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BIRS

Contents

Five-day Workshop Reports

Chapter 1

Extremal Problems in Combinatorial Geometry (18w5058)

February 4 - 9, 2018

Organizer(s): János Pach (École Polytechnique Fédérale de Lausanne), József Solymosi (University of British Columbia), Andrew Suk (University of California - San Diego)

Field overview and objectives

The workshop on Extremal problems in combinatorial geometry focused on the algebraic and combinatorial properties of points, lines, and other simple geometric objects in Euclidean space. The goal was to gather experts and promising young researchers in combinatorial geometry and related areas, to discuss the recent developments of algebraic and combinatorial methods used in the field. Over the past 6 years in particular, several ground-breaking results have been discovered, answering some of the oldest problems in the field. This workshop was a timely event to capitalize on this momentum.

Problems in combinatorial geometry are often simply described, and usually involve finite set of points, lines, convex sets, and other geometric objects in Euclidean space. Extremal problems in the field asks how large or small a finite set of geometric objects can be under certain restrictions. For example, given a set of n points in the plane, how often can the unit distance occur among them, or what is the size of the largest subset in convex position? Many questions in the field are very natural and worth studying for their own sake, while others are fueled by the more recent development of computational geometry. Over the past 6 years, in particular, combinatorial geometry has seen tremendous growth, and numerous unexpected connections to other fields of mathematics are being discovered. Two notable examples using algebraic geometry are the works of Guth and Katz [6], who solved the Erdos distinct distances problem, and of Green and Tao [5], who solved the long-standing conjecture of Dirac and Motzkin on the number of ordinary lines.

The workshop focused on several areas in combinatorial geometry, such as incidence geometry, intersection graphs, graph drawing, Erdos-Szekeres-type theorems, and combinatorial number theory. One of the major goals was to study the interplay between algebraic and combinatorial methods used in the field. Some of the key topics that the workshop covered are:

1. **The polynomial method and its applications in incidence geometry and combinatorial number theory**. Guth and Katz [6] invented, as a step in their nearly complete solution of Erdős's distinct distances problem, a new method for partitioning finite point sets in $\mathbb{R}^d$, based on the Stone-Tukey polynomial ham-sandwich theorem. This method has had numerous applications in incidence geometry. Even more applications were discussed during the workshop.

2. **The container method and its applications in discrete and computational geometry**. This useful method was recently introduced independently by Balogh, Morris and Samotij, and by Saxton and Thomason [1, 64]. Roughly speaking, it says that if a hypergraph H has a uniform edge distribution, then one can find a relatively small collection of sets, containers, covering all independent sets in H. One can also require that the container sets span few edges only. More recently, Balogh and Solymosi [BS] realized that this machinery is useful in discrete geometry. More precisely, the used the hypergraph container method to tackle several longing standing problems for points sets in the plane, including epsilon nets. Further possible applications were discussed during the workshop.

3. **The theory of semi-algebraic hypergraphs: regularity lemmas, VC-dimension arguments, and applications**. Famous Ramsey, Turán, and Szemerédi-type results prove the existence of certain patterns in graphs and hypergraphs under mild assumptions. Recently, several authors have shown that much stronger results hold for semi-algebraic hypergraphs, that is hypergraphs whose vertices are points in $\mathbb{R}^d$ and edges are defined by a semi-algebraic set in $\mathbb{R}^{dk}$ of bounded complexity. These results had several applications in discrete geometry, and more applications and results were discussed at the workshop.

With all of the recent developments and exciting breakthrough results in the field, it was important to bring together prominent experts in the field from all over the world. We believe it is very important to bring together and foster interactions between senior and junior researchers in combinatorial geometry. The workshop had a number of key lectures by international experts, which will survey the state-of-the-art of several long-standing open problems in the field. Other participants had the opportunity to give a 30 minute talk to present their work. The workshop schedule also provided ample time and opportunity for participants to interact and engage in mathematical discussion.

Presentation Highlights

The first plenary talk was given by Frank De Zeeuw, who talked about ordinary lines in space. The Sylvester-Gallai theorem states that if a finite set of points in the real plane is not contained in a line, then it spans at least one ordinary line, i.e. a line containing exactly two of the points. In fact, such a set always spans a linear number of ordinary lines, and that is best possible because there are point sets on cubic curves that determine only a linear number of ordinary lines. One can consider the same question in three-dimensional space. By projection, the results in the plane hold word-for-word in space. But note that the known constructions with a linear number of ordinary lines are contained in a plane. I will show that if one assumes that the point set does not have too many points on a plane, then it spans a quadratic number of ordinary lines. More precisely, for any $a < 1$ there is a $c > 0$ such that if we have n points in space with at most an points on a plane, then there are at least cn^2 ordinary lines. The proof uses projection, Beck's theorem, and a variant of the Sylvester-Gallai theorem. More details can be found in his paper [12].

Joshua Zahl gave a talk on his new result which gives a new bound on the unit distances in three dimensions. In his talk, he talked about a more general problem about cutting curves into pseudo segments and its applications. More details can be found in his paper [4].

Misha Rudnev gave a review on some better or less known results about incidences of sufficiently small non-collinear point sets with straight lines. The two best known and in some sense sharp results are the theorem on distinct directions proved in the 90s by T. Szonyi and the recent Szemeredi-Trotter type incidence theorem by S. Stevens and F. de Zeeuw.

The second plenary talk was given by Orit Raz, who talked about a generalization of Elekes-Rónyai theorem to d variables. This was joint work with Zvi Shemtov.

Balázs Keszegh presented his new result, where he proved that the intersection hypergraph of a finite family of pseudo-disks with respect to another family of pseudo-disks admits a proper coloring with 4 colors. His result serves as a common generalization and strengthening of many earlier results, including ones about coloring points with respect to pseudo-disks, coloring pseudo-disks with respect to points and coloring disks with respect to disks. More details can be found in his paper [2].

The third plenary talk was given by Natan Rubin, who improved the upper bound on weak epsilon nets in the plane. This is the first improvement in over 25 years. More precisely, he showed that for any set P of n points in the plane and $\varepsilon > 0$ there exists a set of $O(1/\varepsilon^{1.7})$ points in the plane that pierce every convex set K with $|K \cap P| \geq \varepsilon|P|$. This improves the previously known upper bound (from 1992) of $O(1/\varepsilon^2)$ by Alon, Bárány, Füredi, and Kleitman.

The fourth plenary talk was given by Nathan Linial, who talked about Hypertrees. In a seminal paper, Kalai (1983) extended the notion of a tree to higher dimensions. Formally, an n-vertex d-dimensional hypertee is a Q-acyclic simplicial complex with a full $(d-1)$ dimensional skeleton and $\binom{n-1}{d}$ d-dimensional faces. In his talk, Nati discussed several of the many open problems that arise here and describe some of the more recent new discoveries.

Radoslav Fulek talked about Z_2-genus drawings of graphs. A drawing of a graph on a surface is independently even if every pair of independent edges in the drawing crosses an even number of times. The Z_2-genus of a graph G is the minimum g such that G has an independently even drawing on the orientable surface of genus g. He showed that the Z_2-genus of graphs in these families is unbounded in t; in fact, equal to their genus. Together, this implies that the genus of a graph is bounded from above by a function of its Z_2-genus, solving a problem posed by Schaefer and Štefankovič, and giving an approximate version of the Hanani-Tutte theorem on surfaces. These results were joint work with Jan Kyncl [3, 4].

Bartosz Walczak talked about a new upper bound on the chromatic number of intersection graphs of L-figures in the plane, which is asymptotically tight. This was joint work with Alexandre Rok.

Lena Yuditsky talked about a structure theorem conjectured by Janson and Uzzell: The vertex set of almost all string graphs on n vertices can be partitioned into five cliques such that some pair of them is not connected by any edge. As a corollary, almost all string graphs on n vertices are intersection graphs of plane convex sets. This was joint work with Bruce Reed and János Pach [8].

Scientific Progress Made

The workshop provided ample free time for participants to work together on joint research projects. Moreover, there were a number of new research projects were initiated during the workshop, while some other researchers used the opportunity to continue to work on projects started earlier. All talks were well received.

Participants

Aronov, Boris (New York University)
Balko, Martin (Charles University)
Bárány, Imre (Alfred Renyi Institute of Mathematics)
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De Zeeuw, Frank (EPFL)
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Ezra, Esther (Georgia Tech)
Fulek, Radoslav (IST Austria)
Furedi, Zoltan (Renyi Institute of Mathematics)
Holmsen, Andreas (KAIST)
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Chapter 2

Modelling Imbalance in the Atmosphere and Ocean (18w5119)

February 18 - 23, 2018

Organizer(s): Bruce Sutherland (University of Alberta), Ulrich Achatz (Goethe Universitaet Frankfurt), Colm-cille Caulfield (University of Cambridge), Jody Klymak (University of Victoria)

PHYSICAL REVIEW FLUIDS **4**, 010501 (2019)

Invited Articles

Recent progress in modeling imbalance in the atmosphere and ocean

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Imbalance refers to the departure from the large-scale primarily vortical flows in the atmosphere and ocean whose motion is governed by a balance of Coriolis, pressure-gradient, and buoyancy forces and can be described approximately by quasigeostrophic theory or similar balance models. Imbalanced motions are manifest either as fully nonlinear turbulence or as internal gravity waves which can extract energy from these geophysical flows but which can also feed energy back into the flows. Capturing the physics underlying these mechanisms is essential to understanding how energy is transported from large geophysical scales ultimately to microscopic scales, where it is dissipated. In the atmosphere, it is also necessary for understanding momentum transport and its impact upon the mean wind and current speeds. During a February 2018 workshop at the Banff International Research Station (BIRS), atmospheric scientists, physical oceanographers, physicists, and mathematicians gathered to discuss recent progress in understanding these processes through interpretation of observations, numerical simulations, and mathematical modeling. The outcome of this meeting is reported upon here.

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I. INTRODUCTION

With some exceptions, the atmosphere and ocean are described by the same equations of motion, the two fluids differing primarily by their equation of state, and so it is not surprising that they exhibit features in common. The most energetic motions of the atmosphere occur at synoptic and planetary scales, on the order of 1000 km and longer, manifest as perturbations of the mean zonal (east-west) winds by cyclonic flows (rotating in the same sense of the Earth's rotation) and anticyclonic flows (rotating in the opposite sense), respectively associated with low- and high-pressure systems. The analogous flows in the ocean occur at the mesoscale, on the order of 100 km, being manifest as cyclonic and anticyclonic eddies embedded in the eastward Antarctic Circumpolar Current and in western boundary currents such as the Gulf Stream and the Kuroshio and Agulhas Currents. Flows such as these are said to be "balanced," meaning that Coriolis forces are equal to pressure-gradient forces such that quasigeostrophic potential vorticity is conserved as expressed through the quasigeostrophic equations [1]. Generally, a suite of balanced models (quasigeostrophy, semigeostrophy, planetary geostrophy, and others) has been devised to account

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for large-scale motion in the tropics, dynamics leading to frontogenesis, and submesoscale motions in the ocean where isopycnals (constant density surfaces) are relatively steep. (See Ref. [2] for a recent review of scalings leading to different balance models of the atmosphere.) Common to all balance models is that they filter out smaller spatial-scale and faster timescale motions associated in particular with internal gravity waves, which are waves that propagate horizontally and possibly vertically, being driven by buoyancy forces where the effective background density decreases with height.

Constantly driven by incoming solar radiation (which itself drives winds that force the upper ocean), an outstanding question for atmospheric scientists and physical oceanographers is how energy at these large scales is transferred progressively to smaller scales until ultimately it is dissipated efficiently by viscosity, closing the global energy balance. One conduit through which these transfers can take place is through direct generation of fully nonlinear turbulence arising when balanced motions interact with solid boundaries, for example, through the atmospheric boundary layer or or when ocean currents and eddies interact with continental margins and, particularly with the Antarctic Circumpolar Current, with the ocean floor. Away from such boundaries, the main conduit for energy transfer from balanced motions to dissipative scales is through internal gravity waves. Although there are similarities, the processes of energy transfer by waves differ significantly in the atmosphere and ocean.

In the atmosphere, observations suggest that internal waves are generated primarily by zonal flows over topography and by nonorographic sources such as convection and the formation of fronts [3,4]. As a consequence of momentum conservation, these waves grow in amplitude as they propagate upward into thinner, less dense air. As a result of such so-called anelastic growth as well as interaction with the large-scale winds, the waves break and deposit their momentum, so decelerating or accelerating the mean wind speeds aloft [5,6]. Breaking waves also vertically mix the air, tending to homogenize it. However, absorption of solar radiation by ozone and other gases readily re-establishes stable stratification.

In the ocean, internal waves are generated primarily as a result of either wind stress on the surface or through the action of tides and eddies embedded within currents that move over bottom topography [7]. Generation and other breakdown processes are illustrated in Fig. 1. The density of the ocean changes little over its depth and so upward-propagating waves do not experience anelastic growth. Except in the equatorial Pacific Ocean, around Antarctica, and at the western boundaries of the ocean basins, ocean currents are generally weak and have negligible influence on wave propagation and breaking. Instead, it appears that the main mechanism leading ultimately to dissipation is through nonlinear wave-wave interactions and wave-induced shear that directly results in turbulent breakdown. Whereas atmospheric scientists are most interested in momentum transport by internal waves, this is less of interest to physical oceanographers because the directionality of the waves is generally horizontally isotropic. Instead, oceanographers are most interested in energy transport by internal waves, which ultimately determines the degree of mixing that occurs as they break down into turbulence. Because sunlight penetrates little below the top 100 m of the ocean surface, the observed stratification of the oceanic abyss can only be explained by internal wave-driven processes.

"Modeling imbalance" typically describes the endeavor to go beyond the balanced (e.g., quasigeostrophic) equations in order to capture the physical processes by which energy is exchanged between balanced flows and smaller scale motions. Here, we take a broader perspective by considering in addition the cascade of energy from inertia-gravity waves to faster and smaller scales through the internal wave spectrum and then onward to dissipation via turbulence, which itself is typically affected nontrivially by stratification. While we do not include consideration of the direct dissipation of energy due to balanced motions interacting with solid boundaries, the reader is referred to recent reviews of research on atmospheric boundary layers [9] and the oceanic kinetic energy budget [10].

Guiding this review are the talks and discussions that took place during the Workshop on Modelling Imbalance in the Atmosphere and Ocean [11], which was held at the Banff International

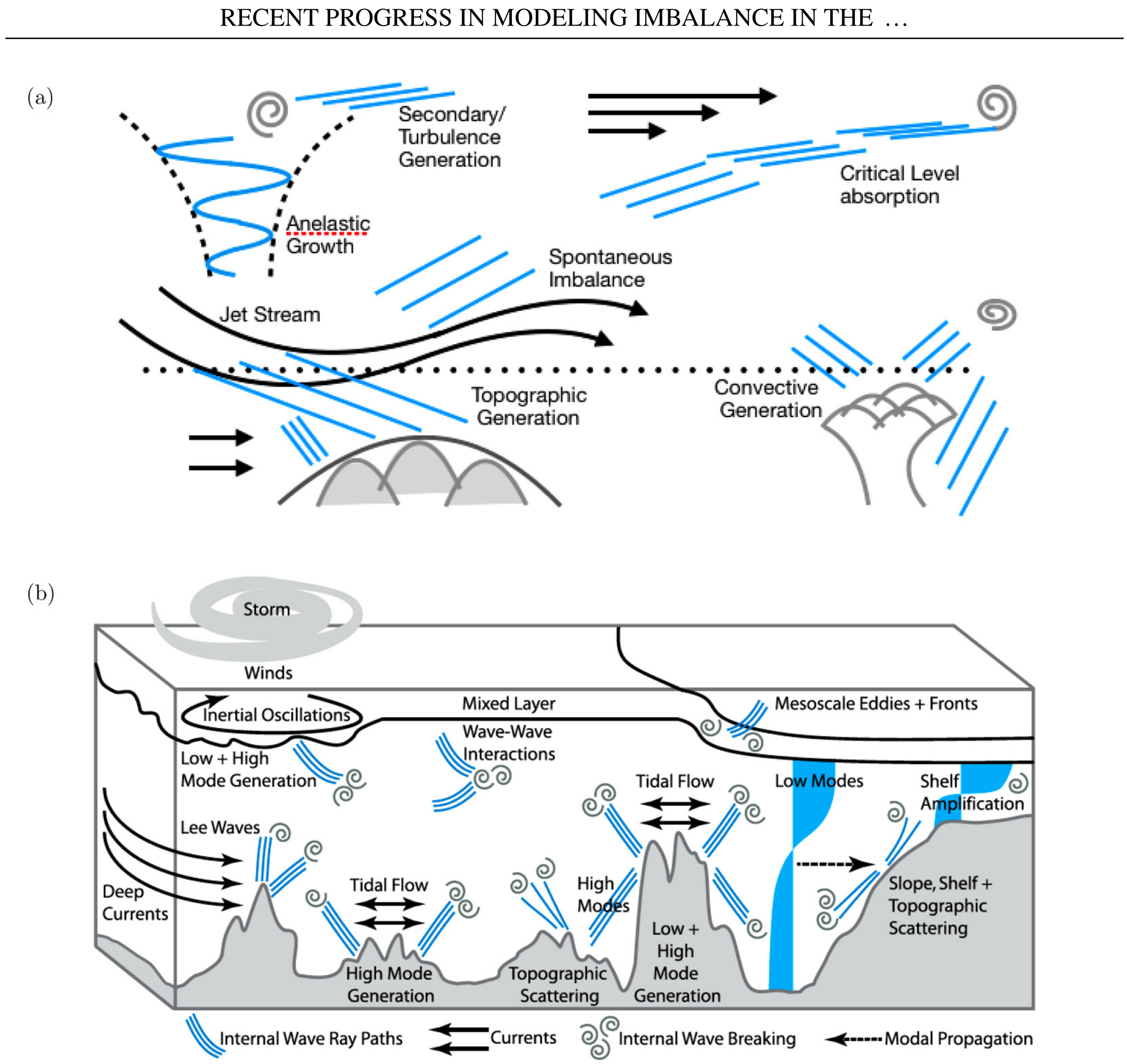

FIG. 1. Schematics illustrating the myriad processes that generate internal waves and which ultimately lead to breaking in (a) the atmosphere and (b) the ocean (the latter, copyright © American Meteorological Society, is used with permission from Fig. 1 of MacKinnon *et al.* [8]).

Research Station (BIRS) during February 19 to 23, 2018. Therein presenters described recent breakthroughs realized through advances in observational technologies, increased computing power, and newly developed mathematical modeling techniques. Crucially, it is through the combination of these resources that advances have taken place. For example, now observational campaigns in the ocean are often guided by numerical simulations that predict where dynamics of interest may be taking place. Mathematical methods are now being applied to observations to distinguish balanced vortical motions from waves. Simulations have improved to the extent that they can now begin to capture the observed spectra of internal gravity waves as well as the processes of turbulent mixing and dissipation in stratified fluids at geophysically realistic parameter values. Just as models are being created to adapt quasigeostrophy to include unbalanced motions that are less influenced by rotation, higher resolution global simulations are now beginning to resolve such small scales that hydrostatic models need to be adapted to account for nonhydrostatic effects.

All of these advances have the ultimate goal of developing parametrizations of energy and momentum transport from large to small scales in atmospheric and oceanic general circulation models. Here again the emphasis of atmosphere and ocean modelers differ. While internal wave dynamics are important for short-term weather forecasts and predictions of clear-air turbulence, climate models of the atmosphere are less concerned about the details of transport by internal waves. Typically their influence is parameterized by assuming they propagate purely in the vertical and deposit all their momentum where they break, as estimated by linear theory. That said, the cumulative impact of internal waves on the middle atmosphere is known to be important. It virtually controls the mean circulation in the mesosphere and leaves significant traces in the stratosphere, e.g., by contributing to the quasibiennial oscillation in the equatorial stratosphere [12–15] and the formation and breakdown of the ozone hole in the southern hemisphere [16]. Since middle-atmosphere dynamics is essential for weather predictions on the seasonal timescale [17] as well as climate simulations [18,19], middle-atmosphere internal-wave dynamics and its correct handling in models is important for these issues as well. By contrast, internal waves are thought to be of primary importance to the ocean's long-term climatology, particularly in the abyss [7]. With increasing observational data and through insights gained by theoretical and numerical modeling of idealized circumstances, ocean general circulation models are only now beginning to develop parametrizations of internal wave-induced mixing [8]. But it is clear that a deeper understanding of the various breakdown mechanisms is required before such parametrization schemes can be agreed upon.

The principal aim of this review is to report recent advances, as discussed in the workshop, rather than to present a comprehensive historical survey. Therefore, the references presented herein are inevitably incomplete, yet may act as a useful starting point for exploring this very important topic. We begin in Sec. II by describing recent progress in distinguishing balanced from imbalanced flows in observations and in representing such processes by a reduced set of equations. Significant advances have been made in this area with the recognition that internal waves interacting with balanced flows may enhance the generation of internal waves through the process of stimulated imbalance. Other mechanisms for extraction and transport of energy from balanced flows through interaction with topography, convection, and turbulence are discussed in Sec. III. Primarily through numerical simulations, insights have been gained into the final stages of breakdown into turbulence, momentum deposition, and mixing. These are presented for the atmosphere in Sec. IV and for the ocean in Sec. V. In light of this progress, the most promising directions for future advances are discussed in Sec. VI.

II. CHARACTERIZING BALANCE AND IMBALANCED FLOWS

Earth-observing satellites readily visualize synoptic-scale cyclonic motions in the atmosphere through the structure of clouds as shown, for example, in the left image of Fig. 2. Their counterpart in the ocean, manifest as mesoscale eddies, can be visualized through satellite imagery of the sea-surface temperature, as shown in the right image of Fig. 2. With some further processing that includes sea surface height data and the assumption of geostrophic balance, global surface currents at the mesoscale can be revealed as derived, for example, by the Ocean Surface Current Analyses Real-time (OSCAR) product [20]. These large-scale motions are said to be "balanced," meaning that their motion is determined by a combination of pressure gradient and Coriolis forces as well as the influence of vortex stretching. These dynamics are captured by the so-called quasigeostrophic (potential vorticity) equations. In the atmosphere, these describe the synoptic scale motions which vary over distances of about 1000 km and greater. In the ocean, these describe the mesoscale motions which vary over distances of about 100 km and greater.

While large-scale motions are clearly distinguished qualitatively from finer strained structures, it is more challenging quantitatively to partition the energy associated with the balanced motions and the unbalanced motions, which occur at smaller scales. *In situ* observations can be gathered in the atmosphere, for example, of wind speed and temperature from airplanes and radiosonde balloons, and in the ocean, for example, of speed, temperature, and salinity from shipboard acoustic Doppler current profilers (ADCPs) and conductivity, temperature, and depth (CTD) profiles. However, these provide limited spatial information.

