theorem). Further (great) effort by many researchers has come close to pinning down a complete classification of the primitive distance-transitive graphs. It is also known that an arbitrary graph in the family will be either a bipartite double or an antipodal cover of a basic graph.

In the case of s-arc-transitive graphs, additional structure is required, because a quotient graph of an s-arc-transitive graph need not itself be s-arc-transitive. However, if the partition $\mathcal{P}$ comes from the orbits of a normal subgroup of an s-arc-transitive group having at least three orbits, then Praeger showed in 1985 [48] that the quotient graph will be s-arc-transitive, and the original graph will be a cover of the quotient. Such a quotient graph is called a normal quotient.

When we use normal quotients to reduce, the reduction comes to an end when there are no further normal subgroups of G whose orbits form a nontrivial partition of Γ - that is, when every nontrivial normal subgroup of G has at most two orbits. Then by definition, G is quasiprimitive if each normal subgroup is transitive, or G is biquasiprimitive if G has a normal subgroup with two orbits and all nontrivial normal subgroups have at most two orbits. In every other case, there is a normal subgroup of G with at least 3 orbits. Thus, the "basic" graphs in the family are those on which the group action on the vertices is quasiprimitive or biquasiprimitive, and arbitrary graphs are covers of the basic graphs. In 1993, Praeger [49] produced a classification of quasiprimitive permutation groups along similar lines to the O'Nan-Scott classification of primitive permutation groups. This can be used to help us further understand the "basic" graphs in a family after normal quotient reduction.

Further work by a variety of researchers has moved towards a classification of the "basic" s-arc-transitive graphs, using this strategy.

Cheryl Praeger presented an overview of the quotient and normal quotient strategies, and discussed the kinds of families of graphs on which these strategies are likely to work well (locally Q graphs for various group-theoretic symmetry properties Q, for example). She presented the example of locally s-arc-transitive graphs, which have been fairly well classified using this approach (cf. [29, 30]). At the end of her talk, she suggested that this approach might be productive in determining the structure of half-arc-transitive graphs, and asked for guidance from people who had worked with these graphs, on how the reduction could best be adapted to avoid reducing to graphs that are fully arc-transitive.

Schur Rings

Although Schur Rings have been used extensively to prove very deep results about vertex-transitive graphs, very few of the researchers who work in vertex-transitive graph theory understand them well. István Kovács gave an introductory talk about Schur rings, and how they have been and can be used to prove results about vertex-transitive graphs.

Determining the Schur rings over a particular group G provides extensive information about the possible automorphism groups of Cayley graphs of G. Schur rings have been used to determine the full automorphism groups of certain classes of graphs (see Subsection 40), and extremely effectively in determining what groups have the CI (Cayley Isomorphism)-property. The CI-property is the property that an arbitrary pair of isomorphic Cayley graphs on a fixed group G, must be isomorphic via an automorphism of G. The property can be restated as the property that any 2-closed group that contains a regular representation of G, has just one conjugacy class of regular subgroups isomorphic to G. Several of the most significant results in proving that families of groups have the CI-property, have involved classifying Schur rings over that family of groups.

Association Schemes

Association schemes are a generalisation of Schur Rings. Again, few of the researchers in vertex-transitive graph theory know much about them, although they are starting to appear more and more often in deep results. Chris Godsil gave an introductory talk about association schemes. He considered the natural special case of association schemes as sets of matrices, and focused on the massive quantity of information that is encoded in the spectrum of an association scheme. As an example to illustrate the techniques of association schemes and the information that can be obtained from them, he considered the Johnson scheme and ended with the result that no automorphism of the Petersen graph maps each vertex to a neighbor.

Open Problems

The following lists some of the open problems that were presented and discussed at the workshop.

1. Find the full automorphism group of every vertex-transitive graph whose order is a product of three (not necessarily distinct) primes.
2. Prove that for any group G that admits a GRR, almost every Cayley graph on G is a GRR.
3. Prove that almost every Cayley graph on G has $G \triangleleft \mathrm{Aut}(\Gamma)$.
4. Prove that almost every Cayley graph on G whose automorphism group is not as small as possible, has $G \triangleleft \mathrm{Aut}(\Gamma)$.
5. Determine whether or not there is any vertex-transitive graph with no semiregular automorphism.
6. Determine whether or not there is any 2-closed permutation group with no semiregular element.
7. Determine whether or not there is any arc-transitive graph with no semiregular automorphism.
8. Determine whether or not there is any distance-transitive graph with no semiregular automorphism.
9. Find new constructions of "elusive" groups.
10. For which degrees do elusive groups exist? (Answer is known up to degree 40.)
11. Does the set of all degrees of elusive groups have density 0?
12. Is every self-complementary vertex-transitive graphs on fewer than 45^2 vertices, a Cayley graph?
13. Determine fixed-point-free automorphisms of $\mathbb{Z}_p^d$ that have 2-power order.
14. Study transitive permutation groups that have an orbital-fixed-free automorphism of prime-power order.
15. Characterise vertex-transitive graphs that have a homogeneous factorisation.
16. Characterise vertex-transitive graphs that occur as a factor of a homogeneous factorisation.
17. Classify arc-transitive graphs that have an arc-symmetrical factorisation whose factors are connected and cubic.
18. Characterise arc-transitive graphs that arise as arc-symmetrical factors of a given arc-transitive graph.
19. Does every connected vertex-transitive graph have a Hamilton path?
20. Does every connected Cayley graph have a Hamilton cycle?
21. Determine whether the number of connected vertex-transitive graphs without a Hamilton cycle is finite, or infinite.
22. When is a vertex-transitive cover of a hamiltonian graph, also hamiltonian?
23. Use normal quotients to determine the structure of families of arc-transitive graphs.
24. Work out how to use normal quotients to determine the structure of families of (bipartite) vertex-intransitive, edge-transitive graphs.
25. Work out how to use normal quotients to determine the structure of families of half-arc-transitive graphs.
26. Is every direct product of two CI-groups of coprime orders, itself a CI-group?
27. Classify all p-Schur Rings over $\mathbb{Z}_p^4$.

Outcomes of the Meeting

All of the participants were vocal in their appreciation of the workshop. The organisers are aware of several new collaborations that began at the workshop and seem likely to produce exciting new results, particularly on using normal quotients to classify families of graphs. Progress on a number of other problems has also been reported to us, though it is too early for any proofs to have been polished. One young post-doc referred to this as his "best-ever" conference, and a student reported that she had made progress on a problem as a result of discussions at the workshop, so will be able to include additional results in her thesis.

The workshop brought together major teams of researchers from Australia and Slovenia, with more isolated vertex-transitive graph theorists who work in North America, China, etc. Even though a number of researchers from Israel and China were forced to decline our invitations due to work or (in one case) health considerations, we were very fortunate in the people who were able to attend the meeting. We are also pleased to be able to say that despite the theme of the workshop being a field that remains fairly male-dominated, 5 of our 20 participants were women, and another 2 women were invited but had to decline.

The organisers have created a web page of resources from the workshop, that includes the slides from all of the talks, and Magma code from Marston Conder's talk. Preprints may also be posted there as they are produced. The url of this web page is www.cs.uleth.ca/˜morris/banff-symmetries/.

A special issue of *Ars Mathematica Contemporanea* will publish papers that were presented at the workshop, or that are closely related to the themes of the workshop.

Dragan Marušič has agreed to host a conference in Slovenia in 2010, to build on the success of this workshop and to maintain the relationships that have been created.

It seems fair to say, then, that the workshop accomplished all of its major goals:

- to bring together experts in the field, who would be able to share their methods, approaches, recent results, and favourite problems and help each other make progress in their research;
- to include dynamic young researchers, who could both help the more established experts, and learn from them; and
- to provide the connections and impetus to begin a regular series of conferences focussed on vertex-transitive graph theory.

List of Participants

Alspach, Brian (University of Newcastle)
Conder, Marston (University of Auckland)
Devillers, Alice (University of Western Australia)
Dobson, Edward (Mississippi State University)
Du, Shaofei (Capital Normal University)
Giudici, Michael (University of Western Australia)
Godsil, Chris (University of Waterloo)
Kovacs, Istvan (University of Primorska)
Kutnar, Klavdija (University of Primorska)
Li, Cai Heng (University of Western Australia)
Malnic, Aleksander (University of Ljubljana)
Marusic, Dragan (University of Ljubljana and University of Primorska, Koper)
Morris, Joy (University of Lethbridge)
Morris, Dave (University of Lethbridge)
Potocnik, Primoz (University of Ljubljana)
Praeger, Cheryl (University of Western Australia)
Sparl, Primoz (University of Ljubljana)
Spiga, Pablo (University of Padova)
Thomson, Alison (University of Melbourne)
Zhou, Sanming (University of Melbourne)

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Chapter 41

Arithmetic of K3 Surfaces (08w5083)

Nov 30 - Dec 5, 2008

Organizer(s): Jean-Louis Colliot-Thél‘ene (Centre National de la Recherche Scientifique et Université Paris-Sud), Adam Logan (University of Waterloo), David McKinnon (University of Waterloo), Alexei Skorobogatov (Imperial College London), Yuri Tschinkel (Courant Institute NYU and University of Goettingen), Ronald van Luijk (Universiteit Leiden)

Overview of the Field

Understanding Diophantine equations is one of the fundamental goals of mathematics. Algebraic geometry has proved to be indispensable in the study of Diophantine problems. It is therefore no wonder that throughout history the geometric complexity of the Diophantine problems in focus has been increasing steadily. While the arithmetic of curves has been studied for a long time now, only fairly recently has there been substantial progress on that of higher-dimensional varieties. Naturally, this started with the easier varieties, such as rational and abelian varieties. K3 surfaces, where many basic problems are still wide open, are the next step in complexity.

In the last five years the rate of progress on the arithmetic of K3 surfaces has increased dramatically. However, before this workshop, not a single international meeting had been held to join the forces of the people involved. The purpose of this workshop was to combine the many lines of research in this new area. The big open problems can only be tackled by combining different strengths, both computational and theoretical. The fields of specialization of the participants include the following.

- Modularity of K3 surfaces
- Potential density of rational points
- Brauer-Manin obstructions
- Weak approximation
- Growth of the number of rational points of bounded height
- Computability of the Picard group
- Applications to curves
- Universal torsors
- K3 surfaces in positive characteristic

- Enriques surfaces

Quite a few of the participants were young researchers, both new postdocs and graduate students. For this reason, and because the participants all come from different backgrounds, the workshop started with several survey lectures on the topics mentioned above. The participants were then able to form small groups to focus on more specialized issues, which were complemented by more specialized talks as the workshop progressed.

The name "K3 surfaces" refers to the three algebraic geometers Kummer, Kähler and Kodaira, but also alludes to the mountain peak K2, which had recently been climbed for the first time when the name was given during the 1950s. By having this workshop at Banff, K3 surfaces are once again linked to the mountains.

Recent Developments and Open Problems

Our understanding of the arithmetic of K3 surfaces has expanded extremely rapidly in the past five years, and the workshop reflected the broad diversity of the advances in the field. At the workshop, there was a one hour session dedicated to describing some of the many open problems in the field. The session was extremely successful, lasting well past its appointed end and into dinnertime, and resulted in 26 open problems, many of which have related subquestions. The list of open problems was compiled by Bjorn Poonen, Anthony Várilly-Alvarado, and Bianca Viray and is reproduced below.

Unless otherwise specified, X is an algebraic K3 surface and k is a number field.

1. (McKinnon) Given X/k and $P \in X(k)$, determine if there is a non-constant map $f\colon \mathbb{P}^1_k \to X$ such that P is in the image.

   (Beauville) Same question over $\overline{k}$.

   (Colliot-Thélène) Related conjecture by Beilinson: $\mathrm{CH}_0(\overline{X})$ should be $\mathbb{Z}$.

2. Given X/k, compute the rank of $\operatorname{Pic} X$. Same question for $\operatorname{Pic} \overline{X}$.

   (Poonen) If one can determine $\operatorname{Pic} \overline{X}$, then one can determine $\operatorname{Pic} X$.

3. Given $L \in \operatorname{Pic} X$ and $m > 1$, determine if $L = mM$ for some $M \in \operatorname{Pic} X$. Given a nonzero L, determine an upper bound for $\{m : L \in m \operatorname{Pic} X\}$.

   (Baragar) Given $\Lambda \subset \operatorname{Pic} X$, decide if $\Lambda = \operatorname{Pic} X$. Determine if Λ is saturated in $\operatorname{Pic} X$. This is equivalent to determining if Λ is saturated in $H^2(X, \mathbb{Z})$.

4. (McKinnon) Given $L \in \operatorname{Pic} X$, decide if $L = [C]$ for some *integral* curve C.

5. (Poonen) Given $D \in \operatorname{Div} X$, can one compute $H^0(X, \mathcal{O}(D))$? The answer seems to be yes.

6. (Silverman) Suppose that X is defined over $\mathbb{C}$ and $\operatorname{Aut}(X)$ is infinite. Let C be an integral curve on X and $P \in X$. Suppose that $(\operatorname{Aut}(X) \cdot P) \cap C$ is infinite. Does this imply that there exists a non-trivial automorphism σ of infinite order mapping C to itself? This is an analogue of Mordell-Lang for K3 surfaces.

   (Beauville) If C is an integral curve on $X/\mathbb{C}$ and σ is an automorphism of infinite order such that $\sigma C = C$, then $g(C) \leq 1$.

7. Let σ be an automorphism of infinite order of X and let $C \subset X$ be a curve. Assume that the set of periodic points of σ contained in C is infinite. Does this imply that C is periodic, i.e. $\sigma^n C = C$ for some n?

8. (Skorobogatov) What does the Bloch-Beilinson conjecture say explicitly for a K3 over $\mathbb{Q}$? What interesting numbers should appear in special values of L-functions?

9. (Bogomolov and Tschinkel) Given $X/\overline{\mathbb{F}}_p$, is there a rational curve through every $\overline{\mathbb{F}}_p$-point? Same for $\overline{\mathbb{Q}}$? There is a positive result due to Bogomolov and Tschinkel for the first question for Kummer surfaces over $\overline{\mathbb{F}}_p$.

   (McKinnon) Over $\overline{\mathbb{Q}}$, this is equivalent to the K3 being "rationally connected" over $\overline{\mathbb{Q}}$.

10. (Skorobogatov) Find a formula for

$$\#\frac{\operatorname{Br} A}{\operatorname{Br}_1 A} = \#\operatorname{im}(\operatorname{Br} A \to \operatorname{Br} \overline{A})$$

for an abelian surface A. This is finite (proved by Skorobogatov and Zarhin). Same question for K3s. Given a fixed A (or X), the size can be made arbitrarily large by making a suitable extension of the base field.

11. (Wittenberg) Is there a K3 surface X over a number field k such that

$$\frac{\operatorname{Br} X}{\operatorname{Br} k} = 0?$$

12. (McKinnon) Find X/k with geometric Picard rank 1 and an accumulating curve over k, i.e., 100% of k-points of X lie on the curve (asymptotically, ordered by height). There are examples of K3s with accumulating curves, but all have large geometric Picard rank.

13. (Silverman) Find an example of a K3 surface with an interesting automorphism of infinite order (e.g., excluding composition of involutions).

14. (Poonen) Describe the possibilities for $\operatorname{Aut}(X/\mathbb{C})$ as an abstract group. Sterk proved that $\operatorname{Aut}(X/\mathbb{C})$ is finitely generated.

    (Kumar) Can one compute generators for $\operatorname{Aut}(X)$? Is there an upper bound on the number of generators?

    (Poonen) Can one compute the relations?

    (Bender) Can one compute the minimum number of generators?

    (Silverman) Is there an upper bound on the number of generators of the subgroup of $\operatorname{Aut}(X)$ generated by all the involutions?

15. (Poonen) Given K3 surfaces X and Y over $\overline{\mathbb{Q}}$, can one decide if $X \cong Y$?

    (McKinnon) Given K3 surfaces X and Y over $\overline{\mathbb{Q}}$, can one decide if $\operatorname{Aut} X \cong \operatorname{Aut} Y$ as abstract groups?

16. Is there a K3 surface X over a number field k such that $X(\mathbb{A}_k) \neq \emptyset$ and X satisfies weak approximation? If so, find it.

    (Colliot-Thélène) Is there a K3 surface X over a number field k such that $X(k) \neq \emptyset$ and X satisfies weak weak approximation?

17. Is there a K3 surface X over a number field k with $X(k)$ nonempty and finite? Nonempty and not Zariski dense? What about over an arbitrary infinite field? Is there a K3 surface X having only finitely many points over its own function field?

18. (Poonen) Given $X/\mathbb{F}_p$ is $X(\mathbb{F}_p(t))$ finite?

    (Beauville) Not always.

    (Poonen) Can you compute $X(\mathbb{F}_p(t))$? Is $X(\mathbb{F}_p(t))/\operatorname{Aut}(X)$ finite?

19. Find a K3 surface over a number field with geometric Picard rank 1 for which one can either prove that the rational points are potentially dense or prove that they are not potentially dense.

20. (Cantat) Suppose that $X(k)$ is Zariski dense. Must there exist a finite extension L/k and an embedding $L \subseteq \mathbb{C}$ such that $X(L)$ is analytically dense in $X(\mathbb{C})$?

    (Cantat) This is true for Abelian varieties.

21. (Cantat and Silverman) Suppose that $X(k)$ is Zariski dense and v is a place of k. Must there exist a finite extension L/k and a place w over v such that $X(L)$ is w-adically dense in $X(L_w)$? Must there exist a finite extension L/k such that $X(L)$ is w-adically dense in $X(L_w)$ for all w over v? Must there exist a finite extension L/k such that $X(L)$ is dense in $X(\mathbb{A}_L)$?

22. Is $X(k)$ always dense in $X(\mathbb{A}_k)^{\mathrm{Br}}$, i.e., is the Brauer-Manin obstruction the only one to weak approximation? To the Hasse principle?

23. (Cantat) Let X be defined over $\mathbb{C}$. Does there exist $\mathbb{C}^2 \dashrightarrow X$ meromorphic and generically of maximal rank?

24. (Colliot-Thélène and Ojanguren) Let Y be an Enriques surface and X be the associated K3 double cover. Is the map
$$\frac{\mathrm{Br}\,\overline{Y}}{\mathrm{Br}\,k} \longrightarrow \frac{\mathrm{Br}\,\overline{X}}{\mathrm{Br}\,k}$$
always injective? If not, how can one determine if it is injective in any given example?

25. (Baragar) Find a K3 surface X over a number field k such there are infinitely many orbits of k-rational curves under the action of $\mathrm{Aut}\,X$.

26. In the following all K3 surfaces S are embedded in $\mathbb{P}^2 \times \mathbb{P}^2$ such that the projections do not contract any curves and $\mathcal{A}$ is a subset of the automorphism group. We are still assuming k is a number field. We define
$$S[\mathcal{A}] = \{P \in S : \mathcal{A}(P) \text{ is finite}\}.$$

    (a) K3 Uniform Boundedness Conjecture:
    There is a constant $c = c(k)$ such that for all K3 surfaces S/k,
    $$\#S[\mathcal{A}](k) \leq c.$$

    (b) K3 Manin-Mumford Conjecture:
    Let $C \subset S$ be a curve such that $\phi(C) \neq C$ for all $C \subseteq A$. Then $C \cap S[\mathcal{A}]$ is finite.

    (c) (Weak) K3 Lehmer Conjecture:
    Fix S/k. There are constants $c = c(S/k) > 0$ and $\delta = \delta(S/k)$ so that
    $$\hat{h}(P) \geq \frac{c}{[L:k]^{\delta}} \text{for all } L/k \text{ and } P \in S(L) \setminus S[\mathcal{A}].$$

    (d) K3 Lang Height Conjecture:
    There is a constant $c = c(k)$ such that for all K3 surfaces S/k,
    $$\hat{h}(P) \geq c \cdot h(S) \quad \text{for all } P \in S(k) \setminus S[\mathcal{A}].$$
    (Here $h(S)$ is the height of S as a point in the moduli space of K3 surfaces.)

    (e) K3 Serre Image-of-Galois Conjecture:
    For any subgroup $\mathcal{B} \subseteq \mathcal{A}$, let
    $$S_{\mathcal{B}} := \left\{P \in S(\overline{k}) : \mathcal{B} \text{ is the stabilizer of } P \text{ in } \mathcal{A}\right\},$$
    and define
    $$\rho_{\mathcal{B}} \colon \mathrm{Gal}(k(S_{\mathcal{B}})/k) \to \mathrm{SymGp}(S_{\mathcal{B}}).$$
    There is a constant $c = c(S/k)$ so that for all subgroups $\mathcal{B} \subset \mathcal{A}$ of finite index,
    $$(\mathrm{SymGp}\,(S_{\mathcal{B}}) : \ \mathrm{Image}\,(\rho_{\mathcal{B}})) < c.$$

Presentation Highlights

There were 18 talks at the workshop, on a variety of topics related to the arithmetic of K3 surfaces. Some of these explored algebro-geometric techniques that have applications to arithmetic. For example, Arnaud Beauville described the Chow ring, which is a fundamental object describing algebraic cycles on an algebraic variety such as a K3 surface. Unfortunately, the Chow ring is known to be very unwieldy, and so Beauville described a finitely generated subring of the Chow ring which is most relevant for arithmetic, and used it to describe a theorem of Huybrechts. Also in this vein was the talk by Tetsuji Shioda, who demonstrated the structure of the Mordell-Weil lattice of elliptic K3 surfaces in general, and the elliptic K3 surfaces of Inose-Kuwata in particular. Jaap Top, meanwhile, gave a talk which used the framework of his joint work with Bert van Geemen to describe a variety of techniques from algebraic geometry that they successfully applied to study the arithmetic of two families of K3 surfaces with Picard rank 19.

Another way in which algebraic geometry can shed light on the arithmetic of K3 surfaces is to provide other algebraic varieties with analogous properties to K3 surfaces. Ekaterina Amerik, for example, with Claire Voisin, has constructed a Calabi-Yau fourfold of Picard number one with a Zariski dense set of rational points. One of the open problems listed at the workshop was to find a K3 surface of Picard rank one that has a Zariski dense set of rational points. Amerik's result is an answer to a four-dimensional analogue of this question.

Chad Schoen, by contrast, worked with threefolds, but changed the characteristic of the underlying field from zero to $p > 0$, in order to describe Calabi-Yau threefolds with vanishing third Betti number. Such threefolds do not exist in characteristic zero, but in arithmetic considerations they can arise as specializations of Calabi-Yau varieties over number rings, which are of mixed characteristic.

One of the major themes in the arithmetic of K3 surfaces has to do with the distribution of rational points. Many of the fundamental questions about this distribution become more tractable if the K3 surface admits a self-map of some kind, and so many of the talks dealt with this special case. Arthur Baragar's talk, for example, described methods for computing the group of automorphisms of K3 surfaces. This computation is closely linked with the question of finding generators for the nef and effective cones, and involves techniques from hyperbolic geometry and fractals, as well as the usual algebraic geometry and arithmetic.

Serge Cantat also discussed automorphisms, by describing the dynamics of automorphisms on a K3 surface, and giving an overview of what is known about the distribution of periodic points and the closure of the set of periodic points. Joe Silverman's talk pertained to similar subject matter, focussing on the distribution of heights of points in orbits, specifically with reference to K3 surfaces embedded as hypersurfaces in $\mathbb{P}^2 \times \mathbb{P}^2$ and $\mathbb{P}^1 \times \mathbb{P}^1 \times \mathbb{P}^1$.

Alessandra Sarti, by contrast, described automorphisms of prime (and therefore finite) order on K3 surfaces. Such surfaces can be described by moduli spaces, and Dr. Sarti's talk further described the fixed locus of such automorphisms, and contrasted the symplectic and non-symplectic cases.

Self-maps of K3 surfaces need not be defined everywhere, however, and Thomas Dedieu highlighted this fact in his talk, in which he described several examples of rational self-maps of K3 surfaces of degree greater than one. Connected to this are conjectures that a generic K3 surface does not admit such a map, and that the universal Severi variety is irreducible.

Another hot topic in the arithmetic of K3 surfaces is the Brauer group, and its role in the Brauer-Manin obstruction to the existence of rational points. Several of the talks made reference to the Brauer group. An overview of this area was given by Olivier Wittenberg, who described the Hasse principle and weak approximation, and how these do not necessarily apply to K3 surfaces because of the Brauer-Manin obstruction. A view of the computational side of the subject was given by Martin Bright, who gave both the theoretical background and a hands-on demonstration of how to compute the (algebraic) Brauer-Manin obstruction of a diagonal quartic surface in $\mathbb{P}^3$.

Dr. Bright's discussion of the algebraic part of the Brauer group was complemented by Evis Ieronymou's talk on the transcendental part, and the role it plays in the Brauer-Manin obstruction for diagonal quartic surfaces. In particular, Dr. Ieronymou described how to construct transcendental elements of the Brauer group, and the relation of these elements to the problem of weak approximation.

These talks were complemented by Yuri Zarhin's talk, in which he described his and Alexei Skorobogatov's finiteness results for Brauer groups. These results are derived from work relating to various conjectures of Tate and their analogues, relating to the algebraicity of Galois-invariant cohomology classes, homomorphisms of abelian varieties, and their Tate modules.

Another major theme in the arithmetic of K3 surfaces is the question of modularity. Modularity of elliptic curves played a famously important role in the proof of Fermat's Last Theorem, and is closely related to certain two-dimensional representations of the absolute Galois group $G = \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$. To find a suitable two-dimensional representation of G connected to a K3 surface, one must use the transcendental part of the lattice $\mathrm{H}^2(S, \mathbb{Z})$. In order for this to have dimension two, the Picard lattice must have the maximal dimension, 20. Thus, the discussion of the modularity of K3 surfaces begins with those of Picard rank 20, namely, the singular K3 surfaces.

Matthias Schütt explained in his talk that all singular K3 surfaces have been known to be modular for some time. His innovation, in joint work with Noam Elkies, is that every newform of weight three with rational coefficients can actually be associated to a K3 surfaces defined over $\mathbb{Q}$. Noriko Yui's talk went further, and described her joint work with Matthias Schütt and Ron Livné in which they classify complex K3 surfaces with a non-symplectic group acting trivially on algebraic cycles, show that they are all of CM type, and prove that they are all modular.

Michael Stoll's talk was on a slightly more computational bent, and showed how the arithmetic of K3 surfaces can be used to find points of extremely large height on curves of genus two. Such curves can be embedded in their Jacobians, which are two-dimensional and so their associated Kummer variety is a K3 surface. Dr. Stoll described how this Kummer surface can be used to find generators of the Jacobian of logarithmic height nearly 100.

Ronald van Luijk's talk presented an analogue of the Batyrev-Manin conjectures for K3 surfaces. The original conjectures predict the number of rational points of bounded height on rational surfaces, and do not generalize in a straightforward way to K3 surfaces. However, Dr. van Luijk's talk gave some precise conjectures about the number of points of bounded height on K3 surfaces and certain open subsets of them, and he presented considerable numerical data to support his conjectures.

Website

For preparation for the conference and for future reference, a website

`www.math.leidenuniv.nl/~rvl/K3Banff`

was set up where all speakers suggested literature related to the subject of their talks. All other participants were also invited to present their papers. The website will continue to exist.

Outcome of the Meeting

It is too early to say what the final outcome of the meeting will be, ultimately, but it is clear that the workshop was a success. Participants in the workshop had many good things to say:

It was really a nice workshop! Even the weather, quite chilly, helped us to stay inside and share more time together. I liked most talks. The nice set of open problems formulated in the problem session seems to play for a few years an important guiding role in this topic of research. It was also a rare opportunity for me, an algebraic geometer, to meet experts from friendly neiboring areas such as number theory and complex dynamics. – Jonghae Keum

It was a great conference. I learned a tremendous amount about the geometry of K3 surfaces that I hadn't known, being primarily a number theorist myself. It was an amazing group of people and I had a lot of helpful math conversations with people at meals and in the common room. And even the cold temperatures were okay (-8 Fahrenheit one morning). – Joe Silverman

I enjoyed the workshop very much. It was a good mix of mathematicians, young and senior, geometry and arithmetic, computational and theoretical. You should try to apply for another one in two years time, again at BIRS. By then the campus reconstruction will be completed. – Noriko Yui

Perhaps the best thing I can say about BIRS is that even the stunning natural beauty or the impressive resources of the musical department of the Banff Centre could not distract me from focussing on our subject and on taking the opportunity to exchange ideas with the other participants. This was my first visit to BIRS and I sincerely hope it will not the be last. – Andreas Bender

I really enjoyed to be at BIRS, it is a very good place to work, find new ideas and discuss with many experts on the field, and of course the location is also great. – Alessandra Sarti

Thank you very much for organizing such a successful conference! I certainly enjoyed the conference very much, and I am sure many others did, too. This was my first conference in Banff, and it is difficult for me to distinguish whether this particular conference was well organized, or the environmental BIRS provides is very good in general. I think both contribute. The best point of this conference, "Arithmetic of K3 surfaces" was that the theme was well focused, and most speakers gave a talk on the topics surrounding this theme, even though most speakers do research in a wider area of mathematics. It was amazing that so many experts in this area were assembled in this conference. It was also nice to see that young active mathematicians are pushing the frontier of the subject very far. The web site you set up helped very much, and will be useful in the future too. I hope one day that many of us gather once again to discuss on the progress in the subject inspired by this conference. – Masato Kuwata

I truly apreciated this conference in BIRS, and I want to thank you for this. This was the occasion for me to learn more on certain areas, with which I am not very familiar. I really benefited from meeting some of the great specialists in number theory, and the very friendly atmoshpere of this conference eased the contacts between all people present. I can say that this conference will have a positive impact on my forthcoming research. – Thomas Dedieu

During the workshop, the BIRS lounge was constantly abuzz with mathematical conversation, and the discussion was lively and productive. BIRS is a fantastic place to do and discuss mathematics, and our workshop took full advantage.

List of Participants

Amerik, Ekaterina (Université Paris-11)
Baragar, Arthur (University of Nevada Las Vegas)
Beauville, Arnaud (University of Nice)
Bender, Andreas (Korea Institute for Advanced Study)
Bright, Martin (University of Bristol)
Bruin, Nils (Simon Fraser University)
Cantat, Serge (Université de Rennes)
Colliot-Thélène, Jean-Louis (Centre National de la Recherche Scientifique et Université Paris-Sud)
Corn, Patrick (St. Mary's College of Maryland)
Dedieu, Thomas (Universität Bayreuth)
Demarche, Cyril (Université Paris-Sud)
Doran, Charles (University of Washington)
Hutz, Benjamin (Amherst College)
Ieronymou, Evis (Ecole Polytechnique Fédérale de Lausanne)
Ingram, Patrick (Waterloo)
Jain, Sonal (New York University)
Keum, Jong Hae (Korea Institute for Advanced Study)
Kisilevsky, Hershy (Concordia University)
Kloosterman, Remke (Leibniz Universitaet Hannover)
Kumar, Abhinav (Massachusetts Institute of Technology)
Kuwata, Masato (Chuo University)
Levin, Aaron (Scuola Normale Superiore di Pisa)
McKinnon, David (University of Waterloo)
Poonen, Bjorn (Massachusetts Institute of Technology)
Salgado, Cecilia (Jussieu)
Sarti, Alessandra (University of Poitiers)
Schoen, Chad (Duke University)
Schuett, Matthias (Leibniz University Hannover)
Shioda, Tetsuji (Rikkyo University)
Silverman, Joseph (Brown University)

Skorobogatov, Alexei (Imperial College London)
Stoll, Michael (Bayreuth)
Testa, Damiano (Oxford University)
Top, Jaap (University of Groningen, Department of Mathematics)
van Luijk, Ronald (Universiteit Leiden)
Varilly-Alvarado, Anthony (University of Carlifornia, Berkeley)
Viray, Bianca (University of California Berkeley)
Wittenberg, Olivier (Centre National de la Recherche Scientifique -École normale supérieure)
Woo, Jeechul (Harvard University)
Yui, Noriko (Queens University)
Zarhin, Yuri (Penn State University)

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Chapter 42

Computability, Reverse Mathematics and Combinatorics (08w5019)

Dec 07 - Dec 12, 2008

Organizer(s): Peter Cholak (University of Notre Dame), Barbara Csima (University of Waterloo), Steffen Lempp (University of Wisconsin–Madison), Manuel Lerman (University of Connecticut-Storrs), Richard Shore (Cornell University), Theodore A. Slaman (University of California at Berkeley)

Measuring the Strength of Theorems

Mathematicians all know what it means to prove a theorem from some set of axioms. In Reverse Mathematics we reverse the process and study what axioms are actually required to prove a theorem. If we can omit some of the axioms and assume instead the "theorem" and use this to prove the omitted axioms, then we know that the omitted axioms were really needed to prove the theorem. Thus Reverse Mathematics addresses the natural and philosophically important question of comparing the relative difficulty (or strength) of theorems by showing that some proofs need stronger axioms than others. Another approach to measuring relative complexity of mathematical notions is to use results from Computability Theory. Can we for example, go from an effective procedure in the finite case of a combinatorial problem to one in the countable case? If not, will a compactness argument suffice or do we perhaps need a transfinite induction?

This subject provides ways to compare the complexity of theorems by precisely calibrating the strength of each theorem along standard axiomatic (proof theoretic) and computational yardsticks. There are, moreover, intimate connections between the computational and proof-theoretic measures, and results from one approach often carry over to, or have consequences for, the other.

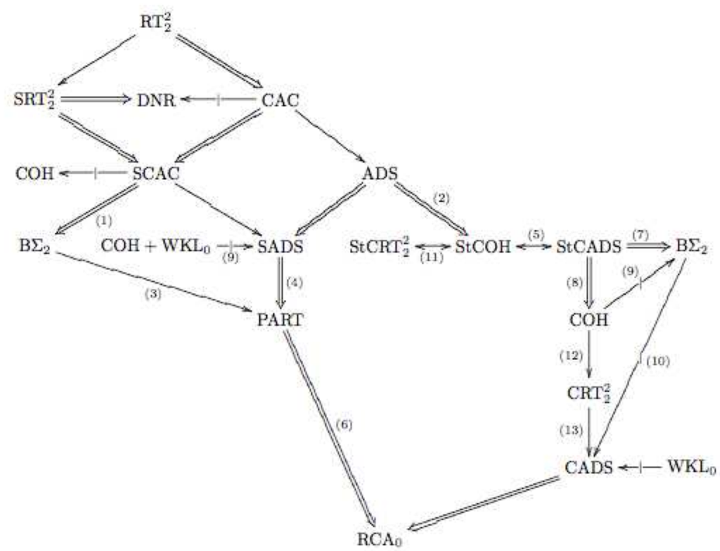
There are five standard levels on the proof-theoretic yardstick. Each represents an increasing level of set existence axioms and has a computational analog. The first (RCA_0) is a system of recursive (computable) mathematics. The existence of a proof in this system of a theorem of the form "for every A of some kind, there exists a B with some properties" implies there is a Turing machine M that, given access to information about an instance A, can compute a corresponding solution B. Generally, the converse holds as well. The second system (WKL_0) includes a weak version of König's Lemma: every infinite binary branching tree has an infinite path. It essentially adds the power of compactness arguments to the elementary effective procedures available in RCA_0. Computationally, it corresponds to the Jockusch-Soare low basis theorem that bounds the complexity of the path in terms of its halting problem. The third system (ACA_0) asserts that every set definable in (first order) arithmetic exists. It corresponds to being able to solve the halting problem (construct the Turing jump, X') relative to any set X. The last two systems (ATR_0 and Π^1_1-CA_0) are more powerful systems with second order existence axioms. The first of them corresponds to (effectively) iterating the Turing jump into the transfinite. The last adds the power to determine if a given ordering is a well ordering.

How then do we show that one of these systems or types of extra computational power is actually necessary to prove a theorem or compute a solution. Proof-theoretically, this is done by showing that (relative to some weak base theory), the theorem in question actually implies the axioms of the stronger system used to prove it. (Thus the name, reverse mathematics.) Computationally, we can show, for example, that given any set X there is an instance of the problem computable from X such that any solution computes the halting problem relative to X or decides if a linear ordering computable from X is well founded. Such investigations show, in one direction, that certain problems cannot be solved without additional (perhaps unexpected) information. In the other direction, they often provide sharper proofs with more precise computational information than had been previously known. Nonimplications between various principles can also be established by both computational and proof-theoretic methods.

The flavor of the calibrations is suggested by some examples from the realms of countable algebra and combinatorics (with their equivalent systems): in general, algebraic and combinatorial existence theorems with algorithmic solutions are in RCA_0; every n-regular bipartite graph (any $n > 0$) has a perfect matching (WKL_0); every vector space has a basis, every Abelian group has a unique divisible closure, every finitely branching infinite tree has an infinite path, Ramsey's theorem giving homogeneous sets for m-colorings of n-tuples for any $n > 2, m > 1$, various marriage/matching theorems such as Hall's (ACA_0); Hindman's theorem is at or slightly above ACA_0; Ulm's theorem on reduced Abelian p-groups, König's duality theorem (ATR_0); every tree has a largest perfect subtree, every Abelian group is the direct sum of a divisible and a reduced group (Π^1_1-CA_0).

Several theorems about or using Nash-Williams's well (or better) quasiordering theory by Kruskal, Laver, Robertson-Seymour, etc., are known to be at levels around Π^1_1-CA_0 but their precise strengths have not been determined. Other new examples at this level have recently come to light and need to be studied. In addition, many questions remain about combinatorial principles that are known to inhabit the area strictly below ACA_0 such as RT^2_2 (Ramsey's theorem for pairs and two colors), CAC (Dilworth's theorem that every infinite partial order has an infinite chain or antichain), and ADS (the Erdős-Szekeres theorem that every infinite linear order contains an infinite sequence which is strictly ascending or descending). The last two, which are easy consequences of Ramsey's theorem for pairs, are also known to be incomparable with WKL_0. Whether Ramsey's theorem for pairs implies WKL_0 is, however, an open problem.

Though the five standard levels on the proof-theoretic yardstick are linearly ordered, the situation is much more complicated in general. Here is a diagram of some combinatorial principals weaker than Ramsey's Theorem for pairs, as taken from Hirschfeldt and Shore [4]. Double arrows indicate a strict implication and single ones an implication that is not known to be strict. Negated arrows indicate known nonimplications.



Outcome of the Meeting

In Stephen Simpson's introductory talk "The Gödel Hierarchy and Reverse Mathematics", he roughly separated the Gödel Hierarchy (a linear order of foundational theories) into three levels: weak (eg. bounded arithmetic), medium (eg. 2nd order arithmetic) and strong (eg. ZFC). At this meeting, we had the rare opportunity of interacting with researchers whose combined studies represent the full realm of the Hierarchy. Through the talks and the open problem session, participants were able to share their approaches to major known problems, and also to invite others to consider questions that they had encountered through their work. In some cases questions posed at the meeting have already been answered; please see the "Scientific Progress Made" section of this report.

Presentation Highlights

Many of the talks included slides that are available at the BIRS page for the workshop, under the tab "Workshop Files".
Speaker: **Sam Buss** (Univ. of Calif., San Diego)
Title: *Polynomial Local Search higher in the Polynomial Hierarchy and Bounded Arithmetic* (slides available)
Summary: Buss presented joint work with Arnold Beckmann, discussing provably total functions of bounded arithmetic, and recent characterization of the Σ^b_i definable functions of S^{k+1}_2 (or T^k_2), for all $i \leq k$. The main tool is extensions of polynomial local search problems to higher levels of the polynomial time hierarchy, where the feasible set is defined by a Π^b_k predicate but the cost and neighborhood functions are definable by polynomial time terms. These higher level PLS problems can be used to determine the truth of Π^b_k properties and also allow "witness doubling". These results can be formalized and then Skolemized with a weak base theory such as S^1_2 — the stronger theory S^{k+1}_2 (or T^k_2) is needed only to prove the existence of a solution. The Skolemization allows us to define sets of clauses that are refutable in a depth m propositional refutation system (a Tait style system for propositional logic), but are conjectured not to be provable in a depth $m - 1/2$ system. Related open problems and future directions for research were discussed.

Speaker: **Timothy J. Carlson** (Ohio State)
Title: *Combinatorics of Words* (slides available)

Summary: Carlson discussed some results on the infinite combinatorics of words and their connection to idempotent ultrafilters.

Speaker: **Douglas Cenzer** (University of Florida)
Title: *Space Complexity of Abelian Groups* (slides available)
Summary: Cenzer presented joint work with Rodney G. Downey, Jeffrey B. Remmel, and Zia Uddin in which they develop a theory of $LOGSPACE$ structures and apply it to construct a number of examples of Abelian Groups which have $LOGSPACE$ presentations. They show that all computable torsion Abelian groups have $LOGSPACE$ presentations and we show that the groups $\mathbb{Z}$, $Z(p^\infty)$, and the additive group of the rationals have $LOGSPACE$ presentations over a standard universe such as the tally representation and the binary representation of the natural numbers. They also study the effective categoricity of such groups. For example, they give conditions are given under which two isomorphic $LOGSPACE$ structures will have a linear space isomorphism.

Speaker: **Chi Tat Chong** (National University of Singapore)
Title: Π^1_1 *conservation of the COH Principle over models of* $B\Sigma_2$ (slides available)
Summary: Chong reported on joint work with Ted Slaman and Yue Yang. Given a model M of RCA$_0$ + BΣ_2 and $R \subset M$, a set G is R-cohesive if for all s, G is either contained in R_s, modulo M-finite sets, or disjoint from R_s modulo M-finite sets, where R_s is the sth co-ordinate set of R. The principle COH states that for all R in M, there is an R-cohesive set for R in M. Chong gave a sketch of the proof that RCA$_0$ + COH + BΣ_2 is Π^1_1 conservative over RCA$_0$ + BΣ_2. He also discussed some open problems related to the existence of solutions for Δ_2 sets A (i.e. those contained in or disjoint from A) that preserve RCA$_0$ + BΣ_2. The existence of such solutions will point a way towards solving the problem of resolving the complexity of Ramsey's theorem for pairs (whether it implies Σ_2 induction) and separating it from Stable Ramsey's Theorem for pairs.

Speaker: **Valentina Harizanov** (George Washington University)
Title: *Computability and orders on structures* (slides available)
Summary: A magma is left-orderable if there is a linear ordering of its domain, which is left invariant with respect to the magma operation. If the ordering is also right invariant, then the magma is bi-orderable. For arbitrary magmas (not necessarily associative), there is a natural topology on the set of all left orders, and this space is compact. Harizanov presented results on computable orderable groups, in particular, free groups, and computability theoretic complexity of their orders.

Speaker: **Denis Hirschfeldt** (University of Chicago)
Title: *The Atomic Model Theorem and Related Model Theoretic Principles* (slides available)
Summary: Hirschfeldt reported on the complexity of several classical model theoretic theorems about prime and atomic models and omitting types. Some are provable in RCA$_0$, others are equivalent to ACA$_0$. One, that every atomic theory has an atomic model, is not provable in RCA$_0$ but is incomparable with WKL$_0$, more than Π^1_1 conservative over RCA$_0$ and strictly weaker than all the combinatorial principles of Hirschfeldt and Shore [2007] that are not Π^1_1 conservative over RCA$_0$. A priority argument with Shore blocking shows that it is also Π^1_1-conservative over BΣ_2. We also provide a theorem provable by a finite injury priority argument that is conservative over IΣ_1 but implies IΣ_2 over BΣ_2, and a type omitting theorem that is equivalent to the principle that for every X there is a set that is hyperimmune relative to X. Finally, we give a version of the atomic model theorem that is equivalent to the principle that for every X there is a set that is not recursive in X, and is thus in a sense the weakest possible natural principle not true in the ω-model consisting of the recursive sets.

Speaker: **Jeffry L. Hirst** (Appalachian State University)
Title: *Two variants of Ramsey's theorem* (slides available)
Summary: This talk explored the computability theory and reverse mathematics of some versions of Ramsey's theorem, including Ramsey's theorem on trees (TT^n_k) and the polarized Ramsey's theorem (PT^n_k). Here are statements of those theorems:

TT^n_k: Let $2^{<\mathbb{N}}$ denote the full binary tree and $[2^{<\mathbb{N}}]^n$ denote all n-tuples of comparable nodes in $2^{<\mathbb{N}}$. If $f : [2^{<\mathbb{N}}]^n \to k$, then we can find a $c < k$ and a subtree S such that S is order isomorphic to $2^{<\mathbb{N}}$, and $f(\sigma) = c$ for every n-tuple σ of comparable nodes in S.

PT^n_k: If $f : [\mathbb{N}]^n \to k$, then we can find a $c < k$ and a sequence $H_1, H_2, \ldots H_n$ of infinite sets such that $f(\{x_1, x_2, \ldots, x_n\}) = c$ for every nonrepeating n-tuple $(x_1, x_2, \ldots, x_n) \in H_1 \times \cdots \times H_n$.

Speaker: **Carl Jockusch** (UIUC)
Title: *Bounded diagonalization and Ramseyan results on edge-labeled ternary trees* (slides available)
Summary: Jockusch discussed recent joint work with Rod Downey, Noam Greenberg, and Kevin Milans. The class of weakly 1-random sets is not strongly (or Medvedev) reducible to DNR_3, the class of diagonally noncomputable functions taking values in 0,1,2. The key element of the proof is a new Ramseyan result on rooted ternary trees with certain edges having labels in 0,1. In fact a family of related results on this topic is obtained.

Speaker: **H. Jerome Keisler** (UW–Madison)
Title: *Nonstandard Arithmetic, Reverse Mathematics, and Recursive Comprehension* (slides available)
Summary: In the paper "Nonstandard Arithmetic and Reverse Mathematics" (Bull. Symb. Logic 2006), it was shown that each of the five basic theories of second order arithmetic that play a central role in reverse mathematics has a natural counterpart in the language of nonstandard arithmetic. This lecture surveyed the results in that paper, and then gave an even more natural counterpart of the weakest the basic theories, the theory RCA_0 of Recursive Comprehension.

The language L_2 of second order arithmetic has a sort for the natural numbers and a sort for sets of natural numbers, while the language ${}^*L_1$ of nonstandard arithmetic has a sort for the natural numbers and a sort for the hyperintegers. In nonstandard analysis one often uses first order properties of hyperintegers to prove second order properties of integers. An advantage of this method is that the hyperintegers have more structure than the sets of integers. The method is captured by the Standard Part Principle (STP), a statement in the combined language $L_2 \cup {}^*L_1$ which says that a set of integers exists if and only if it is coded by a hyperinteger. We say that a theory T' in $L_2 \cup {}^*L_1$ is conservative with respect to a theory T in L_2 if every sentence of L_2 provable from T' is provable from T.

For each of the basic theories $T = \mathsf{WKL}_0, \mathsf{ACA}_0, \mathsf{ATR}_0, \Pi^1_1\text{-}\mathsf{CA}_0$ in the language L_2 of second order arithmetic, the 2006 paper gave a theory U of nonstandard arithmetic in the language ${}^*L_1$ such that:

(1) $U + \mathsf{STP}$ implies T and is conservative with respect to T.

The nonstandard counterpart for RCA_0 in that paper does not have property (1), but instead has a weakened form of the STP. In this lecture we give a new nonstandard counterpart of RCA_0 which does have property (1). That is, we give a theory U of nonstandard arithmetic in ${}^*L_1$ such that $U + \mathsf{STP}$ implies and is conservative with respect to RCA_0.

Speaker: **Hal Kierstead** (Arizona State University)
Title: *Recursive and On-line Graph Coloring* (slides available)
Summary: A survey of results on recursive and on-line graph coloring. A recursive graph is a graph whose vertex and edge sets are both recursive. The basic question is whether for a class $\mathcal{C}$ of graphs there exists a function f such that every recursive k-colorable graph $G \in \mathcal{C}$ has a recursive $f(k)$-coloring. In order to prove positive results, early researchers strengthened the requirements for the effective presentation of graphs under consideration. One method was to restrict to *highly recursive* graphs. A graph is highly recursive if it is recursive, every vertex has finite degree, and its degree function is recursive. Another method was to consider digraphs, and in particular posets. Here the additional structure of the orientation of an edge provides useful information. Later, more sophisticated methods from graph theory led to positive results for the original problem.

At the same time, computer scientists began considering the problem of on-line coloring. An on-line graph coloring algorithm receives the vertices of a graph one at a time. When a vertex is received, the algorithm also learns the edges between it and the previous vertices. At this time it must irrevocably color it. There is an obvious, although not exact, correspondence between on-line and recursive coloring algorithms. However, there are many interesting results concerning on-line coloring finite graphs that have no recursive version, because the performance is measured not only in terms of chromatic number, but also in terms of the number of vertices. Moreover, there are some real world motivations for considering on-line coloring.

Speaker: **Hal Kierstead** (Arizona State University)
Title: *The Survival Game* (slides available)
Summary: The following (p, s, t)-*survival game* plays a critical role in my analysis with Konjevod of on-line Ramsey theory. The game is played by two players Presenter and Chooser. It begins with presenter choosing a positive integer n and fixing a hypergraph $H_0 = (V_0, E_0)$ with n vertices and no edges. The game now proceeds in rounds. Let $H_{i-1} = (V_{i-1}, E_{i-1})$ be the hypergraph constructed in the first $i - 1$ rounds. On the i-th round Presenter plays by presenting a p-subset $P_i \subseteq V_{i-1}$ and Chooser responds by choosing an s-subset $X_i \subseteq P_i$. The vertices in $P_i - X_i$ are discarded and the edge X_i is added to E_{i-1} to form E_i. So $V_i = V_{i-1} - (P_i - X_i)$ and $E_i = E_{i-1} \cup \{X_i\}$. Presenter wins the survival game if for some i, the hypergraph H_i contains a copy of the complete s-uniform hypergraph K_s^t on t vertices. Kierstead discuss a proof that Presenter has a winning strategy for all positive integers p, s, t with $s \leq p$. The case $s = 2$ is an entertaining puzzle, but for larger s the only known strategy uses finite model theoretic techniques and requires more than $n = A(2^s - 1, t)$ starting vertices, where A is the Ackermann function.