One advance in the interpretation of velocity measurements along a given line (e.g., taken from ship or aircraft tracks) is the use of the Helmholtz decomposition, which separates the fields in

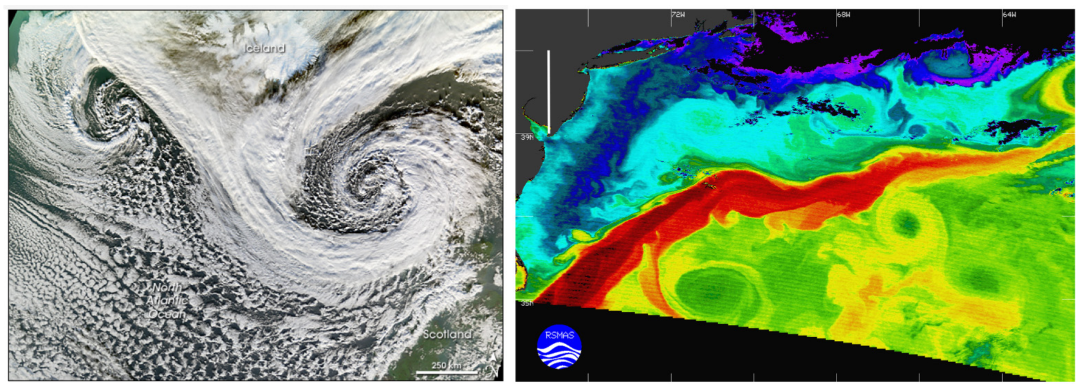

FIG. 2. Images acquired from the Moderate Resolution Imaging Spectroradiometer on NASA's Terra satellite showing (left) atmospheric cyclones between Iceland and Scotland visualized by clouds on November 20, 2006 [NASA image by Jesse Allen, Earth Observatory], and (right) anticyclonic and cyclonic eddies interacting with the Gulf Stream on May 8, 2000, and visualized by sea surface temperature [created at the University of Miami using the 11- and 12-μm bands, by Evans, Minnett, and coworkers]. The horizontal white bar to the lower right in the left image indicates a length of 250 km. The vertical white bar to the upper left of the right image indicates a length of 222 km.

terms of their vertically rotational and horizontally divergent components [21–24]. Significantly, Bühler *et al.* [22] and Callies *et al.* [23] showed how to separate geostrophic from internal wave motions while Bühler *et al.* [24] extended the method to account for the anisotropy in the spectra resulting from eddies and waves being embedded within mean winds and currents. Through these methods, as shown in Fig. 3, it is clear that the power spectrum as a function of horizontal wave number, k, varies as k^{-3} at mesoscales in the ocean, as predicted by Charney [25] (corresponding to a downscale transfer of enstrophy) and that the energy at these scales can be attributed almost entirely to balanced (rotational) motion. At mesoscales in the atmosphere ($\lesssim$100 km) and at the submesoscale in the oceans ($\lesssim$50 km), the spectrum varies as $k^{-5/3}$. The $-5/3$ spectrum is predicted for the downscale cascade of energy in three-dimensional turbulence and the upscale transfer of energy in two-dimensional turbulence [26]. If indeed this spectral slope is associated with two-dimensional turbulence, as has been proposed for the atmosphere [27,28], this suggests that energy at mesoscale ranges in the atmosphere and submesoscale ranges in the ocean is driven "inversely"

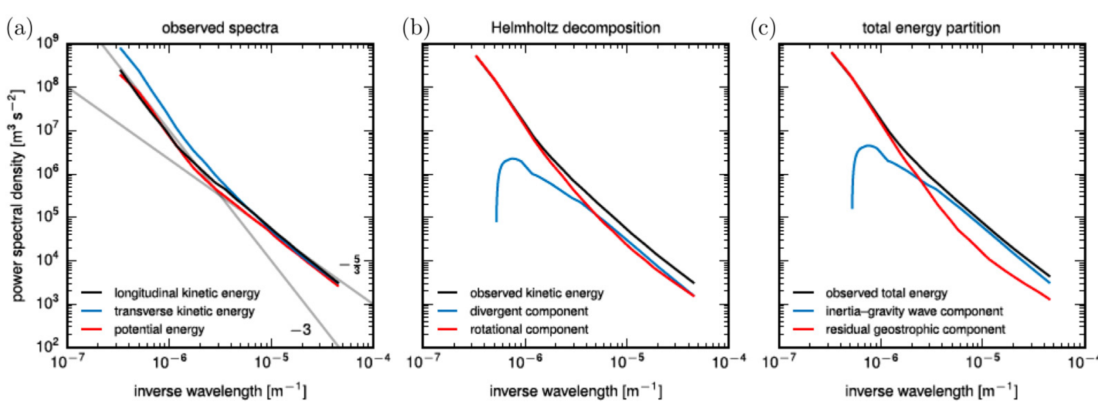

FIG. 3. (a) Spectra of along-track and across-track velocities determined from a collection of aircraft flights in the lower stratosphere, (b) Helmholtz decomposition of the spectra into rotational and divergent components, and (c) adjustment for spectra accounting for internal gravity wave polarization relations. (Reproduced with permission from Fig. 1 of Callies *et al.* [23].)

to large rather than dissipative scales. Other processes must operate in order to provide a global energy balance. These include mechanisms, discussed below, in which internal gravity waves are generated by balanced motions and, by interacting either with these motions or with themselves, energy is carried to small scale, either indirectly via weakly nonlinear interactions or directly by wave breaking. Another possible mechanism not involving waves is through vertical shear, which develops naturally in stratified quasi-two-dimensional turbulence.

As a first theoretical step to understand how energy is extracted from balanced flows in the absence of boundaries, attempts have been made to extend the balanced (e.g., quasigeostrophic) equations to introduce the influence of divergent processes associated with inertia-gravity waves [29–34]. Conceptually, these processes can be broken down into triad interactions between vortical modes (V) and waves (W) acting through the nonlinear advection terms of the fully nonlinear equations of motion [35].

The quasigeostrophic equations can be represented by the triad VVV, meaning that two vortical modes interact (first two letters) to put energy into another vortical mode (the last letter). The triad VVW represents the equations describing the spontaneous generation of internal waves from interactions between vortical modes [30]. Because of the corresponding eigenfrequencies, only nonresonant interactions are allowed. Indeed, analysis of these equations in comparison with observations suggest that this mechanism for wave generation is relatively weak. That said, a recent breakthrough has been the demonstration that stimulated emission of internal waves, represented by the triad VWW, may provide an efficient mechanism through which waves interacting with the vortical modes produce more waves. The question remains as to whether these excited waves in the ocean are able to propagate away from the generation site and so remotely cause mixing elsewhere in the ocean. A recent study by Nagai *et al.* [36] suggests this is not the case: After the waves are generated, it appears they are reabsorbed into the large-scale balanced flows, as represented by the triad VWV. A particular mechanism for reabsorption of waves by large-scale flows through the straining motion between vortices was formulated by Bühler and McIntyre [37]. Another possibility in the ocean is for waves to become trapped in anticyclonic eddies [38–40], eventually redepositing their energy there.

In the context of reduced models, the triad WWV describes waves interacting with themselves without breaking in a way that transfers energy to large-scale flows. For vertically propagating waves, this is manifest as the (Eulerian) induced mean flow [6,41–44] that, for a localized wave packet, can be responsible for creating a circulation far from the wave packet itself [45]. Of course, another mechanism by which waves can affect the large-scale flow, particularly in the atmosphere, is through momentum deposition caused by breaking. However, the process of breaking does not involve a resonant wave-wave interaction, as implied by the triad WWV. Instead, it involves a cascade of energy to the small scales of turbulence, the detailed description of which lies outside the realm of reduced models. Some aspects of such turbulent processes are discussed below.

The last of the interaction triads, WWW, corresponds with weakly nonlinear interactions between waves. This can involve refraction of waves by other waves of different scale [46], the self-interaction of waves in a spanwise-wide wave packet that resonantly generates long waves [44,47–49], or wave-wave interactions leading to parametric subharmonic instability [50–52]. In particular, it has been proposed that the last process may be important for the breakdown of the M2 internal tide at the critical latitude of 29°, where the subharmonic wave frequency equals the background Coriolis frequency [53–55]. However, *in situ* measurements did not reveal as strong a signal of breakdown as suggested by numerical models [56]. It is likely that processes described by the WWW triad will explain the prevalence of the universal spectra for internal waves observed in the abyssal ocean [57–59], and possibly also in the middle atmosphere, whether through the downscale transport of energy through scattering and parametric subharmonic instability or through the upscale transport of energy from small-scale wave packets generated, for example, in the atmosphere through convection [27,28,60] or by localized turbulent patches associated with wave breaking [61], mechanisms that will be discussed below. While much has yet to be explored regarding upscale energy transfers in the context of two-dimensional turbulence or otherwise, numerical models are now able to achieve resolutions capable of reproducing these spectra from the balanced flows to the inertia-gravity wave (low-wave-number) end of the internal wave spectrum.

Apart from triad interactions, energy may be dissipated directly through wave breaking. This can occur due to anelastic growth of atmospheric waves propagating upward into thinner air, due to waves approaching a critical level where their horizontal phase speed matches the background flow speed, or due to other interactions that drive the waves to shear or convective instability. Observations of overturning in the oceanic thermocline suggest that wave packets interacting with large-scale flows overturn predominantly due to convective rather than shear instability [62] though shear instability may play a more important role for inertia gravity waves (cf. Sec. 4.6.3 of Sutherland [63]).

Despite the upscale transfer of energy in two-dimensional turbulence, quasi-two-dimensional turbulence in nonrotating stratified fluid may nonetheless develop structures leading to efficient dissipation in the absence of waves. Here it is important to note that while a power spectrum of an idealized two-dimensional turbulence field inevitably and naturally reveals a spectrum, it is incorrect to interpret this spectrum physically as a pure superposition of waves: Vortices develop naturally in two-dimensional turbulence, and a power spectrum loses the information of such coherent, spatially localized structures. Stratification can render incoherent the vertical structure of vortices in quasi-two-dimensional turbulence: Columnar vortices naturally devolve into "pancake" eddies [64].

This suggests an alternative framework to model quasi-two-dimensional turbulent flow in stratified fluid, which still leads to $-5/3$ slope of the energy spectrum by relying on strong anisotropy in the flow [65] to give a forward cascade of energy consistent with numerical evidence [66]. It is important to appreciate that this argument inherently assumes that rotation plays no dynamical role. As recently demonstrated by Kafiabad and Bartello [67], this places an upper bound of $O(10\,\text{km})$ in the atmosphere where this regime might be expected to be observable. Analogously in oceanographic contexts, this regime is only expected to occur at below submesoscales, with horizontal scales $O(1\text{–}10\,\text{km})$ or less.

As demonstrated by the self-similar scaling analysis of Billant and Chomaz [68], such nonrotating layered anisotropic stratified turbulence (LAST) [69] is inevitably and inherently three-dimensional. Although the horizontal scales L are at least in some sense large, though not too large for rotation to play a dynamical role as characterized by the horizontal Froude number $\text{Fr}_h \equiv U/(NL) \ll 1$, the vertical structure scales as $H \sim U/N$ such that the vertical Froude number $\text{Fr}_v = U/(NH)$ is order unity. In effect, this introduces a different mechanism for energy dissipation whereby, as two pancakes slide over each other, the vertical shear over the small distance between them can result in shear-driven turbulence and mixing if the Richardson number, $\text{Ri} \equiv N^2H^2/U^2$, is sufficiently small, which is certainly possible if $\text{Fr}_v = \text{Ri}^{-1/2} \sim O(1)$.

For shear instability to occur between pancakes, the flow must be of sufficiently high Reynolds number $\text{Re} = UL/\nu$, based on the (largest) horizontal scale such that the combination $\text{ReFr}_h^2 \gg 1$. With a further inertial scaling for the turbulent dissipation rate $\epsilon \sim U^3/L$, this scaling for the onset of instability corresponds to the requirement that the quantity conventionally referred to as the "buoyancy Reynolds number" [70] $\text{Re}_b \equiv \epsilon/(\nu N^2)$ is much larger than unity [71,72]. The quantity Re_b can also be expressed in terms of the ratio of the Ozmidov scale $\ell_O \equiv (\epsilon/N^3)^{1/2}$, which is the largest vertical scale of turbulence not strongly affected by stratification, and the Kolmogorov scale $\ell_\nu \equiv (\nu^3/\epsilon)^{1/4}$, which is the smallest turbulence scale at which dissipation occurs. Explicitly, $\text{Re}_b = (\ell_O/\ell_\nu)^{4/3}$, thus implying that high-Re_b flows, as observed geophysically, have a very high dynamic range over which the flow is inherently nonlinear and turbulent, with no significant role played by the internal wave field. Large values of Re_b thus imply a fivefold hierarchy of scales for the LAST regime to exist such that [66] $L_R \gg L \gg H \gg \ell_O \gg \ell_\nu$, where L_R is an appropriate characteristic horizontal scale above which rotational effects can no longer be ignored. As a consequence, this phenomenon, if it even occurs, is difficult to replicate in the laboratory and to simulate numerically, although high-resolution simulations are beginning to access this regime [73]. Furthermore, though there is observational evidence (see, for example, Falder *et al.* [69]) that this regime occurs, a key outstanding challenge is to understand how it is connected to and interacts with rotationally or wave-dominated dynamical processes. At the moment, the fluid-dynamical research in this area is inevitably somewhat disconnected from oceanic and atmospheric flows, and there is a pressing need to bridge this gap, both in terms of constructing (and testing) new theories and generating numerical and observational data sets capturing the transition (or indeed transitions) in flow dynamics. As perhaps a first step on the theoretical side, some progress has been made in developing a reduced equation set that exploits the large horizontal to vertical scale separation to allow for a quasilinear yet still nontrivial coupling between such widely separated scales [33], constituting a very interesting advance on classical approaches leading to pure hydrostatic flow.

III. INTERNAL WAVE GENERATION BY TOPOGRAPHIC, CONVECTIVE, AND TURBULENT PROCESSES

Besides spontaneous and stimulated generation of internal waves by large-scale flows, there are several other mechanisms by which internal waves can be excited. One of the most significant of these is that of flow over topography, although the main processes of generation and consequent evolution once again differ qualitatively in the atmosphere and ocean.

In the atmosphere, observations suggest that the largest source of internal waves results from the unidirectional flow of mean zonal winds over mountain ranges [3]. Whether or not internal waves are generated depends upon four factors: the characteristic flow speed at the mountain height, U, the characteristic horizontal length scale of the topography, L, the stratification as characterized by the buoyancy frequency, N, and the Coriolis frequency, f. From linear theory, vertically propagating waves exist only if their intrinsic frequency, estimated by U/L, lies between N and f, with typical values of $N \simeq 10^{-2}\,\mathrm{s}^{-1}$ being two orders of magnitude larger than $f \simeq 10^{-4}\,\mathrm{s}^{-1}$ at midlatitudes [1,63]. Waves generated on the scale of mountain ranges have frequencies close to f and so should be classified as inertia-gravity waves. (Waves generated at very large horizontal scales are also influenced by the change in the Coriolis frequency with latitude, the so-called β effect. Study of these waves, known as planetary or Rossby waves, lies beyond the scope of this review.) General circulation models of the atmosphere are now beginning to resolve such small scales that they must begin to include nonhydrostatic effects associated with waves having frequency moderately below N. Being nonhydrostatic means that buoyancy forces are not balanced by vertical pressure gradients and so can lead directly to vertical accelerations.

The amplitude of topographically generated internal waves is set by the height, H, of the topography. This is a crucial parameter since it influences the height at which the waves ultimately break in the absence of encountering a critical level, which is where the upper-level winds change their zonal direction so that the wind speed equals the (ground-based) zero-horizontal phase speed of the waves. Because the density of the atmosphere decreases approximately exponentially with height, the amplitude of the waves grows as they propagate upward in order to conserve momentum. Because of this anelastic growth, the waves ultimately break when they grow to such large amplitudes that they overturn. Waves actually generated at large amplitude can overturn in the upper troposphere irrespective of anelastic effects, sometimes leading to downslope windstorms, and in the lower stratosphere, potentially leading to clear-air turbulence, which is a hazard to aircraft.

A recent comprehensive observational campaign called the Deep Propagating Gravity Wave Experiment (DEEPWAVE) used ground-based lidar, radar, and airglow images as well as *in situ* aircraft measurements to make unprecedented measurements of the life cycle of internal waves generated by flow over mountains in southern New Zealand and extending into the ionosphere situated above 85 km from the surface [74], as shown in Fig. 4. Energy fluxes by internal waves were found to be highly variable in part owing to the pre-existence of large-scale internal waves in the middle atmosphere generated by other sources. Some of the fluxes were the largest ever recorded, with values over 20 times typical values. This campaign also made observations of small-horizontal-scale and small-amplitude waves penetrating through the middle atmosphere to the ionosphere. In some instances, wave breaking was so large as to mix sodium ions in the ionosphere downward by 10 km. It has also been found that from the total spectrum of waves emitted by flow

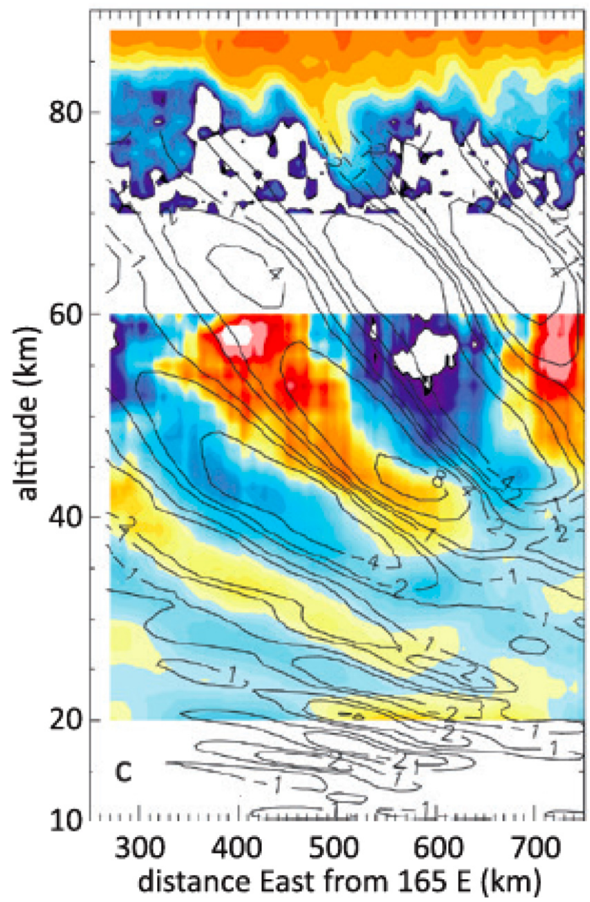

FIG. 4. Composite of temperature observed by lidar below 60 km altitude and sodium ion density in upper mesosphere measured during the DEEPWAVE campaign on July 13, 2014, above Lauder, New Zealand. (Copyright © American Meteorological Society. Used with permission from Fig. 9 of Fritts *et al.* [74].)

over topography the less energetic components are most important for the mesosphere, since the more energetic components already break at lower altitudes.

Conversely, in the ocean it is believed that most of the energy put into the internal wave field results from the oscillatory flow of the barotropic tide (i.e., the tide with virtually no vertical structure) over submarine ridges and at the continental shelves [75], a process sometimes described as baroclinic conversion. More recently, observations and modeling efforts suggest that significant internal waves may also be generated by mesoscale eddies interacting with topography or by the flow of the Antarctic Circumpolar Current over rough bottom topography, resulting in lee waves [76–80]. The efficiency by which energy from the barotropic tide is converted into internal waves is set by the tidal frequency relative to the buoyancy and Coriolis frequencies and the maximum topographic slope, $s^\star$. Independent of their wave number, internal waves with frequency ω propagate with lines of constant phase, forming an angle to the horizontal of $\alpha = \tan^{-1}[(\omega^2 - f^2)/(N^2 - \omega^2)]$, provided $f < \omega < N$. The barotropic tide of frequency ω efficiently generates internal waves with the same frequency if $s^\star > \tan\alpha$ in which case the internal waves emanate as beams originating from the topography where its slope equals $\tan\alpha$. Such topography is said to be supercritical [81].

Comprehensive observational studies of internal wave generation by the barotropic tides in the ocean have been carried out at a few sites in the open ocean [82,83]. These studies provided evidence for enhanced mixing near topography due to breaking internal tides [84]. However, most energy appears to escape the hot spots of generation. The lifecycle of these radiating waves remains poorly understood. There is no anelastic growth of waves in the ocean and, except for the transient occurrence of eddies, critical levels play little role in wave breaking. Far from topographic sources, internal waves are manifest as mode-1 internal waves, characterized by sinusoidal oscillations of the thermocline. Sometimes these mode-1 waves steepen, as observed west of Luzon Strait in the South China Sea, and form solitary wave trains [85,86] that eventually shoal and break. Otherwise, it remains unclear how these mode-1 waves ultimately deposit their energy into turbulence and mixing. Studies examining mode-1 waves incident upon continental shelves indicate that most of the energy is reflected back to the open ocean with dissipation recorded in a few localized regions [87,88], though the proportion reflected is thought to be quite variable [89].

Mean and eddying flows in the ocean also generate internal waves and are thought to be a substantial sink to such flows [80,90]. Linear lee waves are believed to radiate from topographic roughness with modest topographic height, as represented by the inverse vertical Froude number or Long number $\mathrm{Lo} \equiv Nh/U \lesssim 1$, and with horizontal scales smaller than $\simeq$6 km. These lee waves are then envisioned to undergo wave-wave interactions that drive the cascade to turbulence [76], though empirical evidence of this process has been hard to detect [78,91]. Larger scale topography is expected to exert blocking effects, a process that has been realized to be important for parametrizing mountain drag in the atmosphere [92,93], and for generating low-mode internal tides in the ocean [94–96]. This blocking and its effects on mean flows is only beginning to be looked at in the oceanic context [79,97,98].

Convection is understood to be another important source of atmospheric internal waves, particularly above the equatorial oceans and in the southern midlatitudes in summer, but possibly also in northern midlatitudes [4,99,100]. The waves can be excited by vertical motions within storm clouds or induced by latent heating, flow over the cloud tops, or the vertical oscillations of the cloud tops [101]. In addition, wave generation is influenced by the collective behavior of merging convective cells, frontogenesis, and the thermodynamics of moist convection [102,103]. Recent numerical models that capture internal waves generated at the submesoscale by these processes demonstrate that injection of energy into waves at these small scales contributes to the observed $-5/3$ kinetic energy spectrum in the mesoscale through upscale energy transfers [60,102]. One global-scale manifestation of these small-scale processes is the Quasibiennial Oscillation (QBO) in which stratospheric winds above the equator alternately flow eastward and westward on an approximately two-year timescale. The QBO is understood to result from momentum deposition of vertically propagating eastward and westward Kelvin, Rossby-gravity, and internal waves where they encounter critical levels [104]. While general circulation models of the atmosphere are able qualitatively to reproduce the QBO, the details of its amplitude and period differ between different models, which is an indication of the sensitivity of the results due both to the convective parametrization scheme used by each [105] and to the gravity-wave parametrization [15].

The role of convection in exciting internal waves in the ocean is unclear at present. In part, this is because rapid cooling of the ocean surface, as occurs beneath a hurricane or by low-pressure systems passing over the Labrador Sea in winter, is associated with strong surface wind stress, which itself acts as a significant hydrodynamic rather than thermodynamic source of waves [106]. Observations of processes occurring directly underneath the storms remains challenging, though progress may be made as more autonomous vehicles are being deployed in the world's oceans. Besides such extreme events, there is some evidence that Langmuir circulations (counter-rotating cells aligned with the wind) may generate internal waves at scales between meters and kilometers [107].

Indeed, turbulence itself can act as a source of internal waves as observed in laboratory experiments [108,109] and through simulations and observations in the atmosphere of secondary generation of internal waves resulting from the breaking of primary waves [61,74,110,111]. Investigations of the coupling between turbulence and internal waves remains active research.

IV. DRAG PARAMETRIZATIONS IN THE ATMOSPHERE

Climate simulations necessarily are run at relatively coarse resolution so that predictions on decadal and century timescales can be produced in reasonable time. Although such models are

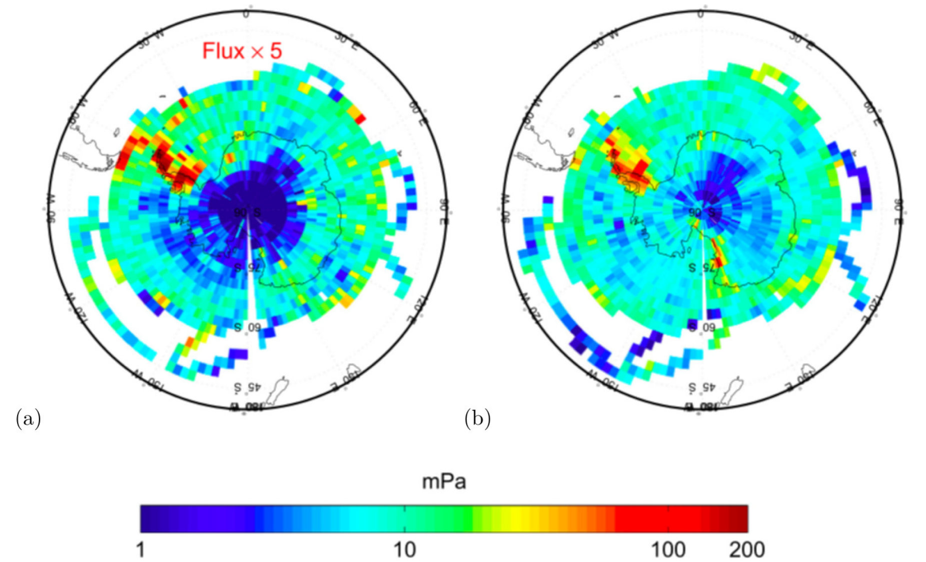

FIG. 5. Comparison between simulations (left) and radiosonde balloon observations (right) of 5-month time-averaged momentum fluxes at 19 km altitude in the Southern Hemisphere. The simulations from ECMWF have had their spatial resolution downgraded to correspond to that of the balloon data and their values have been multiplied by 5. Although the spatial pattern of the fluxes is similar, the simulation underpredicts observations by a factor of 5. (Copyright © American Meteorological Society. Used with permission from Figs. 1(c) and 1(d) of Jewtoukoff *et al.* [121].)

beginning to capture mesoscale horizontal motions with scales on the order of 50–200 km, they are unable to capture the dynamics of the generation, propagation, and breaking of mesoscale ($\simeq$100 km) and submesoscale ($\simeq$10 km) internal waves despite observational evidence that suggests such dynamical behavior has a non-negligible influence upon synoptic scale motions in the middle atmosphere [112–114]. By not appropriately incorporating the effects of subgrid-scale waves, general circulation models fail to reproduce realistic zonal mean winds and temperatures in the middle atmosphere [112,115–117], which affects seasonal and climate forecasts.

Guided by observations and the results of high-resolution numerical simulations, gravity wave drag parametrization schemes have progressively improved over the years through better representation of topographic and nonorographic sources. However, general circulation models continue to underpredict the temperature of the southern-hemisphere winter polar night jet in the middle atmosphere, which crucially influences accurate predictions of the ozone hole evolution over Antarctica. While the southern tips of Chile and New Zealand are significant topographic sources of internal waves, recent evidence suggests that islands in the southern ocean whose sizes lie below the climate model resolutions may nonetheless contribute non-negligibly to the total momentum flux [118,119]. Moreover, especially intermittent wave generation from nonorographic sources, particularly strong winds, constitute an important source of waves [120]. In particular, the comparison shown in Fig. 5 between measurements of momentum fluxes inferred by radiosonde balloons and those predicted and resolved by the European Centre for Medium Range Forecasts (ECMWF) operation model indicate that modeled fluxes can be a fifth of what is observed. This hints at excessive damping of internal waves resolved in the ECMWF model at the respective altitudes in the lower stratosphere. However, it might also indicate that further improvements are necessary to account for nonorographic and transient wave sources, as well as other effects.

The discrepancies between observed and modeled internal-wave momentum fluxes seem indirectly to point at other fundamental problems of present-day gravity-wave parametrizations. A model analysis of parameterized gravity-wave drag in spring during southern stratospheric final warming [16] showed that these events were simulated in a realistic manner though with gravity-wave momentum fluxes similar to those diagnosed from the above-mentioned ECMWF simulations. As the latter, however, are known to be too weak in comparison to measurements, only with a very weak input of internal-wave fluxes at launch altitude can the effects at higher altitude be captured well. As well as improving parametrizations of sources for internal waves, the representation of their propagation should be improved. Idealized theoretical models and simulations suggest that the effect of time-transient background winds, wave energetics, and lateral propagation of the waves as well as weakly nonlinear effects acting upon moderately large-amplitude waves may need to be incorporated into the next generation of parametrization schemes [6,37,45,122–125]. Further corresponding indirect observational evidence is provided again from radiosonde balloons, showing a conspicuous dependence of the intermittency of internal-wave momentum fluxes on the large-scale wind strength that parametrizations cannot reproduce [120]. Finally, in all parametrizations, the handling of internal-wave breaking is still very crude and often in considerable disagreement with findings from direct simulations of this process [126–128].

V. MIXING PARAMETRIZATIONS IN THE OCEAN

The ocean is driven at the boundaries by surface winds and tides, and some of this energy is carried into the interior by internal waves. Through most of the ocean, the mean flow of currents is weak and the propagation of waves is horizontally isotropic. Thus, the influence of drag is generally less important. However, there is a growing appreciation that drag may play a role where mesoscale eddies in strong currents such as the Antarctic Circumpolar Current and the western boundary currents interact with topography [97,129]. Here, the drag more likely acts on the eddy field itself, rather than the large-scale circulation. Because ocean climate models do not yet resolve mesoscale eddies, parametrization of drag presently is not an important issue but likely will become one as the resolution of these models increases. Anticipating this eventuality, idealized studies of lee wave drag are being revisited in the context of oceanography [130].

At present, general circulation models of the ocean are primarily concerned with mixing as a result of breaking waves. Only through such mixing can the observed abyssal stratification of the ocean be explained [7]. Physical oceanographers remain actively engaged in observational and modeling efforts in order to understand the energy cascade so that better parametrizations can be formulated [8].

As in the atmosphere, significant advances have been made through detailed *in situ* and satellite observations as well as numerical models that capture both mesoscale and submesoscale dynamics [131,132]. However, there are many mechanisms through which energy at large scales ultimately results in mixing at small scales, and the relative importance of these processes depends upon spatial location and temporal forcing that varies between diurnal and seasonal timescales [133]. As a consequence, turbulence is intermittent and inhomogeneous. The most important outstanding issue in the improvement of ocean general circulation models is to develop a better understanding of the connection between the large-scale flows and stratification captured by the simulations and the subgrid-scale location and time of occurrence of turbulence, and in particular the cumulative diapycnal mixing induced by such inherently spatiotemporally intermittent turbulent events. Although it may yet be some years before observations and modeling efforts provide better predictions for the onset of turbulence, some progress has been made linking mixing to energy dissipation when turbulence actually occurs.

Most parametrizations of mixing in the ocean quantify the turbulent kinetic energy dissipation rate ϵ as a function of fine- or mesoscale parameters. (It is always important to remember that this quantity is itself highly spatially and temporally intermittent, with growing evidence that it can be elevated by orders of magnitude in the vicinity of rough or ridgelike bottom topography [134], as

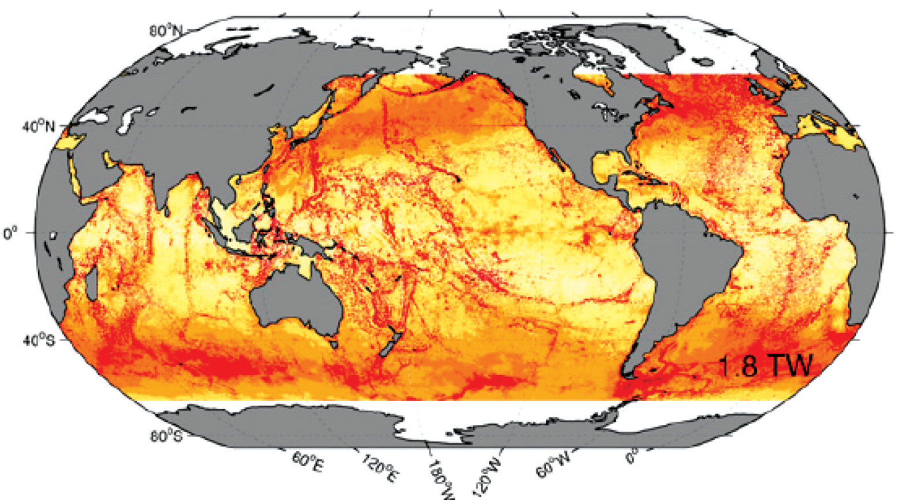

FIG. 6. Estimates of global ocean energy flux inferred from observations. Colors represent a log scale from 10^{-4} (white) to 10^{-1} W/m^2 (dark red). The spidery dark red features correspond to internal modes launched by tidal flow over bottom topography; the remaining light-red zones represent inertia gravity waves launched by wind stress in the ocean. (Copyright © American Meteorological Society. Used with permission from Fig. 2 of Waterhouse *et al.* [134]).

shown in Figs. 6 and 7.) However, what is needed for parametrization in larger scale simulations is a turbulent (vertical, and hence approximately diapycnal) eddy diffusivity for density, $\kappa_\rho \equiv \mathcal{B}/N^2$, in which $\mathcal{B} \equiv (g/\rho_0)\langle w'\rho'\rangle$ is the (vertical) buoyancy flux. Osborn [135] argued that on average, particularly for quasistationary turbulence, it was reasonable to assume that the buoyancy flux is proportional to the dissipation rate, $\mathcal{B} \approx \Gamma\epsilon$, and based on field and laboratory work suggested that the turbulent flux coefficient Γ (often referred to as the "mixing efficiency") may be bounded by $\Gamma \leqslant 0.2$ for a statistically steady state. Studies have shown that during a transient mixing event Γ can be much larger [136,137]. There is also evidence that Γ depends on the nature of the mixing event [138,139], itself being a function of the buoyancy Reynolds number, Re_b, and Richardson number, Ri, and perhaps other parameters (see, for example, Ivey *et al.* [140]). It remains an area of active and somewhat controversial research to capture the fundamental character of different breaking mechanisms, and in particular the effect of those mechanisms on the particular value of the turbulent flux coefficient [141–143]. In particular, plausible interpretation of the observational evidence in the ocean so far indicates that $\Gamma \approx 0.2$ is a reasonable estimate given other uncertainties in measuring and parametrizing ocean mixing [144]. On the other hand, there is accumulating evidence that $\Gamma \propto \mathrm{Re}_b^{-1/2}$ at sufficiently high values of the buoyancy Reynolds number, at least in some circumstances [138,139,141,142]. Clearly, much further interdisciplinary work and collaboration in this area is required, resolving apparent discrepancies between observation, experiment, simulation, and theory. Furthermore, it is important to remember that κ_ρ is the actual quantity of interest for parametrization in larger scale models, and since $\kappa_\rho = \nu\Gamma\mathrm{Re}_b$, understanding whether there is dependence of Γ on Re_b is of leading-order importance. Furthermore, though there is a large amount of research activity attempting to model the properties of Γ, in practice the inherent uncertainty in ϵ and N and hence Re_b plausibly swamps any robust effect of Γ variability on estimation of κ_ρ. Just to mention one (potentially very important) example of profound uncertainty, it is still an open question as to whether Γ and/or κ_ρ have qualitatively different behaviors when the flow is in the LAST regime, as described in Sec. II.

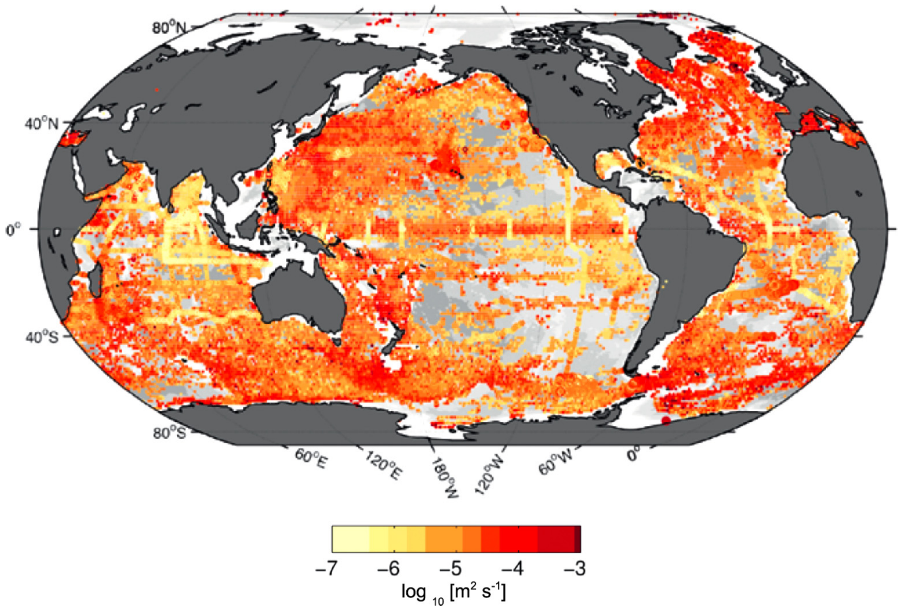

FIG. 7. Global estimates of dissipation in the top 1 km of the ocean. (Copyright © American Meteorological Society. Used with permission, adapted from Fig. 1 of Waterhouse *et al.* [134]).

Issues with the parametrization of Γ aside, substantial recent efforts have been made to develop better parametrizations of ocean mixing [8], leading to spatially variable vertical mixing being included in ocean models in justifiable ways [145]. These methods usually involve as a first step computing the energy that is believed to radiate into the internal wave field either from tides [146] or from mean and eddying flows [76,147]. The simplest of these parametrizations then assume a fixed fraction of the radiated energy goes to turbulent dissipation in a decay scale near the generation site, presumably due to wave-wave interactions. More sophisticated versions assume horizontal isotropy, use wave-wave interaction theory to decide when the wave field is susceptible to breaking, and deposit the radiated energy at those depths [148,149]. These "local" mixing schemes have been found to matter for large-scale modeling [145,150] and deep-water buoyancy budgets [151].

These schemes, however, often do not dissipate all their energy at the generation site, with large vertical wavelength internal waves able to escape the region of generation. This is particularly true of large obstacles like midocean ridges and sea mounts, where most of the internal wave energy generated goes into low-mode waves. For large obstacles, parametrizations have been developed to estimate the local mixing [96,152], but in those cases more than 90% of the energy is still believed to escape the bathymetry. As discussed above, some of this breaks at remote locations. Efforts are under way to track this radiated energy in consistent manner [8,153,154] and decide how it will be dissipated on remote shores [89].

VI. SUMMARY AND FUTURE DIRECTIONS

This review has shown that there remain several open questions regarding fundamental processes involved with energy transfers in the ocean and atmosphere from large scales (>100 km) to dissipative scales (<1 mm, though larger in the upper atmosphere). Theoretical and observational insights have guided the development of parametrizations for these phenomena in general circulation models. However, their limitations are evident.

It remains a challenge in observations, simulations, and theoretical modeling to capture the dynamics occurring in the full range of scales from synoptic and mesoscale through the internal wave spectrum and downward to dissipative scales. Numerical simulations of idealized circumstances (e.g., uniform stratification and zero background flow) are still far from having the resolution to capture the full range. Simulations further suggest that nontrivial effects come into play when the stratification and background flow are not uniform [155].

As well as building a better database of observations and improving the resolution of simulations, there may be other processes important to understanding the global energy budget. For example, a recently proposed hypothesis is that mixing and transport in the deep ocean is driven primarily by its sloping boundaries, not least because of the substantially enhanced turbulence there [133,151,156]. It is becoming increasingly evident how important it is to study key processes by idealized and semirealistic simulations, by measurements and observations, and at all stages by critically checking how well internal-wave parametrizations respect corresponding findings. This seems to be the only way to limit the use of overtuned parametrizations that might be insufficiently reliable in climate-change studies where the simulated conditions cannot agree anymore with those used for present-day empirical parameter optimizations. However, with increasing computing power, parametrizations will be able to incorporate and represent more detailed dynamics. More work is to be done in this direction, with interesting prospects ahead.

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Chapter 3

DM-Stat: Statistical Challenges in the Search for Dark Matter (18w5095)

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Organizer(s): Aaron Vincent (Queen's University), Gianfranco Bertone (University of Amsterdam), Jessi Cisewski (Yale University), Roberto Ruiz de Austri (University of Valencia)

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Statistical challenges in the search for dark matter

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The search for the particle nature of dark matter has given rise to a number of experimental, theoretical and statistical challenges. Here, we report on a number of these statistical challenges and new techniques to address them, as discussed in the *DMStat* workshop held Feb 26 – Mar 3 2018 at the Banff International Research Station for Mathematical Innovation and Discovery (BIRS) in Banff, Alberta.[a]

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* Editors

[a] http://www.birs.ca/events/2018/5-day-workshops/18w5095

I. INTRODUCTION

The nature of dark matter (DM) is one of the most pressing puzzles in modern particle physics and astronomy. Overwhelming evidence from galactic dynamics to cosmology tells us that $\sim 85\%$ of the matter content of the Universe is in a very different form from the familiar "baryonic" matter described by the Standard Model (SM) of particle physics. Precision measurements of the cosmic microwave background (CMB) suggest the existence of a new particle that is cold (i.e. non-relativistic at sufficiently early cosmic times), dark (very weakly-interacting with quarks, electrons and photons), and behaved like matter (a pressureless fluid) in the Early Universe [1].

Evidence for dark matter comes to us entirely via its gravitational influence; however, there are many good reasons to believe in a particle physics portal to the dark sector. In fact, many theories of physics beyond the standard model (BSM) such as supersymmetry naturally predict a nonzero relic abundance of "dark" particles.

In the absence of a definitive non-gravitational signal of DM, the space of possible models of particle dark matter has also thrived. Theoretical motivations such as the "WIMP miracle," the "baryon disaster," the Peccei-Quinn solution to the strong CP problem, and the neutrino mass problem motivate such candidates as the WIMP, asymmetric dark matter, the axion or the sterile neutrino. The full list of DM candidates is as varied as it is extensive.

Following several decades of searches, it has become increasingly clear that discovery is less likely to happen via a single "smoking gun" signal, but rather by scrutinizing data from many experiments in many disparate fields. The main searches for dark matter are broadly categorized into direct detection, indirect detection, and production at colliders.

The next decade will present us with major advances in experiments designed to search for dark matter, as well as experiments with a broader focus on searches for BSM physics. Even though current and past searches have thus far come up empty, the parameter space that has been explored pales in comparison with what will become available in years to come. This includes an unparalleled quantity of astrophysical data, from e.g. the Square Kilometre Array (SKA) radio telescope [2] that will map the distribution of matter in the dark ages before the formation of the first galaxies via the 21 cm spin transition line of the hydrogen atom [3]; gamma ray telescopes such as the Cherenkov Telescope Array (CTA) [4] that will yield important information about the highest energies in the universe; and the next generation of galaxy surveys (eBOSS [5], DESI [6]) which will map the distribution of structure in the universe. Starting in 2022, the Large Synoptic Survey Telescope (LSST) [7] will survey the southern sky to unprecedented depth, allowing for the discovery of new ultra-faint dwarf galaxies [8] and increasing the sample of known galaxy-scale strong gravitational lenses by a factor of 10 [9]. Taken together, these new observations will dramatically improve our knowledge of dark matter structure on kiloparsec scales and below, hence stress-testing the standard cold dark matter paradigm in a new regime. Concurrently, space based missions such as Gaia [10, 11] will map the distribution of dark matter in our own neighbourhood for the first time, with the promise of sub-milliarcsecond astrometry. The PINGU upgrade to the IceCube neutrino detector at the South Pole [12] will be able to detect light DM candidates, as we embark on the first decade of neutrino astronomy.

Meanwhile, DM-specific searches such as XENONnT [13], LUX-ZEPLIN [14] and ADMX [15] (along with DM-focused analyses of collider data) will provide the best sensitivity for testing a large variety of hypotheses regarding the particle properties of DM.

Reconciling the vast landscape of theoretical models and the many disparate data sets is not an easy task, and it inevitably leads to a number of statistical challenges on scales that range from the interpretation of a single experiment, all the way to combination of models and large datasets with one another.

Our aim in this short review is to outline major statistical challenges that came up over the course of the *DMStat* workshop[1], along with proposed approaches and

[1] Held Feb 26 – Mar 3 2018 at the Banff International Re-

solutions including software developed by the community. We begin with a brief review of the problem of dark matter (Sec. II), followed in Sec. III by a description of current strategies for experimental dark matter searches and some challenges those searches have encountered. We then outline and discuss several statistical approaches (Sec. IV), including some novel techniques, and present some simple examples in Sec V.

A. Disambiguation

Although statistics acts in some sense as a lingua franca across the sciences, there are certain "regional dialects" that should be noted: we have identified a few terms in particular that have very different meanings when used by the astroparticle physics community versus statisticians.

Model: In physics, the word "model" may be entirely synonymous with "theory", in the sense of referring to an entire physical theory that one may wish to test with statistics – or it may refer to a specific realisation of a theory. This can be a restriction of the theory to a particular subspace of its possible forms, or very often, a specific numerical choice for all values of the free parameters of a theory. In contrast, in the field of statistics, the term "model" refers to an incompletely-specified probability distribution; draws from this distribution are meant to replicate the processes that generated the observable data. Data are used to *estimate* the missing components of the model, typically a vector of unknown parameters. Such estimation problems are fundamental in *statistical inference*.

Simulation: In statistics, this usually refers to the process of generating a large number of random realizations from a probability model by Monte Carlo methods, in order to characterize the distribution of a quantity of interest, e.g. an estimator or a test statistic. In physics, the word simulation will usually refer to modeling the outcome of a physical experiment based on the model parameters (for example, the angular power spectrum of the cosmic microwave background, given a set of cosmological parameters). A physicist's simulation may or may not be deterministic in nature.

Coverage: Often (mis)used in particle physics as a loosely defined qualitative notion of the completeness with which a theoretical parameter space has been sampled. In statistics, coverage has a very specific and well-defined meaning, referring to the fraction of repeated experiments in which the true value of a quantity actually appears inside a confidence interval/region. A 90% confidence interval/contour is said to undercover if the true value would actually appear inside the interval in less than 90% of repeated experiments, or to overcover if the true value would appear within the interval in more than 90% of repeats. Overcoverage is inefficient but relatively benign, as it increases the probability of a type II error (failure to reject a false null hypothesis, a "false negative" finding); undercoverage leads to an increase in the rate of type I error (rejection of a true null hypothesis, a "false positive" finding), so is generally considered more serious.

Machine learning: A field that grew out of computer science and the study of artificial intelligence, but is concerned with many of the same challenges faced by statisticians. Indeed, the line between these fields is quite blurry, although each uses its own terminology, e.g., *supervised learning* problems in machine learning are closely aligned with *regression* problems in statistics. Methods developed within machine learning tend to be more focused on broad applicability with computational efficiency, while statisticians will often tailor their models more to a particular application, and place more emphasis on theoretical properties of methods.

II. THE DARK MATTER PROBLEM

While the flat rotation curves of spiral galaxies [16] are often held up as conclusive evidence for a missing matter component in the Universe, equally strong evidence for dark matter arises over a range of scales: the motion of nearby stars above and below the galactic plane [17, 18]; the velocities of galaxies within clusters [19]; gravitational lensing by galaxies and clusters [20–23]; the rapid formation time of galaxies [24, 25], as well as the angular power spectrum of the cosmic microwave background [26]. Each of these points to a large nonbaryonic component of matter in the Universe – about 85% of the total matter, or ∼25% of the total energy density. If this missing matter is in the form of particles, it should be (almost) electrically neutral [27] and have only very weak interactions with ordinary matter [28].

The Standard Model of particle physics does not provide a suitable particle to play the role of dark matter. However, a number of BSM theories of physics provide compelling candidates for this nonbaryonic particle. In supersymmetric (SUSY) extensions of the Standard Model, for example, the lightest new SUSY particle is typically stable and can be produced with sufficient density in the early Universe to account for all of the dark matter [29]. Such particles fall into the class of 'Weakly Interacting Massive Particles' (WIMPs) [30]. Another

search Station for Mathematical Innovation and Discovery (BIRS) in Banff, Alberta (http://www.birs.ca/events/2018/5-day-workshops/18w5095).

popular candidate arises in solutions of the strong CP problem, which hint at the existence of a new light pseudoscalar, the axion [31, 32]. Other exotic candidates are also plausible: primordial black holes [33], sterile neutrinos [34], particles in a strongly-interacting dark sector [35], or candidates motivated by potential problems on small astrophysical scales such as self-interacting dark matter [36, 37].