Speaker: **Bjørn Kjos-Hanssen** (University of Hawai‘i at M$\bar{\text{a}}$noa)
Title: *Birth-death processes, bushy trees, and a law of weak subsets* (slides available)
Summary: The proof that every set of integers that is Martin-Löf random relative to $0'$ has an infinite subset that computes no Martin-Löf random set was presented. The relation between this result and the still-open question whether Stable Ramsey's Theorem for Pairs implies Weak Weak König's Lemma was discussed.

Speaker: **Ulrich Kohlenbach** (Technische Universität Darmstadt)
Title: *Tao's correspondence principle, a finitary mean ergodic theorem and conservation results for Ramsey's theorem for pairs.* (slides available)
Summary: In the first part of the talk focussed on the proof theory of a correspondence principle implicit in recent work of T. Tao and apply this principle to study the strength of different finitary versions (one by Tao and another one – inspired by monotone functional interpretation – due to ourselves) of the infinite pigeonhole principle (joint work with J. Gaspar). In the second part we show how recent proof theoretic metatheorems can be used to provide quantitative finitizations even in the absence of compactness. As an example we give a new quantitative form of the mean ergodic theorem for uniformly convex Banach spaces (joint work with L. Leustean). In the third part we calibrate the provable recursive function(al)s of systems that may use fixed sequences of instances of Ramsey's theorem for pairs (joint work with A. Kreuzer).

Speaker: **Alberto Marcone** (Universitá di Udine, Italy)
Title: *An interaction between reverse mathematics and computable analysis* (slides available)
Summary: There is a natural correspondence between subsystems of second order arithmetic and some functions studied in computable analysis, although results cannot be translated automatically in either direction. In recent work with Guido Gherardi we use this correspondence to solve an open problem in computable analysis la Weihrauch. We introduce the computable analysis version of $\mathbf{WKL}_0$, and prove its equivalence with the computable analysis version of the Hahn-Banach theorem.

Speaker: **Antonio Montalbań** (Univerity of Chicago)
Title: *On the Strength of Fraïssé's conjecture.* (slides available)
Summary: Fraïssé's conjecture, which is now Laver's theorem, says that the class of countable linear orderings is well-quasi-ordered by the relation of embeddability. A well-quasi-ordering is a partial ordering with no infinite descending sequences and no infinite antichains. The question of what is the proof theoretic strength of Fraïssé's conjecture has been open for twenty year. Some progress has been made but the question is still open.

In Montalbán's Ph.D. thesis he proved that Fraïssé's conjecture is equivalent to many statements about embeddability of linear orderings. This shows the statement is robust in the sense that is equivalent to many theorems in a certain area of math, and equivalent to all small variations of these theorems. Only the big five systems are known to be robust.

Montalbán also talked about the plan of attack that he and Alberto Marcone have, which involves ordinal notations up to the ordinal Γ_0.

Speaker: **Jim Schmerl** (UCONN)
Title: *Grundy colorings of graphs* (slides available)
Summary: A Grundy coloring of a graph is a special kind of proper coloring. Chromatic numbers of graphs are defined in terms of proper colorings, and Grundy numbers are defined using Grundy colorings. These concepts were discussed in the context of Reverse Mathematics.

Speaker: **Stephen G. Simpson** (Pennsylvania State University)
Title: *The Gödel Hierarchy and Reverse Mathematics* (slides available)
Summary: The Gödel Hierarchy is an array of foundationally significant theories in the predicate calculus. The theories range from weak (bounded arithmetic, elementary function arithmetic) through intermediate (subsystems of second-order arithmetic), through strong (Zermelo/Fraenkel set theory, large cardinals). The theories are ordered by inclusion, interpretability, and consistency strength. Reverse Mathematics is a program which seeks to classify mathematical theorems by calibrating their places within the Gödel Hierarchy. The theorems are drawn from core mathematical areas such as analysis, algebra, functional analysis, topology, and combinatorics. Remarkably, the Reverse Mathematics classification scheme exhibits a considerable amount of regularity and structure. In particular, a large number of core mathematical theorems fall into a small number of foundationally significant equivalence classes (the so-called “big five”). There are close connections with other foundational programs and hierarchies. In particular, concepts and methods from degrees of unsolvability play an important role.

Speaker: **Reed Solomon** (UCONN)
Title: *Classically equivalent definitions of well quasi-orders*
Summary: There are several classically equivalent ways to define a well quasi-order. The equivalence of these definitions follows from Ramsey’s Theorem for Pairs and we explore the reverse mathematical strength of these equivalences. This work is joint with Alberto Marcone and Peter Cholak.

Speaker: **Frank Stephan (NUS)**
Title: *Implementing Fragments of ZFC within an r.e. Universe*
Summary: Rabin showed that there is no r.e. model of the axioms of Zermelo and Fraenkel of set theory. In the present work, it is investigated to which extent one can have natural models of a sufficiently rich fragment of set theory. These models are generated by considering the relation $x \in A_y$ to be generated from a Friedberg numbering $A_0, A_1, A_2, \ldots$ of all r.e. sets and then a member A_x of this numbering is called a set in the given model iff the downward closure of the induced ordering from x is well-founded. It is shown which axioms and basic properties of set theory can be obtained and which cannot be obtained in such a model. The major short-coming is that the axioms of comprehension and replacement do not hold in full generality, as, for example, the r.e. sets are not closed under complement and therefore differences of sets might not exist. Furthemrmore, only partial-recursive functions can be used in the axiom of replacement. The existence of transfinite ordinals depends on the model; some Friedberg models do not contain any of them while other Friedberg models contain all recursive ordinals. The axioms of pair, union and similar set constructions are satisfied, but not in a uniform way. That is, the union of two sets is a set but one cannot find the index of it effectively. For the power set axiom, one can find a Friedberg model where for every set there is a further set consisting of all the (r.e.) subsets of the first set. This is the best possible result which one can obtain and the operation is again not effective. Besides these constructions, it has been determined which sets exist in all Friedberg models. Some sets like the set V_ω of all hereditarily finite sets does not exist in any Friedberg model.

Speaker: **Henry Towsner** (UCLA)
Title: *How Constructive is Furstenberg’s Multiple Recurrence Theorem?* (slides available)
Summary: On its face, Furstenberg’s method for proving Szemeredi’s Theorem seems to be as non-constructive as possible, with multiple applications of compactness and a transfinite induction. Yet other proofs, such as those by Szemeredi and Gowers, show that these theorems can be proven by explicit combinatorial means. The use of a “partial Dialectica translation” to eliminate the transfinite aspects of the argument was discussed, as was how conventional unwinding methods suffice to eliminate the other non-constructive aspects.

Speaker: **Andreas Weiermann** (Ghent University)
Title: *Well partial orderings and their strengths in terms of maximal order type* (slides available)
Abstract: A well partial ordering (wpo) is a partial ordering which is well-founded and which does not admit infinite anti-chains. Famous examples for wpo's are provided by results of Higman, Kruskal, Friedman and Kriz. Every wpo can be extended to a well-ordering on the same domain such that the resulting order type is maximal possible and we may call this order type the maximal order type of the wpo under consideration. The reverse mathematics strengths of assertions about a wpo can typically be measured in terms of its maximal order type. It might therefore be of some interest to get a "formula" providing in natural situations the maximal order type of a wpo. In our talk we will suggest a general principle which yields appropriate maximal order types for the standard trees classes. The conjecture is that it also applies to the tree classes (equipped with an ordering fulfilling a certain gap condition) studied by Harvey Friedman. For classes of trees labeled with two labels some first results have been obtained and we believe that a general result will soon be available. Parts of the talk are based on joint work with A. Montalban, H. Friedman, and M. Rathjen.

Speaker: **Keita Yokoyama** (Tohoku University)
Title: *Non-standard analysis within second order arithmetic* (slides available)
Summary: Some systems of non-standard second order arithmetic and their interpretation to second order arithmetic were introduced. Then, he showed some Reverse Mathematics for non-standard analysis. For example, a non-standard version of the Weierstraßapproximation theorem is equivalent to ns-WKL$_0$, which is a conservative extension of WKL$_0$, and Σ^0_1-transfer principle for real numbers is equivalent to ns-ACA$_0$, which is a conservative extension of ACA$_0$. We can apply non-standard arguments in non-standard systems to standard Reverse mathematics. For example, we can show that the Riemann mapping theorem for Jordan region is provable within ns-WKL$_0$, thus, it is provable within WKL$_0$.

Open Problems

Probably the most famous open problem in the field is to determine the strength of Ramsey's Theorem for Pairs. In particular, does Ramsey's theorem for pairs imply Weak König's Lemma over RCA$_0$? There are many related open problems who's aim is to get a handle on this question.

During the meeting there was a Problem Session where many open problems were presented, far too many to include with context into this report. We are compiling these problems into a paper that we will make available to participants and also perhaps publish.

Scientific Progress Made

Stephen Simpson solved a problem that was presented by Keita Yokoyama in the problem session. Simpson showed that if (M, S) is a countable model of WWKL$_0$, then we can find $\overline{S} \supseteq S$ such that $(M, \overline{S})$ is a countable model of WKL$_0$ and every closed set of positive measure which is coded in $\overline{S}$ contains points in S. Yokoyama needed this result in order to prove that his formal system for nonstandard analysis with Loeb measures, ns-BASIC + LMP, is conservative over WWKL$_0$.

At the meeting, Denis Hirschfeldt raised the question of whether the principle PART, which arose in his work with Richard Shore, is not just implied by BΣ_2 but actually equivalent. Since the meeting, Chi Tat Chong, Steffen Lempp and Yue Yang have shown these to be equivalent, thus showing that BΣ_2 is very robust over IΣ_1 in both first-order and second-order arithmetic.

List of Participants

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Cholak, Peter (University of Notre Dame)

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Csima, Barbara (University of Waterloo)
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Greenberg, Noam (Victoria University of Wellington–New Zealand)
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Two-day Workshop Reports

Chapter 43

Ted Lewis Workshop on SNAP Math Fairs 2008 (08w2021)

Apr 18 - Apr 20, 2008

Organizer(s): Tiina Hohn (Grant MacEwan College), Ted Lewis (University of Alberta), Andy Liu (University of Alberta)

This was the sixth 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 thirty-seven participants at this year's workshop in spite of the bad weather and driving conditions on the highways were educators of all types, from teachers to grad students to expert puzzle and game designers. Our keynote speaker this year was Kate Jones.

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 learned from Ontario teachers Tanya Thompson and Troy Comish the top ten reasons why not to do math fair and their counterproofs. Kate Jones, puzzle designer in her company Kadon Enterprices, presented how simple shapes and combinations of different shapes lead to very interesting puzzles and beautiful patterns with mathematical properties. Gordon Hamilton from Calgary brought variety of games and problems. The teachers from Woods School in Calgary shared her excellent presentation how math fair is helping to reach students who are already fallen out of the reach of traditional teaching methods. Bill Ritchie from Thinkfun explained math Gamerooms in a school. Grad student from University of Alberta Trevor Pasanen shared his experiences with math fairs and how to teach difficult concepts in a puzzle environment. He also told us about the GAME organization at the University of Alberta. Dr. Jim Timourian connected the math fair concept with other benefits of student learning and then on Sunday we also touched a very hot topic for teachers, assessment. The newest project that was discussed extensively at BIRS was a video trailer about SNAP math fairs that had been produced by the Capillano College in B.C.

The concept of the SNAP math fair originated in Edmonton with Andy Liu and Mike Dumanski, and it has proved so successful that it led to the formation of a non- profit organization, the SNAP mathematics foundation, which has helped promote mathematics in schools around the world. As well as the SNAP foundation, the Calgary-based Galileo Education Network Association (GENA) helps schools organize math fairs, and provides valuable lesson-study follow-ups.

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.

List of Participants

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Comish, Troy (Simcoe County District School Board)
Creary, John (George Wood Learning Centre)
Cunningham, Valerie (Queen Elizabeth High School)
Dumanski, Micheal (SNAP Foundation)
Francis-Poscente, Krista (St. Mary's University College)
Hamilton, Gordon (Masters Academy and College)
Hamnett, Jacqueline (BC Schools (Dr A.R.Lord))
Hassenstein, Ray (Clearview Schools)
Hodgson, Jon (West Point Grey Academy)
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Hummel, Allen (DS MacKenzie School EPSB)
Jones, Kate (Kadon Enterprises, Inc.)
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McCaffrey, Allison (Father Doucet School)
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Nichols, Ryan (Edmonton Schools)
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Chapter 44

Recent Progress in Rigidity Theory (08w2137)

Jul 11 - Jul 13, 2008

Organizer(s): Robert Connelly (Cornell University), Bill Jackson (Queen Mary College, University of London), Tibor Jordan (Eotvos University, Budapest), Walter Whiteley (Department of Mathematics and Statistics York University)

Overview of the Field

Mathematicians have been interested in the rigidity of frameworks since Euler's conjecture in 1776 that 3-dimensional polyhedra are rigid. The conjecture was verified for convex polyhedra by Cauchy in 1813 and for generic polyhedra by Gluck in 1975. Connelly constructed a counterexample to Euler's original conjecture in 1982. Interest and developments in rigidity have increased rapidly since the 1970's, motivated initially by the combinatorial characterization of rigid 2-dimensional generic bar-and-joint frameworks by Laman in 1970, and also by applications in many areas of science, engineering and design. This 2-day workshop was preceded by a 5-day workshop 'Rigidity, Flexibility, and Motion: Theory, Computation and Applications to Biomolecules' which concentrated on one such application. Discussions begun at that workshop, in particular on global rigidity, played an essential role in the momentum carried into this workshop and into the progress reported below. The applications have encouraged mathematicians not only to develop theoretical results but also fast algorithms for determining whether a framework is rigid, and more generally calculating its rigid components and degrees of freedom. See [9] for definitions and a survey of results on the rigidity frameworks.

Open Problems and Recent Developments

Two fundamental open problems are to determine when a 3-dimensional generic bar-and-joint framework is either rigid or globally rigid. An important special case of the first problem, which has applications to the rigidity of molecules, is the 'Molecular Conjecture' of Tay and Whiteley [8]. This would characterize when a 3-dimensional generic bar-and-joint realization of the 'square' of a graph is rigid. A conjectured characterization of when an arbitrary 3-dimensional generic bar-and-joint framework is rigid is given in [6].

The 2-dimensional version of the second problem, i.e. characterizing when a 2-dimensional generic bar-and-joint framework is globally rigid, was solved in [5]. Gortler, Healy, and Thurston [4] recently completely the proof that the d-dimensional version of this problem is equivalent to determining the generic rank of a 'stress matrix' associated to the underlying graph. This result verifies a conjecture of Connelly and is analogous to a result of Gluck which connects the rigidity of a generic framework to the rank of the 'rigidity matrix' of its underlying graph. It implies, in particular, that the global rigidity of generic d-dimensional bar-and-joint frameworks is completely determined by the underlying graph.

Other open problems and results concern the rigidity and global rigidity of different types of frameworks, e.g. symmetric frameworks, body-and-bar frameworks, as well as angles and directions as constraints, alone or with added distance constraints. All of the above topics were addressed during the workshop.

Scientific Progress Made During the Workshop and Future Outcomes

Sitharam presented an algorithm which she conjectures could determine whether a 3-dimensional generic bar-and-joint framework is rigid. This generated much discussion, particular between Jackson, Jordán and herself, and will lead to future research collaboration.

There were many discussions on various aspects of global rigidity. Connelly and Whiteley [3] began work on using the above mentioned result of Gortler at al to show that a d-dimensional generic framework is globally rigid if and only if its $(d + 1)$-dimensional 'cone' is globally rigid, and also derive a random algorithm for determining whether a d-dimensional generic bar-and-joint framework is globally rigid. Jordán and Whiteley formulated a conjectured characterization of d-dimensional globally rigid generic body-and-bar frameworks. Follow up work of Connelly, Jordán and Whiteley has confirmed this conjecture, and has led them to a closely related conjectured characterization of global rigidity in molecular frameworks [2]. Whiteley asked whether the 'X-replacement' operation preserves global rigidity in 3-space and Jordán constructed an example to show that this is not always the case.

Jackson and Jordán [7] completed their work on showing that the '1-extension' operations preserve global rigidity in 2-dimensional generic direction-length frameworks, and began work with Connelly [1] on determining when redundant rigidity is a necessary condition for global rigidity in these frameworks. Sitheram and Whiteley each spoke about angle constraints in 2-D and 3-D. The resulting conversations of Servatius, Sitheram, Whiteley, have continued around these topics and also analogs of direction-length frameworks for the sphere.

Schulze and Whiteley began a collaborative research project with Watson, combining their independent results on the rigidity of bar-and-joint frameworks under symmetry, and dependence which is implied by flatness, which also follows from flatness.

Servatius, Shai, and Whiteley continued their investigation of Assur Graphs and extending the algorithms for decomposition of mechanisms (one-degree of freedom frameworks).

List of Participants

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Thorpe, Michael (Arizona State University)
Watson, Adam (Queen Mary, University of London)
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Chapter 45

CARP User Meeting (08w2131)

Sep 05 - Sep 07, 2008

Organizer(s): Gernot Plank (Medical University of Graz/Oxford University), Edward Vigmond (University of Calgary)

Overview of the Field

Heart disease is the number one killer in the industrialized world. Modelling cardiac electrical phenomena is attractive since it allows complete control of the system and one has full knowledge of all components in the system, unlike animal experiments. Cardiac bioelectricity is described by the bidomain equations[1] which links current flow in the extracellular space to current flow within cells through current flowing through the cell membranes:

$$\nabla \cdot (\bar{\sigma_i} + \bar{\sigma_e})\nabla\phi_e = -\nabla \cdot \bar{\sigma_i}\nabla V_m - I_e \tag{45.1}$$

$$\nabla \cdot \bar{\sigma_i}\nabla V_m = -\nabla \cdot \bar{\sigma_i}\nabla\phi_e + \beta I_m(V_m, \zeta) \tag{45.2}$$

which is a parabolic and an elliptical equation which depend on the voltage across the cell membrane, V_m, and the extracellular electric potential, ϕ_e. While the media are linear, a highly nonlinear source source term, I_m, links solutions in the two media.

Simulations of cardiac electrophysiology are becoming increasingly sophisticated and more quantitative. This has arisen as a result of faster computing hardware, better imaging and experimental methodology, and advances in scientific computation. However, simulation of a human heart at a near real time performance is still a challenge as the size of the system is currently prohibitive. Solving the bidomain equations is an inherently expensive procedure since the involved space constants are small (some tens of μm up to 1 mm) and the time scales are very fast. At the same time, domain sizes which are sufficiently large to maintain arrhythmias or to observe wavefront propagation free of boundary effects, is large, at the order of centimetres, and the observation periods are long (some hundreds of milliseconds up to minutes). The dynamics of charge transport across the membrane and between intracellular compartments is described by a set of non-linear ODEs. In general, the set of ODEs is quite stiff. This is particularly true for very recent formulations that rely on Markov state models to describe the cellular dynamics. In these models, the intrinsic time scales vary from the sub-microsecond scale for the fastest processes up to hundreds of milliseconds for the slowest processes. The fast onset of the cellular excitation process, referred to as upstroke of the action potential, leads to potential variations over fairly small spatial domains when electrical wavefronts are traversing the heart (within less than 1 mm the transmembrane voltage covers the full physiological range). That is, discretizations of the bidomain equations using anatomically realistic representations of the whole heart together with recent mechanistically realistic models of the cellular dynamics typically lead to systems of millions of degrees of freedom and hundreds of thousands of time steps. Therefore, even when simulations are executed using the most powerful HPC hardware available today, execution times impede fine-grained explorations of the parameter space of interest.

Finally, the heart is an electrically activated mechanical pump. While electrical pathologies have been recognized as lethal and been the subject of much research, the role of electromechanical coupling and mechano-electric feedback has been receiving less attention. For many clinically relevant scenarios, both aspects, electrical activation as well as mechanical contraction, have to be accounted for in computer modelling studies to contribute additional information. Recent therapeutical strategies aim at improving cardiac output in patients suffering from an impaired synchronization of the ventricles by implanting devices which pace the heart to improve synchrony between the two main pumping chambers, the ventricles. This therapeutical approach is referred to as Cardiac Resynchronization Therapy (CRT). Although quite successful with quantifiable survival benefits for patients, the therapy is expensive and the percentage of non-responders is too high. Computer simulations will be helpful to investigate the mechanisms which determine whether CRT improves cardiac output or not. Such simulations can be used to sweep the parameter spaces (electrode locations, timing and delay for delivery of pacing pulses, etc) to determine optimal configurations.

Our software, CARP, is among the fastest and most versatile for simulating cardiac electrophysiology. With a growing user base of about 50 spread throughout several universities including Johns Hopkins and Oxford, a reexamination of the code was necessary, in order to keep at the forefront in terms of computational efficiency as well as flexibility with particular focus on multiphysics simulations.

Recent Developments and Open Problems

Current trends in cardiac modelling are aiming at developing simulation environments that enable researchers to perform “in-silico” experiments. It is expected that the increased level of anatomical and functional detail will contribute to further increase the predictive value of computer simulations which will make simulators an indispensable complementary clinical modality over the next few years. A further important trend is to add mechanical movement to electrical heart models. This is a significant advancement and opens new and exciting perspectives for basic research and clinical applications. Finally, in many recent studies not only the physics of the heart is modelled, but also the experimental techniques employed to observe bioelectrical phenomena to better understand how the physical quantities behave and how they appear to behave when being measured with a particular modality. Such approaches have demonstrated that experimentally measured signals suffer from substantial distortions and are related to the actual physical quantity in a non-trivial manner. Such “secondary” simulations include the simulation of the processes underlying the signal acquisition in mapping techniques such as optical mapping, electrical mapping, the computation of magnetocardiograms, etc.

Great challenges are offered by these current trends that cardiac modelling is becoming *multiphysics*, incorporating electrical and mechanical activity and, at a later stage, also fluid-structure interaction, as well as *multiscale*, where subcellular processes are modeled which seem to have an impact at the tissue and organ level. Besides the constant scientific challenge to improve, develop and validate the quantitative descriptions of cardiac phenomena upon which current simulators are built, dealing with the computational burden and the complex software engineering involved in the development of “in-silico” simulators is probably the most difficult obstacle to overcome on the quest to establish cardiac modeling in new application areas where modeling is not an option today. A major open problem is to increase computational efficiency and speed. Although many problems of practical interest can be tackled today using the fastest HPC facilities available, execution times remain to be a limiting factor that impede quick parameter sweeps. To be of relevance in a clinical context, an increase in computational efficiency of 3-4 orders or magnitude is required. Parallel and scalable implementations that take advantage of upcoming PetaFLOPS computing hardware are sought after to achieve these speedups. Optimizing codes for novel hardware is likely to take cardiac modelling a major step forward, nonetheless, numerical techniques including spatiotemporal adaptivity, linear solver and preconditioning techniques, custom-tailored cache optimized ODE solver techniques for extremely stiff sets of ODEs which are required to better describe the cellular physiology may contribute to further reduce the computational burden and/or increase the efficiency of “in-silico” simulators. A major concern is the scalability of numerical methods. Although it can be expected that the available computational power will increase substantially over the next few years, it is unclear to which degree current simulators will benefit.

For instance, with the CARP simulator the entire numerical scheme shows excellent scaling up to 128 processors for problem sizes of 1e6 degrees of freedom or more. Using more processors is inefficient, since scaling efficiency saturates and, when more processors are added a critical number of processors, N_{crit}, will be eventually hit where execution time starts to increase. However, for many applications execution times are too slow even when using $_{crit}$ processors. Using the anatomically most realistic model of the rabbit ventricles available today [6] with 4.3 million degrees of freedom, solving the monodomain equations with 128 processors is about 4000 times slower than real time. This is a hard limit that cannot be overcome with current computing hardware and currently implemented numerical techniques. When considering human heart, the critical number of processors N_{crit} will be much larger, but the same scalability issue will eventually kick in when the problem sizes per partition are becoming sufficiently small leading to a less favourable ratio between local computational load and communication. No matter how powerful PetaFLOPS computers are, current simulators will not benefit and it appears that near real-time performance is not within reach without a shift in paradigm.

Currently, reliable predictions on which hardware and computing paradigms will prevail, are difficult to make. Regarding classical CPUs, further increases in clock frequency cannot be expected, but rather an increase in the number of available cores. A major bottleneck with multicore processors using the CPU is the limited memory bandwidth which prevents data from being transferred sufficiently quickly from memory to the CPU. Accelerator cards, although unlikely to be suited for all relevant aspects of cardiac modeling, bear significant promise to overcome some of these limitations. To our understanding, the most promising technologies include: i) general purpose graphical processing units (GP-GPU), promoted mainly by NVidia and, to a lesser extent, by AMD, ii) cell processors, promoted by IBM, and iii) the Larrabee processor, promoted by Intel.