Each of these models and candidates comes with its own set of parameters: particle masses, interaction strengths, etc. While these parameters can in principle be constrained by experiment, there is often little theoretical guidance as to which values should be preferred and so choosing appropriate priors is often a challenge [38–40]. Each model also provides its own set of experimental signatures, requiring an ability to sort signal from background, as we discuss shortly.

In what follows, we will focus on the standard WIMP paradigm for DM, but of course many of the statistical challenges we discuss are relevant also for other candidates. Indeed, an interesting question arises if we remain agnostic about the nature of the dark matter particle: how do we compare models with very different parameter spaces and observational signatures? Most commonly used tools for model comparison require them to be *nested*, so that a modification of the parameters of one model yields the second model. We must therefore be careful if we choose to compare fundamentally distinct models such as the WIMP and the axion.

III. CONTEMPORARY CHALLENGES IN DARK MATTER

Here we summarise some of the key observational challenges in the search for DM. This includes searches for DM scattering of Standard Model particles (Sec. III A), searches for the products from DM annihilation (Sec. III B) and searches for DM production in colliders (Sec. III C). We also discuss the impact of DM on galaxy formation and the challenge of constraining its properties with astronomical observations (Sec. III D). Our goal is not to provide a thorough review of these topics but to point out some of the statistical issues involved and to provide a backdrop for the more detailed discussion of statistical challenges in Sec. IV.

A. Direct searches

Direct searches are experiments searching for evidence of interactions of individual dark matter particles in terrestrial detectors. This type of experiment can be carried out for most dark matter candidates (except for very light particles which have energies that are below the threshold of existing particle detectors, and extremely heavy particles where the number density becomes too small and interactions are too rare even in the case of high cross sections).

1. WIMP Signatures

Here we concentrate on experiments originally developed for the detection of WIMPs or WIMP-like particles. Due to simple scattering kinematics and the fact that particles we can hope to detect would be gravitationally bound to our galaxy (and thus must have a velocity of less than $\sim$600 km/s [41]), the energy transfer through interactions with electrons is at most in the eV range, while interactions with nuclei yield typical recoil energies in the keV range. Thus, most of these experiments concentrate on the identification of nuclear recoils (NR), while discarding electron recoils (ER). However, recent developments have yielded detectors with very low energy thresholds capable of detecting energies in the range that can be expected from electron interacting dark matter [42, 43].

Other signatures that have been proposed for the identification of dark matter interactions include modulations of the detected signal with time. Due to the motion of the earth about the Sun and the Sun about the galaxy, the relative velocity of the detector and the dark matter particles changes over the course of the year, leading to a weak modulation of the interaction rate [44].

If the direction of the incoming dark matter particles can be identified in a detector, one would also expect a modulation over the course of the day, since the rotation of the earth about its axis leads to a change of the orientation of the detector relative to the flux of incoming dark matter particles [45].

2. Detection Channels

There are three main ways of detecting particles:

1. Particle interactions may ionize the target, and the liberated charges can be collected; the amount of charge detected allows for an estimate of the deposited energy. However, the amount of charge produced is usually very different for different interactions (ER interactions are usually much more efficient in ionizing than NR interactions).

2. In some cases excited electrons de-excite via the emission of photons in a process called *scintillation*. The fraction of energy converted to scintillation light is usually small (few percent) and again the scintillation efficiency is usually much higher for ER than for NR interactions.

3. Eventually, most of the energy of the interaction is converted into thermal energy. This provides an opportunity to measure the total energy transfer of the interaction independent of the interaction type.

Experiments have been designed to take advantage of each of the detection channels, and in many cases two of the channels are combined, allowing for the discrimination between ER background events and NR dark matter candidate events.

Below we list a selection of current experiments, to give an idea of the range of techniques:

- *Inorganic scintillating crystals* are used by the DAMA/LIBRA experiment [46–48] which relies on the annual modulation discussed above for signal identification. Such a signal as indeed been observed beyond any statistical doubt, but its interpretation in terms of dark matter interactions is inconsistent with the absence of a compatible signal in other experiments. SABRE [49] and COSINE [50] are upcoming attempts to test the DAMA signal using the same technique.

- *Semiconductor detectors* made out of Si (DAMIC [51, 52]) and Ge (CoGeNT [53]) benefit from low thresholds and very high intrinsic material purity. CoGeNT observed a statistically significant rise of the observed event rate towards low energy and hinted at a possible interpretation as a dark matter signal. However, a careful reanalysis with a more realistic background model was able to explain the observation with conventional interactions [54]. This highlights that statistical significance must be accompanied with a very good understanding of background and detector response in order to avoid misinterpretations.

- *Super-heated liquid detectors* were developed by COUPP [55] and PICASSO [56], now combined to form the PICO collaboration [57]. The level of superheat in these detectors is adjusted such that they are insensitive to ER background and only NR interactions trigger a phase transition.

- *Cryogenic detectors* combine the detection of thermal energy with the measurement of a charge signal (SuperCDMS [58–61], EDELWEISS [62, 63]) or scintillation light (CRESST [64, 65] and COSINUS [66]) for an effective reduction of ER background.

- *Gaseous detectors* are either designed to reach very low thresholds and thus access dark matter particles down into the sub-GeV mass range (NEWS-G [67]) or aim at identifying the recoil direction (DRIFT [68], MIMAC [69], DMTPC [70] and NEWAGE [71]).

- *Noble liquid detectors* often use dual-phase time projection chambers, taking advantage of the high scintillation light yield of Xe (LUX [72], XENON1T [73, 74], PANDA-X II [75]) and Ar (DarkSide [76, 77]) and the fact that electrons liberated in an interaction can be drifted over long distances in the inert material. Comparison of the initial scintillation light and the secondary scintillation produced by the charges that are extracted from the liquid into the gas phase allow for an effective ER background discrimination. In argon, an excellent ER discrimination can also be achieved by just looking at the pulse-shape of the scintillation light in a simple liquid detector (DEAP [78]).

Finally, upcoming generations of these detectors (e.g. LZ [79], XENONnT [80], DarkSide [81], PICO-500L [82], SuperCDMS SNOLAB [83]) are aiming to push the sensitivity to the ultimate limit given by NR interactions from solar or atmospheric neutrinos.

3. Statistical methods in direct detection

A very good tool for the analysis of data from experiments with very low background is the Optimum Interval Method [84–86]. This gives the best sensitivity in the presence of an unknown background. Since no assumption is required about the origin or spectral shape of the background, this is also a very conservative method. Instead of spectral information, other parameters (timing, pulse shape parameters, etc.) could be used and it would be very useful to have an expansion of this method to a 2- or more-dimensional parameter space. This method can by construction only produce limits on the dark matter interaction rate and does not allow signal extraction.

Recently, many experiments have adopted an analysis method in which known backgrounds are explicitly taken into account. The spectral shapes of these backgrounds are determined and included in a Maximum Likelihood fit. This provides better sensitivity in the presence of a background, but requires that the background features be determined independently. It also allows the extraction of a dark matter signal. A problem arises if there are backgrounds whose distributions are not known, or not well known.

Combining results from different experiments or in some cases from different detectors in the same experiment may also cause a challenge. In particular if the performance and the backgrounds of the different detectors are different, it is non-trivial to find an unbiased method that extracts the best joint sensitivity (see Sec. V B for a simple toy example).

B. Indirect searches

Indirect searches for DM mainly rely on a search for the high-energy products of DM self-annihilation into Standard Model particles (for a dedicated review, see Ref. [87]). The WIMP hypothesis has been a compelling driver of these searches, since thermal production through annihilation in the early Universe implies ongoing (albeit suppressed) annihilation today. Nonetheless, WIMPs are not the only DM candidates that are expected to yield an indirect signal: asymmetric DM can annihilate with a relic symmetric DM component, and axions and sterile neutrinos can decay or oscillate to standard model particles. Indirect searches make use of the large DM concentrations present in astronomical bodies including the Galactic centre, dwarf satellite galaxies, galaxy clusters, as well as the full isotropic background at high redshifts.

Signals of DM annihilation or decay can include:

1. Cosmic rays produced by nearby DM annihilation in the MW halo can be detected by space observatories including PAMELA [88, 89] and AMS-02 [90], or balloon experiments such as ATIC [91, 92], HEAO [93], TRACER [94], and CREAM [95]. Cosmic rays mainly probe local (within ∼1 kpc) cosmic ray sources. Because they are composed of charged particles, their arrival directions do not point back towards their sources; rather, they diffuse through the turbulent magnetic structures of the interstellar medium (ISM).

2. Gamma rays, produced copiously by internal bremsstrahlung, decay of heavy unstable DM annihilation products, or interactions with the ISM, are searched for with space-borne experiments such as Fermi-LAT [96], DAMPE [97], INTEGRAL/SPI [98] and Chandra [99] (among others). At very high energies (and thus very high DM mass), ground-based air Cherenkov telescopes such as MAGIC [100], VERITAS [101], HESS [102] and in the future CTA [4] can constrain signals from high-mass DM.

3. Neutrinos from DM annihilation and decay can be searched for at neutrino telescopes such as SuperKamiokande [103], IceCube [104] and ANTARES [105]. Because of the difficulty in detecting neutrinos, these bounds are fairly weak. However, neutrino telescopes are sensitive to DM which is captured in the Sun via elastic scattering. Since these particles sink to the Solar centre and annihilate, the neutrino signal (or lack thereof) from $>$ GeV dark matter becomes one of the cleanest (if model-dependent) indirect signals of DM [106].

4. Finally, DM annihilation at high-redshift into photons and charged particles change the ionization floor during the post-recombination dark ages [107]. This extra fraction of free electrons rescatters CMB photons, leading to a suppression in the angular power spectrum at high multipoles, akin to a "blurring" of the last scattering surface. Energy injection at lower-redshift (e.g., from DM decay or annihilation in clusters) leads to an increase in correlation on large scales. The polarization of the CMB signal is particularly sensitive to this effect, because Thomson scattering is polarized.

A common issue that plagues indirect searches for DM is the simple fact that astrophysical backgrounds are quite poorly understood. A DM-like signal will inevitably come with a number of plausible astrophysical interpretations.

Given known backgrounds, indirect searches nevertheless provide strong and fairly model-independent constraints on new physics. CMB bounds from Planck [26], gamma ray observations of the Milky Way's dwarf satellite galaxies (e.g. [108]), and low-energy (∼10 GeV) positron observations by AMS-02 [109] provide some of the strongest limits on WIMP dark matter. Solar neutrino observations provide the best limits on spin-dependent WIMP-nucleus scattering [110, 111].

C. Collider searches

If non-gravitational interactions between DM and the Standard Model (SM) exist, particles of DM could be produced in proton-proton collisions at the Large Hadron Collider (LHC) [112]. The LHC operates at the highest center of mass energy and provides the highest luminosity in current high energy experiments. Therefore, sensitivity to very low production cross-sections of DM particles can be achieved at general purpose experiments like ATLAS [113] and CMS [114], while sensitivity to certain DM models can be also obtained at specialized experiments like LHCb [115] and ALICE [116]. As DM particles are not expected to interact with the detector material, the typical signature will have missing transverse energy in the detector. The main backgrounds for the analyses come from limited detector resolution, neutrinos in the final states of SM processes, and non-collision background processes.

Several approaches in DM searches are used at LHC experiments [117]. The DM particles are not expected to leave a signal in interaction with the material of the detectors, but they can be observed if they are produced in association with a visible SM particle $X(= g, q, \gamma, Z, W, h)$. These are the so-called "mono-X" or $\not{E}_T{+}X$ searches, where $\not{E}_T$ is the missing transverse energy in the detector. Another approach in DM searches is to use effective field theories (EFT). They rely on the assumption that production of DM occurs through a contact interaction, involving a quark-antiquark pair (or two gluons) and two DM particles. Kinematics of $\not{E}_T{+}X$ models can significantly differ from the contact interaction approach. EFT assumes a heavy mediator in the interaction of DM and SM particles, but if the mediator is not heavy, models that explicitly include mediators need to be used. They provide an extension to the EFT approach, and use "simplified models", constructed for specific particles and their interactions. Models using a mediator can predict significantly different signals, where decays back to SM particles are viable. In this context, due to different kinematics, analyses can be optimized for two types of signatures. The first use the $\not{E}_T{+}X$ signature, and can be interpreted using both the EFT and simplified models, and the second use simplified models that probe DM – SM couplings. A number of additional physics scenarios account for DM. These include e.g. the two Higgs doublet model (2HDM) [118], or various models in the framework of Supersymmetry (SUSY) [119–124].

A few assumptions are made in DM searches at LHC experiments. To ensure that DM particles are produced in p-p collisions, it is assumed that interactions between SM and DM particles exist. Most of the analyses assume DM to be a weakly interacting massive particle (WIMP), which is stable on collider time scales and does not interact with the detector material. Typically, minimal flavor violation (MFV) is assumed [125], which results in the same flavor structure of couplings of DM to ordinary particles as in the SM. Results of $\not{E}_T$+X and simplified models that probe DM – SM couplings are typically presented using vector and axial-vector mediators; fixed values of mediator couplings to quarks, leptons and DM; mediator width set using the minimal width formula; and the mediator and DM particle masses as free parameters [126]. Other physics scenarios have their results presented as a function of free parameters in the model under study, e.g. Higgs branching ratio or SUSY particle masses, for 2HDM and SUSY models respectively.

1. *Collider signatures*

A wide range of models are tested and dedicated DM searches are performed at ATLAS and CMS. These include the $\not{E}_T$ + X and searches using simplified models that probe DM - SM couplings. Since the interactions of DM with SM particles are not known, a number of additional scenarios are considered:

- In the $\not{E}_T$+X search, DM is produced in association with the particle X coming from an Initial State Radiation (ISR) jet, photon, W boson or Z boson. The DM production cross-section scales with quark-X coupling, and the signal is expected as an excess in the tail of the $\not{E}_T$ distribution. The analysis typically has a requirement on $\not{E}_T$, and a selection for the particle X, and the interpretation is done for different mediator and DM particle mass. The highest cross-section is for gluon ISR, and the highest sensitivity in the mediator and DM particle mass can be achieved using the $\not{E}_T$+jet analysis, compared to $\not{E}_T+\gamma$, $\not{E}_T+Z$ and $\not{E}_T+Z$ searches.
- In analyses that probe the DM - SM couplings, the mediator can decay back to SM particles. Then the signal appears as a localized excess in the invariant mass distribution of two fermions. Typical searches perform a scan on a di-fermion invariant mass distribution. The search for dijet resonance represents one of the most important analyses due to the high production cross-section and a number of approaches are used, while the dilepton resonance search is well motivated by the clean signature which provides strong constraints for small mediator-lepton couplings. The exclusion is done using different sets of assumptions on the DM, mediator and couplings. For an axial-vector mediator, dijet searches have smaller sensitivity for very low mediator masses, but very high exclusion for high mediator masses, for any mass of DM particles.
- At LHC energies there is no top quark content in protons, and a mono-top final state is a clear signature of new physics, and represents an important scenario in DM searches.
- DM can be produced in association with heavy flavor particles, and interesting searches are $\not{E}_T+t\bar{t}$ and $\not{E}_T+b$.
- Since ISR of Higgs bosons is strongly suppressed, models where the Higgs couples to DM represent an interesting scenario. The typical signature has visible decays of the Higgs (e.g. $H \to bb$ or $H \to \gamma\gamma$) and $\not{E}_T$.
- Invisible Higgs decay occurs for a model where DM couples to the Higgs boson, and the mass of the DM particle is smaller than half of the Higgs boson mass. This gives rise to an 'invisible' branching fraction for the Higgs boson.
- The two Higgs doublet model with a light pseudoscalar mediator which decays to DM produces an enhanced $\not{E}_T$+X signature. Due to resonant production of heavy scalar and heavy pseudoscalar Higgses, enhancement occurs in the $\not{E}_T+Z$ and $\not{E}_T+h$ channels.
- Supersymmetry (SUSY) predicts a DM candidate (e.g. neutralino, gravitino), and systematic searches are done for different productions of SUSY particles. A typical signature has a long chain of cascade decays of SUSY particles, with the lightest SUSY particle (LSP) at the end of the chain.

2. *Statistical approaches at the LHC*

In LHC searches analyses are optimized to maximize signal and reduce the background in the signal region (SR) selection [127]. The SM background is estimated using data-driven techniques, from the control region (CR) selections, designed to be dominated by one type of SM background, and orthogonal to the SRs, where normalization factors for each background are estimated using data. Statistical interpretation is performed using the frequentist approach, where a hypothesis is tested using statistics only. For an analysis with multiple bins in the discriminating variable distribution, the likelihood for the observed number of events is modeled by the Poisson distribution, which considers the expected and observed number of events in each bin, and nuisance parameters to account for uncertainties in each bin as:

$$L(\mu, \theta) = \prod_{i=1}^{N} P(\mu s_i(\theta) + b_i(\theta)) \times \prod_{j=1}^{M} P_j(\theta)\,, \qquad (1)$$

where μ is the signal strength, s is the expected number of signal events, b is the expected number of background events, θ are the nuisance parameters, N is the number of signal region bins, and M is the number of backgrounds considered.

In order to quantify a possible excess, a local p-value is calculated using the profiled log-likelihood ratio test statistic

$$q_\mu = -2 \ln \frac{L(\mu, \hat{\hat{\theta}})}{L(\hat{\mu}, \hat{\theta})}\,, \qquad (2)$$

where $L(\mu, \hat{\hat{\theta}})$ maximizes the likelihood for a specific signal strength μ, and $L(\hat{\mu}, \hat{\theta})$ is the global maximum likelihood. For the case of a statistical test for the discovery of a positive signal, a one-sided likelihood for the background hypothesis only ($\mu = 0$) is used:

$$q_0 = \begin{cases} -2 \ln \lambda(0) & \hat{\mu} \geq 0\,, \\ 0 & \hat{\mu} < 0\,, \end{cases} \qquad (3)$$

where λ is the likelihood ratio [128]. The test statistic's distribution asymptotically follows a χ^2 distribution [129], and the p-value is calculated as an integral for values higher than the observed test statistic $q_{0,obs}$. The significance is calculated using the inverse Gaussian cumulative distribution function ($Z = \Phi^{-1}(1-p)$). For a case of high significance, the global significance needs to be calculated, as a probability for finding such an excess from statistical fluctuations of the background when looking in a large number of SR bins. As the number of SR bins considered increases, the global significance becomes smaller.

If no significant excess is observed, upper limits on the visible production cross-section are set using the one-sided profile log-likelihood (with the signal strength μ as a free parameter) using the test statistic:

$$q_\mu = \begin{cases} -2 \ln \lambda(\mu) & \hat{\mu} \leq \mu, \\ 0 & \hat{\mu} > \mu. \end{cases} \qquad (4)$$

To set exclusion limits, the CL_S technique [130] is used. It accounts for a small number of expected signal events compared to the number of expected background events. Exclusion limits are calculated using:

$$CL_s = \frac{p_{s+b}}{p_b}\,, \qquad (5)$$

where $p_{s+b} = P(q \geq q_{obs}|s+b)$ using $\mu = 1$, and $p_b = P(q \geq q_{obs}|b)$ for $\mu = 0$. The p_b is a conditioning factor to account for the goodness of fit of the background-only hypothesis, designed to prevent downwards fluctuations in the background leading to the unreasonably strong exclusion of signal models. The exclusion limits are typically set at 95% CL, for each DM model point, and exclusion regions are drawn for $CL_s \leq 0.05$.

With recent developments of machine learning (ML) techniques, a number of improvements are being developed in DM searches. Firstly, performance in object reconstruction can be improved using ML which allows for better signal separation. A number of applications are being implemented for e.g. lepton reconstruction or b-jet tagging. Secondly, signal separation in the analyses can be improved using ML techniques with a number of new methods being investigated for DM searches, e.g. Boosted Decision Trees [131], Deep-learning Networks [132], Generative Adversarial Networks [133], etc. Further details of ML techniques in DM searches can be found in Sec. IV B 3.

Collider searches represent an important avenue in DM searches, as they provide precise constraints on DM masses, for given assumptions on the mediator and couplings. The $\not{E}_T + jet$ and a dijet resonance searches are expected to have good sensitivity to many DM models using the full Run 3 integrated luminosity [134]. If DM is not found, this would represent an important constraint. Current analyses use simplified models for optimization but more complex models of DM interactions need to be considered for the future. Additionally, initial assumptions on the DM particles need to be relaxed, e.g. additional scenarios with long-lived DM particles need to be considered to extend the reach of DM searches. Statistical interpretation represents a crucial aspect in quantifying the significance of a potential excess and for setting exclusion limits. In addition, better sensitivity can be achieved through improved object reconstruction and signal separation by using modern machine learning techniques.

D. Gravitational probes and structure formation

Predictions for the distribution of large scale structure from cold dark matter (CDM) cosmology are in excellent agreement with observations on large scales [135]. On smaller scales, it may be possible to probe the microphysics of DM by studying the properties of galaxies and comparing with the results of numerical simulations of galaxy formation [136].

For around a decade, a number of discrepancies between the results of numerical simulations and observations of galaxies have been put forward as indicators of physics beyond the standard CDM paradigm. These "small-scale" problems include the presence of bulge-less disk galaxies [137], the core-cusp problem [138, 139], the missing satellites problem [140] and the Too-Big-To-Fail problem [141, 142]. However, many of these issues were first observed in DM-only simulations. The inclusion of gas and stars (and associated feedback mechanisms) in more realistic hydrodynamical simulations has alleviated many of these "small-scale" tensions (see e.g., [143–150]).

The effects of baryonic feedback must be included in any realistic simulation of galaxy formation, even those which include non-standard dark matter models. These include Self-Interacting dark matter [151–154] (originally invoked to solve the core/cusp problem [155, 156]) and warm dark matter [157–159] (which may suppress structure on small scales). Simulations involving even more exotic models, such as ultra-light fuzzy dark matter [160, 161], could yield testable predictions but are still in their infancy. In all cases, the complicated (and sometimes poorly understood) sub-grid physics of baryonic feedback can make it difficult to derive strong constraints on the DM properties from galaxy simulations.

Perhaps the most promising probe will be in the properties of ultra faint dwarf galaxies, many more of which will be detected and studied in the LSST-era [162–164]. In such galaxies, the effects of baryonic feedback tend to be less pronounced, and thus small-scale problems (such as the presence of cored density profiles) in ultra faint dwarfs would be strongly suggestive of new physics beyond the CDM paradigm [165, 166]. Unfortunately, modeling uncertainties in dwarf galaxies means that detecting the presence of large cores may be difficult. In particular, different approaches, assumptions and priors tend to produce different estimates for the density profiles of dwarfs [167, 168], even when the same data set is used. Reconciling these estimates in a statistically meaningful way represents a key challenge for using galaxy formation to probe the properties of DM (see Sec. IV B 1).

This challenge has motivated the development of new techniques to probe even smaller DM structures. Due to their small masses and shallow gravitational potentials, these structures are likely to be devoid of stars and gas, and are thus essentially dark [8, 169]. Techniques to detect these small DM subhalos thus rely on the latter's gravitational influence on their surrounding. These include phase-space perturbations to local stellar streams [170–184], to the Milky Way disk [185, 186], or to halo stars [187] that could be detected with precise astrometric observations such as those enabled by the Gaia satellite [10, 11]. Other techniques rely on the gravitational lensing signatures of these small, dark subhalos, both in our local neighborhood [188–190], and at cosmological distances from our galaxy (see e.g. Refs. [191–206]). Although promising, these different methods of probing the small-scale DM structure all come with their own statistical challenges, including the delicate balance between allowing for enough model complexity while avoiding over-fitting the noise.

IV. STATISTICAL CHALLENGES AND APPROACHES

The two important reasons for scientists to turn to statistics can be summarized as 1) discovery and 2) parameter estimation. In this review, we will focus mainly on the first question, that of discovery, since it is obviously the ultimate goal of dark matter searches. The question therefore becomes one of *model comparison*, i.e., answering the question: given available data, does this theory of dark matter do better than the null hypothesis H_0?

The statistical approach to such a problem then depends on a number of criteria: whether H_0 is the presumed model, or if we are comparing two equally "plausible" alternatives (for example, the normal vs inverted neutrino mass hierarchies); whether H_0 is a special case of – nested within – the alternative; whether parameters have unknown or meaningless values under H_0, and finally whether one adopts a Bayesian or frequentist framework.

The p-value is the most commonly used discovery criterion. In this framework, the conclusion of the statistical test for discovery is based on a test statistic TS which has the property that larger values of TS represent stronger evidence against H_0 and in favor of H_1. The p-value has the intuitive definition

$$p = Pr(TS(y) \geq TS(y_{obs})|H_0), \tag{6}$$

or: the probability that the test statistic $TS(y)$ is more extreme than the observed $TS(y_{obs})$ under the null hypothesis. The logarithm of the likelihood ratio

$$-2\log\frac{\max_\theta P_{H_0}(y|\theta)}{\max_\theta P_{H_1}(y|\theta)} \tag{7}$$

is a convenient test statistic, since Wilks' theorem tells us that for nested models, and under certain regularity conditions, its probability distribution follows a chi-squared distribution with degrees of freedom equal to the difference in the dimension of the parameter space under H_0 and H_1 [207].

More often than not, Wilks' theorem will not be applicable. This is usually due to comparison between non-nested models, or boundary issues where a given parameter has no meaning under H_0. In these cases, the "bootstrap" method of generating a PDF via Monte Carlo simulation must be used, which can be prohibitively expensive when searching for a 5-sigma effect.

The question that a phenomenologist seeks to answer when performing a statistical analysis is: how likely is the model to be true, given the data. However, p-values do not measure the relative likelihood of hypotheses, nor do they accurately reflect $P(\theta|y)$. Instead, they can be viewed as a measure of the "false alarm" rate: how often one should expect data this extreme if the null hypothesis is true. However, a large p-value does not validate the null hypothesis H_0, nor does a small p-value, in itself, suggest that $P(H_0|y)$ is small. In this sense, the p-value is anti-conservative: typically $p \ll P(H_0|y)$, meaning that interpreting the p-value as the probability that the null hypothesis is true may significantly overstate evidence for New Physics.

One way to help reduce this confusion is to report (in addition to the p-value) what is referred to as

$P(H_0|y)_{\min}$. Here, $P(H_0|y)_{\min}$ is a lower bound on the probability of the null hypothesis given the data $P(H_0|y)$: the smallest possible value of $P(H_0|y)$ which can be obtained over a large class of priors. These two summary statistics provide different information about the problem at hand. In addition, reporting both numbers – p and $P(H_0|y)_{\min}$ – highlights to the reader that they are *not the same thing* and encourages a more careful interpretation of the results. We present a toy example of this in Sec. V C.

On the practical side, it is not always trivial to find the maximum likelihood, especially when the parameter space is complicated and high-dimensional. A number of tools are available for efficiently exploring parameter spaces and calculating likelihoods, posterior probabilities and Bayesian evidences. These include: Markov Chain Monte Carlo samplers such as `CosmoMC` [208] and `GreAT` [209]; ensemble samplers such as `emcee` [210]; nested samplers such as `MultiNest` [211–213] and `POLYCHORD` [214]; differential evolution samplers such as `Diver` [215]; and global optimizers such as AMPGO[2] [216]. A number of these were compared in Ref. [215] but in general the best tool will depend (unfortunately) on the particular problem under investigation.

The rest of this section is split into two subsections. First we describe the details of a number of novel techniques that were primarily developed to overcome issues in modern DM data analysis. Second, we discuss recent progress in tackling some specific statistical problems in DM searches, as well as a number of opportunities and challenges that still remain in the field.

A. Novel Techniques

1. Selecting between non-nested models

How do we perform model selection between wildly different, non-nested models? For example, how do we choose which DM model (axions vs. WIMPs; scalar vs. fermion) is preferred by the data when the parameter spaces differ? In a frequentist framework, Wilks' theorem fails in this setting, and thus comparisons based on the χ^2 approximation of the Likelihood Ratio Test (LRT) become meaningless. In a Bayesian framework, comparing evidences can be misleading, as the comparison between prior volumes becomes arbitrary. For example, the weight of a decade in axion masses versus a decade in WIMP masses are certainly not equivalent to one another.

One proposed solution is to make the models nested by means of a comprehensive model which includes the models to be tested as special cases [217, 218]. For instance,

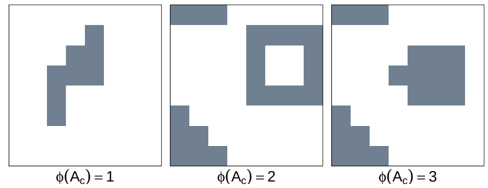

FIG. 1. From Ref. [217]. Euler characteristic in two dimensions.

let $f(y, \boldsymbol{\psi})$ and $g(y, \boldsymbol{\theta})$ be the models to be compared with vectors of parameters $\boldsymbol{\psi}$ and $\boldsymbol{\theta}$ respectively. Consider the mixture model

$$(1 - \eta) f(y, \boldsymbol{\psi}) + \eta g(y, \boldsymbol{\theta}) \tag{8}$$

where $\eta \in [0, 1]$. Despite the fact that η does not have any physical interpretation (as the data are assumed to be generated by either f or g), the asymptotic normality of its Maximum Likelihood Estimate (MLE) allows one to approximate the distribution of the LRT when testing

$$H_0 : \eta = 0 \quad \text{vs} \quad \eta > 0. \tag{9}$$

Specifically, as described in Refs. [219, 220], in order to circumvent the problem of non-identifiability of $\boldsymbol{\theta}$, one can construct the profile LRT statistic for each value of $\boldsymbol{\theta}$ fixed, i.e.,

$$LRT(\boldsymbol{\theta}) = -2 \sum_{i=1}^{n} \log \frac{f(y_i, \hat{\boldsymbol{\psi}}_0)}{(1 - \hat{\eta}_{\boldsymbol{\theta}}) f(y_i, \boldsymbol{\psi}_{\boldsymbol{\theta}}) + \hat{\eta}_{\boldsymbol{\theta}} g(y_i, \boldsymbol{\theta})}\,, \tag{10}$$

where $\hat{\boldsymbol{\psi}}_0$ is the MLE of $\boldsymbol{\psi}$ under H_0, $\hat{\eta}_{\boldsymbol{\theta}}$ and $\boldsymbol{\psi}_{\boldsymbol{\theta}}$ are the MLEs of η and $\boldsymbol{\psi}$ under H_1 with $\boldsymbol{\theta}$ fixed. Letting $\boldsymbol{\theta}$ vary, $\{LRT(\boldsymbol{\theta})\}$ corresponds to a random field[3] with index $\boldsymbol{\theta}$. A p-value for the test in (9) is given by $P(\sup_{\boldsymbol{\theta}}\{LRT(\boldsymbol{\theta})\} > c)$, where c is the maximum of (10) observed over a grid of values for $\boldsymbol{\theta}$. Although the asymptotic distribution of $LRT(\boldsymbol{\theta})$ is known to be a 50:50 mixture of χ^2_1 and zero [221], we can only approximate the asymptotic distribution of the supremum of the random field $\{LRT(\boldsymbol{\theta})\}$.

One possible way to do so is to consider the so-called Euler characteristics of the set $\mathcal{A}_c$ of points $\mathcal{A}_c = \{\boldsymbol{\theta} \in \boldsymbol{\Theta} : LRT(\boldsymbol{\theta}) > c\}$. We denote with $\phi(\mathcal{A}_c)$ the Euler characteristic of $\mathcal{A}_c$. In two dimensions, $\phi(\mathcal{A}_{c_k})$ corresponds to the numbers of connected components less the number of holes (see Figure 1). In an arbitrary number of dimensions one can consider a quadrilateral mesh over $\mathcal{A}_c$. In this case, $\phi(\mathcal{A}_c)$ is computed by adding and subtracting

[2] See http://infinity77.net/global_optimization/ampgo.html for an implementation.

[3] A random field is a stochastic process where the index is multi-dimensional.

hypercubes of increasing dimensionality (i.e., number of points − number of edges + number of squares − number of cubes + number of 4-dimensional hypercubes etc). The p-value of interest can then be computed as

$$P(\sup_{\boldsymbol{\theta}}\{LRT(\boldsymbol{\theta})\} > c) \approx E[\phi(\mathcal{A}_c)]. \quad (11)$$

As originally investigated by Ref. [220], the advantage of referring to the expected Euler characteristic $E[\phi(\mathcal{A}_c)]$ in Eq. (11) is that it can be estimated via a small Monte Carlo simulation of $\{LRT(\boldsymbol{\theta})\}$ under H_0 as described below. Following Ref. [222], we write $E[\phi(\mathcal{A}_c)]$ as

$$E[\phi(\mathcal{A}_c)] = \sum_{d=0}^{D} \mathcal{L}_d(\boldsymbol{\Theta})\rho_d(c), \quad (12)$$

where D is the dimensionality of $\boldsymbol{\theta}$, and the functionals $\rho_d(c)$, namely the Euler characteristic densities, are known in the statistical literature and only depend on the marginal distribution of each component of $\{LRT(\boldsymbol{\theta})\}$, i.e., the above-mentioned 50:50 mixture of χ^2_1 and zero. For instance, if $D = 2$, Eq. (12) takes the form

$$E[\phi(\mathcal{A}_c)] = \frac{c^{\frac{1}{2}} e^{-\frac{c}{2}}}{(2\pi)^{\frac{3}{2}}}\mathcal{L}_2(\boldsymbol{\Theta}) + \frac{e^{-\frac{c}{2}}}{2\pi}\mathcal{L}_1(\boldsymbol{\Theta}) + \frac{P(\chi^2_1 > c)}{2}\mathcal{L}_0(\boldsymbol{\Theta}).$$

(see Ref. [217] for more details.) The functionals $\mathcal{L}_d(\boldsymbol{\Theta})$ in Eq. (12) are known as the Lipschitz-Killing curvatures and their analytical expression for $d > 0$ is typically hard to compute in practice. However, this problem can be overcome using the following steps:

- **Step 1:** Simulate $y_1, \ldots, y_n$ from $f(y, \boldsymbol{\psi})$ 100–1000 times via Monte Carlo.
- **Step 2:** For each Monte Carlo replicate in Step 1 compute (10) over a grid of values for $\boldsymbol{\theta}$.
- **Step 3:** Select $c_1, \ldots, c_D$ arbitrary small thresholds.
- **Step 4:** For each c_k, $k = 1, \ldots, D$, in Step 1 compute $E[\phi(\mathcal{A}_{c_k})]$ over the Monte Carlo simulation obtained in Steps 1-2.
- **Step 5:** Obtain the solutions $\mathcal{L}^*_d(\boldsymbol{\Theta})$ of the system of D linear equations

$$\begin{cases} E[\phi(\mathcal{A}_{c_1})] - \mathcal{L}_0(\boldsymbol{\Theta})\rho_0(c_1) &= \sum_{d=1}^{D} \mathcal{L}_d(\boldsymbol{\Theta})\rho_d(c_1) \\ E[\phi(\mathcal{A}_{c_2})] - \mathcal{L}_0(\boldsymbol{\Theta})\rho_0(c_2) &= \sum_{d=1}^{D} \mathcal{L}_d(\boldsymbol{\Theta})\rho_d(c_2) \\ &\vdots \\ E[\phi(\mathcal{A}_{c_D})] - \mathcal{L}_0(\boldsymbol{\Theta})\rho_0(c_D) &= \sum_{d=1}^{D} \mathcal{L}_d(\boldsymbol{\Theta})\rho_d(c_D). \end{cases}$$

- **Step 6:** Compute $E[\phi(\mathcal{A}_c)]$, and consequently $P(\sup_{\boldsymbol{\theta}}\{LRT(\boldsymbol{\theta})\} > c)$, as

$$E[\phi(\mathcal{A}_c)] = \frac{\mathcal{L}_0(\boldsymbol{\Theta})P(\chi^2_1 > c)}{2} + \sum_{d=1}^{D} \mathcal{L}^*{}_d(\boldsymbol{\Theta})\rho_d(c),$$

  where $\mathcal{L}_0$ is the Euler characteristic of $\boldsymbol{\Theta}$, (e.g. it is one if $\boldsymbol{\Theta}$ is a disc, a square, a cube or it is zero if $\boldsymbol{\Theta}$ is a circle).

A more detailed discussion on the computation of the expected Euler characteristics $E[\phi(\mathcal{A}_{c_k})]$ is given in Ref.[217]. Applications to realistic simulated data from the Fermi LAT are discussed in Refs. [217, 218].

2. *Exploiting the count statistics of the signal*

DM detectors are typically counting experiments, i.e. looking for signal events above a background.

In the case of DM indirect detection the observed signal is pixelized observed counts, *e.g.* as seen in data from the *Fermi*-LAT gamma-ray telescope. In this case the data would be a Poisson realization of the modeled dark matter signal, which could represent emission from large-scale structures such as the smooth Galactic halo, as well as point/extended structures such as dwarf spheroidal galaxies, extragalactic halos and Galactic subhalos.

The associated likelihood is then a product of the Poisson probabilities associated with the observed counts n_i^p in each pixel of the region-of-interest:

$$\mathcal{L}(d|\boldsymbol{\theta}) = \prod_p \frac{\mu^p(\boldsymbol{\theta})^{n^p} e^{-\mu^p(\boldsymbol{\theta})}}{n^p!}\,, \quad (13)$$

where d denotes the data, $\boldsymbol{\theta}$ represents the set of model parameters (e.g. modeled backgrounds or signal) and $\mu^p(\boldsymbol{\theta})$ is the number of expected counts in a given pixel and energy bin, usually characterized through spatial templates which model the emission associated with one or more physical process and/or source class.

A particular problem with indirect detection is distinguishing the signal events on top of a complex and uncertain background. One particular background of common interest comes from point sources in the signal region of interest, for example millisecond pulsars, which have non-power-law gamma-ray spectra similar to those expected from annihilation of weak-scale DM. Typically, known point sources are masked or individually modeled in an analysis, but this cannot be done when point sources cannot be detected individually. In this case, the collective emission of dim, sub-threshold point sources could be confused with a diffuse DM *signal*.

In the presence of unresolved sources with unknown positions, detections of multiple photons from the same pixel no longer behave as independent events, as the detection of one photon increases the probability that a source is present in the pixel. The likelihood consequently deviates from the Poissonian form, and is instead characterized by non-Poissonian noise in the data. Following [223], the non-Poissonian likelihood can be conveniently cast in the language of probability generating functions, which for a discrete probability distribution with p_k with $k = 0, 1, 2, \ldots$ are defined as $P(t) \equiv \sum_{k=0}^{\infty} p_k t^k$ and allows us to recover the associated probabilities as $p_k = \frac{1}{k!}\left.\frac{d^k P(t)}{dt^k}\right|_{t=0}$. Exploiting the fact that the probability generating function for a sum of independent random variables is simply the product of the respective generating functions, the generating function for a smooth (Poissonian) template (associated with the likelihood in Eq. 13) takes the form

$$P_{\rm P}(t;\boldsymbol{\theta}) = \prod_p \exp\left[\mu_p(\boldsymbol{\theta})(t-1)\right], \qquad (14)$$

while for a non-Poissonian template characterizing the distribution of an underlying unresolved point source population this takes the form

$$P_{\rm NP}(t;\boldsymbol{\theta}) = \prod_p \exp\left[\sum_{m=1}^{\infty} x_{p,m}(\boldsymbol{\theta})(t^m-1)\right], \qquad (15)$$

where the $x_{p,m}$ have the interpretation of being the average number of point sources contributing m photon counts within a pixel p. Further details on characterizing the non-Poissonian likelihood associated with a point source population, and numerical recipes, may be found in [224–226].

While DM emission from individual sources has been traditionally studied in the context of Poissonian template fitting [108, 227–232], a comprehensive study taking into account all potential DM emitters (dwarf galaxies, sub- and above-threshold extragalactic halos, sub-threshold subhalos as well as the smooth Galactic halo) would require accurate modeling of the underlying sources and robust characterization of the (non-)Poissonian signal likelihood.

3. *Euclideanized signals*

Efficient forecasting of experimental sensitivities is key for developing the most relevant searches for dark matter particles. The sensitivity of future experiments can be quantified in various ways. This includes the discovery reach, expected exclusion limits, and — assuming a significant detection has been made — the ability to discriminate various models and regions in the model parameter space. Traditionally, the latter is done by defining a number of 'benchmark points' in the model parameter space of interest, and studying with simulated mock data how well this scenario – if realized in nature – could be constrained with the experiment at hand.

The 'Euclideanized signals' approach that was introduced in Ref. [233] provides a way to study the model discrimination power of future instruments in a fundamentally *benchmark-free* way. This is achieved by efficient approximation methods for calculating the expected log-likelihood ratios, which in turn allow us to consider a very large number of reference points in the parameter space simultaneously. Instead of considering, say, 10 benchmark points, one would consider thousands or millions of points, covering the entire parameter space of interest exhaustively.

Euclideanized signals are a mapping of a complicated model parameter space into a (typically high-dimensional) space where statistical distinctness corresponds to the Euclidean distance. Various clustering algorithms allow for the efficient pair-wise comparison and grouping of points according to their Euclidean distance, even for millions of points. Once the mapping is done, it is then easy to study which parts of the parameter space are in principle distinguishable from other regions.

In Ref. [234] a mapping of model parameters $\theta \mapsto x$ was defined, which allows one to approximate the log-likelihood ratio with Euclidean distances,

$$\mathrm{TS}(\vec{\theta}')_{\mathcal{D}(\vec{\theta})} \equiv -2\ln\frac{\mathcal{L}(\mathcal{D}(\vec{\theta})|\vec{\theta}')}{\max\limits_{\vec{\theta}''}\mathcal{L}(\mathcal{D}(\vec{\theta})|\vec{\theta}'')} \simeq \|\vec{x}(\vec{\theta})-\vec{x}(\vec{\theta}')\|^2 \,. \qquad (16)$$

This mapping is valid for Poisson likelihoods (which trivially includes also Gaussian likelihoods), with arbitrary signal parameterization, and general background uncertainties modelled as Gaussian random fields. In Ref. [234] it was shown with randomly generated signal and background models that the approximation technique yields estimates for the log-likelihood ratio that are correct to within 20% (for up to 5σ distances).

The Euclideanized signal method makes two analyses computationally possible:

- *Benchmark-free forecasting:* an exhaustive study of the model-discrimination power of experiments without resorting to a small number of benchmark scenarios,
- *Signal diversity:* estimating the number of discriminable signals that are predicted by a specific model.

We further discuss these in detail below focusing primarily on benchmark free forecasting.

Benchmark-free model comparison — Here we want to calculate, based on the collection of Euclideanized signals, whether two subsets of a global model can exist within a confidence region, with radius r, of each other. We define the radius as $r_\alpha(\mathcal{M}) = \sqrt{\chi^2_{k=d,\mathrm{ISF}}(1-\alpha)}$ where $\chi^2_{k=d,\mathrm{ISF}}$ is the inverse survival function of the Chi-squared distribution with $k = d$ degrees of freedom such that for $k = 2$ and $\alpha = 0.046$ (corresponding to 95.45% CL) $r_{0.046}(\mathcal{M}) = 2.486$. Here the two subsets of the global model correspond to the distinct models (A and B) we wish to compare and distinguish. Both model A and B are nested within (subsets of) the global model.

If within $r_{0.046}(\mathcal{M})$ of a parameter point from model A there exists a parameter point from B, then the point in A is not discriminable from B. On the other hand, if there exists no point from model B within $r_{0.046}(\mathcal{M})$ then the models can be in principle distinguished at 95% CL. Here is a step by step guide to performing these calculations with reference to a direct detection (DD) example as presented in Ref. [233].

- **Step 1:** Sample the parameter space of $\mathcal{M}$, calculating signals for each point. For the problem at hand, we found that one obtains stable results if there are more than around 10 points within every 1σ (68% CL) confidence contour. In the case of DD, the global model $\mathcal{M}$ may correspond to the non-relativistic effective field theory operators $\mathcal{O}_1$ and $\mathcal{O}_4$ (these are simply the usual spin independent and dependent interactions, respectively) [235]. We then have a three-parameter model i.e. the mass of the dark matter particle and the two individual DM-nucleon couplings to each operator. The sub-models A and B then correspond to two boundaries of $\mathcal{M}$ where one or the other of the DM-nucleon couplings is set to zero.

- **Step 2:** Euclideanize the signals using experimental parameters such that each parameter point has an associated new vector $\vec{x}_i$. This step can be done using `swordfish` [234].

- **Step 3:** For each point i in model A (i.e. points with model parameters $\vec{\theta}_i$ corresponding to model A), find all points within $r_{0.046}(\mathcal{M})$. We denote the set of model parameters for these neighboring points as $\{\vec{\theta}_j^{(i)}\}$.

  The number of degrees of freedom used to calculate $r_{0.046}(\mathcal{M})$ for model comparison is equal to the difference in the dimensionality of the models of interest. If we consider comparison of the overall model $\mathcal{M}$, which has d degrees of freedom, with the sub-model A with d′ then k = d − d′. For the DD example, d = 3 and d′ = 2 therefore $k = 1$ and $r_{0.046}(\mathcal{M}) = 2.0$.

- **Step 4:** Each point i is then defined as discriminable or not according to the list of parameter points $\{\vec{\theta}_j^{(i)}\}$. If $\{\vec{\theta}_j^{(i)}\}$ contains a point from model B then i is not discriminable and vice versa.

In this way we are able to make benchmark-free statements about the discriminability of models such as those presented in Ref. [233] and shown in Fig. 2.

Signal Diversity — The number of discriminable models is approximately defined as the number of points one could fit in to a parameter space whilst maintaining 2σ discrimination between all points. We can visualize these regions by tightly packing confidence contours into the parameter space, as is shown in Fig. 3 for the case of a typical direct detection experiment. As can be seen in Fig. 3, this number is $\mathcal{O}(10-100)$ but calculating $\nu^{\alpha}_{\mathcal{M},X}$ (defined below) in higher dimensional models with multiple experiments can be difficult. We therefore estimate the quantity using the following method:

- **Step 1:** Same as previous step 1

- **Step 2:** Same as previous step 2

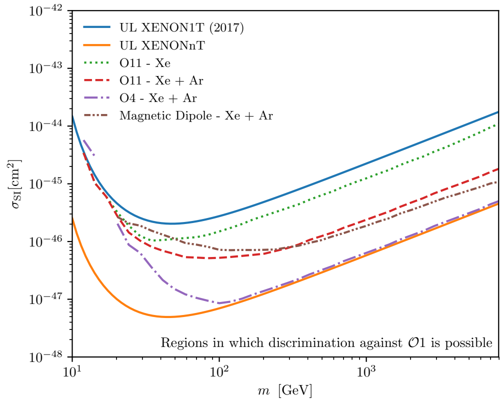

FIG. 2. Taken from Ref. [233]. *Blue and Orange Lines:* 90% confidence limits (CL) on the standard spin-independent cross section for XENON1T (2017) [73], and a future experiment with 100 times the exposure. To the left/below each broken line, it is not possible to discriminate an $\mathcal{O}_1$-signal (with the indicated cross-section and DM mass) from the corresponding best-fit $\mathcal{O}_4$, $\mathcal{O}_{11}$ or magnetic dipole signal. Above/right of each broken line, such a discrimination is possible with at least 2σ significance. All lines include DM halo uncertainties.

- **Step 3:** Calculate the number of points w_i within $r_{0.046}(\mathcal{M})/2$ of the point $\vec{x}_i$. The number of degrees of freedom is equal to the number of free parameters of the model. Again, for the DD example we have a three parameter model therefore $k = 3$ and $r_{0.046}(\mathcal{M}) = 2.833$.