Porting an “in-silico” simulator as complex as CARP to a novel non-standardized computing platform entails major coding efforts. Although efforts are under way to develop high-level interfaces, designed to hide differences between different accelerator technologies, it can be expected that the technology will not be in place soon enough, or at least not a the level of maturity required to support software development endeavours as complex as “in-silico” multiphysics simulators. Hence, not all new paradigms can be supported and decisions have to be made which platforms to support. Performance charts over the last few years clearly indicate that GPUs increase their performance at a faster rate than CPUs. The software development kit CUDA, provided by NVidia to develop software for their GPUs, is at a reasonably mature stage and facilitates a fairly smooth migration pathway to run entire software packages such as CARP, or at least specific aspects of it, on a GPU. Based on these observations we decided to invest major efforts into developing GPU based codes to replace or complement specific aspects of CARP. While remarkable speedups with GPU based implementations have been achieved for some classes of problems at a fraction of the cost of a supercomputer, they have yet to be applied to solution of the bidomain problems.

Producing a tractable heart simulator will only result from the collaboration of experts at every level, from computer hardware, to computer scientists, to mathematicians, software engineers, experts in mesh generation, physiologists, and clinicians. To succeed in the quest of developing an efficient, flexible general purpose simulator that can be employed to execute “virtual experiments” without any or very little trade-offs in terms of accounting for anatomical or functional details of the heart, a major shift in the academic approach to software engineering is required. Unlike in the past, where fairly simple simulators were developed in a single laboratory within the course of a single PhD thesis that were quite often custom-tailored for a single specific problem, endeavours such as the development of the CARP simulator require a distributed network based approach to reflect the multifaceted challenges where several groups make longterm commitments to further advance the code to ensure the long-term sustainability of the code development process and to steer the development effort into directions that support those applications that are of particular interest to the research community. The development of the CARP simulator started in 2002. The development process has been set up as a distributed effort.

This workshop invited specialists from all disciplines relevant to the development and application of “in-silico” modeling tools with a focus on application to building a virtual human heart. It was a first step towards building a larger community that Further, despite major advancements, reflected in an increase in the number of users by an order of magnitude over the last 3 years, Not all aspects of “in-silico” modelling can be addressed easily within an academic environment and may be in an non-academic setting. Interestingly, in the field of mechanics, most research groups rely on commercial modeling tools which seem to be well suited. This may be a viable option in the field of cardiac modeling as well as soon as commercial modeling packages become available. Industrial partners were invited to discuss and explore future directions.

Presentation Highlights

The workshop was organized to cover three main topics which were *Geometric Modelling*, *Numerical Techniques and Novel Computing Paradigms for Large-scale Bidomain Simulations* and *Modelling Applications within an Experimental and Clinical Context*.

Geometric Modelling

Numerical Techniques and Novel Computing Paradigms for Large-scale Bidomain Simulations

To address the challenge of reducing execution times two major themes were discussed. First, what are the bottlenecks in current codes and which algorithms are suited to overcome current limitations. Secondly, since it is unlikely that major increases in computational efficiency can be achieved by novel numerical techniques alone, particular attention has to be paid to explore in which way novel computing paradigms can be exploited, which gains in efficiency can be expected and how well these paradigms are suited for cardiac modeling applications.

Both themes cannot be seen in isolation. One of the major themes presented was that algorithms need to be developed which are parallel from the beginning and not as an afterthought. Computers are not getting faster, but we are getting many more cores. Novel numerical approaches that are not well suited to execute efficiently on upcoming computing platforms, are of limited interest. Highly sophisticated spatio-temporal modeling approaches, although of great interest from a numerical point of view, are a candidate to fall into this category and, consequently, were not considered at the workshop.

The computationally most expensive portion of a numerical scheme to solve the bidomain equations is the solution of the elliptic PDE. The fastest known solver for this problem relies on using a multilevel preconditioner for the conjugate gradient (CG) iterative solver. Our group demonstrate the efficiency of this technique for both a geometric variant [4] as well as an algebraic (AMG) variant [3] which is better suited for "in-silico" modeling where complex grids are considered. Dr. Gundolf Haase presented a novel AMG implementation which was implemented by his group as part of their Parallel Toolbox (PT) solver library. Relative to the Boomer-AMG method used in previous studies, the PT implementation is more lightweight and the multilevel strategy is simpler. First benchmarks suggest that the PT implementation, although requiring about twice the number of iterations over Boomer AMG to converge, results in a three-fold increase in terms of execution time. A further advantage of the PT implementation of AMG is the option to compile for execution on a GPU. Dr. Liebmann presented impressive performance results for the AMG-PT solver running on a GPU. He presented results measured on a Quad GPU server costing $4000 to perform 2.5 times faster than 32 traditional CPUs in a cluster interconnected by a low-latency Infiniband network costing $200.000. The other major contributor to the overall workload is the solution of the system of ODEs. The numerical technique implemented in CARP, essentially, a non-standard finite difference technique based on the work of Rush and Larsen[], seems to be sufficiently simple and thus very well suited for being executed efficiently on a CPU. Dr. Leon presented first results measured with a GPU implementation of a very recent rabbit ventricular ionic model [5]. The reported speedups on the GPU were equally impressive. Preliminary results suggest that GPUs are very well suited for solving the two computationally most burdensome components of bidomain simulations, the solution of the elliptic PDE and the set of ODEs.

Dr. Kickenger summarized his meshing mesh method. Using an Octree approach and a dual mesh, he is able to rapidly mesh segmented medical images into computationally usable grids. His software is among the best available commercially, in terms of the size of the meshes he can generate, the time in which he can do it, and the accurate surface representations.

Modelling Applications within an Experimental and Clinical Context

Dr. Albert Kim gave an overview of clinical approaches for the treatment of arrhythmias. He outlined the shortcomings of current approaches and advocated the use of computer simulations to explore more targeted and less destructive therapies.

Dr. Trayanova showcased work performed in her lab which is cutting edge in terms of application to clinical issues. One member of her lab, Dr. Gurev, presented his work on electromechanics. He showed his simulations, which are a first, involving defibrillation and a mechanically contracting heart, based on electrical propagation with mechanoelectric feedback. His work further emphasized the need for including mechanical activity, since it is ultimately a major clinical measurand as well as has a profound influence on cardiac electrical activity through feedback of stretch-sensitive channels.

Scientific Progress Made

For the first time, many people working on specific aspects of the cardiac electrophysiology simulator were able to see how their contribution fit into the whole scheme.

Outcomes of the Meeting

Several potential collaborations also became apparent. Dr. DiMartino work had concentrated on mechanical aspects only. She will now work with Drs. Vigmond and Comtois to integrate electrical activity with mechanical.

Representatives from the medical device companies were impressed with the level of sophistication that cardiac modelling had reached. There was interest in pursuing licensing of the CARP software so that it could be used for device design.

Drs. Vigmond and Plank were able to have discussions with researchers involved at all levels of the software. Several aspects became apparent after the meeting:

- the software needs to remain flexible and not be tied into any one computing paradigm or numerical technique
- ease of use is paramount as the software becomes more wide spread, with more automatic setting of parameters needed
- in the immediate future, GPU computation will be very attractive. As such, we will need to rethink algorithms to be parallel from the beginning, and match algorithms to the hardware.
- geometrical models will continue to become more detailed as imaging improves, necessitating greater heterogeneity that our software must be able to capture

List of Participants

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Chapter 46

Second Graduate Research Summit of the International Graduate Training Centre (IGTC) in Mathematical Biology (08w2141)

Sep 19 - Sep 21, 2008

Organizer(s): Alejandro Adem (PIMS), Gustavo Carrero (Athabasca University / University of Alberta), Leah Keshet (University of British Columbia), Mark Lewis (University of Alberta), Pauline van den Driessche (University of Victoria)

The International Graduate Training Centre (IGTC) in Mathematical Biology is an initiative sponsored and funded by the Pacific Institute for the Mathematical Sciences (PIMS). Its focus is the training of graduate students of PIMS associated universities in the field of Mathematical Biology.

The IGTC Annual Research Summit Theme: Communicating Mathematical Biology

The 2-days workshop served as one of the fundamental training elements of the IGTC programme, namely the Annual Graduate Research Summit. The main theme of the Summit was Communicating Mathematical Biology. Given the fact that Mathematical Biology is an interdisciplinary field, scientists in it face real challenges at the time of communicating research ideas and scientific findings to audiences whose specific research areas are solely in Mathematics or in Biology.

A mathematical biologist should be able to bridge these two scientific areas and make his/her research accessible to both mathematicians and biologists. The theme of the Summit aimed at training IGTC students to face successfully this particular communication challenge.

The Professional Development Seminars and Talks

The workshop had three professional development talks/seminars focusing on the oral and written aspects of communication in mathematical biology.

Inspired by the book ”Scientists must speak: bringing presentations to life” [1], Dr. Gerda de Vries (University of Alberta) gave a presentation on how to structure a good mathematical biology talk entitled ”Mathematicians Must Speak: The DOs and DON’Ts of Giving Effective Mathematical Presentations”. The talk not only gave a very positive tone to the rest of the workshop, but it also provided a fundamental analogy between a regular narrative ”story” and a mathematical biology ”story” that was practically followed by the rest of the speakers in the workshop. The story-like way of presenting a research topic to an audience is not conventional among mathematicians, but the participants seemed to agree that is an effective way of communicating mathematical biology.

The nature of the second professional development seminar given by Dr. Betty Moulton from the Department of Drama, University of Alberta was a unique experience for the audience. Everyone, including the graduate students and the Faculty participated in actual physical and vocal exercises that showed the importance of coordinating body and voice with the research messages needed to be conveyed.

A common experience among science graduate students is the difficulty they face when the time of writing their first paper comes. Questions such as how should the paper be structured? how long should it be? which title is appropriate? which Journal should I submit the paper to? Which order should be followed in a multiple author paper? are examples of questions that all IGTC students faced, are facing or will face. Dr. Eric Cytrynbaum from University of British Columbia presented a series of ideas [2] answering these relevant questions.

The real outcome of these series of professional seminars will be seen in the quality of future presentation given and papers written by the IGTC students. Also, having experienced IGTC faculty members interested in guiding graduate students in communicating mathematical biology effectively will have a positive effect on the image of Mathematical Biology in the scientific world.

The Mathematical Biology Presentations

IGTC graduate students were exposed to current mathematical biology research topics, ranging from research at the cellular level to research at the ecological level.

In particular, current models for influenza developed by Pauline van den Driessche (University of Victoria) and colleagues were introduced. The importance of calculating the basic reproduction number R_0, defined as the number of secondary infections caused by introducing one infective into a susceptible population, was stressed.

At the macro level, models concerning the spatio-temporal dynamics of predator-prey models were presented by Dr. Rebecca Tyson (University of British Columbia-Okanagan) and Dr. Jeremy Fox (University of Calgary). At the micro level, models in cellular biology were presented by Dr. Adriana Dawes (University of Alberta) leaving in evidence the incredibly wide range of research possibilities within the field of Mathematical Biology.

Also, there was a talk on data and statistical analysis for dynamical systems. This talk, presented by Dr. Dave Campbell (Simon Fraser University) was crucial for showing students how the link between real data and mathematical models can be carried out. This last talk gave a flavor of a course that Dr. Campbell will offer in the Summer. The interest in the topic had such an impact that it made the IGTC Steering Committee to consider this course as a Mathematical Biology course to be advertised and partially funded by the IGTC. This is a important outcome of having a valued visitor presenting a relevant topic during the IGTC Summit.

The wide range of talks was intended to satisfy the various research interests from IGTC students. Of course, productive discussions were generated after each presentation.

Students challenged the speakers by asking questions related to the real application of the models and more specific ones related to the mathematical techniques used.

The Poster Session

During the workshop the both the IGTC and invited students had the chance to present their current research in a poster format. There was a poster competition and the best two posters were awarded. The poster evaluation criterium was based on written communication skills, an oral presentation of the research, and mathematical biology content.

The first poster awarded was by Sandra Merchant, an IGTC student working under the supervision of Dr. Wayne Nagata. Her research is on wavetrains, periodic traveling waves exhibited by natural populations. She proposes that a possible mechanism for the generation of these patterns is predator invasion and her work has been submitted for publication. The second poster awarded was by Diana White (University of Alberta), who presented her previous work with Dr. Gerda de Vries on the effect that gender and ethnicity can have on body composition when there are changes in diet.

The poster judges felt that the quality of all poster were so high that they decided to give the third place in the competition to all the other posters.

The poster session allowed IGTC students not only to share their research knowledge and excitement but to experience the inspiring theme of the Summit: Communicating Mathematical Biology.

List of Participants

Ashander, Jaime (University of Alberta)
Brydges, David (University of British Columbia)
Campbell, David (Simon Fraser University)
Carrero, Gustavo (Athabasca University / University of Alberta)
Cooper, Jane (University of Alberta)
Cytrynbaum, Eric (University of British Columbia)
Dawes, Adriana (University of Alberta)
Dawson, Andria (University of Alberta)
de Vries, Gerda (University of Alberta)
Dushek, Omer (University of British Columbia)
Fox, Jeremy (University of Calgary)
Gong, Jiafen (University of Alberta)
Jacobsen, Jon (University of Alberta)
Lewis, Mark (University of Alberta)
Lindquist, Jennifer (University of Victoria)
Lukeman, Ryan (University of British Columbia)
Ma, Junling (University of Victoria)
Marleau, Justin (University of Alberta)
Martin, Jonathan (University of Alberta)
Mckenzie, Hannah (University of Alberta)
Merchant, Sandra (University of British Columbia)
Morrison, Jennifer (University of British Columbia)
Prosk, Erin (University of British Columbia)
Rajakaruna, Harshana (University of Alberta)
Rajani, Vishaal (University of Alberta)
Strohm, Shaun (University of British Columbia-Okanagan)
Tyson, Rebecca (University of British Columbia, Okanagan)
van den Driessche, Pauline (University of Victoria)
Wheeler, Jeanette (University of Alberta)
White, Diana (University of Alberta)
Wilson, Ben (University of British Columbia-Okanagan)
Wittmann, Meike (University of Alberta)
Wong, Rita (University of Alberta)

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Chapter 47

Singular Phenomena in Nonlinear Optics, Hydrodynamics and Plasmas (08w2133)

Oct 24 - Oct 26, 2008

Organizer(s): (Alejandro Aceves (Southern Methodist University), Pavel Lushnikov (University of New Mexico), Vladimir Zakharov (University of Arizona)

Overview of the Field

Nonlinear wave phenomena arising in the areas of optics, hydrodynamics and plasmas have led to fundamental discoveries in applied mathematics. This is mainly due to the universality of the governing equations such as the nonlinear Schrödinger equation (NLS),

$$i\psi_t + \triangle\psi + |\psi|^2\psi = 0,$$

which describes nonlinear interaction of waves. It is a common trend that solutions of the governing nonlinear equations result in the formation of singularities. This has been observed for example in the filamentation of laser beams in nonlinear media, wave breaking in hydrodynamics, collapse and Langmuir waves in plasmas. Analytical and numerical models continue to evolve to allow deeper understanding of these phenomena at fine spatial and temporal scales. The workshop brought some of the leading scientists in these fields combining theoretical, numerical and experimental studies.

Recent Developments

This field experiences rapid developments in analytical, numerical and experimental directions. It includes new results from the more theoretical side such as standing ring solutions to a super critical NLS, recent discovery of ground state selection and energy equipartition in NLS and Gross Pitaevskii Equation, lattice solitons, orbital instabilities, and the band-gap interface, as well as new bounds on Kolmogorov spectra for the Navier - Stokes equations. These results are complemented with growing achievements in numerical simulations of strongly nonlinear phenomena, examples include the modeling of freakons which is a new type of soliton, simulation of quasisolitonic turbulence in the Majda-McLaughlin-Tabak equation, modelling of weak electron-phase space holes, regularized point vortex simulations of vortex sheet roll-up. Another important development is the necessity of combining theoretical and numerical results to achieve better understanding of experiments. Experimental studies are now becoming much more elaborative; this allows to distinguish relative contributions from different types of strongly nonlinear processes. Examples are the use of femtosecond bullets for laser inscription of photonic structures, study of mixing transitions and oscillations in low-Reynolds number viscoelastic fluids.

Presentation Highlights

We had many excellent presentations at the workshop. Here we highlight some representative presentations:

Walter Craig found new bounds on Kolmogorov spectra for the Navier - Stokes equations. An argument involving scale invariance and dimensional analysis given by Kolmogorov in 1941, and subsequently refined by Obukov, predicts that in three dimensions, solutions of the Navier - Stokes equations at large Reynolds number and exhibiting fully developed turbulent behavior should obey *energy spectrum*

$$E(\kappa, t) \sim C\kappa^{-5/3},$$

at least in an average sense. A global estimate on weak solutions in the norm $|\mathcal{F}\partial_x u(\cdot, t)|_\infty$ was found which gives bounds on a solution's ability to satisfy the Kolmogorov law. The result gives rigorous upper and lower bounds on the inertial range, and in the unforced case an upper bound on the time of validity of the spectral regime.

Philippe Guyenne presented numerical simulations of 3D overturning water waves over bottom topography. The numerical model solves the fully nonlinear potential flow equations using a 3D high-order boundary element method combined with an explicit time integration scheme, expressed in a mixed Eulerian-Lagrangian formulation. Results on wave profiles and kinematics were presented as well as comparisons with 2D results as well as with theoretical predictions.

Mark Hoefer considered a dispersive regularization of degenerate rarefact ion wave Interactions. In an Eulerian fluid, shock waves do not propagate into a region of zero density. Instead, degenerate rarefaction or expansion waves describe the fluid behavior. The interaction of two such waves does however generate gradient singularities which must be regularized. A dissipative regularization for this problem leads to two counter-propagating shock waves moving away from the initial interaction point. A dispersive regularization for this problem was presented using the Whitham averaging method which gives rise to an oscillatory interaction region described by a modulated train of solitons decaying to small amplitude linear waves. Viewed in the context of dispersive shock waves (DSWs), the interaction region can be thought of as two expanding DSWs placed back-to-back. A comparison of the asymptotic results with numerical simulations and experiments demonstrates that this interaction region corresponds to the macroscopic, quantum mechanical interference of matter-waves in a Bose-Einstein condensate.

Boaz Ilan investigated positive soliton solutions of nonlinear Schrodinger equations with periodic and irregular-lattice potentials. Using rigorous, asymptotic and computational methods he showed that the solitons are (un)stable precisely whenever they (violate) satisfy the power-slope (Vakhitov-Kolokolov) and lesser-studied spectral condition. Violations of the power-slope and spectral conditions induce focusing and drift instabilities, respectively. This unified approach predicts the strength of the instabilities as well. These results are elucidated by computation of soliton dynamics with periodic, defect, and quasi-crystal lattice structures.

Robert Krasny considered vortex sheets as weak solutions of the incompressible fluid equations describing velocity fields with a tangential discontinuity. Physically, a vortex sheet represents a thin shear layer in slightly viscous flow. The initial value problem for vortex sheets is ill-posed due to the Kelvin-Helmholtz instability. Moore showed that a curvature singularity forms in finite time in a perturbed vortex sheet. To go past the critical time, it is necessary to regularize the principal value integral defining the sheet velocity. This talk presented regularized point vortex simulations of the problem. For a large value of the regularization parameter, the sheet rolls up into a smooth spiral past the critical time. As the regularization parameter is reduced, the onset of chaotic dynamics due to resonances in the vortex core was observed.

Brenton LeMesurier developed a new approach for generating time discretizations for a large class of Hamiltonian systems which exactly conserve the energy and other quadratic conserved quantities of the corresponding differential equations. An essential feature is a procedure for constructing discrete approximations of partial derivatives in a way that mimics essential properties of derivatives, in particular for the quadratic forms of most "momenta". The approach is applied to a class of systems which includes models of energetic pulse propagation in protein due to Davydov, Scott et al. These models have the integrable nonlinear

Schrödinger equation as a continuum limit, with sech pulse solutions. Extensions will be shown to systems like coupled systems of discrete nonlinear Schrödinger equations and oscillators. The discrete models have self-focusing effects not seen in the 1D cubic NLS.

Pavel Lushnikov derived a regularization of collapse in cellular dynamics. In this case biological cells interact through chemotaxis when cells secret diffusing chemical (chemoattractant) and move towards the gradient of the chemoattractant creating effective nonlocal attraction between cells. Macroscopic description of cellular density dynamics through Keller-Segel model has striking qualitative similarities with the nonlinear Schrödinger equation including critical collapse in two dimensions and supercritical in three dimensions. Critical collapse has logarithmic corrections to $(t_0 - t)^{1/2}$ scaling law of self-similar solution. Microscopic motion of eucaryotic cells is accompanied by random fluctuations of their shapes. A nonlinear diffusion equation was derived coupled with chemoattractant from microscopic cellular dynamics in dimensions one and two using excluded volume approach. The nonlinear diffusion coefficient depends on cellular volume fraction and it provides regularization (prevention) of cellular density collapse. A very good agreement is shown between Monte Carlo simulations of the microscopic Cellular Potts Model and numerical solutions of the macroscopic equations for relatively large cellular volume fractions.

Vladimir Mezentsev presented a full vectorial modeling of femtosecond bullets for laser inscription of photonic structures. This means that the full set of Maxwell's equations coupled to standard Drude model of the generated plasma is modeled. The results are compared with orthodox models based on the paraxial envelope approximation.

Pierre Raphaël discussed the description of singularity formation for some focusing nonlinear Schrödinger equations $iu_t + \Delta u + u|u|^{p-1} = 0$ in N dimensions. He used the analysis of the stable "log-log" blow up regime for the L^2 critical case $p = 1 + \frac{4}{N}$ to prove the existence of standing ring blow up solutions in the super critical case. In particular, for $p = 5$ and *any* $N \geq 2$, he proved the existence of radially symmetric blow up solutions which concentrate their L^2 mass on the unit sphere N dimentions and the stability of this singularity formation in the radial class.

Benno Rumpf addressed important issues of strong turbulence by studying quasisolitonic turbulence in the Majda-McLaughlin-Tabak equation which is a simple one dimensional model system for turbulence. He discussed formation of collapses and of quasisolitons from a weakly turbulent background in this system.

Catherine Sulem discussed the problem of nonlinear wave motion of the free surface of a body of fluid over a variable bottom. The objective was to describe the character of wave propagation in a long wave asymptotic regime, under the assumption that the bottom of the fluid region is described by a stationary random process whose variations take place on short length scales. The principal result is the derivation of effective equations and a consistency analysis. The effects of random modulations on the solutions was computed giving an explicit expression for the scattered component of the solution due to waves interacting with the random bottom.

Becca Thomases studied mixing transitions and oscillations in low-Reynolds number viscoelastic fluids. In the past several years, it has come to be appreciated that in low Reynolds number, the flow the nonlinearities provided by non-Newtonian stresses of a complex fluid can provide a richness of dynamical behaviors more commonly associated with high Reynolds number Newtonian flow. For example, experiments by V. Steinberg and collaborators have shown that dilute polymer suspensions being sheared in simple flow geometries can exhibit highly time dependent dynamics and show efficient mixing. The corresponding experiments using Newtonian fluids do not, and indeed cannot, show such nontrivial dynamics. To better understand these phenomena, a computational study of the Stokes-Oldroyd-B viscoelastic model in 2D was performed. For low Weissenberg number, flows are "slaved" to the four-roll mill geometry of the fluid forcing. For sufficiently large Weissenberg number, such slaved solutions are unstable and under perturbation transit in time to a structurally dissimilar flow state dominated by a single large vortex, rather than four vortices of the four-roll mill state. The transition to this new state also leads to regions of well-mixed fluid and can show persistent oscillatory behavior with continued destruction and generation of smaller-scale vortices.

Natalia Vladimirova investigated the qualitative behavior of solutions of a Burgers-Boussinesq system – a reaction-diffusion equation coupled via force to a Burgers equation – by a combination of numerical and asymptotic techniques. When the force is small, the solutions decompose into a traveling wave and an accelerated shock wave moving in opposite directions. When the force exceeds some critical value, the solutions are composed of three elementary pieces: a wave fan, a reaction traveling wave, and an accelerating shock, with the whole structure traveling in the same direction. With further increase of the force, the wave fan catches up with the accelerating shock wave – the solution drops below reaction threshold and reaction is ceased. Extinction results irrespective of the size of initial data – a major difference with what happens in advection-reaction-diffusion equations where an incompressible flow is imposed.

Michael Weinstein discussed ground state selection and energy equipartition in the NLS and the Gross Pitaevskii Equation which are central equations to the mathematical description of nonlinear optical and macroscopic quantum systems. It was shown that NLS/Gross Pitaevskii systems support multiple families of nonlinear bound states ("solitons") that (i) the generic evolution is towards a nonlinear ground state and (ii) in the weakly nonlinear regime an energy equipartition law holds.

Scientific Progress Made and Outcome of the Meeting

This workshop provided a unique opportunity for the advancement and understanding of strongly nonlinear phenomena in nonlinear optics, biology, hydrodynamics and plasma through the integration of theoretical, numerical and experimental studies. Cross-fertilization of these interdisciplinary approaches allowed achieving a new level of understanding of nonlinear phenomena. Because of the diversity of the underlying nonlinear phenomena, correct models require good understanding of the underlying physics and the recognition of characteristic dominant scales and effects so that asymptotic methods could lead to tracktable models. An important outcome of the workshop was the study of mechanisms of regularization of strongly nonlinear solutions which depend on the particular application, but show many universal features such as dissipative anomaly in Navier-Stokes turbulence when regularization does not depend on the exact value of the dissipative regularization provided viscosity of fluid is small enough. An example is the formation of freak waves and wave breaking which are described by nondissipative Euler's equations up to point of formation of white caps which are responsible for dissipation.

The workshop brought together many leading researchers in the field of strongly nonlinear phenomena and we only regret that we applied for a 2-days workshop instead of a 5-days workshop, because in the shorter workshop was really a stretch to cover such a large number of important results. The workshop allowed active engagement of junior faculty and researchers to what is the happening in this interdisciplinary area. A total 8 junior researchers and 3 women participated and their contribution was crucial for the success of the workshop.

List of Participants

Balk, Alexander (University of Utah)
Craig, Walter (McMaster University)
Goldman, Martin (University of Colorado at Boulder)
Guyenne, Philippe (University of Delaware)
Hoefer, Mark (Columbia University)
Ilan, Boaz (University of California, Merced)
Krasny, Robert (University of Michigan)
LeMesurier, Brenton (College of Charleston)
Lushnikov, Pavel (University of New Mexico)
Mezentsev, Vladimir (Aston University)
Raphael, Pierre (Paul Sabatier University)
Rumpf, Benno (Chemnitz University of Technology)
Sulem, Catherine (University of Toronto)
Thomases, Becca (University of California, Davis)
Vladimirova, Natalia (University of New Mexico)
Warchall, Henry A. (National Science Foundation)
Weinstein, Michael (Columbia University)
Yu, Xinwei (University of Alberta)
Zakharov, Vladimir (Lebedev Physics Institute of the Russian Academy of Sciences / University of Arizona)

Focused Research Group Reports

Chapter 48

Water Movements in Biological Tissue and Diffusion-Weighted Imaging (08frg113)

May 11 - May 18, 2008

Organizer(s): Jin Cheng (Fudan University), Huaxiong Huang (York University), Robert Miura (New Jersey Institute of Technology)

Introduction

This Focussed Research Group (FRG) was organized with two goals. The first goal was to facilitate the interpretation of results from the state-of-the-art diffusion-weighted magnetic resonance imaging (DWI) technique by using a multi-scale mathematical modeling approach to study the transport of ions and water in biological tissue. The second goal was to utilize more realistic models of water transport in tissues, such as the brain-cell micro-environment, to develop methodologies to refine imaging techniques such as DWI. At the FRG, we took initial steps to achieve these goals by focussing on simple models of apparent diffusion coefficient (ADC) and on cell swelling associated with the clinically important problem called cortical spreading depression (CSD). Cell swelling serves as a case study to explore the issues related to co-transport of ions and water as well as those associated with DWI.

The FRG included applied mathematicians involved in modelling, mathematical analysis, and scientific computing of fundamental problems in fluid dynamics and neuroscience (Huang, Lewis, Miura, Wylie) and biomedical and mechanical engineers and a biomechanician involved in applications to mammalian biological tissue (Sotak, Takagi, Yao).

Overview of the Field

Diffusion-Weighted Magnetic Resonance Imaging (DWI) is a powerful tool for the non-invasive measurement of the apparent diffusion coefficient (ADC) of tissue water. The ADC is directly related to the Brownian motion of an ensemble of water molecules and reflects the specific characteristics of the tissue micro-architecture that impose restricting barriers to water diffusion. In addition to normal anatomy, DWI is often used to visualize disease states that affect the tissue micro-architecture in ways that change the net displacement of water molecules (and hence the ADC value).

For example, immediately following the onset of acute ischemic stroke, the rapid failure of high-energy metabolism and associated ionic pumps leads to the migration of sodium and calcium into the cell. The subsequent influx of osmotically-obligated water results in cellular swelling (cytotoxic edema) and a decrease in the extracellular volume fraction. The ADC of brain water declines over the first 1-2 h following stroke onset [6] and allows visualization of the ischemic territory as a hyperintense region on the DW image. In addition to acute ischemic stroke, transient ischemic attack (TIA), ischemic depolarizations (IDs), cortical spreading depression (CSD), status epilepitcus, and hypoglycemia also exhibit cellular swelling (cytotoxic edema) that reduces the net displacement, and hence the ADC of the tissue water molecules as measured by DWI [11]. Water ADC values are also affected by the presence and orientation of barriers to translational water movements (such as cell membranes and myelin fibers) and thus MRI measures of anisotropic diffusion are sensitive to more chronic pathological states where the integrity of these structures are compromised by disease.

The biophysical mechanisms responsible for these ADC changes are still not well understood. However, the water ADCs are temporally well correlated with the relative changes in intra- and extracellular volume fraction and increased extracellular tortuosity, e.g., as measured independently by electrical conductivity and real-time iontophoretic methods [7]. Furthermore, the transient water ADC changes measured during CSD and IDs suggest that MRI diffusion measurements are also sensitive to chemical communication (e.g., via K^+ or glutamate) between cells through the extracellular space (i.e., extrasynaptic or volume transmission, VT).

Recent Developments and Open Problems

The exact connection between cellular swelling and decrease in overall water ADC has not been quantified. Various mechanisms have been proposed to explain changes in tissue water ADC [1, 4], and some analytical models have previously been presented to study restricted water self-diffusion [12, 13]. However, earlier attempts to relate MR signals in DWI with morphologic changes have been either qualitative or based on simple non-realistic geometries, such as cylinders and spheres. For better understanding of the factors that affect water diffusion in biological tissues with more complex morphologies, numerical models have been proposed, such as Monte Carlo (MC) [13] and image-based finite difference (FD) methods [3, 15].

In spite of the theoretical models that have been proposed to date, the fundamental biophysical mechanism responsible for the water ADC changes observed during cerebral ischemia, cortical spreading depression, ischemic depolarizations, status epilepticus, and hypoglycemia remains uncertain. However, it is clear that all of these conditions share the common features of acute cell membrane depolarization and subsequent cell volume changes (cytotoxic edema). A more quantitative understanding of how the underlying tissue pathology manifests in the measured water ADC would be important for clarifying the role of these measurements in characterizing the severity of disease as well as the potential outcome in response to treatment. In this regard, improved theoretical modeling of water diffusion in tissue may play an important role in improving the diagnosis and treatment of these diseases using DWI.

Some open questions

Model Cell Swelling

1. What is the sensitivity of water ADC changes on parameters such as: intracellular diffusion coefficient (D_{int}), extracellular diffusion coefficient (D_{ext}), cell-membrane permeability, volume fraction, geometry (cell size)? How does the underlying tissue geometry affect the sensitivity analysis of the parameters?

2. Can cell volume changes alone account for all of the percentage-reduction in water ADC observed during CSD or stroke? Can such an analysis be done without making any particular assumptions about the underlying tissue geometry?

3. Given the changes in membrane permeability to ions that accompany CSD, could it be inferred what changes occur in the effective membrane permeability to water that accompanies the osmotic water shifts?

4. From the Goldman-Hodgkin-Katz equation used to model cell membrane potential in CSD, is it possible to get the correct changes in relative volume fraction (due to osmotic swelling) from just the shifts in ions alone (knowing all of the intra- and extracellular ion concentrations both before and after depolarization as well as the channel permeabilities both before and after depolarization)?

5. Based on the volume of the region where reduced ADC is observed by DWI during CSD, it is possible to incorporate this information into a model such that the length scale of the cellular depolarization could be determined? From this length scale, could a ”‘syncytium size”’ be estimated which would correspond to the size of the cell population that is depolarized at any one time during CSD. This would require that both the temporal and spatial aspects of the CSD depolarization be incorporated into the model.

q-Space Analysis

1. Apply the Tanner model to the *q*-space problem.

2. How should *q* be chosen, e.g., to estimate higher-order moments?

3. What is the sensitivity of the second-order moment to D_{int}, D_{ext}, permeability, and volume fraction?

4. How can the relationship between the diffusion time and *q* be exploited to provide additional information about the underlying tissue geometry?

5. What is the effect of noise on the *q*-space analysis?

Diffusion and Displacement Distribution Profile of Water

The data obtained from DWI techniques have typically been interpreted using ideas from diffusion in isotropic homogeneous materials. This effectively means that the techniques are used to estimate a single ‘effective’ diffusion coefficient that represents an ’effective medium’ approximation to the complicated inhomogeneous and anisotropic structure in tissues. This method has been extremely useful in application.

In biological applications, such as the brain, the complex intracellular and extracellular regions that are separated by permeable membranes represent a medium that is far from being either homogeneous or isotropic. Therefore, diffusive processes in the brain differ significantly from those that would be observed in homogeneous and isotropic media. In principle, it is possible to use the data from DWI measurements to determine much more detailed information about the diffusive processes. The natural questions then arise of how much information about the complex structure of the brain can be extracted from the data and how robust is this information to measurement errors. There is also the important question of whether it is possible to extract this information in an acceptable image acquisition time.

One-, two-, and three-dimensional models

To investigate these questions, we will consider a simple one-dimensional model that contains intra- and extracellular regions that have different sizes and diffusivities and are separated by permeable membranes, and use this as a model for brain tissue. We will determine an exact solution to the diffusion of water in this model environment, and then use this solution to determine the DWI measurements that one would obtain. We will use this data to attempt to reconstruct the parameters that characterize the model system. We will also determine the robustness of this approach when noise is added to the signal. This will allow us to determine what type of information can realistically be obtained from the DWI measurements.

Subsequently, we will extend this model by coupling it to a one-dimensional region of uniform diffusivity containing no boundaries. This region will represent the connected component of the extracellular space, while the original portion of the model will represent the contribution from the diffusive particles that move within and between cells. With this model, it will be possible to separate out the relative importance of the intracellular and extracellular spaces in determining the value of the ‘effective diffusion coefficient’, and thus, we may use the model to provide insight into the process of cell swelling that occurs in brain ischemia and cortical spreading depression.

We will also consider the diffusion of water in fully two- and three-dimensional cellular media. We will use closed regions within the domain to model the intracellular space. A permeable boundary will separate these regions from a continuously connected region that represents the extracellular space. In this case, it will not be possible to derive an exact solution, and thus numerical approximations will be made. With this model, we can consider further the questions discussed above. In particular, we will consider how the variation of the anisotropy, in addition to the inhomogeneities, affects the value of the 'effective diffusion coefficient'. Furthermore, we can extend the discussion to include Diffusion Tensor Imaging (DTI), which is an extension of the effective medium assumption that drops the assumption of isotropy while maintaining the assumption of homogeneity.

Displacement distribution profile

By Fourier transformation of the decay of the DWI signal for water, it is possible to extract the displacement distribution profile. Some models have been set up to simulate water diffusion in tissues, but it is difficult to solve the inverse problem for these models. Since the displacement distribution profile is determined by the movement of intracellular or extracellular molecules, we set up a compartmental (lumped parameter) model based on molecular thermodynamics theory. This model allows us to simulate the displacement distribution profile and to solve the inverse problem.

Suppose the tissue consists of two compartments: the intracellular and extracellular spaces, and water molecules can move between these two compartments. Then the velocity distribution of the water in the tissue can be simplified to give

$$\alpha f(\alpha, v) + (1-\alpha) g(\alpha, v) + \beta h(v) = P(v) \tag{1}$$

where α is the intracellular volume fraction and β is the fraction of water molecules exchanged between the intracellular and extracellular spaces. $f(\alpha, v)$ is the velocity distribution of the intracellular water molecules, and $g(\alpha, v)$ is the velocity distribution of the extracellular water molecules. $h(v)$ is the tissue water molecules without considering cell boundaries. $P(v)$ is the velocity distribution profile that can be inferred from the distribution profile of the DWI, i.e., by dividing the displacement by time t. If we know these velocity distributions, then we can get the optimum values of α and β.

Theoretical velocity distribution

If these two compartments are homogeneous, then from our knowledge of statistical mechanics, the velocity distribution can be defined by a Maxwell-Boltzmann distribution

$$\phi(v) = C \exp((-Kv^2)/2) \tag{2}$$

where C and K are constants. Obviously, C and K are affected by the volume (or boundary) of the compartment and the tortuosity within the compartment. Therefore, $f(\alpha, v), g(\alpha, v)$, and $h(v)$ can be defined as

$$f(\alpha, v) = C_I(\alpha) \exp((-K_I(\alpha) v^2)/2), \tag{3}$$

$$g(\alpha, v) = C_E(\alpha) \exp((-K_E(\alpha) v^2)/2), \tag{4}$$

$$h(v) = C_W \exp((-K_W v^2)/2). \tag{5}$$

If we can determine expressions for the parameters, $C_I(\alpha), C_E(\alpha), C_W, K_I(\alpha), K_E(\alpha)$, and K_W, and obtain the velocity distribution profile over a short enough time, then we should be able to solve the inverse problem for this model.

Comparison of the Predicted Apparent Diffusion Coefficient Using Three Different Models

Although the apparent diffusion coefficient (ADC) is often used to characterize water movement in brain-tissue, the actual phenomenon is not dominated only by the diffusion process. The permeability of water

Table 48.1: Parameter values from Latour et al. [4]. a: radius of sphere (cell), ϕ: volume fraction of the extracellular region, c_{int}: water concentration in intracellular region, D_{int}: diffusion coefficient of the intracellular region, D_{ext}: diffusion coefficient of the extracellular region.

Sample	a	ϕ	c_{int}	D_{int}	D_{ext}	Permeability
	μm			$\times 10^{-5}$ cm^2/s	$\times 10^{-5}$ cm^2/s	$\times 10^{-3}$ cm/s
A	2.1	0.19	0.71	1.56	2.12	6.3±1.4
B	2.1	0.19	0.71	1.56	2.12	3.7±1.4
C	2.3	0.00	0.78	1.64	2.12	1.1

molecules through cell membranes also is an important factor. Since the spatial scale of MRI measurements is much larger than the cell size, the measured ADC is just an indicator to show how far water molecules can spread. There exist several simple models for evaluating macroscopic water movement that take into consideration the water permeability through membrane. Here, we discuss and evaluate the ADCs obtained using different phenomenological models.

Latour et al. [4] obtained time dependent ADCs based on experiments using red blood cells. They evaluated the permeability of water through cell membranes from the long time asymptotic behavior of ADC. They used Effective Medium Theory and called this long time ADC an effective diffusion coefficient (D_{eff}). The parameters they used and the estimated permeabilities are shown in Table 48.1.

Estimation of D_{eff}

Using these values, we evaluated the ADCs using two other models, given in Szafer et al. [13], which are called the Parallel-Series Approximation and the Series-Parallel Approximation. In these models, the ADCs are computed as follows. Let the volume fraction of the intracellular region be $f = 1 - \phi$, and the length of the periodic volume is given by

$$L = \frac{2a}{g} \tag{48.1}$$

where $g = f^{1/3}$. Define

$$D_{\text{c}} = \left(\frac{2}{PL} + \frac{1}{D_I c_{\text{int}}} \right)^{-1}. \tag{48.2}$$

The ADC using the Parallel-Series Approximation ADC$_{\text{ps}}$) is given by

$$ADC_{\text{ps}} = g^2 \left(\frac{g}{D_C} + \frac{1-g}{D_E} \right)^{-1} + (1-g^2)D_E \tag{48.3}$$

and that using the Series-Parallel Approximation (ADC$_{\text{sp}}$) is given by

$$ADC_{\text{sp}} = \left(\frac{g}{g^2 D_C + (1-g^2)D_E} + \frac{1-g}{D_E} \right)^{-1}. \tag{48.4}$$

It is noted that these formulas, (48.3) and (48.4), are slightly different from the original ones, since they have the effect of water concentration in the cell (c_{int}) in D_c given by Eq.(48.2). This c_{int} is not taken into account in the original formula given in [13]. The comparisons of the effective diffusion coefficients (D_{eff}), i.e., ADCs at large time, are shown in Table 48.2.

It can be seen that the differences in D_{eff} is less than 5% in Sample A and B, and 20% in Sample C. Since the differences between the models is primarily in the geometric shapes of the cells, these values indicate that the D_{eff} is insensitive to the geometric shape of the cells, provided the same physical parameters are used.

Estimation of Permeability Coefficients

We also did another type of analysis; namely, we used D_{eff} obtained from Latour et al. [4] to estimate the permeability coefficients using the models given by Eqs. (48.3) and (48.4). The results are shown in Table 48.3. Interestingly, the estimation of permeability coefficients has a larger error than that in the effective diffusion coefficients. There is more than a 20% difference in some cases.

Table 48.2: Effective diffusion coefficient (D_{eff}) based on three models using permeability coefficient [10^6 cm^2/s] estimated by Latour et al. [4].

Diffusion model	Sample A	Sample B	Sample C
Latour et al.	4.2	3.50	2.70
ADC_{ps}	3.95 (3.71-4.17)	3.50 (3.26-3.73)	2.25
ADC_{sp}	4.10 (3.87-4.32)	3.66 (3.42-3.88)	2.25

Table 48.3: Permeability (10^{-3} cm/s) estimation based on three different models using the same effective diffusion coefficient obtained by Latour et al. [4]

Diffusion model	Sample A	Sample B	Sample C
Latour et al.	6.3±1.4	3.7±1.4	11
ADC_{ps}	7.90	3.70	13.9
ADC_{sp}	6.94	2.81	13.9

Discussion

From the results given above, it is concluded that the estimation of D_{eff} using the same permeability coefficients is less sensitive to the models than is the permeability coefficients when using the same D_{eff}. This characteristic suggests that obtaining the permeability by different experimental means and using them to evaluate apparent diffusion coefficient is a more robust way to probe into scales smaller than the MRI resolution allows.

Cell Swelling in CSD

Under pathological conditions such as stroke, the depletion of oxygen due to reduced blood supply leads to failure of ion pumps and a resulting depolarization of the cell membrane potential. Consequently, the intracellular ion concentration increases and water moves into cells due to osmotic pressure and the cells swell. This has been observed by diffusion weighted MRI measurements since cell swelling reduces extracellular space and restricts water diffusion [10]. Understanding the relationship between these pathological conditions and restricted diffusion due to cell swelling could help us to identify regions in the brain at risk and limit further damage. However, since complex biological and biochemical processes typically occur during dramatic pathological conditions, such as stroke, it is difficult to identify cell swelling as the single most important factor to affect the MRI signals. On the other hand, less severe physiological phenomena, which do not involve energy failure, also could lead to cell swelling and alter the characteristics of water movement in the brain-cell microenvironment. Studying these phenomena could provide useful clues for us to understand the underlying biological and biochemical processes involved in cell swelling. Cortical spreading depression is one such phenomenon and is relatively easy to study using diffusion-weighted-imaging (DWI) techniques such as MRI [11].

Cortical spreading depression

Cortical spreading depression (CSD) is a slowly propagating chemical wave phenomenon observed in the cortex of various brain structures in a diverse set of experimental animals. CSD 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 during CSD. The primary clinical interest in CSD is due to its presence in the visual cortex of humans during migraine with aura (aka classic migraine). Although CSD was discovered in 1944 by the Brazilian neurophysiologist, A.A.P. Leão [5], the mechanisms producing CSD and their quantitative explanations remain elusive.

Some of the mechanisms that are believed to be of importance in CSD instigation and propagation are ion diffusion, cell (neuronal and glial) membrane electrical activities (ionic channels and metabolic pumps), release of neurotransmitter (due to increased extracellular potassium), spatial buffering (effects of electrotonic spread of depolarization along glial cell syncytia), and cell swelling due to osmotic effects. While several of these effects have been considered in different models, all of them have not been incorporated into a comprehensive model, see [9, 14]. The need for parameter values in quantitative modeling motivates the use of DWI in helping to establish upper and lower bounds on these parameter values.

Spatially independent model of CSD

During the FRG, it was decided that a first step in a more comprehensive study of CSD would be to construct a spatially independent compartmental model of Hodgkin-Huxley (HH) type. This model would include water movement in the direction of osmotic pressure differences between the intra- and extracellular compartments. The basic model takes the following form

$$\frac{dC_j^E}{dt} = I_j + P_j; \quad \frac{dC_j^I}{dt} = -(I_j + P_j), \tag{48.5}$$

where C_j^E and C_j^I are the extra- and intracellular ion concentrations, respectively, with j=Na, K, Cl, and Ca for sodium, potassium, choride, and calcium ions, respectively. The ion channel fluxes for Na and K are given by,

$$I_K = g_K(V - V_K), \quad I_{Na} = g_{Na}(V - V_{Na}) \tag{48.6}$$

where

$$V_j = \frac{RT}{Fz_j} \ln \frac{C_j^E}{C_j^I} \tag{48.7}$$

is the Nernst potential and R, T, F, and z_j are the universal gas constant, the temperature, Faraday constant, and the valence for ion j, respectively. The cell membrane potential can be computed using either the Goldman-Hodgkin-Katz (GHK) formula

$$V = \frac{RT}{F} \ln \frac{g_{Na}C_{Na}^E + g_K C_K^E + g_{Ca}C_{Ca}^E + g_{Cl}C_{Cl}^I}{g_{Na}C_{Na}^I + g_K C_K^I + g_{Ca}C_{Ca}^I + g_{Cl}C_{Cl}^E} \tag{48.8}$$

or the Hodgkin-Huxley (HH) equation

$$\begin{aligned} V &= \frac{RT}{F(g_{Na} + g_K + g_{Ca} + g_{Cl})} \\ &\quad \times \left(g_{Na} \ln \frac{C_{Na}^E}{C_{Na}^I} + g_K \ln \frac{C_K^E}{C_K^I} + g_{Ca} \ln \frac{C_{Ca}^E}{C_{Ca}^I} + g_{Cl} \ln \frac{C_{Cl}^I}{C_{Cl}^E} \right). \end{aligned} \tag{48.9}$$

For the conductance, we use the Hodgkin-Huxley formulas for g_{Na} and g_K given by

$$g_{Na} = \bar{g}_{Na} m^3 h, \quad g_K = \bar{g}_K n^4 \tag{48.10}$$

where m, h, and n are given by equations in the form

$$\frac{du}{dt} = \frac{u_\infty - u}{\tau_u} \tag{48.11}$$

with coefficients

$$\tau_u = \frac{1}{\alpha_u + \beta_u}, \quad u_\infty = \tau_u \alpha_u \tag{48.12}$$

for $u = m$, h, and n, respectively. As a simplification, we assume that the conductance for Cl is a constant, $g_{Cl} = 0.5\bar{g}_K n_\infty^4$ and the calcium conductance is zero, i.e., $g_{Ca} = 0$.

The ion pumps play a crucial role in maintaining homeostatic ion concentrations and cell membrane potential. The basic ion pump is the sodium-potassium exchange pump, which is modeled as

$$P_{Na} = 3\hat{P}, \quad P_K = -2\hat{P} \tag{48.13}$$

where

$$\hat{P} = 2.01 \times 10^{-3} \left(\frac{C_K^E}{C_K^E + 176.5} \right)^2 \left(\frac{C_{Na}^I}{C_{Na}^I + 0.6} \right)^3 \frac{0.052 \sinh(\gamma)}{0.026 \exp(\gamma) + 22.5 \exp(-\gamma)} \tag{48.14}$$

with

$$\gamma = \frac{F(V + 176.5)}{RT}.$$

Finally, the volume fraction of the extracellular space, α_E, can be computed using

$$\frac{d\alpha_E}{dt} = g_w \alpha_E^{\frac{2}{3}} \left(\sum_j c_j^E - \sum_j c_j^I - \frac{A_i}{1 - \alpha_E} \right) \tag{48.15}$$

where g_w is the conductance and A_i is the number of immobile anions inside the cell.

In summary, the above system of ordinary differential equations can be used to compute the evolution of the ion concentrations and membrane potential from a given set of initial data.

Numerical tests

We use the parameter values, $R = 8.31$, $T = 310$, and $F = 95$, specify the initial conditions as $c_{Na}^E = 145$, $c_{Na}^I = 10$, $c_K^E = 2$, $c_K^I = 140$, $c_{Ca}^E = 1.8$, $c_{Ca}^I = 2 \times 10^{-4}$, $c_{Cl}^E = 110$, $c_{Cl}^I = 5$, $\alpha_E = 0.2$, and set $A_i = (1 - \alpha_E) \sum_j \left(c_j^E - c_j^I \right)$, $g_{Na} = 0.01 g_K$, $g_{Cl} = 0.5 g_K$. Since the effect of calcium on the osmotic pressure is small, we have neglected the effects of Ca by setting $g_{Ca} = 0$, and the conductance for Cl is assumed to be fixed. Finally, we set $\bar{g}_{Na} = 120$ and $\bar{g}_K = 3.6$. The water conductance is set at $g_w = 0.1$.

The numerical results show that using the GHK formula, the membrane will automatically depolarize from about -95 mV to a much higher value and the cell swells. The behavior of the system changes little when KCl is injected except that the cell shrinks initially before swelling. The HH formula for membrane potential, on the other hand, maintains the resting membrane potential (computed based on the initial ion concentrations). Furthermore, when we inject KCl, the membrane depolarizes as expected. However, the cell shrinks instead of swells. Note that there is no recovery in these results because spatial diffusion is not included.

Discussion

The preliminary studies conducted during the FRG suggest that further modeling is needed. As shown in [8], the GHK and HH formulas for membrane potential are two asymptotic limiting equilibrium cases. Therefore, a dynamic approach which yields more consistent equations for membrane potential and ionic currents is desirable, as indicated by [2].