- **Step 4:** The volume (here defined) is then approximated by $\nu^{0.046}_{\mathcal{M},X} = c_{ff}\sum_i w_i$ where c_{ff} is a filling factor dependent on the dimensionality.

We can visualise the diversity and global degeneracy breaking abilities of experimental configurations (for nested models) using Infometric Venn diagrams as introduced in Ref. [233].

4. ABC: when you can't actually afford a likelihood

The increasing complexity of the models we use to describe physical processes have made the computation of a likelihood often difficult to handle or even impossible. Fortunately many methods have been developed to allow for the forward simulation of these complex situations, for example calculating the end state observables from an LHC event or the distribution of galaxies from a ΛCDM cosmological simulation.

Approximate Bayesian Computation (ABC) is a computationally-intensive framework for approximating

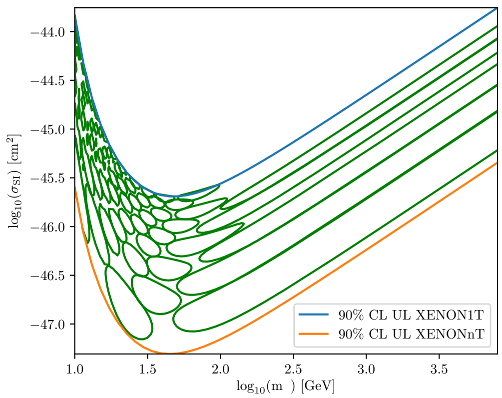

FIG. 3. Taken from Ref. [233]. *Blue and Orange Lines:* 90% confidence limits (CL) on the standard spin-independent cross section for XENON1T (2017) [73], and a future experiment with 100 times the exposure. *Green Ellipses:* 68% confidence contours for tightly packed set of points. Approximately describes the number of discriminable signals in the parameter space between blue and orange lines.

a Bayesian posterior distribution when a likelihood function is not available or intractable [236, 237]. The basic ABC algorithm was introducted in [238, 239], but was also hinted at conceptually in [240]. ABC has proved to be a useful tool for several problems in astronomy (e.g. [241–244]).

The basic ABC algorithm proceeds simply, with only a few steps. The overall idea is to use a forward model to generate a simulated dataset given draws from the prior distribution(s). If that simulated dataset is "close enough" to the real observations, then the draws from the prior(s) that produced the simulated dataset are considered "good" draws, and those values are retained. If not, the values are discarded. This is repeated until enough draws from the prior are accepted, and those values are used to approximate the Bayesian posterior.

More precisely, the steps of the basic ABC algorithm proceed as follows given unknown parameter(s) θ, prior(s) $p(\theta)$, observations y_{obs}, and forward model $F(y \mid \theta)$:

(i) sample $\theta_{\text{prop}} \sim p(\theta)$,

(ii) compute $y_{\text{prop}} \sim F(y \mid \theta_{\text{prop}})$,

(iii) if $y_{\text{prop}} = y_{\text{obs}}$, then keep θ_{prop}, if not, discard θ_{prop},

(iv) repeat until desired number of values of θ_{prop} have been accepted.

Rather than waiting until y_{prop} is equal to y_{obs} exactly, lower-dimensional summary statistics are used. For example, rather than comparing the full set of observations, one could compare only their sample means. The summary statistics are crucial for good performance of the ABC algorithm. The summary statistics will only be as good as the amount of information they contain about the data. There are some methods for developing summary statistics (e.g. [245, 246]), but physically-motivated summary statistics can also be effective. The performance of the summary statistics and distance functions should be checked in a similar scenario where the true posterior is available (which will likely require a simplified model).

In order to define what is meant by "close enough", a tolerance (or tolerances) ϵ is set. Then for distance function Δ, θ_{prop} is accepted if $\Delta(y_{\text{obs}}, y_{\text{prop}}) \leq \epsilon$. The desire is for ϵ to be small.

For observations y_{obs} with summary statistic(s) $S(y_{\text{obs}})$, distance function Δ, (small) tolerance ϵ, and desired particle sample size N, an ABC posterior can be based on $\{\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(N)}\} = \{\theta^{(i)}\}_{i=1}^{N}$ $\{\theta^{(i)}\}_{i=1}^{N}$ from Algorithm 1.

Algorithm 1 Basic ABC Algorithm

for $i = 1$ to N **do**
while $\Delta\left(S(y_{\text{obs}}), S(y_{\text{prop}})\right) > \epsilon$ **do**
Propose θ_{prop} by drawing θ_{prop} from prior $p(\theta)$
Generate y_{prop} from forward process $F(x \mid \theta_{\text{prop}})$
Calculate summary statistics $\{S(y_{\text{obs}}), S(\theta_{\text{prop}})\}$
end while
$\theta^{(i)} \leftarrow \theta_{\text{prop}}$
end for

Selecting a small enough ϵ can be challenging because setting ϵ too low leads to a lower acceptance rate and hence (possibly significantly) more computational resources and time. One popular option for getting around this issue is to use the ABC-Population Monte Carlo (ABC-PMC) algorithm proposed in [247]. The general idea with ABC-PMC is to set up a sequential version of ABC that uses the accepted particles from the previous iteration as the proposal for the current iteration, rather than drawing from the prior distribution. This provides improved proposals at each iteration, which is coupled with a shrinking tolerance at iteration t, ϵ_t. The important point is that in order to target the correct posterior distribution (assuming everything else is selected correctly), importance weights need to be computed at each iteration. Details about the importance weights and the specific steps of the algorithm can be found in [247]. Ref. [244] also has a nice overview of the ABC-PMC with an astronomy application and a Python implementation. There are other sequential extensions of the ABC algorithm (e.g. [248, 249]).

B. Progress and Challenges

1. Quantifying nuisances

The signal expected in both direct and indirect searches depends sensitively on quantities of astrophysical nature: for indirect searches the DM distribution within the target (along the line of sight), and for direct searches, the amount of DM in the proximity of the Sun/Earth, as well as its velocity distribution (in principle also important for indirect searches, but generally ignored in simplified scenarios). The lack of knowledge (i.e. uncertainties of statistical and/or systematic nature) on these quantities can be considered as "nuisances" for the interpretation of the signal in terms of DM particle properties (mass, self-annihilation, or scattering cross section). The local DM density can be extracted from local and global measurements [17, 250, 251], while recent state-of-the-art hydrodynamical simulations of galaxy formation provide information on the local DM velocity distribution [252–255], as well as the DM density profile of Milky Way-like galaxies [256]. Each of these astrophysical quantities are estimated with their associated uncertainties, yet little work has been done to properly quantify all known astrophysical uncertainties in the interpretation of DM signals. The impressive precision and refinement of both statistical tools, and searches at colliders, to which direct and indirect searches must be coupled, compel us to cope with these issues by addressing the state of our ignorance, and to properly treat the impact of astrophysical uncertainties within the budget of overall nuisances affecting the signal.

One example of quantifying nuisances is the case of how uncertainties on quantities in our own Galaxy, the Milky Way, affect particle DM constraints: how can we quantify the effect of astrophysical uncertainties in the determination of new particle physics parameters?

The reconstruction of the DM distribution in the entire Galaxy –when obtained through a method based on global properties such as the "Rotation Curve"– relies on a host of ancillary measurements and determinations, among which are those related to the motion of the Sun within our own Galaxy (the Local Standard of Rest, and the relative motion between the Sun and the Galactic Centre, in the following generically referred to as "Galactic Parameters"), and the spatial distribution of the visible component of the Milky Way (stars and interstellar gas). The latter is affected by a statistical uncertainty related to the overall normalization of the stellar mass, and from a (currently) irreducible systematic on the determination of the shape of stellar morphological components (disc-s, and bulge). The impact of both classes of uncertainties on the determination of the DM profile (expressed in terms of the local DM density, and the inner slope of a generalized NFW profile) has been assessed in recent studies [250, 257], with the conclusion that although none of them can hinder the certainty of the presence of a *dark* component of matter in the Galaxy – even within the solar circle – the effect of both classes of uncertainties is sizable in the actual determination of the local DM density and its distribution, especially towards the region of the Galactic bulge. These analyses have compelled a study of how such uncertainties propagate in the determination of DM parameters, in the case of model-specific analysis: in Ref. [258] the authors considered the effect of Galactic uncertainties on two minimal extensions of the Standard Model, in the context of direct and indirect DM searches: the Singlet Scalar (SSDM) and the Inert Doublet (IDM) DM models. The phenomenologies of these two particular models have a simple dependence on a limited set of parameters, which makes them ideal cases for quantifying the effect of Galactic uncertainties on the determination of their parameters.

The following constraints from DM direct and indirect detection in the parameter space of the SSDM and IDM were taken into account: the 2015 LUX exclusion limit on the spin-independent elastic WIMP-nucleon cross section [259], and the Fermi-LAT limit on the averaged velocity annihilation cross section from the analysis of dwarf spheroidal galaxies in the Milky Way [260]. The authors also considered the parameter space favored by the DM interpretation of the Galactic Centre GeV excess [261]. In particular, it was studied how the LUX exclusion limit and the region favored by the GeV excess vary in the available parameter space of the SSDM and IDM, for three different cases of variation of astrophysical uncertainties: a) the statistical uncertainty on one "reference" baryonic morphology, b) the variation of the Galactic parameters for the reference morphology, and c) the baryonic morphologies that maximize or minimize the local DM density.

It was found that for the SSDM case, the statistical uncertainty on the reference morphology has a very small effect on the LUX limit, while the uncertainties on the values of the Galactic parameters or the baryonic morphology have large effects on the LUX constraint. The largest variation in the exclusion limit is due to the variation in the Galactic parameters which leads to the largest variation in the local DM density (varying from $0.055 \pm 0.004\,\mathrm{GeV\,cm^{-3}}$ to $1.762 \pm 0.017\,\mathrm{GeV\,cm^{-3}}$; see Table 1 in Ref. [258]). For the region favored by the GeV excess, again the statistical uncertainty on the reference morphology has a minor effect. However, varying the Galactic parameters and considering different baryonic morphologies have large effects on the favored region and can relieve or worsen the tension with the constraints from dwarf spheroidals. The largest shift in the GeV excess region is due to the variation of the baryonic morphologies.

For the IDM case, it was found that the effects of Galactic uncertainties on the LUX exclusion limit are similar to those discussed for the SSDM. The variation of the local DM density causes the largest uncertainty in direct detection limits, and hence the variation in the Galactic parameters for the reference morphology has the largest effect in the IDM parameter space. The analysis also showed that the regions which can simultaneously explain the GeV excess and reproduce the measured DM relic abundance are small and in most cases in tension with the dwarf spheroidal constraints. Varying the Galactic parameters or baryonic morphology shifts the GeV excess region such that the DM relic abundance cannot be reproduced.

In summary, the statistical uncertainties in the observed Milky Way rotation curve and the normalization of the baryonic mass component do not affect the constraints on the parameters of new physics models, while the uncertainties in the Galactic parameters and the baryonic morphology can significantly impact the allowed model parameter space. Quantifying astrophysical uncertainties will be especially important in case a DM signal is discovered in future direct and indirect experiments, and is required to accurately determine the particle physics nature of DM.

2. *Global fits: let's just do everything (and worry later about trying to afford it)*

The profusion of experiments hunting for DM in the last decade has left us with an enormous amount of complementary data on its possible identity. Unfortunately, the heterogeneity of that data makes it difficult to apply to the DM problem in a cohesive, efficient and consistent way. Different experiments are optimised to look for different types of dark matter, involve entirely different (but sometimes correlated) experimental methods and uncertainties, make different (but related) theoretical assumptions in the analysis of their data, and take different attitudes to sharing their data with the rest of the community. Most experimental collaborations looking for DM have apparatuses that in principle are sensitive to many different variants, but only have the resources to analyse their own data, in the context of a small number of well-chosen theories.

Experimental constraints on theoretically well-justified theories help theorists to efficiently construct new models, based on some real picture of physical quantities such as masses or couplings. The converse is also true: theoretical predictions for observable quantities in concrete and complete models help experimentalists to build powerful cuts, choose the right energy range to search, and estimate the exposure required for a statistically-significant measurement. Ideally, this process should be a circular feedback loop. This loop has become difficult to implement in modern times, because of the growing number and complexity of DM models, and the great number of different experiments searching for them.

Global fits in particle and astroparticle physics are the means by which we can use the full treasure-trove of existing data to analyse a broad range of theories, and thereby complete the traditional scientific feedback loop. Working with the experimental collaborations to define forms of their likelihood functions applicable to a broad range of DM theories (e.g. [262–265]) and then combining them into composite likelihood analyses, teams of theorists, phenomenologists and experimentalists have successfully produced broad-ranging analyses of many popular theories for DM. These include a number of different versions of supersymmetry [266–283], extra dimensions [284], Higgs portal and other minimal WIMP DM models [285–289], axions [290] and DM effective field theories [291, 292].

Care needs to be taken when combining data from different experiments. In particular, consistent theoretical calculations and assumptions must be applied to all predictions (and even experimental likelihoods) in a global fit, along with the same assumptions about Standard Model parameters, nuclear physics and astrophysical aspects like the density and velocity distributions of DM [293–295]. Similarly, different theoretical calculations and experimental analyses must be invoked for different theories, alternative theoretical calculations should be considered for the same model in order to estimate theory errors accurately, sophisticated statistical sampling schemes must be employed for analysing high-dimensional parameter spaces [296–298] and coverage properties need to be checked carefully [299–301]. Ideally, the global fitting framework itself should automatically ensure that all of these requirements are satisfied. This is something that has only recently become possible [302]; future work is focussed on extending this rigorous consistency-checking and automation as far as the Lagrangian level.

Once a new DM model is proposed, an initial choice of priors on its parameters must be made, based on some theoretical constraints or preferences of the researcher. If the likelihoods are strong, the final fitted result will not be dependent on the chosen prior. However, because only the *Planck* [303] relic density measurement provides a clear "signal" amongst the different DM experiments, the likelihoods for DM searches are very often too weak to dominate over the impact of the prior on the posterior. Such prior dependence is therefore difficult to avoid until more constraining experimental data become available. On the other hand, it is still not clear what kind of prior distribution – if any – is more objective and therefore preferable. At this stage, showing results based on both Bayesian and frequentist statistics is generally considered best practice in global fits, as they provide complementary information about the impacts of priors, fine-tuning and the quality of sampling and fit available in different parts of the parameter space.

A comprehensive global fit requires a lot of CPU time for many likelihoods, such as the simulation of signals at the LHC. If good sampling is required of the entire likelihood surface, it can be extremely difficult to study collider signatures in models with more than a few degrees of freedom. Nevertheless, considering DM models in neighbouring parameter regions, and the similarity of their respective likelihood computations, it might not be necessary to perform full signal simulations across entire parameter spaces. Some simplifications can be used in the global analysis, based on simplified modelling of detector effects [304], the similarity of kinematics, some mathematical tricks, or model configurations (e.g. [288, 291, 294, 305–308]). Of course, such simplifications could introduce some systematic uncertainties or limitations on the applicability of the resulting constraints, which must be carefully checked before performing the fit.

Treating different *theories* on the same footing, and comparing them both rigorously and quantitatively, was one of the major topics of discussion at this workshop. Indeed, this is of particular difficulty and importance for global fits, given their comprehensiveness and the fact that they purport to provide a complete and accurate summary of the current status of the search for different theories of DM, and the identity of DM more broadly. Possible approaches include mixture models (Sec. IV A 1), comparison of global p-values, the use of Bayes factors, or some extension of the Euclideanized signals approach (Sec. IV A 3). These have their own challenges: global p-values are notoriously difficult to obtain in complicated high-dimensional parameter spaces, Bayes factors come with attendant prior dependence – which in general only gets worse for non-nested models – and application of Euclideanized signals to model selection first requires that the method be developed further.

3. Machine Learning in DM Physics

Machine Learning (ML) techniques have already been widely adopted throughout the high energy, astro, astroparticle, and particle physics communities. We here briefly comment on some use cases for DM physics and provide useful references. Details are beyond the scope of this work, but we point the interested reader to darkmachines.org for a community effort to increase the use of ML in DM physics (an associated white paper is in preparation). Also, see Refs. [309, 310] for recent publications in high energy physics.

Direct Detection — The simplicity of direct detection experiments and their low background design has made the procedure of data analysis relatively simple. They have therefore been robust to the revolution of ML techniques. Nevertheless some progress has been made in improving the efficiency of posterior sampling when considering the large number nuisance parameters associated with galactic halo uncertainties [311]. Boosted decision trees have also be used to improve traditional cut and count analyses by optimally and automatically selecting the most promising signal events [312, 313].

Indirect Detection — Unlike DD, a large variety of ML techniques have been widely adopted throughout the indirect detection (ID) community. For concreteness we mention three major applications here. Firstly, Neural Networks (NNs) have been used to assess the probability of the galactic center gamma-ray excess [261] being produced by a population of unresolved point sources [314]. Unlike the characterization of the likelihood proposed in Sec. IV A 2, the approach of Ref. [314] relies on many simulated realizations of a population of Millisecond Pulsars towards the galactic center. Secondly, the Fermi-LAT has provided the first view into the varied population of gamma ray point sources. Classification of these point sources has proven to be a complicated task typically involving dedicated follow-up studies from telescopes in other wavebands [315]. There are close to 1000 objects in the 3FGL source catalog which have yet to be associated to any source type. For DM searches these point sources are of great interest when looking for low mass sub-halos that would appear as point sources for Fermi-LAT resolution ($< 0.15^\circ$ above 10 GeV) [316]. Much progress has been made in classifying these unassociated sources using different methods such as random forests and logistic regression [317] with searches for novel source classes such as sub-halos also being performed in Ref. [318]. Finally, lensing signatures from sub-halos on a variety of scales, as those mentioned in Sec. III D, can be sensitive to DM physics. Progress has been made primarily in finding strong lens candidates from the large volume of incoming data, see Ref. [319] for an example using Convolutional Neural Networks.

Collider Searches — There is an ongoing and dedicated effort to improving the use of machine learning techniques throughout the collider physics community, see https://iml.web.cern.ch and http://diana-hep.org for details. Specifically for DM searches, see Ref. [320] where distributed Gaussian processes and NNs were used to increase the speed of likelihood evaluations to a computationally feasible rate for parameter inference.

4. The statistical interpretation of fine-tuning

A theoretical model presents fine-tuning (or, equivalently, the absence of naturalness) when the observable quantities depend critically on fine adjustments of the fundamental parameters. For example, in the minimal supersymmetric standard model (MSSM) the Higgs mass, m_h, is related to the initial soft mass m_{H_u} and the $\mu-$parameter by $-m_h^2/2 \simeq m_{H_u}^2 + \mu^2$. Hence, if these initial parameters are $\mathcal{O}(1)$ TeV, the Higgs mass is fine-tuned by $\sim 1\%$.

Beyond amusing (and unlikely) coincidences, the presence of severe fine-tuning is a warning that the model is implausible in the way it is formulated. The detection of fine-tuning is always interesting because it is telling us something potentially highly non-trivial about the model. There are three possible attitudes in the presence of fine-tuning: *(i)* discard the model as implausible; *(ii)* complete the model, i.e. find a reason for the apparently improbable correlations; *(iii)* ignore the fine-tuning, i.e. assume a fortunate coincidence or, alternatively, hope that someone else will find a reason for the odd correlations, as in attitude *(ii)*.

Fine-tuning is an important but, admittedly, slippery and debatable subject. There are two reasons for that. First, it is not easy to quantify the fine-tuning in a universal, model-independent way (ideally with a sound statistical meaning). Second, once the amount of fine-tuning has been established, it is a subjective matter how much fine-tuning one should accept; after all, coincidences happen. These difficulties (which may seem Bayesian, due to their implicit subjectivity) do not contradict the fact that fine-tuning (or naturalness) is a deep, relevant issue for the structure of a theory.

Consequently, the first and most important matter is how to quantify fine-tuning. Let $F(\theta_i)$ be the fine-tuned (observable) quantity, where θ_i are the fundamental (independent) parameters of the theory. Generically, this means that F is very sensitive to small variations of one (or several) θ_i. This has inspired the most popular (and perhaps standard) 'measure' of fine-tuning [321]:

$$\Delta \equiv \max |\Delta_{\theta_i}|, \quad \text{with} \quad \Delta_{\theta_i} = \frac{\partial \log F}{\partial \log \theta_i} \; . \qquad (17)$$

It is understood that $\Delta \sim 10, 100, \cdots$ amounts to $\sim 10\%, 1\%, \cdots$ fine-tuning. While this seems reasonable, it would be nice to find a probabilistic interpretation of (17). Let us call θ and θ_0 the parameter responsible for the tuning and the value that reproduces the experiment, $F(\theta_0) = F^{\rm exp}$. Suppose, for the sake of argument, that F has to be fine-tuned to a small value. Then θ_0 should lie at a small distance, $\delta\theta$, from the value that fully cancels F. Assuming that the natural range of θ is $\sim [0, \theta_0]$ with a flat prior, and that the expansion of $F(\theta)$ at first order captures its behavior in the neighborhood of interest, then it is straightforward that Δ^{-1} has the statistical meaning of a $p-$value [40, 322, 323]:

$$P(F \leq F^{\rm exp}) = \frac{\delta\theta}{\theta_0} \simeq \Delta^{-1} \; . \qquad (18)$$

The previous assumptions are reasonable, but may be inappropriate in particular theoretical scenarios. Suppose for instance that the dependence of F on θ is the one depicted in Fig. 4. Clearly, the standard criterion (17) underestimates the real fine-tuning, as it overestimates the actual interval of θ where $F \leq F^{\rm exp}$. This is not just an academic example. If the dark matter relic density is controlled by annihilation through some funnel (like Higgs or Z funnels), the dependence of $\Omega_{\rm DM}$ on the DM-mass is exactly as in Fig. 4. In the borderline case, where the previous interval tends to zero, the actual fine-tuning tends to infinity, whereas the standard criterion gives $\Delta \to 0$! The general lesson is that, before applying (17) blindly, one should check that the conditions for its validity are met. It is normally more sensible (and easier) to directly apply a $p-$value criterion to the parameter considered, instead of using the approximate expression (17). Examples of this, in the context of supersymmetric mechanisms for DM, can be found in [323]. A more sophisticated way of giving an statistical meaning to fine-tuning, in a fully Bayesian spirit, would be the following. Pretend that the fine-tuned quantity, $F(\theta_i)$ has not been measured yet. Then, evaluate the Bayesian probability that $F \leq F^{\rm exp}$. A similar-in-spirit procedure was applied in [324] to the electroweak fine-tuning of the MSSM.

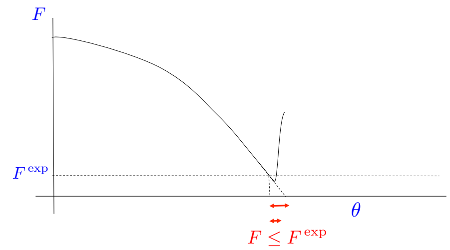

FIG. 4. An example of a fine-tuned quantity where the standard criterion (17) cannot be applied.

5. *Global significance for overlapping signal regions*

When high local significance is observed in LHC searches for new physics, the probability of seeing such an excess only from statistical fluctuations of the background in *any* of the analysis signal regions (SRs) needs to be quantified. This is described by the global significance, which takes into account trial factors, often called the "look-elsewhere effect" in physics. For a large number of signal regions, the probability of seeing a "signal-like" fluctuation in any one of them is higher. The probability p_0 of seeing one such high significance excess anywhere in a number of signal regions (assuming the background-only hypothesis H_0) is given as:

$$p_0 = P(q_x \geq q_{x,obs} | H_0) \, , \qquad (19)$$

for some test statistic q_x. The global significance is obtained from the probability of observing a maximum local significance (across the $N_{\rm SR}$ signal regions considered) greater than the *observed* maximum local significance. This is typically estimated using a number of pseudo-experiments $N_{\rm toy}$. A number of aspects in this calculation are described in [325–327] for the case of non-overlapping SRs. However, if SRs in the analysis have overlap in their discriminating variable selections, the correlations of SR selections need to be taken into account.