Scientific Progress and Outcome of the Meeting

Comparison of the continuous medium theory of Latour et al. [4] with that of Szafer et al. [13] showed a good correspondence using the permeability data from the Latour et al. paper to predict the water ADC values from the Szafer et al. model. The results of this comparison will be considered for a conference abstract.

The FRG has proved to be a very effective way to bring our group of researchers to a common level of understanding and competence to work together on several different projects related to Water Movements in Biological Tissue and Diffusion-Weighted Imaging. We have identified several interesting problems that will continue to be studied. The group worked together very well and had a very productive week.

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Chapter 49

Hausdorff geometry of complex polynomials, positive charge distributions and normal operators (08frg121)

Jun 29 - Jul 06, 2008

Organizer(s): Julius Borcea (University of Stockholm), Rajesh Pereira (University of Guelph), Mihai Putinar (University of California at Santa Barbara)

Overview

The intensive week spent at the Banff Research Center was focused on discussions of a series of precise quantitative conjectures and pointed questions referring to the Euclidean distance geometry of the critical points of complex polynomials versus the locations of their zeros. The subject goes back to some early studies in electrostatics by Gauss and Maxwell and has penetrated into modern mathematics via approximation theory, specifically the Ilieff-Sendov conjecture.

Open Problems

We have begun our attempt at solving the following three conjectures [1,2], the first of which is a strengthening of Sendov's conjecture.

Conjecture 1 [Variance conjecture for complex polynomials]: If $p \in \mathbb{C}[z]$ with $deg(p) \geq 2$ then $H(p) \leq \sigma_2(p)$, where $H(p)$ denotes the symmetrized Hausdorff distance between the zero sets of p and p' while $\sigma_2(p)$ is the standard deviation of the zero set of p.

During the focused research group, we formulated some sufficient conditions for the truth of this conjecture. Before we give an example, we need the following terminology.

Let $p(z) = \prod_{k=1}^{m}(z - z_k)^{m_k}$ where the z_k are distinct. Let $\{w_k\}_{k=1}^{m}$ be the roots of p' which are not also roots of p. We define the Gauss-Lucas matrix of p to be the m by n matrix G with entries $g_{ij} = \frac{|w_i - z_j|^{-2}}{\sum_{k=1}^{n} |w_i - z_k|^{-2}}$. This matrix is a stochastic matrix; a fact which was used by Cesaro in his proof of the Gauss-Lucas theorem [5, pg. 93]. It can be shown that the variance conjecture holds for p if every column of the Gauss-Lucas matrix has an entry greater than or equal to $1/n$. This observation gives us a nice proof of the conjecture for polynomials with at most three distinct roots. The conjecture also holds for polynomials with all roots real. This approach cannot be used to prove the conjecture in general since there are high degree polynomials whose Gauss-Lucas Matrices do not satisfy the above column property. (The 19th degree polynomial from [4] is one such example).

A similar conjecture can be stated for the zeros of the Cauchy transform of compactly supported probability measures. We first need the following notation. Given $K \Subset \mathbb{C}$, let $\mathcal{P}(K)$ be the set of all probability measures μ on $\mathbb{C}$ supported on K. For $\mu \in \mathcal{P}(K)$ denote by $E(\mu)$ and $\sigma_2(\mu)$ the barycenter and the standard deviation of μ, respectively. Let $\mathcal{W}(\mu)$ be the set of finite zeros of the Cauchy transform of μ (i.e., the equilibrium points of the logarithmic potential associated with μ) and let $\mathcal{W}_e(\mu) = \mathcal{W}(\mu) \cup E(\mu) \cup \partial K$. One can show that the minimal radius of the circle containing K (the circumradius) $\rho(K)$ equals the maximal variance of K, that is, $\rho(K) = \sup_{\mu \in \mathcal{P}(K)} \sigma_2(\mu)$.

Conjecture 2 [Variance conjecture for probability measures]: For any $K \Subset \mathbb{C}$ and $\mu \in \mathcal{P}(K)$ one has $H(K, \mathcal{W}_e(\mu)) \leq \rho(K)$, where H is the symmetrized Hausdorff distance.

We have also formulated an operator-theoretic conjecture which is roughly analogous to conjectures 1 and 2.

The solution to these and other related problems would almost certainly involve novel techniques which could be useful in solving other problems in complex analysis, potential theory and operator theory. Progress on the stated conjectures and related results may have implications in numerical analysis, in the study of the propagation of singularities of solutions to linear PDE's in the complex domain, in astrophysics (such as the recent solution to the long standing open question about the number of images in gravitational lensing by Khavinson and Neumann [3]), in statistical physics (e.g. Lee-Yang type results on the zeros of the partition function), in combinatorics as well as to matrix models in quantum field theory and fluid mechanics.

Outcome of the Meeting

During the focused research group, we have identified the following five topics for further study.

We have been able to reformulate some of our questions about the Gauss-Lucas matrix in terms of a related dynamical system. We will continue our analysis of the dynamics (such as fixed points, basins of attraction, singular points) of this system. We will work towards a better understanding of the potential theoretic parallel/contrast between finitely many sources and continuous densities, incorporating known phenomena into the larger theory of value distribution for meromorphic functions. We will further examine the statistical interpretation of the Hausdorff distance between critical points and zeros of a polynomial in terms of invariant dispersion measures. We will attempt to construct and solve a hyperbolic version of the Sendov or variance conjecture by elaborating in terms of the hyperbolic distances the relationship between various configurations of the critical points versus the zeros of finite Blaschke products in the hyperbolic metric of the unit disk. It would also be worth considering the spectral analysis of central truncations of Toeplitz matrices as a two dimensional analog of the classical Padé approximations of Markov functions.

Because of the diverse research backgrounds of the group, we were able to find connections among and acquaint one another with many different areas of mathematics. In one case this extended beyond our focused research group. Julius Borcea gave a talk entitled ”Negative correlations, phase transitions and zeros of multivariate polynomials” to the BIRS workshop in Recent progress in two-dimensional statistical mechanics which was taking place at the same time.

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Chapter 50

Traceability of Graphs and Digraphs (08frg134)

Aug 03 - Aug 10, 2008

Organizer(s): Marietjie Frick (University of South Africa), Ortrud Oellermann (University of Winnipeg)

Overview of the Field, Recent Developments and Open Problems

A graph or digraph is *hamiltonian* if it contains a cycle that visits every vertex, and *traceable* if it contains a path that visits every vertex. A (di)graph D is *hypotraceable* if D is nontraceable but $D - v$ is traceable for every $v \in V(D)$. A (di)graph is k*-traceable* if each of its induced subdigraphs of order k is traceable. Clearly, a nontraceable digraph of order $k+1$ is k-traceable if and only if it is hypotraceable.

An *oriented* graph is a digraph without 2-cycles. Our interest in k-traceable oriented graphs stems from the following conjecture, which is stated in [1].

The Traceability Conjecture (TC): *For $k \geq 2$, every k-traceable oriented graph of order at least $2k-1$ is traceable.*

It has been proved that the TC holds for $k \in \{2, 3, 4, 5, 6\}$ (see [1] and [8]). The TC was motivated by the OPPC, an oriented version of the Path Partition Conjecture, which can be formulated as follows.

OPPC: *If D is an oriented graph with no path of order greater than λ and a is a positive integer such that $a < \lambda$, then $V(D)$ contains a set A such that the oriented graph induced by A has no path of order greater than a and $D - A$ has no path of order greater than $\lambda - a$.*

If the TC is true, it would imply that the OPPC is true for every oriented graph whose order is exactly one more than the order of its longest paths. Directed versions of the PPC are considered in [4], [5], [6], [7], [9] and [10]. Results supporting the TC are proved in [1], [2] and [8].

Clearly, 2-traceable oriented graphs are tournaments, i.e. their underlying graphs are complete. It is well-known that every strong tournament is hamiltonian. In [1] we extended this result by showing that every strong k-traceable oriented graph of order greater than k is hamiltonian for every $k \in \{2, 3, 4\}$. However, when $k \geq 5$ the situation changes dramatically. We showed in [1] that for every $n \geq 5$ there exists a strong nonhamiltonian oriented graph of order n that is k-traceable for every $k \in \{5, \ldots, n\}$. Thus for $k \in \{2, 3, 4\}$ there are no strong nonhamiltonian k-traceable oriented graphs of order greater than k, while for each $k \geq 5$ there are infinitely many.

It is also well-known that every tournament is traceable, i.e., every 2-traceable oriented graph is traceable. It is therefore natural to ask: What is the largest value of k such that every k-traceable oriented graph of order at least k is traceable? And, are there nontraceable k-traceable oriented graphs of arbitrarily large order for some $k \geq 3$?

It is shown in [8] that for $k \geq 2$ every nontraceable k-traceable oriented graph of order $n > k$ contains a hypotraceable oriented graph of order h for some $h \in \{k+1, \ldots, n\}$ and also that there does not exist a hypotraceable oriented graph of order less than 8. In [3] it is shown that there exists a hypotraceable oriented graph of order n for every $n \geq 8$ except, possibly, for $n = 9$ or 11 and also that no hypotraceable oriented graph of order 8 is 5-traceable or 6-traceable. These results, together with the fact that the TC holds for $k \leq 6$, imply that for $k \in \{2, 3, 4, 5\}$, every k-traceable oriented graph of order at least k is traceable and every 6-traceable oriented graph of order n is traceable if $n = 6, 7$ or 8 or $n \geq 11$. Moreover, for every $k \geq 7$ except, possibly, for $k = 9$ or 11, there exists a nontraceable k-traceable oriented graph of order $k+1$. During the workshop we addressed the following two questions.

Question 1 Does there exist a nontraceable 6-traceable oriented graph of order 9 or 10?

Question 2 Do there exist nontraceable k-traceable oriented graphs of arbitrarily large order for some $k \geq 7$?

The underlying graph of a k-traceable oriented graph is, obviously, also k-traceable, so we also considered the following two questions during the workshop.

Question 4 What is the structure of k-traceable oriented graphs?

Question 5 Which k-traceable graphs have k-traceable orientations?

Outcome of the Focussed Research Workshop

We answered Question 1 by proving that there does not exist a 6-traceable oriented graph of order 9 or 10. Thus we conclude that for each $k \in \{2, 3, 4, 5, 6\}$ every k-traceable oriented graph of order at least k is traceable.

We answered Question 2 in the negative by establishing an upper bound in terms of k on the order of nontraceable k-traceable oriented graphs. We proved that the order of nontraceable k-traceable oriented graphs is at most $6k - 21$ for $k = 7, 8$ and at most $2k^2 - 20k + 58$ for every $k \geq 9$.

We made progress on Questions 4 and 5 by characterizing k-traceable graphs for $k = 3, 4, 5, 6$ and also characterizing k-traceable orientations of k-traceable graphs for $k = 3, 4$.

The results of our Workshop are written up in the two attached papers.

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Chapter 51

Differential equations driven by fractional Brownian motion as random dynamical systems: qualitative properties (08frg140)

Sep 29 - Oct 04, 2008

Organizer(s): Frederi Viens (Purdue University), David Nualart (University of Kansas), Björn Schmalfuß(University of Paderborn)

Outcome of the Meeting

The focused research group on Stochastic Differential Equations driven by Fractional Brownian Motion as Random Dynamical Systems met from around 9:30am to around 5pm from Monday September 29 to Saturday October 4, 2008. It included 8 participants and one observer.

The goal of the group was to exchange ideas between two largely distinct aspects of differential systems driven by self-similar stochastic processes: the stochastic analysis angle and the theory of random dynamical systems. Each of the 9 people gave talks on various topics in each of these aspects. These talks were not aimed at presenting individual research results, rather they were meant to introduce the audience to the general theory, and to present the most current tools being used. Thereafter, the 9 met in smaller groups to discuss ways of exploiting synergies within the collective expertise, defining strategies for solving major problems in stochastic differential equations with fractional Brownian motion.

The expository talks covered the following topics on fractional Brownian motion (fBm) and random dynamical systems:

- **Ciprian A. Tudor** (U. Paris 1 Pantheon-Sorbonne, France): fBm as a Gaussian process, Malliavin calculus for fBm, including the divergence (Skorohod) integral.

- **Fabrice Baudoin** (Purdue University, USA): Rough path theory for integration with respect to fBm, limits of the integration theory for small Hurst parameter.

- **David Nualart** (University of Kansas, USA): Fractional calculus and fBm, Stochastic differential equations driven by fBm, solutions in the rough path sense, estimates of the solutions using a fractional calculus reinterpretation of the rough path theory.

- **Ivan Nourdin** (U. Paris 6 Jussieu, France): Gubinelli's version of rough path theory; integration against fBm via regularization and via Riemann-sum approximations, limits of this integration theory.

- **Maria-Jose Garrido-Atienza** (U. Sevilla, Spain): random dynamical system property for stochastic differential equations driven by fBm, finite-dimensional cases.

- **Björn Schmalfuß** (U. Paderborn, Germany): random dynamical system property for stochastic differential equations driven by fBm, infinite-dimensional cases: results and questions.

- **Jinqiao Duan** (Illinois Institute of Technology, USA): application of fBm-driven stochastic partial differential systems to climate modeling and other physical systems with colored noise, long memory, or self-similarity.

- **Frederi Viens** (Purdue University): Wiener chaos calculus, characterization of normal convergence via Malliavin derivatives, and application to Hurst (self-similarity) parameter estimation.

- **Kening Lu** (Brigham Young University): Formulation of linearized or linear-multiplicative random dynamical systems as products of random matrices, and infinite-dimensional version of the Oseledets theorem for Lyapunov exponents.

All participants used the expository talks to ask many questions of the expositors, in order to enhance their understanding of areas with which they were less familiar. One main topic of investigation that came out of these discussions early on was to seek to prove that the solution of a nonlinear stochastic differential equation driven by fBm in the rough-path sense, with Hurst parameter between 1/4 and 1/2, is in fact a random dynamical system in the sense that the solution satisfies a cocycle property that holds for all starting points simultanously, almost surely (and not merely almost surely for a fixed starting point). This can be done for finite-dimensional systems with Hurst parameter larger than 1/2, working "omega-wise" via standard estimates from the pathwise (Young-type) integration theory; a similar effect should exist when using rough paths. At the moment, the consensus appears to be that the new explicit estimates for rough-path integrals discovered and used by David Nualart and Yaozhong Hu, may provide the best hope for completing this initial problem. Using rough path estimates from Gubinell's theory may also be useful, although this was less clear in our minds. There was a general agreement that the divergence-integral interpretation of fBm-driven stochastic differential equations would not lead to new developments in the study of random dynamical systems.

Other discussions pertained to more specific questions on random dynamical systems for fBm, including existence of stable manifolds, and random attractors, for non-trivial systems, such as those infinite-dimensional ones driven by fBm. We speculate that many fBm-driven systems in infinite dimensions should have finite-dimensional random attractors, a very desirable property from the standpoint of quantitative analysis. Some of us also discussed extensions of the ergodic property to non-Gaussian self-similar and long-memory processes, as well as the question of how to determine statistically the long-memory parameter for such processes, in the non-Gaussian contexts of Wiener chaos or of non-linear time series.

FBm, long-memory processes, self-similar processes, and other colored noises are becoming very popular in the applied sciences. We have had several discussions along these lines on several models. In climate modeling, the atmospheric advection-diffusion-condensation equation is shown empirically to contain long memory; we have discussed estimating the humidity parameter or function via variations methods similar to those that can yield the long-memory parameter itself. Joint estimation of these two parameters should also be possible. Other real-world problems we discussed addressed long memory and self-similarity in financial econometrics, internet traffic, DNA sequencing, and polymers.

List of Participants

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Research in Teams Reports

Chapter 52

Higher Resonance Varieties (08rit129)

May 04 - May 11, 2008

Organizer(s): Graham Denham (University of Western Ontario), Hal Schenck (University of Illinois)

Scientific Progress Made

The purpose of this meeting was to describe some qualitative properties of the higher resonance varieties of hyperplane arrangements and related topological spaces. Our starting point was the Bernstein-Gel'fand-Gel'fand (BGG) correspondence, an equivalence of bounded derived categories of graded modules over a polynomial algebra and an exterior algebra, respectively. By using Eisenbud, Fløystad and Schreyer's [3] explicit formulation of the BGG correspondence, we were able to generalize some previous work of Schenck and Suciu [6] from the first to the higher resonance varieties: definitions follow below.

Various interrelated spectral sequences appear when the BGG correspondence is applied. In particular, these give convenient language to talk about syzygies in minimal, graded free resolutions. On the other hand, work of Jan-Erik Roos [5] and Maurice Auslander[2] gives a filtration of a module over a regular ring with supports that decrease in dimension, via a suitable Grothendieck spectral sequence. We considered the interplay between this filtration (in the case of polynomial algebras) and the BGG correspondence. We obtained some specific results that, in particular, relate the growth of Betti numbers in free resolutions of cohomology algebras (as modules over the exterior algebra) to the dimensions of components of resonance varieties.

More precisely, a hyperplane arrangement $\mathcal{A}$ is a finite collection of n hyperplanes in some fixed (usually complex) vector space V of dimension ℓ. The complement $X = V - \mathcal{A}$ can be viewed as the intersection of a torus $(\mathbb{C}^*)^n$ with a linear space: accordingly, for any field $\Bbbk$, there is a map onto $A = H^*(X, \Bbbk)$ from the cohomology ring of the torus, the exterior algebra $E = \Lambda(\Bbbk^n)$. A result of Eisenbud, Popescu and Yuzvinsky [4] shows that the cohomology algebra A, regarded as a graded E-module, has a minimal injective resolution which is linear, in the sense that the differentials in the resolution can be expressed as matrices with degree-1 entries. Interpreted via the BGG correspondence, there is a certain "dual" module $F(X)$, over the polynomial algebra $S = \mathrm{Sym}((\Bbbk^n)^*)$, which also possesses a linear resolution

$$0 \leftarrow F(X) \leftarrow H^{\ell}(X, \Bbbk) \otimes_{\Bbbk} S \leftarrow H^{\ell-1}(X, \Bbbk) \otimes_{\Bbbk} S \leftarrow \cdots \leftarrow H^0(X, \Bbbk) \otimes_{\Bbbk} S \leftarrow 0 \tag{52.1}$$

where the differential is given by multiplication by a tautological element of degree $(1, 1)$.

By definition, the kth resonance variety (over $\Bbbk$) of a space X having the homotopy type of a finite CW-complex is given pointwise by

$$R^k(X) = \{a \in A^1 \colon H^k(A^{\cdot}, a) \neq 0\},$$

where $(A^{\cdot}, a)$ denotes the cochain complex obtained from the cohomology algebra A of X with differential given by multiplication by the 1-cocycle a. Under certain hypotheses, the resonance varieties parameterize (infinitesimal versions of) one-dimensional local systems on X with non-vanishing cohomology. If the exterior algebra acts on A, as it does in the cases we consider, these are also the rank varieties of A, as introduced by Avramov, Aramova and Herzog in [1].

For spaces X possessing a linear complex of the form (52.1) (such as arrangement complements or the classifying spaces of certain right-angled Artin groups), one can extract information about the resonance varieties by specializing the complex (52.1). This was first noticed in [6], where Schenck and Suciu prove that, for arrangements, the first resonance variety is given by

$$R^1(X) = V(\mathrm{ann}(\mathrm{Ext}_S^{\ell-1}(F(X), S))).$$

More generally, we noted that the higher resonance variety

$$R^k(X) = \bigcup_{p \leq k} V(\mathrm{ann}(\mathrm{Ext}_S^{\ell-p}(F(X), S))).$$

for $k \geq 1$. Since the modules $\mathrm{Ext}^{\cdot}_S(F(X), S)$ are, roughly speaking, BGG-dual to a minimal free resolution of A as an E-module, we obtain a link between syzygies of A and the geometry of higher resonance varieties. Going somewhat further, we see that for certain classes of arrangements, some syzygies can be understood in terms of the combinatorics of the hyperplane arrangement. Correspodningly, this leads to an explicit description of the resonance varieties in those cases. A preprint is in preparation.

List of Participants

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Chapter 53

Investigating graphs with odd cycles via commutative algebra (08rit124)

May 25 - Jun 01, 2008

Organizer(s): Chris Francisco (Oklahoma State University), Tai Ha (Tulane University), Adam Van Tuyl (Lakehead University)

Background

Our work over the last few years has focused on building bridges between commutative algebra and graph theory. We associate monomial ideals to graphs to try to understand the structure of graphs and algebraic implications of different features of graphs [7, 8, 11], and this correspondence helps us use knowledge of graphs to study purely algebraic questions [6]. As a result of this work and computational experiments using computer algebra systems, we became interested in questions related to perfect graphs.

We recall a few terms from graph theory. We will work with simple graphs, i.e., those with no loops or multiple edges. A subgraph H of a graph G is an induced subgraph if for any vertices x and y of H, x and y are connected by an edge in H if and only if they are connected by an edge in G. The chromatic number of a graph G, denoted $\chi(G)$, is the smallest number of colors needed to color the vertices of G so that no two adjacent vertices have the same color. The clique number of a graph G, denoted by $\omega(G)$, is the number of vertices in the largest complete subgraph of G. Combining these notions, a perfect graph is a graph in which every induced subgraph has its clique number equal to its chromatic number.

Perfect graphs are a focal point of research in graph theory. Not only do they provide the setting for theoretical results about cliques and colorings, but they also represent efficient networks. A *Science* article [15] gives the following explanation: Let the vertices of a graph be cell-phone transmitters in a network with two transmitters connected by an edge if and only if their ranges overlap. One wants to use different channels when the ranges overlap, and this is equivalent to assigning different colors to adjacent vertices. A perfect graph has the smallest possible number of colors, maximizing efficiency.

Attempts to characterize perfect graphs occupied graph theory for over four decades, culminating in the proof of the Strong Perfect Graph Theorem in 2002 [3]; this theorem says that a graph is perfect if and only if neither G nor its complement G^c contains an odd hole, i.e., an odd induced cycle of cardinality at least five. Subsequently, Chudnovsky, Cornuéjols, Liu, Seymour, and Vušković proved the existence of a polynomial time algorithm to determine if a graph is perfect [2]. If G is not perfect, however, this algorithm does not tell whether it is G or G^c that contains an odd hole, and it is still not known whether one can detect the existence of an odd hole in polynomial time.

We began to investigate related questions in our paper [8]. The edge ideal of a graph G is a monomial ideal $I(G) \subset R = k[x_1, \ldots, x_n]$ generated by all x_ix_j such that the vertices x_i and x_j are connected by an edge in G. (We use x_i to denote both a vertex of G and an indeterminate in $k[x_1, \ldots, x_n]$ for notational convenience to make the correspondence between G and $I(G)$ clear.) The Alexander dual of $I(G)$ is an ideal J formed by intersecting all ideals (x_i, x_j), where $\{x_i, x_j\}$ is an edge of G; the minimal generators of J correspond to the minimal vertex covers of G, and thus J is often called the cover ideal of G. The set of associated primes of an R-module M, denoted by Ass(M), are the prime ideals P of R such that P is the annihilator of some element of M. When $M = R/I$, where I is a monomial ideal, all associated primes are generated by subsets of $\{x_1, \ldots, x_n\}$. Our main result in [8] is:

Theorem 1. Let G be a simple graph with cover ideal J. Then $P \in$ Ass(R/J^2) if and only if:

- $P = (x_i, x_j)$, where $\{x_i, x_j\}$ is an edge of G, or
- $P = (x_{i_1}, \ldots, x_{i_{2b+1}})$, where the induced graph on $x_{i_1}, \ldots, x_{i_{2b+1}}$ is an odd cycle.

This enables us to detect all odd induced cycles and, in particular, all odd holes of a graph using a simple algorithm from commutative algebra. Consequently, we can determine immediately whether a graph is perfect, and if it is not, our algorithm tells explicitly where the odd hole is in G or G^c. The paper [8] also contains other algebraic means for detecting odd holes, including using colon operations, arithmetic degree, and regularity.

Scientific Progress Made

The Research In Teams week enabled the three of us, who live far enough apart that we are rarely all together, to spend an intensive week working in a collaborative environment. We found that we made progress much more quickly with all three of us in the same room rather than trying to attack the problems on our own and sending incremental accomplishments to each other via e-mail.

In our paper [8], we emphasized finding algorithms using algebra that enabled us to study important properties of graphs related to the Strong Perfect Graph Theorem. While at BIRS, we took a different approach, trying to understand how to interpret underlying structure of perfect graphs (or obstructions to being perfect) algebraically. In particular, we were interested in how the notion of colorability appears in the algebra. Our first major result gives a simple algebraic method for determining the chromatic number $\chi(G)$ of a graph G.

Theorem 2. Let G be a simple graph with cover ideal $J \subset k[x_1, \ldots, x_n]$, and let $m = x_1 \cdots x_n$. Then $\chi(G) \leq d$ if and only if $m^{d-1} \in J^d$.

Consequently, to compute the chromatic number, one needs only to find the smallest d for which $m^{d-1} \in J^d$. This is easy to do for graphs with a reasonable number of vertices in a computer algebra system like Macaulay 2 [14].

We were particularly interested in finding generalizations of Theorem 1 by understanding the associated primes of R/J^s for $s > 2$. When G is an odd cycle, we have Ass(R/J^2) =Ass(R/J^s) for all $s > 2$, but in general, one can get additional associated primes for higher powers. Computational experiments in Macaulay 2 suggested that the new primes were related to the chromatic number of induced subgraphs of G, and we made significant progress in determining how these primes arise. We have two main results relating the chromatic number and the associated primes of R/J^s.

Theorem 3. Let G be a simple graph with cover ideal J. Suppose $P \in$ Ass(R/J^d), and let G_P be the induced subgraph of G on the vertices that correspond to minimal generators of P. Then $\chi(G_P) \leq d + 1$.

Thus the associated primes of G_P cannot show up "too early," meaning that a prime corresponding to an induced subgraph with large chromatic number is never associated to R/J^s for small s. Conversely, we can also tell exactly at which power some primes are first associated.

Theorem 4. Let G be a simple graph with cover ideal J. Let P be a monomial prime ideal such that $\chi(G_P) = d + 1$.

(a) If all induced subgraphs of G_P have chromatic number $\leq d$, then $P \in$ Ass(R/J^d), and $P \notin$ Ass(R/J^e) for $e < d$. In addition, if G_P is a clique, odd hole, or odd antihole, then $P \in$ Ass(R/J^s) for all $s \geq d$.

(b) If there exists $x \in P$ such that $\chi(G_{P\setminus\{x\}}) = d+1$, then $P \notin \mathrm{Ass}(R/J^d)$.

We are working on extending these results to understand completely which primes are associated to R/J^s, but this seems to be a difficult problem. Two particularly interesting questions are whether $\mathrm{Ass}(R/J^s) \subseteq \mathrm{Ass}(R/J^{s+1})$ for all s, and what is the smallest integer a such that

$$\bigcup_{s=1}^{\infty} \mathrm{Ass}(R/J^s) = \bigcup_{s=1}^{a} \mathrm{Ass}(R/J^s);$$

such an integer must exist by a theorem of Brodmann [1]. We know what happens in special cases, particularly in cases where we can use degree arguments because the structure of the graph is relatively simple, but not for arbitrary graphs. Initially, we hoped that the chromatic number might provide a bound for the power at which the associated primes stabilize, but during our week at BIRS, we found some counterexamples, and we are trying to prove that we have an infinite family of examples showing that the value of a can be arbitrarily larger than the chromatic number. We believe that when G is perfect, the situation is much nicer, and one should get no associated primes other than those described in Theorem 4(a). Ultimately, we hope to understand underlying characteristics of perfect graphs from a more algebraic perspective, and we think Theorems 2-4 are the foundation for such an approach.

In a different direction, we took some time at the end of our stay at BIRS to find combinatorial applications of some ideas we had first thought about in 2006. Our goal was to generalize work of Eliahou and Kervaire from 1990 [4] that has been used to study, for example, stable ideals [4], ideals of fat points [5], and ideals corresponding to graphs and hypergraphs [12, 13]. We had earlier found convenient sufficient conditions on monomial ideals $I = J + K$, where the minimal generators of I are the disjoint union of those of J and K, such that for all i and multidegrees j, we have a formula for the graded Betti numbers:

$$\beta_{i,j}(I) = \beta_{i,j}(J) + \beta_{i,j}(K) + \beta_{i-1,j}(J \cap K).$$

This "splitting" formula enables one to compute graded Betti numbers recursively, and the fact that all the coefficients are positive makes this approach particularly useful for computing bounds on the Betti numbers. We discovered an iterative method of computing the graded Betti numbers of cover ideals of Cohen-Macaulay bipartite graphs using this splitting technique; it appears in our paper [10].

Our work is often inspired by computer experiments, and thus we thought it would be helpful to make the code we have written available to other researchers with similar interests. With Andrew Hoefel, a PhD student at Dalhousie University, Francisco and Van Tuyl are writing a package for Macaulay 2 entitled "EdgeIdeals." The package contains methods for working with graphs and, more generally, hypergraphs, using algorithms from commutative algebra. We have a number of functions that are based on our work both in [8] and [9]; in particular, the method we use for computing the chromatic number was developed while at BIRS. Researchers will be able to use our code as the basis for their own experiments on graphs and hypergraphs without having to develop from scratch methods of handling these combinatorial objects in a computer algebra system originally written primarily for commutative algebra and algebraic geometry.

We have three papers that arose at least partially from this meeting. We were able to finish our paper [8] on algebraic methods for detecting odd holes in graphs, and we have since submitted it for publication. Having all three coauthors in the same room made it much faster to discuss revisions to a draft we had written prior to the meeting. We also added a section to the paper that led directly to the work on which we spent the majority of our RIT week. We are continuing our work on algebraic aspects of vertex colorings of graphs and have much of a paper written [9]. We will likely submit it by the end of the year. The combinatorial applications of our splitting ideas enabled us to finish the paper [10], and it has been submitted for publication. We also anticipate the Macaulay 2 EdgeIdeals package will be ready by the end of this year.

We had an exciting and productive stay at BIRS, and we greatly appreciate both the opportunity to come to BIRS and the outstanding hospitality of the BIRS staff. It is truly a magnificent place to do mathematics, and the RIT program fit our needs perfectly.

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Chapter 54

Discrete integrable systems in projective geometry (08rit125)

May 18 - May 25, 2008

Organizer(s): Valentin Ovsienko (Centre National de la Recherche Scientifique, Institut Camille Jordan, Universite Claude Bernard Lyon 1), Sergei Tabachnikov (Pennsylvania State University)

The notion of integrability is one of the central notions in mathematics. Starting from Euler and Jacobi, the theory of integrable systems is among the most remarkable applications of geometric ideas to mathematics and physics in general.

Discrete integrable systems is a new and actively developing subject, hundreds of new articles in this field are written every year by mathematicians and physicists. However, geometric interpretation of most of the discrete integrable systems considered in the mathematical and physical literature is unclear.

The main purpose of this Workshop was to study one particular dynamical system called the *pentagram map*. The interest in this map is motivated by its natural geometric meaning and aestetical attractiveness. The pentagram map was introduced in [2], and further studied in [3] and [4]. Originally, the map was defined for convex closed n-gons. Given such an n-gon P, the corresponding n-gon $T(P)$ is the convex hull of the intersection points of consequtive shortest diagonals of P. Figure 54.1 shows the situation for a convex pentagon and a convex hexagon.

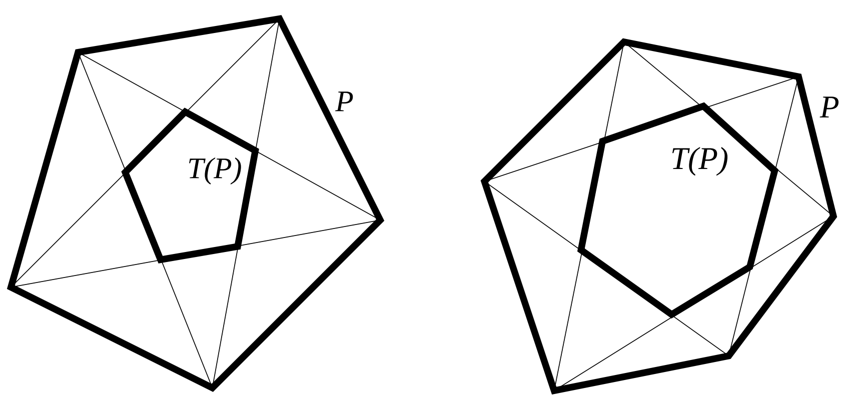

Figure 54.1: The pentagram map defined on a pentagon and a hexagon

Computer experiments suggested that the pentagram map is a completely integrable systems. Indeed, this was conjectured in [4].

The goal of this Workshop was to prove the integrability conjecture, but first one had to develop an adequate framework. Rather than work with closed n-gons, we worked with what we call *twisted n-gons*. A twisted n-gon is a map $\phi : \mathbb{Z} \to \mathbb{R}P^2$ such that that

$$\phi(k+n) = M \circ \phi(k); \quad \forall k.$$

Here M is some projective automorphism of $\mathbb{R}P^2$ called the *monodromy*.

It is a powerful general idea of projective differential geometry to represent geometrical objects in an algebraic way. It turns out that the space of twisted n-gons is naturally isomorphic to a space of difference equations. Given two arbitrary n-periodic sequences $(a_i),\ (b_i)$ with $a_i, b_i \in \mathbb{R}$ and $i \in \mathbb{Z}$, such that $a_{i+n} = a_i,\ b_{i+n} = b_i$, one associates to these sequences a difference equation of the form

$$V_{i+3} = a_i\, V_{i+2} + b_i\, V_{i+1} + V_i,$$

A solution $V = (V_i)$ is a sequence of numbers $V_i \in \mathbb{R}$ satisfying this equation. Such an interpretation provides a global coordinate system $(a_i,\ b_i)$ on the space of twisted n-gons.

The main result obtained during and in the summer after the Workshop is as follows. It is proved that there exists a Poisson structure on the space of twisted n-gons, invariant under the pentagram map. The monodromy invariants Poisson-commute. This provides the classical Arnold-Liouville complete integrability of the pentagram map.

The pentagram map is expressed in the coordinates $(a_i,\ b_i)$ by a beautiful combinatorial formula:

$$T : a_i \mapsto a_{i+2} \prod_{k=1}^{m} \frac{1 + a_{i+3k+2}\, b_{i+3k+1}}{1 + a_{i-3k+2}\, b_{i-3k+1}}, \qquad T : b_i \mapsto b_{i-1} \prod_{k=1}^{m} \frac{1 + a_{i-3k-2}\, b_{i-3k-1}}{1 + a_{i+3k-2}\, b_{i+3k-1}}.$$

The T-invariant Poisson bracket is defined on the coordinate functions as follows.

$$\begin{aligned} \{a_i, a_j\} &= \sum_{k=1}^{m} (\delta_{i,j+3k} - \delta_{i,j-3k})\, a_i\, a_j, \\ \{a_i, b_j\} &= 0, \\ \{b_i, b_j\} &= \sum_{k=1}^{m} (\delta_{i,j-3k} - \delta_{i,j+3k})\, b_i\, b_j. \end{aligned}$$

It is also proved that the continuous limit of the pentagram map is precisely the classical Boussinesq equation which is one of the most studied infinite-dimensional integrable systems. Moreover, the above Poisson bracket is a discrete analog of the well known first Poisson structure of the Boussinesq equation.

The results obtained during the Workshop and developed after led to a preprint [1].

List of Participants

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Tabachnikov, Sergei (Pennsylvania State University)

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Chapter 55

Derived Category Methods in Commutative Algebra (08rit132)

Jun 01 - Jun 08, 2008

Organizer(s): Lars Christensen (Texas Tech University), Hans-Bjorn Foxby (University of Copenhagen)

This is our report on the Research in Teams Workshop "Derived Category Methods in Commutative Algebra" held at Banff International Research Station (BIRS), 1–8 June 2008.

Background

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.

History of the book project

As one of the pioneers in the applications of derived category methods in commutative algebra, Foxby has previously circulated two sets of lecture notes on the topic [17, 13].

In 2006 Christensen and Foxby started the current project. The book in progress offers a systematic development of hyperhomological algebra. This includes the construction of the derived category of a general (associative) ring and a careful study of the functors of importance in ring theory. To demonstrate the strength and utility of the theory, and to motivate the choice of topics, the book includes an extensive course in central homological aspects of commutative ring theory. This part includes many recent results, which were discovered by means of derived category methods, and gives valuable new insight into the theory of commutative rings and their modules.

Based on four peer reviews, Springer-Verlag offered to publish the book, and a contract was signed in late 2007.

For health related reasons, Foxby has been unable to work on the project for some time. To ensure timely completion of the book, Christensen and Foxby decided to add a third author, and in April 2008 Holm accepted to joint the project.

Aim and results of the workshop

The workshop at BIRS had two purposes. To introduce the new coauthor Holm to the project, and to complete a first rough draft of the manuscript—taking into account the extensive comments in the reports solicited by Springer-Verlag.

The first three days of the workshop were spent on a major reorganization of the manuscript based on the referees' suggestions and feedback from students and colleagues. This reorganization serves two purposes:

- To make the book more useful as a reference to derived category methods also for researchers in non-commutative algebra.
- To structure the applications to commutative algebra in a fashion more familiar to researchers in that field.

This process was an excellent way to introduce Holm to the scientific as well as the technical and administrative aspects of the book project.

The balance of the workshop was spent on discussions and "prototyping" aimed at merging contributions from the different authors into a coherent text. This includes

- Laying down principles for indexing and cross-referencing
- Standardizing formulations of mathematical statements
- Homogenizing levels of abstraction between chapters
- Homogenizing levels of details in proofs

As the workshop participants live on different continents, and in different time zones, face-to-face meetings as provided by this workshop are of utmost importance for solving scientific as well as editorial problems. We thank BIRS sincerely for providing us with this opportunity.

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Christensen, Lars (Texas Tech University)
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Chapter 56

String Cosmology (08rit128)

Jun 15 - Jun 22, 2008

Organizer(s): Cliff Burgess (Conseil Européen pour la Recherche Nucléaire, McMaster University and Perimeter Institute)

Overview of the Field

String cosmology has experienced an explosion of interest over the past few years, partly because of the recent flood of precise cosmological observations, and partly due to the advent of new theoretical tools for fixing moduli in string vacua.

The new observations have pinned down the properties of the observed early universe and in so doing have revealed two startling features. First, by allowing for the first time the measurement of the total energy budget of the universe, these observations have revealed the existence of two new, still not understood, forms of matter (Dark Matter and Dark Energy) which together make up 95% of what is out there. Second, they provide the beginnings of hard evidence for the existence of a previously-undetected very early 'inflationary' epoch of the universe, during which its size increased in an accelerated way.

Both of these discoveries potentially change our picture of the laws of nature in a fundamental way, since both imply the existence of new kinds of particles and interactions that have hitherto gone undetected in experiments on Earth. As a result they have engaged the attention of string theorists, who study our best-formulated theory of how nature works at its most fundamental level. The relatively new field of string cosmology aims to try to see if string theory can explain the Dark Matter and Dark Energy, and to see if it can account for why the universe might have undergone a very early epoch of inflationary expansion. Success in either of these directions could provide the first real experimental tests of string theory, which are so far lacking in particle physics experiments.

Because string theory is such a tightly constrained mathematical structure it has proven to be very challenging to build successful models of cosmology within the framework of reliable and fully consistent calculations. Although it is unlikely that the observations by themselves can decisively determine whether it is string theory or another more conventional field theory that is at work in cosmology, the preliminary goal in the meantime is to better focus the strategies for experimental verification by seeing what is suggested by a combination of the known experimental constraints and those imposed from the need for internal mathematical consistency. It is also hoped that this process will shed further light on the difficult and more general problem of finding time-dependent solutions to the string equations.

Considerable progress in both of these directions has been made over the last few years (partly by the participants in the present application) in building inflationary models based on specific Calabi-Yau threefold compactifications of the extra dimensions of string theory. The key for making this progress has been the newly developed understanding of how moduli can be stabilized in string theory, since the understanding of the low-energy scalar potential to which this leads is a prerequisite for developing an understanding of cosmology. The most rigorous calculations yet made of the inflationary potential have been done in this framework, and bring us closer to being able to use cosmology as a test of string theory (as opposed to merely 'string-inspired' models).

Recent Developments and Open Problems

There were two lines of development that were the most pertinent for the purposes of our workshop. The first of these was the improving precision with which it has been possible to construct viable brane inflationary models using explicit string constructions. The second concerns the emergence of potentially 'stringy' predictions that might be used to characterize string-generated inflation from inflation obtained from other sources.

Regarding the precision of the explicit models, the most precise of existing constructions use branes that roll down the extended warped geometrical throats that often arise in Type IIB string compactifications with fluxes [1]. However problematic issues still do arise even in this case, such as to do with the manner in which supersymmetry is broken. In particular, breaking supersymmetry using an antibrane can lead to loss of control over some of the approximations made, placing a premium on the search for supersymmetry breaking mechanisms (such as breaking using D-branes) that do not rely on the use of antibranes.

A related issue asks how generic inflation is for such vacua, and seeks to extend our understanding in two ways. First, one can further explore the known parameter space in warped-throat models to seek to identify whether parameters in the scalar potential must be finely tuned to achieve a slow enough cosmic expansion. Second, one can try to extend the tools used in warped-throat models to other systems for which similar calculational control might be possible, to see how representative the warped-throat situation really is.

Regarding the issue of observable signals, it was recently observed that all of the extant string-inflationary models predict an unobservably small amplitude of primordial gravitational waves, suggesting that any eventual detection of these waves could be used as a way to falsify the string-inflationary picture.

Scientific Progress and Outcome of the Meeting

Our daily discussions of these issues was very spirited and stimulating. We decided to divide our time between thrashing out the various conceptual issues in group discussions, and time spent separately calculating in order to take advantage of the lack of other distractions while at BIRS. This proved to be a very fruitful way to proceed, as we all have slightly different and very complementary expertise. We were able to identify several ways forward on all of the above issues. These ultimately led to several calculations that we have since carried through together and with other collaborators.

- Regarding the issue of the robustness of warped-throat inflationary models, two papers emerged from our discussions. The first of these [2] pursues the precise models explored earlier, in ref. [1], but extends the breadth of the parameter space that was compared with cosmological observations, applying the COBE normalization and constraint on the spectral index. This paper improves on previous treatments of uplifting by antibranes, and show that the contributions from noninflationary throats play an important role in achieving a flat inflationary potential. To quantify the degree of fine-tuning needed by the model, an effective volume is defined in the part of parameter space which is consistent with experimental constraints, and using Monte Carlo methods to search for a set of optimal parameters, it is shown that the degree of fine-tuning is alleviated by eight orders of magnitude relative to a fiducial point which has previously been considered. In fact, close to the optimal parameter values, fine-tuning is no longer needed for any of the parameters. In this natural region of the parameter space, larger values of n_s close to 0.99 (still within 2 sigma of the WMAP5 central value) are favored, giving a new aspect of testability to the model.
- The related issue of how to use D-terms to break supersymmetry in these throats, rather than using antibranes, was explored in ref. [3]. This paper tries to embed this kind of breaking more explicitly into string-generated throats, without concentrating directly on the cosmological implications. In particular, it derives a novel deformation of the warped resolved conifold background with supersymmetry

breaking ISD (1,2) fluxes by adding D7-branes to this type IIB theory. Spontaneous supersymmetry breaking is found without generating a bulk cosmological constant. In the compactified form, the background geometry is not a Calabi-Yau manifold, since it allows a non-vanishing first Chern class. It is the presence of the (1,2) fluxes in the presence of D7-branes that gives rise to non-trivial D-terms. The Ouyang embedding of D7-branes is studied in detail and it is found that in this case the D-terms are indeed non-zero. In the limit where the singular conifold is approached, the D-terms vanish for Ouyang's embedding, although supersymmetry appears to be broken nevertheless. The F-theory lift of this background is also constructed, and demonstrates how these IIB (1,2) fluxes lift to non-primitive (2,2) flux on the fourfold. The seven branes correspond to normalizable harmonic forms. A possible way to attain an inflaton potential in this background is briefly described once extra D3-branes are introduced, and some possibilities for restoring supersymmetry in the background are also considered that could in principle be used as the end point of an inflationary set-up.

- Our attempts to generalize the constructions to other string vacua led us to investigate in detail the motion of D3 branes within a K3 x T2/Z2 compactification in the presence of D7 and O7 planes, since this does not involve warped throats but the flatness of the T2 does give the potential for accommodating shallow potentials. Our paper exploring this system [4] works within the effective 4D supergravity describing how the mobile D3 interacts with the lightest bulk moduli of the compactification, including the effects of modulus-stabilizing fluxes. Inflationary solutions to the resulting equations were sought numerically, in order to avoid resorting to approximate parameterizations of the low-energy potential. We considered supersymmetry breaking from both D-terms and from anti-D3 branes. Examples of slow-roll inflation (with anti-brane uplifting) were found with the mobile D3 moving along the toroidal directions, falling towards a D7-O7 stack starting from the antipodal point. The inflaton turns out to be a linear combination of the brane position and the axionic partner of the K3 volume modulus, and the similarity of the potential along the inflaton direction with that of racetrack inflation led to the prediction $n_s \leq 0.95$ for the spectral index. The slow roll is insensitive to most of the features of the effective superpotential, and requires a one-in-10^4 tuning to ensure that the torus is close to square in shape. We also considered D-term inflation with the D3 close to the attractive D7, but found that for a broad (but not exhaustive) class of parameters the conditions for slow roll tended to destabilize the bulk moduli. In contrast to the axionic case, the best inflationary example of this kind required the delicate adjustment of potential parameters (much more than a part in a thousand, and gave inflation only at an inflection point of the potential (and so suffered from additional fine-tuning of initial conditions to avoid an overshoot problem).

- Finally, we pursued two lines of inquiry to determine whether string models really do preclude the existence of primordial gravitational waves. We were able to find two classes of examples which do. One of these, as described in ref. [5], examines wrapped branes in string compactifications where a monodromy is introduced that extends the field range of individual closed-string axions to beyond the Planck scale, but uses approximate shift symmetries of the system to control corrections to the axion potential. The result is a general mechanism for chaotic inflation driven by monodromy-extended closed-string axions. This possibility was systematically analyzed, with the result that the mechanism was shown to be compatible with moduli stabilization and could be realized in many types of compactifications, including warped Calabi-Yau manifolds and more general Ricci-curved spaces. In this broad class of models, the effective low-energy potential turns out to be linear in the canonical inflaton field, predicting a tensor to scalar ratio r=0.07 accessible to upcoming observations.

  The other approach [6] instead uses a class of vacua that arise naturally in large-volume compactifications of IIB string theory with moduli stabilisation, and takes advantage of the generic existence there of Kahler moduli whose dominant appearance in the scalar potential arises from string loop corrections to the Kahler potential. The inflaton field is taken to be a combination of Kahler moduli of a K3-fibered Calabi-Yau manifold. There are likely also to be a great number of models in this class in which the inflaton starts off far enough up the fibre to produce observably large primordial gravity waves.

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Chapter 57

Schur quasisymmetric functions and Macdonald polynomials (08rit138)

Jul 20 - Jul 27, 2008

Organizer(s): Jim Haglund (University of Pennsylvania), Stephanie van Willigenburg (University of British Columbia)

Overview of the Field

The study of Macdonald polynomials is one of the most active current areas of research in the area of algebraic combinatorics. It exhibits natural ties with many areas of mathematics such as algebraic geometry, representation theory, and quantum computation. For example, in the mid 1990's Cherednik showed that nonsymmetric Macdonald polynomials are intimately connected to the representation theory of double affine Hecke algebras, and resolved the "Macdonald constant term-conjectures" for arbitrary root systems [2]. Another example is the work of Haiman, who showed that there are deep connections between algebraic geometry, the representation theory of the space of diagonal harmonics, and the the theory of Macdonald polynomials. He was awarded the 2004 Moore AMS prize for this work [5].

Quasisymmetric functions, like Macdonald polynomials, is another area of strong activity in algebraic combinatorics that appears in a number of mathematical areas. More precisely, the Hopf algebra Qsym of quasisymmetric functions was introduced by Gessel in the early 1980's as a source of generating functions for Stanley's P-partitions [4]. Since then, quasisymmetric functions have appeared in many contexts. In particular, in the 1990's it transpired that the Hopf algebra of quasisymmetric functions is a terminal object in the category of graded Hopf algebras equipped with a zeta-function [1].

Connecting these two areas in a natural way are the symmetric functions known as Schur functions, which are both refined by quasisymmetric functions and generalized by Macdonald polynomials that are, in fact, symmetric functions with additional parameters that naturally generalize Schur functions. Schur functions are often considered to be the source of the area of algebraic combinatorics since the work of Schur and Frobenius on the representation theory of the symmetric group over 100 years ago. Their impact has been felt in the fields of algebraic geometry via classical Schubert calculus, representation theory through the symmetric group, and enumerative combinatorics as the generating function of tableaux. Their impact continues to be felt today through the work of Field's medalists such as Tao [6].

Recent Developments and Open Problems

Recently Haglund-Mason-van Willigenburg discovered certain linear combinations of nonsymmetric Macdonald polynomials that are quasisymmetric functions, called Schur quasisymmetric functions. These functions not only form a new basis for Qsym, but also naturally refine Schur functions. This raises the exciting question of what properties of Schur functions extend to these Schur quasisymmetric functions? Desirable properties would include combinatorial descriptions of the product of two such functions, in particular, the existence of Pieri rules and Littlewood-Richardson rules that refine the classical rules.

During the BIRS workshop "Applications of Macdonald Polynomials" members of our group discovered a potential Pieri rule for multiplying a simple Schur function and a Schur quasisymmetric function and proved the rule for a special case. From this initial breakthrough we proved such a Pieri rule, and consequently conjectured a Littlewood-Richardson rule for multiplying any Schur function and a Schur quasisymmetric function.

Therefore, our aim for our Research in Teams was to prove the aforementioned Littlewood-Richardson rule, and extend it to the analogous product of a Schur function and a Demazure atom; and to the analogous product of a Schur function and a Demazure character.

Scientific Progress Made

During the week we proved the following three theorems by exploiting the proof of the classical Littlewood-Richardson rule found in [3].