Analyses are often designed to use orthogonal selections in the parameter space of discriminating variables, to avoid considering correlations in the overlapping regions. However, there are cases of analyses that require overlapping selections. An example of such an analysis is the SUSY search for $\tilde{q}$ and $\tilde{g}$ production using a selection with two leptons, jets and missing transverse en-

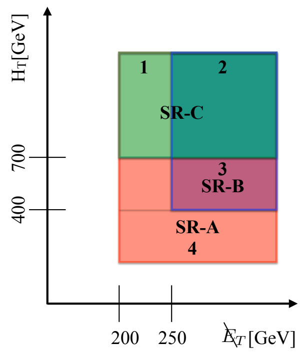

FIG. 5. Overlapping signal regions SR-A, SR-B and SR-C, in the SUSY analysis for $\tilde{q}$ and $\tilde{g}$ production using a selection with two leptons, jets and missing transverse energy [328]. Selections have overlap in the selection of missing transverse energy ($\not{E}_T$), scalar sum of transverse momentum of jets (H_T), and invariant mass of two leptons (m_{ll}). Global significance is calculated using orthogonal sub-regions 1,2,3 and 4.

ergy [328]. The analysis is optimized for $\tilde{q}$ and $\tilde{g}$ decays with jets and two leptons in the decay chain. The signal would produce an excess in the two-lepton invariant mass distribution m_{ll}. Depending on the mass differences of the SUSY particles, the m_{ll} excess appears at different ranges of the distribution. In addition, different mass spectra produce jets of different transverse momentum, and different masses of the $\tilde{\chi}^0_1$ LSP give different sizes of missing energy in the signature, which are considered in the selection. Therefore, to account for a large number of SUSY models, SRs are designed with overlap in the selection. Consequently, when the global significance is calculated, the correlations of the overlap of SRs need to be taken into account.

Here, we briefly describe a novel technique to take overlapping SRs into account. It makes the assumption that systematic uncertainties for all background components are fully correlated across all SRs. First, the N_{SR} considered signal regions are split into non-overlapping sub-regions. An example for the SUSY analysis with two leptons, jets and missing transverse energy is shown in Figure 5. Next, for each non-overlapping sub-region, and for each background component, the yields of events are scaled in the following way:

- To account for systematic uncertainty, scaling is done by the random value obtained from a Gaussian with unit mean and width equal to the systematic uncertainty,

- To account for the statistical uncertainty, scaling is done by the random value obtained from a Gaussian with unit mean and width equal to the statistical uncertainty,

- To produce a pseudo-experiment, a random number from a Poisson distribution is drawn, with mean equal to the yield obtained in the previous steps.

Then the newly obtained yields from corresponding bins are summed into SRs. The p-value and corresponding significance is evaluated for each SR. The procedure is repeated for a large number of pseudo-experiments. The global p-value is then calculated as the fraction of pseudo-experiments in which the largest local significance is higher than the observed maximum local significance. This p-value is then converted into a one-sided significance.

The calculation of global significance represents a computationally demanding task. As a rule of thumb, a number of pseudo experiments $N_{\rm toy}$ is taken of the order of the inverse of the p-value, e.g. for a p-value of 10^{-4}, $N_{\rm toy}$ is of order 10^4. Calculations corresponding to 3-4 σ significance are viable using hundreds of processing units on a modern computing cluster. However, the calculation of significance regions above 5σ becomes computationally intractable. When the number of signal regions is $\mathcal{O}(10)$, the effect of the correction for the global significance becomes negligible at high significance. However, certain aspects of using asymptotic formulae need to be considered when the number of signal regions is large. A viable solution for large number of overlapping signal regions and high maximum local significance could be obtained by developing a method using the counting of up-crossings, as described in the global significance calculation using non-overlapping regions of Ref. [327].

V. EXAMPLES AND TOY MODELS

In this section, we present a number of brief examples, based on statistical issues which arose during discussions at the workshop. While these toy examples represent simplified scenarios, it should be possible to extend them straightforwardly to more realistic applications in the field of DM searches.

A. Parameter limits with non-compact support

Consider the following toy problem: an experimental search for a new signal s with an expected flux $\phi(E)$ as a function of energy E proportional to:

$$\frac{d\phi_s}{dE} = \alpha^2 \frac{E^2}{(E^2 - m^2)^2 + \Gamma^2}. \quad (20)$$

This could parametrize some resonant scattering or annihilation process at $E_{res} = m$, with width Γ and strength α. This search could be performed in the presence of some background event rate:

$$\frac{d\phi_{bg}}{dE} = R_{BG} \left(\frac{E}{E_0}\right)^{\gamma}, \quad (21)$$

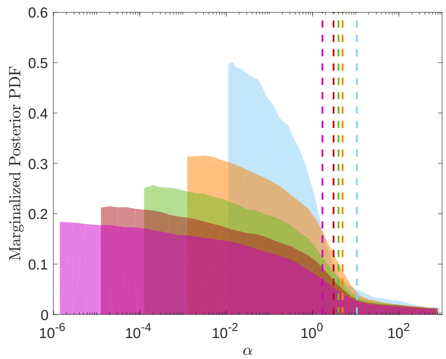

FIG. 6. Marginalized 1D posterior on the parameter α from (20), where the true value falls below the experimental sensitivity. Different colors correspond to lower boundaries on the prior from $\alpha_{min} = 10^{-6}$ to 10^{-2}. Vertical dashed line show the corresponding 95% CL limit inferred in each case.

governed by unknown nuisance parameters R_{BG}, γ. The total events observed in each energy bin i with width ΔE_i of such a search would be:

$$N_i = T\Delta E_i \left(\frac{d\phi_s}{dE}(E_i) + \frac{d\phi_{bg}}{dE}(E_i) \right), \tag{22}$$

where T represents the *exposure* of the experiment. One can then construct a likelihood $\log \mathcal{L} = \sum_i \log P(N_i)$ and proceed with the usual Bayesian analysis.

In the absence of a signal (i.e., the "new physics" rate is lower than the experiment's sensitivity can reach), we would like to place a limit on the (non-background) parameters governing the new physics we have been searching for (20), via the parameters α and m. Our theory does not specify a scale for these parameters, so the correct choice of prior that reflects our understanding of this theory would be log-uniform. Upon inspection of Eq. (20), it is clear that in the absence of a clear signal, α can be arbitrarily small, and m can be arbitrarily large. There is thus no well-motivated choice of a prior boundary.

This leads to the following conundrum: any change, e.g., in the lower prior boundary of α will affect the location of the 95% credibility boundary, because the latter depends on the total posterior volume, even if the likelihood is completely flat down to $\alpha \to 10^{-\infty}$. The limit set on the theory in this way is therefore entirely dependent on the arbitrary size of the prior box. This is illustrated in Fig. 6, where shaded regions represent the marginalized posterior distribution in α, and the vertical lines show the limit set in each case. This inherent fuzziness sends many dark matter phenomenologists (who are currently in the business of setting limits) running towards a more frequentist approach such as a profile likelihood where no such ambiguity exists.

B. Combining two experiments

Combining the evidence produced from N similar experiments (i.e., ones which require only a few, commonly shared nuisance parameters $\boldsymbol{\eta}$) can be a relatively painfree task with a simple product of likelihood functions

$$\mathcal{L}(d|\boldsymbol{\theta}, \boldsymbol{\eta}) = \prod_{i=1}^{N} \mathcal{L}_i(d_i|\boldsymbol{\theta}, \boldsymbol{\eta}) . \tag{23}$$

Here, $\boldsymbol{\theta}$ are the parameters of interest and d_i are the observed data in each experiment.

Complications can arise however when these experiments have many distinct nuisance parameters which may or may not be governed by some common parameters. The overall likelihood function is then instead

$$\mathcal{L}(d|\boldsymbol{\theta}, \boldsymbol{\eta}) = \prod_{i=1}^{N} \mathcal{L}_i(d_i|\boldsymbol{\theta}_i, \boldsymbol{\eta}_i) . \tag{24}$$

In general, there can be a large number of nuisance parameters $\{\boldsymbol{\eta}_i\}$, which may not be independent and which therefore complicate the issue of specifying priors or joint likelihoods on these nuisance parameters. Furthermore, if we want to calculate (for example) posterior distributions for the parameters of interest, the required integrals over (correlated) $\{\boldsymbol{\eta}_i\}$ are high-dimensional and typically intractable.

We discuss here a Bayesian solution to this problem of combining *dissimilar* experiments. More details can be found in [329, 330]. For clarity we discuss a simple setup, namely two toy single bin counting experiments (which we will refer to as DAMU and LAX) with uncertain background components. We assume that each experiment is contaminated with radioactive Unobtainium, governed by a contamination factor $c \in [0, 1]$. The number of expected background events is then $N_{\rm BG} = cR_{\rm Un}T$, where $R_{\rm Un}$ is the background rate expected from a pure Unobtainium source and T is the exposure time (which we set to 1). From calibration using a purely Unobtainium source we can constrain the expected background rate to be

$$P_U(R_{\rm Un}) = \frac{1}{\sqrt{2\pi\sigma^2 R_{\rm avg}^2}} \exp\left(-\frac{(R_{\rm Un}/R_{\rm avg} - 1)^2}{2\sigma^2} \right), \tag{25}$$

where $R_{\rm avg} = 1000$ events per unit time and $\sigma = 10\%$. Unfortunately our purification procedure is not perfect but the contamination in a given experiment can be constrained to be below $c_{\max}$. Below this value we assume a uniform prior on c, therefore the probability for getting a number of background events is described by

$$P_{\rm BG}(N_{\rm BG}) = \int_0^{c_{\max}} P_U\left(\frac{N_{\rm BG}}{c}\right) \frac{{\rm d}c}{c} . \tag{26}$$

Finally, the signal is simply given by a number of events $N_{\rm sig} = \mu$ on which we want to place an informative limit by combining evidence from DAMU and LAX.

Our two toy experiments are now governed by different nuisance parameters $N_{\rm BG}^{\rm (LAX)}$ and $N_{\rm BG}^{\rm (DAMU)}$.

We can deal with this in a Bayesian manner by first identifying the set of parameters common to both experiments - in this case μ and $R_{\rm Un}$. The different contamination factors $c^{\rm (LAX)}$ and $c^{\rm (DAMU)}$ are now independent. We can then calculate the adjusted likelihood functions for each experiment j:

$$\mathcal{L}_j(\mu, R_{\rm Un}) = \int {\rm d}N_{\rm BG}^{(j)}\, \mathcal{L}(N_{\rm obs}^{(j)}|\mu, N_{\rm BG}^{(j)})\, P(N_{\rm BG}^{(j)}|R_{\rm Un})\,, \tag{27}$$

where $P(N_{\rm BG}^{(j)}|R_{\rm Un})$ simply corresponds to the flat prior on the contamination $c^{(j)}$ up to $c_{\rm max}^{(j)}$. We can then calculate the marginal likelihood, incorporating our prior on $R_{\rm Un}$, $P(R_{\rm Un}|\mu) = P_U(R_{\rm Un})$,

$$\mathcal{L}(\mu) = \int {\rm d}R_{\rm Un} \left\{\prod_j \mathcal{L}_j(\mu, R_{\rm Un})\right\} P(R_{\rm Un}|\mu)\,. \tag{28}$$

This likelihood function can now be used as usual, for exploring the parameter space, calculating posteriors and setting limits on the signal strength for the combined experiments. In Fig. 7, we show the marginal likelihood ratio $\hat{\mathcal{L}} = \mathcal{L}/\mathcal{L}_{\rm max}$ (top panel) and cumulative posterior distribution (bottom) for LAX and DAMU separately and combined. We assume that both experiments see a total of 4 events, but that the contamination in LAX ($c_{\rm max} = 0.01$) is more poorly constrained than in DAMU ($c_{\rm max} = 0.005$). The posterior is calculated assuming a flat prior on μ.

As one can see, this parameterization of the problem requires the segmentation of relevant nuisance parameters to different experiments, i.e., $c^{\rm (LAX)}$ and $c^{\rm (DAMU)}$ even though they have a common baseline uncertainty set by the probability of events from pure Unobtainium (Eq. 25). In this way a hierarchical structure can be created for convenient computation of the adjusted likelihood functions per experiment. For more complex situations, this method can make an intractable likelihood calculation possible by reducing the dimensionality of the required integrals to variables associated with each experiment individually.

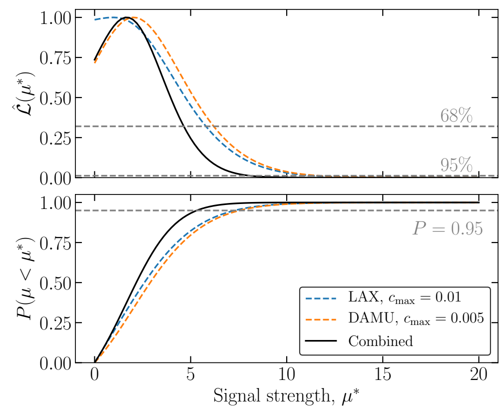

FIG. 7. Marginal likelihood ratio (top) and cumulative posterior distribution (bottom) for the LAX and DAMU toy experiments separately and combined. The combined curves correctly account for the correlation between nuisance parameters in the two experiments and can be used to easily set limits on the signal strength μ.

C. Presenting the p-value and the probability of the null

As discussed in Sec. IV, it is important to emphasize the distinction between the p-value and the probability of the null hypothesis, given the observed data, $\Pr({\rm H_0|y})$. These two numbers quantify different things. Taking the concrete example of looking for a bump-like signal on top of a smooth background (as in the case of the discovery of the Higgs Boson), the p-value gives a measure of the false alarm rate – how often we expect the smooth background to fluctuate upwards to *look* like a signal. Instead, $\Pr({\rm H_0|y})$ gives the probability that the background-only hypothesis is correct (given the observed data), compared with the hypothesis that there is a signal. The probability of the null hypothesis will depend on the our choice of priors (for both the background and the signal). However, by considering a wide range of priors, we can determine a lower bound on $\Pr({\rm H_0|y})$ and therefore the lowest possible probability that the background-only hypothesis is true.

We demonstrate this idea with a simple toy example of a single bin counting experiment. We assume that the expected number of background counts is known, $N_{\rm BG} = 49$. Given a number of observed counts $N_{\rm obs}$, we would like to quantify the level of agreement with the null hypothesis H_0 (that only background events contribute to the rate) and the alternative H_1 (that there is some non-zero signal).

The p-value is obtained as the probability of observing data as extreme or more extreme than what is observed, assuming H_0. Thus, we have:

$$p = \begin{cases} \sum_{k=N_{\rm obs}}^{\infty} P(k|N_{\rm BG}) & \text{for } N_{\rm obs} > N_{\rm BG}\,, \\ \frac{1}{2} & \text{for } N_{\rm obs} \leq N_{\rm BG}\,. \end{cases} \tag{29}$$

Here, $P(k|N_{\rm BG})$ is the Poisson probability of observing k events when $N_{\rm BG}$ events are expected. We set the p-value to $\frac{1}{2}$ for $N_{\rm obs} \leq N_{\rm BG}$ because an under-fluctuation does not correspond to data which is incompatible with

H_0 in favor of H_1.

The probability of the null hypothesis is obtained using Bayes' theorem [331]:

$$P(H_0|N_{\rm obs}) = \frac{P(N_{\rm obs}|H_0)P(H_0)}{P(N_{\rm obs}|H_0)P(H_0) + P(N_{\rm obs}|H_1)P(H_1)}\,. \quad (30)$$

Here, $P(H_0)$ and $P(H_1)$ are the prior probabilities that H_0 and H_1 respectively are true. In the absence of another well-motivated choice, we will assume $P(H_0) = P(H_1) = \frac{1}{2}$. As before, $P(N_{\rm obs}|H_0)$ is simply the Poisson probability of observing $N_{\rm obs}$ events, given $N_{\rm BG}$ expected background events. Instead, $P(N_{\rm obs}|H_1)$ is the probability of observing $N_{\rm obs}$ events, integrated over all possible numbers of signal events $N_{\rm sig}$:

$$P(N_{\rm obs}|H_1) = \int P(N_{\rm obs}|N_{\rm BG} + N_{\rm sig})P_\beta(N_{\rm sig})\,{\rm d}N_{\rm sig}\,. \quad (31)$$

Here, we write the prior on $N_{\rm sig}$ as $P_\beta(N_{\rm sig})$, which we parametrize by β. For concreteness, we will assume an exponential prior on the number of signal events:

$$P_\beta(N_{\rm sig}) = \beta \exp\left(-\beta N_{\rm sig}\right)\,. \quad (32)$$

In Fig. 8, we show the p-value as a function of the number of observed counts in this toy example. We also show $P(H_0|N_{\rm obs})$ for one specific prior on the number of signal counts, set by $\beta = 0.01$. Finally, we show the *lower bound* on $P(H_0|N_{\rm obs})$ obtained by minimizing over a large class of priors (i.e. by minimizing over β). This concrete example highlights what was discussed in Sec. IV: that the p-value is anti-conservative. In this case, when the p-value drops to 5%, the probability of the null hypothesis is always larger than 30%, even in the case of rather extreme priors. By presenting both the p-value and the bound on the probability of the null hypothesis, we give a more detailed picture of the evidence at hand as well as reminding the reader that these two things represent different information about the data.

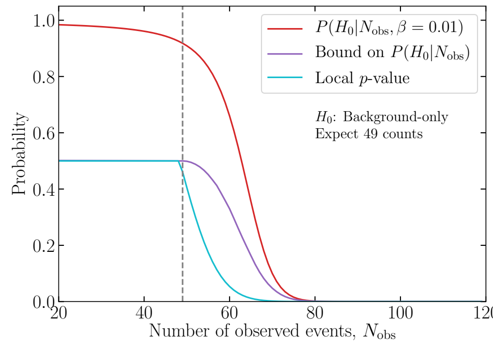

FIG. 8. Compatibility of an observed number of events $N_{\rm obs}$ with the 'background-only' null hypothesis H_0. The p-value quantifies the false alarm rate while $P(H_0|N_{\rm obs})$ quantifies the evidence in favor of H_0, as compared with the 'signal + background' hypothesis H_1. The red line corresponds to the probability of the null hypothesis assuming a particular choice of prior on the number of signal events (see Eq. 32). The purple line shows the lower bound on the probability of the null, over a wide range of priors.

VI. CONCLUSIONS

The search for new physics has become a complex task, with many moving parts. By now, it seems likely that an eventual detection and identification of dark matter through its particle interactions will take place through careful statistical analysis. We have outlined a number of experimental lines of attack in the hunt for particle DM, along with their specific statistical challenges. **Direct detection** experiments search for very rare events by creating a signal region that is as background-free as possible. **Indirect detection** relies on the vast scale of the cosmos, with the drawback of a large and not-so-well understood background from standard model astrophysical processes. Finally, **collider** searches benefit from a very well-understood background, but the tremendous amount of data lead to a challenge of analysis and trials factors.

We have outlined a number of statistical challenges that arise in these areas, and some techniques to help overcome them. The detection of new physics amounts to a challenge of model selection, which comes with a number of pitfalls: the construction of a good test statistic, likelihood function or detection criterion; the choice of physical model parameters and their priors; and the efficient exploration of that parameter space. We have discussed Bayesian methods as well as the dangers of p-values and their misinterpretation. We have also presented a number of novel techniques for dealing with complicated and computationally expensive parameter spaces, such signal euclideanization and likelihood-free approaches (i.e. ABC). Combining experiments and approaches poses additional challenges, as nuisance parameters may or may not overlap, and systematic uncertainties may have varying effects. Approaches such as hierarchical modeling and global fitting help tackle these daunting issues with finite effort. We have also provided a small number of examples or challenges that help illustrate some of the issues of statistics that astroparticle physicists are confronting.

A key goal of the *DMStat* workshop was to single out specific problems in the search for dark matter which present a statistical challenge. As we have seen, such problems are not hard to find. Thankfully, a wealth of advanced statistical tools have made confronting these challenges feasible. Indeed, we have been able to report significant progress in addressing a number of DM-specific problems, as well as highlighting a number of future challenges and avenues for further study. We are confident that the ongoing cooperation between statistics and DM physics will continue to yield progress and, perhaps some day soon, a discovery.

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Chapter 4

Distributionally Robust Optimization (18w5102)

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Overview of the Field

A wide variety of real-life decision-making problems, ranging from managerial planning and governmental policy making to finance, engineering, energy and healthcare, can naturally be formulated as large-scale mathematical optimization problems which seek to determine values for a set of decision variables that optimize a specified objective function, subject to a number of feasibility constraints. These optimization problems are often affected by substantial uncertainty because their parameters are subject to measurement errors or are not yet observable at the planning stage.

Optimization problems under uncertainty have a long history, and they are traditionally solved by methods of stochastic and dynamic programming, both of which have been popularized in the 1950s. Nowadays, the applicability of these methods is challenged for several reasons:

1. **Ambiguity.** In stochastic and dynamic programming, uncertainty is traditionally modeled via probability distributions. However, in many practical decision situations the raw data can be explained by several strikingly different distributions. Naive reliance on a single probabilistic model (e.g., the lognormal distribution underlying the Black Scholes equation of option pricing or the use of the Gaussian copula in the pricing of collateralized debt obligations [24]) can have catastrophic consequences, as has been demonstrated during the recent financial crisis.

2. **"Big Data."** In today's increasingly interconnected world, traditional localized decision problems must be integrated in order to correctly account for all possible synergies and systemic risks. Moreover, through the ongoing proliferation of digital information sources, increasing amounts of decision-relevant data become available (see [15] for a report by McKinsey Global Institute). As a result, modern decision problems have substantially increased in size and often grown beyond the grasp of traditional dynamic and stochastic programming methods.

3. **The Optimizer's Curse.** The solutions of stochastic programming problems parameterized by statistical data tend to display an optimistic bias even if the underlying parameter estimates are unbiased. This phe-

nomenon is referred to as the "optimizer's curse" and can lead to great post-decision disappointment in out-of-sample tests (c.f. [26]).

4. **The Curse of Dimensionality.** In dynamic optimization all future decisions are modeled as contingency plans, that is, as functions mapping observations to actions. In order to solve the emerging functional optimization problems numerically, dynamic and stochastic programming discretize the underlying state space or the probability distribution of the uncertain parameters. In either case, the computation time grows exponentially with the problem size (see [1]), which has been a major impediment to the practical use of classical dynamic and stochastic programming methods.

The new field of distributionally robust optimization (DRO) (as popularized with [8]) aims to remedy both the conceptual and the computational shortcomings of classical stochastic and dynamic programming. The central idea is to represent uncertainty through an ambiguity set, that is, a family of (possibly infinitely many) probability distributions consistent with the available raw data or prior structural information, and to model the decision-making process as a game against "nature." In this game, the modeler first selects a decision with the goal to maximize expected reward, minimize risk or maximize the probability of constraint satisfaction etc., in response to which "nature" selects a distribution from within the ambiguity set with the goal to inflict maximum harm to the modeler. This setup prompts the modeler to select worst-case optimal decisions that offer performance guarantees valid for all distributions in the ambiguity set.

DRO has several striking benefits. It enables modelers to incorporate information about estimation errors into optimization problems. Therefore, it results in a more realistic account of uncertainty and mitigates the optimizer's curse characteristic for classical stochastic programming. Moreover, surprisingly, DRO problems can often be solved exactly and in polynomial time – in marked contrast to the intractable approximate models obtained via discretizations of stochastic problems tailored to a single nominal distribution. Thus, DRO models have the potential to scale to industrially relevant problem sizes and is already being employed in a number of fields of practice including vehicle routing, fleet management, portfolio selection, revenue management, scheduling, environmental policies, smart grid management, etc.