- There exists a Littlewood-Richardson rule for the product of a Schur function and a Demazure atom, in which the fundamental objects of enumeration are all Littlewood-Richardson skyline tableaux of certain extended basement *weak* composition shape whose reading word is contrelattice.

From the natural relationship between Demazure atoms and Schur quasisymmetric functions we were immediately able to deduce

- There exists a Littlewood-Richardson rule for the product of a Schur function and a Schur quasisymmetric function, in which the fundamental objects of enumeration are all Littlewood-Richardson skyline tableaux of certain extended basement composition shape whose reading word is contrelattice.

By constructing a bijection between particular ordered pairs involving Littlewood-Richardson key tableaux, and Littlewood-Richardson skyline tableaux we also proved

- There exists a Littlewood-Richardson rule for the product of a Schur function and a Demazure character, in which the fundamental objects of enumeration are all Littlewood-Richardson key tableaux of certain extended basement weak composition shape whose reading word is contrelattice.

This latter result was particularly exciting as special cases of it include a classical Littlewood-Richardson rule, and a rule for multiplying a Schur function and a Schubert polynomial.

Outcome of the Collaboration

Further to completing our project from which a journal article will result, we also learned a range of techniques and relationships between our areas of expertise, through informal lectures we gave to each other.

Additionally, the concurrent 5-day workshop "Quantum Computation with Topological Phases of Matter" gave our group a rare chance to interact with mathematical physicists whose research also involves specific instances of Macdonald polynomials, known as Jack polynomials. This interaction included both conversing during the lecture breaks and attending relevant seminars.

We would like to thank BIRS for this invaluable Research in Teams opportunity, without which our project would have taken many more months to complete.

List of Participants

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Chapter 58

Finiteness problems in arithmetic deformation theory (08rit135)

Jul 27 - Aug 03, 2008

Organizer(s): Frauke Bleher (University of Iowa), Ted Chinburg (University of Pennsylvania)

Overview of the project

Deformation theory pertains to the local behavior of moduli spaces. One example which has been very fruitful in solving various problems in number theory concerns deformations of Galois representations. Here one starts with a representation of a Galois group over a field of characteristic $p > 0$, and one tries to lift this representation over local rings having this field as their residue field [4].

We have been studying a generalization of this deformation theory in which one replaces a single representation by a complex of modules for an arbitrary profinite group [1]. Such complexes arise naturally in arithmetic geometry, e.g. from the action of Galois groups on the hypercohomology of etale sheaves.

Our main goal has been to prove finiteness theorems for universal deformations arising from arithmetic. We have shown in various interesting cases that the universal deformation of a complex of modules for a profinite group can be realized by a bounded complex of modules having terms which are finitely generated over the associated universal deformation ring. When this is true, one has much stronger methods for determining the deformation ring.

To study such finiteness problems, one would like to have an obstruction theory for deformations of complexes. We have been working on developing such an obstruction theory with Luc Illusie, following a suggestion of Ofer Gabber. Gabber's method is very concrete. Illusie proposed that it should be understood in the context of the low degree terms in a spectral sequence, as in his work on cotangent complexes in [3].

Outcome of the research in teams workshop

We spent most of the week attempting to reconcile Gabber's approach with the spectral sequence method of Illusie. For background on spectral sequences, see [2, §11]. We came to the following conclusions:

A. Usually when one speaks of the exact sequence of low degree terms associated to the spectral sequence of a bicomplex $L^{\bullet,\bullet}$, one assumes that the terms of $L^{\bullet,\bullet}$ are in the first quadrant. However, the $L^{\bullet,\bullet}$ which arises in our problem will not in general have all of its terms in the first quadrant.

B. We found that the correct object to focus on is the 0^{th} term [4]$F_I^0 H^1(\mathrm{Tot}(L^{\bullet,\bullet}))$ of the first filtration of the first cohomology of the total complex of $L^{\bullet,\bullet}$ rather than the entire first cohomology group

$H^1(\mathrm{Tot}(L^{\bullet,\bullet}))$. One does have a short exact sequence of low degree terms

$$0 \to E_\infty^{1,0} \to F_I^0 H^1(\mathrm{Tot}(L^{\bullet,\bullet})) \to E_\infty^{0,1} \to 0$$

arising from the first filtration spectral sequence associated to $L^{\bullet,\bullet}$.

C. We proved that in fact, $F_I^0 H^1(\mathrm{Tot}(L^{\bullet,\bullet}))$ is exactly the subgroup of [4]$H^1(\mathrm{Tot}(L^{\bullet,\bullet}))$ which is defined by exact sequences of the kind considered by Gabber when defining lifting obstructions. This unified the approaches of Gabber and Illusie in a very satisfactory way. The tools we developed for showing this result should be very useful in carrying out computations pertaining to the finiteness problem discussed in §1.

List of Participants

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Chapter 59

The Rate of Convergence of Loop-Erased Random Walk to SLE(2) (08rit136)

Aug 24 - Aug 31, 2008

Organizer(s): Christian Benes (Brooklyn College of the City University of New York), Michael Kozdron (University of Regina)

Overview of the field

In 2000, O. Schramm [4] introduced a one-parameter family of random growth processes in two dimensions which he called the *stochastic Loewner evolution* (now also called the *Schramm-Loewner evolution*) or SLE. In the past several years, SLE techniques have been successfully applied to analyze a variety of two-dimensional statistical mechanics models including percolation, the Ising model, the Q-state Potts model, uniform spanning trees, loop-erased random walk, and self-avoiding walk. Furthermore, SLE has provided a mathematically rigorous framework for establishing predictions made by conformal field theory (CFT), and much current research is being done to further strengthen and explain the links between SLE and CFT.

The importance of proving predictions about such models made by conformal field theory in a rigorous mathematical sense was acknowledged when W. Werner was awarded a Fields medal in 2006 for "his contributions to the development of stochastic Loewner evolution, the geometry of two-dimensional Brownian motion, and conformal field theory." Although there is knowledge of the scaling limit in the aforementioned models, there is essentially nothing known about the rates of convergence of any of these discrete models to SLE. In fact, this mathematically important open problem was communicated by Schramm in his plenary lecture at the International Congress of Mathematicians in Madrid in 2006: "Obtain reasonable estimates for the speed of convergence of the discrete processes which are known to converge to SLE." (See [5], page 532.)

Therefore, the objective of our *Research In Teams* meeting was to study the rate of convergence of loop-erased random walk to $\mathrm{SLE}(2)$ (i.e., SLE with parameter 2). In our opinion, this was the most promising case and the first one that should be considered. Loop-erased random walk has been extensively studied, and there are a number of tools available for analyzing them including a detailed proof of convergence to radial $\mathrm{SLE}(2)$ by G. Lawler, O. Schramm, and W. Werner [3].

In order to determine a reasonable rate of convergence of loop-erased random walk to $\mathrm{SLE}(2)$, it was necessary to first understand Lawler, Schramm, and Werner's original proof of convergence [3]. The following is a description of the two convergence theorems they established for loop-erased random walk. Suppose that D is a simply connected proper subset of the complex plane $\mathbb{C}$ containing 0, and let $\delta > 0$. Denote by μ_δ the law of the loop-erasure of simple random walk on $\delta\mathbb{Z}^2$ started at 0 and stopped at ∂D, and denote by ν the law of the image of the radial $\mathrm{SLE}(2)$ path under a normalized conformal transformation from the unit disk $\mathbb{D}$ onto D fixing 0. Define the metric ρ on the space of unparametrized curves in $\mathbb{C}$ by setting

$$\rho(\beta, \gamma) = \inf \sup_{0 \le t \le 1} |\hat{\beta}(t) - \hat{\gamma}(t)|$$

where the infimum is taken over all possible parametrizations $\hat{\beta}$, $\hat{\gamma}$ in $[0, 1]$ of β, γ, respectively.

The main theorem is a precise statement about what it means for loop-erased random walk to converge in the scaling limit to radial $\mathrm{SLE}(2)$.

Theorem 1.1 (LERW scaling limit). *The measures μ_δ converge weakly to ν as $\delta \to 0$ with respect to the metric ρ on the space of curves.*

An important step in their proof was to establish that the Loewner driving process for the discrete process (loop-erased random walk) converged to a scaled Brownian motion (which is the driving process for SLE).

A *grid domain* is a simply connected subset of the complex plane with a boundary that is contained in the edge set of $\mathbb{Z}^2$.

Theorem 3.7 (Driving process convergence). *For every $T > 0$ and $\epsilon > 0$, there is an $r = r(\epsilon, T) > 0$ such that, for all grid domains $D \ni 0$ with $\mathrm{inrad}(D) > r$, there is a coupling of γ with Brownian motion $B(t)$ starting at a uniform random point in $[0, 2\pi]$ such that*

$$\mathbf{P}[\sup\{|\vartheta(t) - B(2t)| : 0 \le t \le T\} > \epsilon] < \epsilon.$$

Scientific progress made

The primary goal we had for our week at BIRS was to understand the original paper [3] by Lawler, Schramm, and Werner. We knew *a priori* that it would not be possible to establish a rate of convergence without a clear understanding of the convergence itself. After several days of studying their proof, it became clear to us that our first step would be to establish a reasonable rate for the "driving process convergence" (which is Theorem 3.7 in [3]). Indeed, by the end of our week at BIRS, we had an outline of the proof of such a rate.

The original proof of Theorem 3.7 in [3] of the driving process convergence required several preliminary results that together form the proof. These included their Proposition 2.2 ("hitting probability"), Proposition 3.4 ("the key estimate"), and Lemma 3.8 ("Skorohod embedding").

Therefore, in order for us to establish a reasonable rate for the "driving process convergence," the first thing that we had to do was understand in detail these three preliminary results. We eventually discovered how a modification of a result due to Kozdron and Lawler (Proposition 3.10 in [2]) could be used to give a rate in Proposition 2.2 ("hitting probability"). We were then able to use this rate to re-establish Proposition 3.4 ("the key estimate") with a rate of convergence. The final step was to study in detail the Skorohod embedding scheme for martingales. Having done this, we were then able to determine a specific rate for the driving process convergence. We are currently working on a manuscript [1] that writes this proof out carefully with complete details. Once that is complete, we will begin working on establishing a rate in Theorem 1.1 ("LERW scaling limit") of [3].

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Chapter 60

Classification of amalgams for non-spherical Kac-Moody groups (08rit130)

Sep 14 - Sep 21, 2008

Organizer(s): Rieuwert Blok (Bowling Green State University), Corneliu Hoffman (University of Birmingham)

Overview of the Field

Dating back to Felix Klein's Ernlangen's program, mathematicians (and more recently physicists) have used the interplay between a geometric structure and its group of automorphisms.

Some of the most interesting objects in group theory are Lie groups/ algebraic groups and the related finite groups of Lie type. A unifying geometric approach for these groups was proposed by J. Tits (see [25]) in the 60's using combinatorial geometric objects called *spherical buildings*. The approach was extremely successful and gave unifying results for all such groups.

Later Ronan and Tits generalized the notion of a spherical building and introduced the idea of a *twin building*. These objects are more general than spherical buildings but not as general as buildings. Moreover many of the abstract results about spherical buildings could be generalized to twin buildings.

In an apparently unrelated development, Victor Kac [19] and Robert Moody[21] independently considered a class of infinite dimensional Lie algebras that closely resemble the finite dimensional semi-simple ones. These came to be known as Kac-Moody Lie algebras. The usual Chevalley game of exponentiation gave rise to a new series of groups that were called Kac-Moody groups. These objects found applications in various areas of theoretical physics.

In [26], Tits proved that the automorphisms groups of twin buildings are the Kac-Moody groups. This provided a combinatorial framework to the newly discovered class of groups.

The last piece of the puzzle came from the classification of finite simple groups. An important step of the classification of finite simple groups, announced in 1981, and of the ongoing Gorenstein-Lyons-Solomon revision of the classification is the identification of the "minimal counterexample" with one of the known simple groups. This step follows the local analysis step, when inside the minimal counterexample G one reconstructs one or more of the proper subgroups using the inductive assumptions and available techniques. Thus the input of the identification step is a set of subgroups of G that resemble certain subgroups of some known simple group $\hat{G}$ referred to as the target group. The output of the identification step is the statement that G is isomorphic to $\hat{G}$. Two of the most widely used identification tools are the Curtis-Tits theorem (see [13]) and Phan's theorem (see [23]). The Curtis-Tits theorem allows the identification of G with a simple

Chevalley group $\hat{G}$ provided that G contains a system of subgroups identical to the system of appropriately chosen rank-two Levi factors from $\hat{G}$. Phan's theorem is very similar and allows one to identify the group G with a unitary group provided that G contains a set of appropriately chosen rank 2 unitary subgroups. The relation between the two theorems was explained in [1].

Recent Developments and Open Problems

One important result obtained using this point of view is Abramenko and Mühlherr's generalization of the Curtis-Tits theorem which assesses that both the twin building and the associated groups can be recognized by local data. In the same manner the Phan theorem was generalized using results of Devillers and Mühlherr [10]. Another series of important results is the large number of generalizations of Phan's result to many other groups of Lie type [1, 2, 4, 5, 14, 15, 16]

Several important classification results on Kac-Moody groups and twin-buildings have been obtained recently. The classification of twin buildings as proposed by Mühlherr is under way but not published. Criteria for a building to be twin-able have recently appeared in work by Devillers, Mühlherr and Van Maldeghem [11], and Ronan [24]. Mühlherr and Caprace have described automorphisms of twin buildings [7, 8] and Caprace and Remy proved abstract simplicity of non-affine Kac Moody groups [9].

Scientific Progress Made

As put forth in our proposal for this RIT, the main question we have considered is whether the "Curtis-Tits" amalgams determine the groups in the absence of the actual twin building.

A common and elegant way to describe an amalgam $\mathcal{A}$ uses a diagram similar to the Dynkin diagram of a Lie algebra. Nodes represent the "rank 1" groups in $\mathcal{A}$ and edges represent the "rank 2" groups containing the corresponding rank 1 groups in some prescribed way. In the case of spherical and tree-shaped diagrams, this diagram uniquely determines the rank-2 Curtis-Tits amalgam and hence its universal completion. The Curtis-Tits theorem can be interpreted to say that in fact this diagram is equal to the Dynkin diagram of the group, where nodes now represent Levi components rather than the full parabolic subgroups. Similar results are obtained for certain Phan-type amalgams mentioned above. These results motivate the following fundamental question:

> To what extent do diagrams for Curtis-Tits amalgams determine the amalgam?

We study diagrams for which non-isomorphic amalgams exist. This phenomenon can already be studied in the following setting. As a diagram we consider an arbitrary simple graph without triangles. The "rank 1" groups, corresponding to the vertices, are all isomorphic to $SL_2(k)$, where k is a field. The "rank 2" groups are given by the graph as follows: two $SL_2(k)$'s will generate an $SL_3(k)$ (in the "standard" way) if the corresponding vertices are on an edge and an $SL_2(k) \circ SL_2(k)$ if they are not. The first question is to classify such amalgams. That is, for any amalgam with a given diagram, one needs to describe the universal completion. We do this by describing this completion algebraically and, wherever possible, by describing a geometric object on which this completion acts flag-transitively.

The RIT at BIRS was extremely successful. We managed to classify all amalgams in the case of a loop graph and have devised a method to deal with the general case. It turns out that in the case of a loop diagram the set of isomorphism classes of amalgams is in bijection with $Aut(k) \times \mathbb{Z}$. To our surprise we realized that the classes of amalgams corresponding to twin buildings are just those in $Aut(k)$. The others correspond to a new class of groups that generalize Kac-Moody groups that we call *Curtis-Tits groups*.

We intend to publish three papers as a direct result of our collaboration in Banff. I will briefly describe the results in each.

In the first paper we prove the classification of amalgams and consider the twin building amalgams. These were briefly described by Tits in [26] as groups of invertible matrices over a non-commutative polynomial ring. We correct a small error in that paper and give an equivalent description of these twisted Kac-Moody groups as actual subgroups of untwisted Kac-Moody groups fixed by certain automorphisms. On some abstract level, a result by Mühlherr [22] implies the existence of such groups, but no complete classification like ours is available in the literature.

In the second paper we describe the *non-orientable* Curtis-Tits amalgams and the corresponding groups. These groups are not Kac-Moody groups but they appear as fixed subgroups of Kac-moody groups under a certain kind of type-changing automorphism. The automorphism resembles a Phan-type flip as studied for the first time in [5]. The fixed-point result from [22] is not applicable here, and our methods are based on the results of Devillers and Mühlherr [10].

Finally in the third paper we consider a particular example of the non-orientable Curtis-Tits group. It is a unitary group for a non-symmetric sesquilinear form over $k[t, t^{-1}]$. We construct a Clifford-like super-algebra on which this group acts. This is a very interesting algebra. It can be viewed as a generalization of Manin's quantum plane and it is a sort of q-CCR algebra as defined for example in [18]. Moreover if one specializes the group and the algebra at $t = 1$ we get an orthogonal group and its usual Clifford algebra. If we do the same at $t = -1$ we get a symplectic group and its corresponding Heisenberg algebra. In short, our group is related to those algebras that are used by theoretical physicists to study elementary particles and quantum phenomena.

Outcome of the Meeting

The very fact that out of the material developed during the meeting we will be able to publish three separate papers, made the meeting very productive. Scientifically speaking the meeting was very productive in that we have been able to achieve the following goals:

(a) We have been able to give a complete answer to the fundamental question to what extent a Curtis-Tits diagram can determine an amalgam in an important instance, namely that of simply laced diagrams.

(b) We have discovered a new family of groups, namely the non-orientable Curtis-Tits groups.

(c) Although our study of non-orientable Curtis-Tits groups was motivated by pure mathematical considerations, we find that there is a surprising connection between these and certain super-algebras that are used by theoretical physicists to study elementary particles.

Encouraged by these results in (a) we are now in a position to extend our work field to amalgams over other non-spherical diagrams as well as amalgams whose groups are different from $SL_2(k)$'s and $SL_3(k)$'s. In particular, with these results in hand, one can begin to obtain Phan-type amalgams for these groups of Kac-Moody and Curtis-Tits type. Our results in (c) encourage us to seek contact and possible collaboration with colleagues interested in super-algebras and their groups.

List of Participants

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Summer School Reports

Chapter 61

The stable trace formula, automorphic forms, and Galois representations (08ss045)

Aug 10 - Aug 17, 2008

Organizer(s): James Arthur (University of Toronto), Michael Harris (Universite de Paris 7), Eric Urban (Columbia University), Vinayak Vatsal (University of British Columbia)

Overview of the Field

The heart of Langlands' program reinterpreting much of number theory in terms of automorphic forms is his *Functoriality Conjecture*. This is a conjecture associating the automorphic representations on a pair of connected reductive groups over a number field F, say G and H, whenever there is a homomorphism of the appropriate type between the corresponding L-groups

$$h : {}^L H \to {}^L G.$$

The structure of functoriality is largely captured in terms of parametrization of automorphic representations of a given group G by homomorphisms

$$\phi : \mathcal{L}_F \to {}^L G$$

where $\mathcal{L}_F$ is the hypothetical Langlands group.

In the analogous conjectured parametrization of irreducible representations of a reductive group G over a local field K, the Langlands group is replaced by the Weil-Deligne group W_K; in this setting one can state precise conjectures in terms of known objects, and these conjectures were proved when $G = GL(n)$ during the 1990s. This represents the first step to the extension of local class field theory to the non-commutative context, whereas the Langlands functoriality conjectures for automorphic forms are to be understood as generalizations of global class field theory. In particular, the Artin conjecture on holomorphy of Artin L-functions follows from Langlands' Functoriality Conjecture applied when H is the trivial group.

The most comprehensive technique for proving the Functoriality Conjecture in the cases in which it has been established is the Arthur-Selberg trace formula. This was used by Lafforgue to prove the global Langlands conjecture for $GL(n)$ over a global field of positive characteristic, and has had a variety of striking applications to number fields, including the Jacquet-Langlands correspondence and its generalizations in higher dimensions and the Arthur-Clozel theory of cyclic base change for $GL(n)$. Each special case of functoriality has been of enormous importance in number theory. Until recently, applications of the trace formula were limited to the cases in which it could be stabilized. With the proof of the fundamental lemma for unitary groups by Laumon and Ngô, followed by its extension to all groups by Ngô – together with the proof that the fundamental lemma depends only on the residue field, first by Waldspurger, more recently by Cluckers, Hales, and Loeser – Arthur's stabilization of the trace formula is close to being complete, and the simple trace formula can be stabilized in a number of situations. This makes it possible to carry out the applications of the trace formula anticipated more than two decades ago by Langlands, Kottwitz, and Arthur.

Objectives of the Summer School

The primary goal of the summer school was to contribute to creating a situation where number theorists will be able to make use of the most recent developments in the theory of automorphic forms on higher-dimensional groups with no less ease than they have hitherto done with the $GL(2)$-theory. This necessarily involves coming to terms with the stable trace formula. Applications of the stable trace formula of special interest to number theorists include

(i) the determination of multiplicities of automorphic representations;

(ii) the proof of functoriality in the special case when $G = GL(n)$ and H is a classical group (symplectic, orthogonal, or unitary), with the hypothetical Langlands parameter ϕ introduced above replaced by a discrete automorphic representation of $GL(n)$;

(iii) the parametrization of irreducible representations of classical groups over local fields in terms of the local Langlands parametrization for $GL(n)$; and

(iv) the calculation of the zeta functions of Shimura varieties, and the analysis of the corresponding Galois representations.

The first three topics are treated in the book on functoriality and the twisted trace formula that James Arthur is in the process of completing. The fourth topic, together with special cases of functoriality when H is a unitary group, is developed in the series of books in preparation by participants in the Paris automorphic forms seminar. A concrete objective of the summer school, then, was to help prepare participants to read these books. This applies as well to virtual participants who will at some future date be able to watch video recordings of the proceedings online.

Presentation Highlights

The seven-day program was organized as a series of daily themes, beginning with basic facts about automorphic representations of $GL(n)$ and classical groups and leading up to applications of the stable trace formula to functoriality and the cohomology of Shimura varieties. The daily themes are presented in order:

Day 1: Framework of reciprocity and functoriality

(a) Classical modular forms and associated Galois representations in the light of automorphic representations of GL(2) (C. Skinner)

(b) Automorphic representations of GL(n) and classical groups (J. Cogdell)

(c) Introduction to Langlands reciprocity for Galois representations (M. Harris)

(d) Introduction to Langlands functoriality for classical groups (T. Gee)

Day 2: Basic representation theory of GL(n) over local fields and classical groups

(a) Introduction to representation theory of p-adic classical groups (A. Minguez)

(b) Introduction to harmonic analysis on p-adic groups (J. Arthur)

(c) (Tempered) cohomological representations of GL(n) and unitary groups (D. Shelstad)

(d) d. Local Langlands correspondence for GL(n) over p-adic fields (M. Harris)

Day 3: Introduction to the simple trace formula

(a) The trace formula for cocompact groups (J. Bellaïche)

(b) Introduction to the simple trace formula (J.-P. Labesse)

(c) Applications of the simple trace formula (E. Lapid)

Day 4: Introduction to endoscopy

(a) Introduction to stable conjugacy (T. Hales)

(b) The stable trace formula, part I (S. W. Shin)

(c) The stable trace formula, part II (J.-P. Labesse)

(d) Endoscopic transfer of unramified representations (J. Bellaïche)

(e) Endoscopy for real groups (D. Shelstad)

Day 5: Functoriality and the stable trace formula

(a) Introduction to functoriality for classical groups (J. Cogdell)

(b) Functorial transfer for classical groups, statements (J. Arthur)

(c) Functorial transfer for classical groups, sketch of proofs (J. Arthur)

(d) Simple stable base change and descent for $U(n)$ (M. Harris)

Day 6: Shimura varieties

(a) Introduction to Shimura varieties (L. Fargues)

(b) Integral models of PEL Shimura varieties (L. Fargues, in two parts)

(c) Points on special fibers of PEL Shimura varieties, following Kottwitz (S. Morel, in two parts)

Day 7: Shimura varieties

(a) Newton stratification of special fibers of PEL Shimura varieties (E. Mantovan)

(b) Points on special fibers of PEL Shimura varieties and Igusa varieties (S. W. Shin)

Outcome of the Meeting

Registered to attend the meeting was the maximum number of 42 participants, all but one of whom did in fact attend. Among the participants were seven graduate students, ten recent post-docs, and twelve confirmed researchers who are not specialists in the topics of the summer school, primarily number theorists. The remaining participants were speakers either at the summer school or, in a few cases, in the subsequent week's program.

Seven number theorists were invited to organize and moderate evening sessions to review each day's lectures, to answer questions that could not be treated in detail during the formal presentations, and to provide opportunities for the less experienced students and post-docs to familiarize themselves with foundational material. The seven moderators (Darmon, Nekovar, Kisin, Skinner, Iovita, Böckle, and Prasanna) succeeded in convincing most of the day's lecturers to attend the lively evening sessions, which lasted 2-3 hours and represented an important addition to the formal program.

With a view to making the week's lectures available to a broader audience, all lectures were videotaped, with the generous support of the French Agence Nationale de la Recherche as well as NSERC.

List of Participants

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