Recent Developments and Open Problems

A distributionally robust optimization model typically takes the form of :

$$\underset{x\in\mathcal{X}}{\text{minimize}} \quad \sup_{F\in\mathcal{D}} \mathbb{E}_F[h(x,\xi)]\,, \tag{4.0.1}$$

where $x \in \mathbb{R}^n$ is a vector of decision variables, $\mathcal{X} \subset \mathbb{R}^n$ is the set of implementable decisions, $\xi \in \mathbb{R}^m$ is a random vector for which the distribution F is only known to lie inside an ambiguity set $\mathcal{D}$. Finally, one typically refers to $h(x,\xi)$ as a cost function which depends on both the decisions that are implemented and the realized values for ξ.

One can classify some of the main open questions with the use of the DRO framework in the following categories.

Choice of performance measure in DRO: While the DRO paradigm has to this date been heavily used in its classical form (4.0.1), a number of alternative formulations, involving other risk measures than expectation [23], and competing paradigms have recently surfaced (e.g. [5]). This brings the question of how to select the right formulation in any specific context. Perhaps, the pessimistic view is not always the one that should be adopted. Interestingly, Wolfram Wiesemann presented some work establishing an axiomatic motivation for DRO. We also refer to talks summarized in sections 4 and 4 which shed more light on some of these issues.

Choice of ambiguity sets in DRO: While the community has been very successful, both from a numerical and statistical point of view, employing ambiguity sets that are based on perfect or imperfect moment information (e.g. in [8, 18]), or the notion of "distance" from a reference distribution [2, 27, 10, 4, 17], there are still a number of questions that should be addressed by our community. In particular, one may ask:

- What are the approaches that make the "best" use of data in the design of ambiguity sets?

- What type of algorithms might efficiently handle ambiguity sets that describe more structured random variables such as discrete random variables, dependent variables based on copula information, or even a structure as simple as independence?

Both of these questions were the subject of a number of talks during the workshop. In particular, the first question was the main focus on our second day for which highlights are presented in Section 4. One might also be interested by talks from the following presenters regarding the second question: Melvyn Sim, Krzysztof Postek, and Ruiwei Jiang.

Efficiency of solution methods : While, in many cases, it is possible to reformulate DRO problems as tractable mathematical programs (see [11, 19, 30]), there are still a number of DRO models for which high precision solutions are numerically and analytically unattainable. This gives rise to the following questions:

- Can we extend the range of tractable instances?
- Can we design more efficient exact methods or better bounds for approximation algorithms?

In this regard, it is worth examining some of the recent successes achieved in robust optimization (see for instance the talks summarized in Section 4). Moreover, a number of the talks summarized in Section 4 addressed the second questions.

Distributionally robust optimization in multi-stage settings: While the DRO approach has been very useful in the handling of static optimization problems, its use in multi-stage/dynamic problems is more limited (see e.g. [29, 28, 20] for its use within Markov decision processes). In our opinion, this is due to the fact that the community still has not found satisfying answers to the following questions:

- How can we design exact/approximate algorithms with solution time that scale reasonably with the number of periods?
- Following the work in [22, 13, 3], how can algorithms more efficiently handle discrete delayed decision?
- How can ambiguity set account for conditional independence?
- How severe are the time consistency issues that arise as reported in [25]?

We refer the reader to the presentations of Section 4 which shed some light on the first issue.

Applications: We close this section with a brief overview of the areas where distributionally robust optimization as been used: healthcare [16], energy (see [14], portfolio selection [6, 31, 32], statistics [9], vehicule routing [12], etc. A number of new applications were discussed in this workshop and are summarized in Section 4.

Presentation Highlights

Emergent Modeling Paradigms

The first session of the workshop had two talks on the general concepts and modeling issues in distributionally robust optimization (DRO) and was conducted by Yinyu Ye (Stanford University). Professor Ye discussed some of the popular modeling approaches for ambiguity sets in distributionally robust optimization using moment, likelihood and Wasserstein ambiguity sets and some of the corresponding tractability results. A second idea that he discussed was that of addressing ambiguity in high dimensions where only the marginal distributions are known but the joint is unknown. Using an approximation to the problem with independent distributions, he showed that for submodular functions, this approach has a good approximation guarantee which is however not valid for supermodular functions. While the complexity of solving the independence model was not discussed in detail in the talk, an interesting question it naturally raises is if the distributionally robust formulation can be directly solved to optimality. He also discussed generalization to online learning using concepts from DRO.

Melvyn Sim (National University of Singapore Business School) proposed new ambiguity sets in his work by building on a scenario wise representation where in each scenario, the uncertain random variables lies in an ambiguity set defined by moments information. Such an ambiguity set can be defined using clustering methods. The model has nice tractable convex optimization representation using linear programming (LP) and second-order cone programming (SOCP) methods and solving the DRO problem can be done in multi-stage problems using decision rules. He also discussed using infinitely constrained ambiguity sets to characterize information such as independence and algorithms to solve it.

Wolfram Wiesemann (Imperial College London) and Professor Erick Delage (HEC Montréal) gave a sequence of two talks on randomized decision making and the value it provides in distributionally robust optimization. Professor Wiesemann proposed a mathematical framework to define ambiguity averse risk measures and developed a representation theorem for it. He discussed conditions under which randomized decisions might be optimal in such a setting and used a simple facility location example to illustrate this. Professor Delage built on this to show the application of this method to distributionally robust facility location problems and developed tractable bounds for this problem while proposing a column generation method to solve this problem. He also proposed that randomized decision-making might be a useful paradigm particularly if the benefits over deterministic decision-making is significant. The idea of randomization in other decision-making problems such as consumer choice is currently under investigation by economists and this stream of work has interesting connections with it, but in an ambiguity averse setting.

Patrick Jaillet (Massachusetts Institute of Technology) discussed an alternative decision-making criterion under uncertainty where instead of maximizing expected utility, the objective is to have a satisfactory solution. He discussed how the classical chance constraint formulation can be generalized by the satisficing model by focusing on the maximum size of the ambiguity set that leads to satisfactory solution. He used a facility location problem to illustrate the model and this leads to interesting questions on how these techniques can be adapted to other decision-making problems.

Marco Campi (University of Brescia) and Simone Garatti (Politecnico di Milano) presented two talks on scenario optimization which appears to be a powerful mathematical tool for controlling the risk that a solution be infeasible. In particular, they demonstrated that in a decision making problem where the constraint set is indexed by scenarios drawn from a distribution, the infeasibility risk is directly related to what they call "complexity", i.e. the minimum number of scenarios needed to identify the optimal solution. While the distribution of scenarios is typically difficult to identify precisely, "complexity" can numerically be evaluated once the optimal solution to the scenario problem is obtained. It is also possible to explore the trade-off between infeasibility risk and expected performance by employing their theory on a version of the decision problem where violations of the constraints are penalized more or less heavily through a tunable penalty parameter. The use of regularization as a way of controlling risk is also discussed.

The Interplay between DRO and Classical Risk Measures

Jonathan Y. Li (University of Ottawa) reviewed some of the closed form bounds for worst-case conditional value at risk measure under first and second order moment information and showed how it can be generalized to law invariant risk spectral risk measures. His work discusses how for special cases of risk measures, multi-dimensional problems can be reduced to single-dimensional problems. The worst-case distribution in such examples is not two points unlike the classical worst-case conditional value at risk model. A natural question that this work raises is how can these methods be applied to general two stage distributionally robust optimization problems and what are the complexity implications in those cases?

Ruiwei Jiang (University of Michigan) in his talk discussed how DRO chance constraints and conditional value at risk constraints with first and second order moment information can be supplemented with additional structural information such as log-concavity and tail dominance. For the log-concave set of distributions, the results indicate that the DRO constraint with conditional value-at-risk (CVaR) can be formulated in a manner similar to what is currently known but with modified scaling factors for the second order conic terms. In the case of the value-at-risk (VaR) formulation, it is not tight, but it is possible to develop tractable approximations. He discussed applications of the results in optimal power flow problems and appointment scheduling problems.

The Use of DRO in Data-driven Problems

Dimitris Bertsimas (Massachusetts Institute of Technology) provided a survey of recent developments in the field of data-driven optimization. He showed how one can transform predictive machine learning algorithms to prescriptive ones that are useful for two-stage and multi-stage decision-making problems and characterized the rates of convergence of the resulting algorithms. He also described an approach to make prescriptive approaches immune to overfitting phemonema and to improve the performance of parametric methods via kernel techniques.

Anton Kleywegt (Georgia Institute of Technology) showed how distributionally robust optimization can help to regularize algorithms of statistical learning. This is achieved by minimizing the worst-case expected prediction error across all distributions in a ball, sized with respect to the Wasserstein distance, is centered at the empirical distribution. He identified a broad class of loss functions for which the proposed approach leads to a gradient-norm penalty and discussed important applications in deep learning and discrete choice models.

Andrew Lim (National University of Singapore) proposed a theory for calibrating the ambiguity parameter that typically determines the size of the uncertainty set in robust optimization. He showed that the first-order benefit of injecting robustness into a nominal optimization model is a significant reduction in the variance of the out-of-sample reward, while the corresponding impact on the mean reward is almost an order of magnitude smaller. This observation motivated Andrew to introduce a robust mean-variance frontier, which can be used to tune the ambiguity parameter. He also showed that this frontier can conveniently be approximated using resampling methods like the bootstrap. He then provided evidence that solutions of robust optimization problems whose ambiguity parameters are calibrated to ensure a certain coverage probability may be too conservative out of sample, while tuning the ambiguity parameter in view of the out-of-sample expected reward with no regard for the variance may lack robustness.

Vishal Gupta (University of Southern California) pointed out that practical optimization problems often depend on a huge number of uncertain parameters, for each of which there are only very few historical observations leading to imprecise estimates. He then argued that this large-scale, small-data regime is distinct from the large-sample regime usually studied in statistics. Given a fixed class of candidate policies, he then identified a policy that performs best in this class asymptotically as the number of uncertain parameters tends to infinity (while the number of samples per parameter remains small). He further showed that the loss of optimality of the proposed method relative to the best-in-class policy decays exponentially fast in the number of uncertain parameters for two important policy classes inspired by the empirical Bayes and the regularization literature, respectively.

Karthyek Murthy (Singapore University of Technology and Design) investigated distributionally robust optimization problems where the ambiguity sets are defined via optimal transport distances such as the popular Wasserstein distance. He demonstrated that several widely used machine learning algorithms that employ regularization can be recovered as particular examples of this distributionally robust approach. He also developed a method to calibrate the radius of a Wasserstein ambiguity set by leveraging ideas from empirical likelihood theory in statistics that obviates the need to use brute-force cross-validation techniques. Moreover, he proposed a fast stochastic gradient descent algorithm for solving the resulting optimization problems.

Bart Van Parys (Massachusetts Institute of Technology) studied data-driven optimization problems, where the uncertain parameters that impact the problem's objective function depend on observable contextual information captured by a potentially large number of covariates. He emphasized that a naïve use of the training data (independent samples of the uncertain problem parameters and the covariates) may lead to overfitting. To combat the overfitting, he proposed to leverage ideas from distributionally robust optimization, the statistical bootstrap and Nadaraya-Watson or nearest neighbor density estimation. He showed that the proposed approach leads to tractable convex optimization problems that offers rigorous out-of-sample guarantees.

Henry Lam (Columbia University) discussed new methods to calibrate the uncertainty sets in robust optimization and the Monte Carlo sample sizes in constraint sampling or scenario generation. He proposed strategies to select good parameter values based on data splitting and the validation of their performances in terms of feasibility and optimality. He then showcased the effectiveness of these strategies in relation to the dimension of the underlying optimization model.

Nathan Kallus (Cornell University) proposed a new approach to policy learning from observational data (for example, the transformation of electronic health records to personalized treatment regimes). The task is difficult because only outcomes of the interventions performed are observable, and the distribution of units exposed to one intervention or another differs systematically. Nathan described a new distributionally robust approach to policy learning in the context of personalized medicine that offers strong finite-sample guarantees and preserves the asymptotic optimality and convergence rates of naïve traditional plug-in approaches.

Daniel Kuhn (École Polytechnique Fédérale de Lausanne) outlined an abstract perspective on data-driven stochastic programming whereby one should find a procedure that maps time series data to a near-optimal decision (a prescriptor) and to a prediction of this decision's expected cost under the unknown data-generating distribution (a predictor). He proposed a meta-optimization problem, that is, an optimization problem over optimization problems, that identifies the least conservative predictors and prescriptors subject to constraints on their out-of-sample disappointment. He then showed that the best predictor-prescriptor pair is obtained by solving a distributionally robust optimization problem.

Computational Lessons Learned from Robust Optimization

Dick den Hertog (Tilburg University) proposed to tackle a robust optimization problem where the cost function $h(x, \xi)$ is convex with respect to both x and ξ. These are generically difficult problems to handle within a classical robust optimization framework, yet have recently been addressed successfully for special instances of DRO models [30, 21]. The proposed approach applies when the uncertainty set is polyhedral and relies on a series of reformulation that converts the problem into a two-stage robust linear program. The resulting problems can subsequently be approximated via classical approximation schemes for these types of robust optimization models. A set of numerical examples provide evidence that this approach often leads to near-optimal solutions.

Grani Hanasusanto (University of Texas at Austin) studied robust quadratically constrained quadratic programs where the uncertain problem parameters contain both continuous and integer components. Grani showed that these problems can be reformulated as copositive programs of polynomial size, which he subsequently approximated via semidefinite programs. Grani demonstrated the superiority of these approximations over the state-of-the-art solution schemes on several problem classes.

Anthony Man-Cho So (Chinese University of Hong Kong) considered a class of robust quadratic optimization problems that arise in various applications in signal processing and wireless communications (such as robust beamforming with cognitive radio constraints). Due to the NP-hardness of this problem class, Anthony developed an approximate solution scheme that uses the so-called epsilon-net technique from functional analysis to offer rigorous approximation guarantees.

The Use of DRO with Moment Information

A classical form for the DRO problem employs an ambiguity set defined by imposing constraints on moments of the distribution. Typically, these include bounding the mean vector of ξ and its second-order moment matrix $\mathbb{E}[(\xi-\mu)(\xi-\mu)^T)]$. In her talk, Siqian Shen revisited the well-known ambiguity set presented in [8] for the case of a distributionally robust chance constrained (DRCC) optimization problem. She demonstrated that it is possible to reformulate the chance constraint using second-order cone (SOC) constraints instead of linear matrix inequalities (LMI) as was originally proposed. This is interesting since 1) from a numerical perspective, SOC constraints are easier to optimize than LMIs; 2) it somehow ties in together a number of reformulations that are known for these type of constraints and which uses the canonical representation first introduced in [7]. Siqian also presented a branch-and-cut method to improve the solution time in a bin packing problem with these types of constraints. The numerical results were quite promising.

Abdel Lisser (Laboratoire de Recherche en Informatique - University Paris Sud) further presented how the DRCC could be reformulated for a geometric program with uncertainty about the coefficients that multiply each monomial. He also obtained useful reformulation for the cases where the ambiguity set is based on KL-divergence with respect to some reference empirical distribution. While these reformulations were not SOC programs in this case they still could be solved using algorithms that are available for convex optimization problems. Abdel's numerical results involved a shape optimization problem where it appears that there is still important challenges to overcome before large scale problems can be addressed.

Krzysztof Postek (Erasmus University Rotterdam) addresses in his talk the common criticism made against DRO models that they often consider worst-case distribution that are unnatural for the problem at hand. Indeed, it is well known that most moment-based problems have a worst-case distribution that is supported on a handful of scenarios. The proposed remedy consist in using a polynomial function as the density function. In this way, it is possible to control the smoothness of the worst-case density function and prevent it from peaking so significantly at any point of the support set. While a number of numerical difficulties seem to arise when implementing this idea, Krzysztof appeared very resourceful in addressing each of them and will certainly make interesting progress in the months to come.

The talk of Jianqiang Cheng (University of Arizona) proposed methods to improve the computational efficiency in moment-based DRO problems by exploiting principal component analysis (PCA) to reduce the dimensionality of the uncertain vector ξ. This is especially promising in problems that involve covariance information as these problems can take the form of semi-definite programming model where the dimension of ξ has an important effect on solution time. Theoretically, he provides a bound on the size of the approximation error that is introduce through dimensionality reduction which depends on the size of the eigenvalues that are dropped during PCA. The technique is applied on a production-transportation problem where the objective function is a distributionally robust conditional value-at-risk (CVaR) measure. Numerical experiments illustrate the trade-off between the size of the approximation gap and computation time for solving this problem.

Huifu Xu (University of Southampton) presented valuable results concerning the stability of moment-based DRO models. In particular, he considered the case where the moment information is estimated from data and whether the solutions of DRO models constructed based on these estimate converge to a limit solution as more data is used to make the estimation. He also paid special attention to cases where the distribution ambiguity set is designed as decision dependent. Finally, he concluded is presentation with a discussion on the implication of his stability results for a distributionally robust chance constrained problem.

Guzin Bayraksan (Ohio State University) introduced the notion of effective scenarios and ineffective scenarios in the context of a scenario based distributionally robust optimization problem, which is a special case of moment based DRO where the distribution's support is assumed discrete. In particular, she noticed that in some DRO formulations, the optimal solution is not necessarily sensitive to all the scenario with positive probability in a worst-case distribution. For this reason, she considers a scenario to be effective if its removal from the support causes the optimal value of the DRO problem to change, otherwise the scenario is considered ineffective. In some way, these concepts are related to the concept of "complexity" presented by M. Campi and S. Garatti yet the intent here is different. Indeed, Guzin's interest is regarding post-optimization analysis where one can question whether effective scenarios are realistic of perhaps outliers that can be removed from the problem. She also indicates how this information might be helpful from a computational point of view by motivating scenario reduction scheme or provide guidance for improving the effectiveness of decomposition schemes. The applications that illustrates her findings involves a water allocation problem for the Colorado River and where a total variation ambiguity set was used.

Handling Multi-stage problems with DRO

Sanjay Mehrotra (Northwestern University) proposed decomposition algorithms for two-stage distributionally robust optimization problems with continuous and binary decision variables in both the first and the second stage. The algorithms utilize distribution separation procedures and parametric cuts within a Benders' algorithm. The presentation also studied conditions and families of ambiguity set for which the proposed algorithms converge in finite time.

Huan Xu (Georgia Institute of Technology) discussed robust Markov decision process models with parameter uncertainty. His talk discussed how it is possible to learn the uncertainty when a combination of robust and stochastic elements are present in a Markov decision process. He developed an algorithm that combines elements of pessimism and optimism such that it is robust to adversarial uncertainty and optimistic to stochastic uncertainty. This talk discusses new ideas of learning uncertainty sets that might be relevant in other online decision-making problems.

Angelos Georghiou (McGill University) proposed an adaptation of the well-known stochastic dual dynamic programming (SDDP) scheme to multi-stage robust optimization problems. The resulting robust robust dual dynamic programming (RDDP) scheme maintains both inner and outer approximations of the cost to-go for each time stage of the problem. The algorithm converges in finite time, and the presented numerical results show the promise of the proposed scheme.

Vineet Goyal (Columbia University) investigated the performance of affine policies in two-stage robust optimization problems. While it is well-known that their worst-case performance is poor, it has been observed that affine policies perform well in numerical experiments. The presentation has shown that affine policies are a good approximation for two-stage adjustable robust optimization problems with high probability on random instances where the constraint coefficients are generated i.i.d.

Dan Iancu (Stanford University) discussed necessary and sufficient conditions for affine policies to be optimal in multi-stage robust optimization problems. The treatment drew interesting connections with the theory of discrete convexity and global concave envelopes.

Georg Pflug (University of Vienna) in his talk discussed the idea of how distributional robustness might be modeled in multi-stage problems. This is a challenging problem and he proposed an extension of the Wasserstein metric ambiguity set that is relevant for the multi-stage problem using distances between conditional probability measures. The size of the ambiguity sets can be determined from statistical confidence regions. He also discussed applications to the multi-period portfolio optimization using the average value at risk measure under ambiguity.

Recent Applications of DRO

Tito Homem-de-Mello (Universidad Adolfo Ibáñez) used distributionally robust optimization to model a general class of newsvendor problems where the underlying demand distribution is unknown and the goal is to find an order quantity that minimizes the worst-case expected cost among all distributions within some distance from a given nominal distribution. Due to the specific structure, Tito was able to derive explicit formulas and properties of the optimal solution as a function of the level of robustness, determine the regions of demand that are critical to optimal cost and establish quantitative relationships between the distributionally robust model and the corresponding risk-neutral and classical robust optimization models.

Karthik Natarajan (Singapore University of Technology and Design) also revisited the distributionally robust newsvendor problem but this time exploring conditions for which the optimal order quantity that is returned by DRO can be motived using a risk neutral setting where the distribution is known. While an early result from H. Scarf already established that this is the case for mean-variance models, Karthik presented an analysis that extends, in an asymptotic sense, this equivalence to problems where variance information is replaced by any p-th order moment information. The interesting insight from this range of work is the fact that solutions from DRO models might for some family of problems be explained using a stochastic programming model that uses a heavy-tailed distribution which is not even a member of the original distribution set.

Chung Piaw Teo (National University of Singapore) proposed a new method to integrate probabilistic assessment of disruption risks into the Risk Exposure Index approach for supply chains under disruption. His method measures the resilience of a supply chain by analyzing the Worst-case CVaR (WCVaR) of total lost sales under disruptions. Chung Piaw showed that the optimal strategy in this model can be fully characterized by a conic program, which allows managers to focus their mitigation efforts on critical suppliers and/or installations that will have greater impact on the performance of the supply chain when disrupted.

Selin Damla Ahipasaoglu (Singapore University of Technology and Design) proposed novel classes of equilibria in traffic models with relaxed information assumptions. Selin studied conditions under which these equilibria exist and are unique, and she also provided convex programs for determining these equilibria and developed customized algorithms to calculate the equilibrium flows.

Phebe Vayanos (University of Southern California) studied systems that allocate different types of scarce resources to heterogeneous allocatees based on predetermined priority rules, such as the U.S. deceased-donor kidney allocation system or the public housing program. Phebe proposed to estimate the wait times in such systems via the solution of robust multiclass, multiserver queuing systems. Phebe showcased how the methodology can be applied to the U.S. deceased- donor kidney waitlist.

Jin Qi (Hong Kong University of Science and Technology) studied a finite horizon stochastic inventory routing problem where the supplier determines the replenishment quantities as well as the times and routes to all retailers. The probability distribution governing the uncertain demand of each retailer is assumed to be ambiguous, and the goal is to minimize the risk of the uncertain inventory levels falling outside a pre-specified range. Jin provided algorithms to solve the problem exactly, and she compared the performance of her solutions with several benchmarks to show their benefits.

John Gunnar Carlsson (University of Southern California) considered a distributionally robust version of the Euclidean travelling salesman problem and computed the worst-case spatial demand distribution from within a Wasserstein ball centered at an observed demand distribution. Numerical experiments on a districting problem in multi-vehicle routing confirmed that the proposed approach is useful for decision support tools that divide a territory into service districts for a fleet of vehicles when limited data is available.

Outcome of the Meeting

The meeting provided a great opportunity for high quality researchers to meet and discuss some of the most active research directions of this field. Our discussions were particularly enriched by the diversity and range of areas of expertise of the participants. These included experts in optimization, stochastic modeling, game theory, statistics and machine learning, and experts of applications such as financial engineering, vehicle routing, scheduling, health care, to name a few. In the opinion of the organizing committee, there is no doubt that a number of new collaborations have emerged from this event.

Participants

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Chapter 5

Modular forms and Quantum knot invariants (18w5007)

March 11 - 16, 2018

Organizer(s): Kazuhiro Hikami (Kyushu University), Jeremy Lovejoy (CNRS, Université Paris 7), Robert Osburn (University College Dublin)

Overview

A modular form is an analytic object with intrinsic symmetric properties. They have enjoyed long and fruitful interactions with many areas in mathematics such as number theory, algebraic geometry, combinatorics and physics. Their Fourier coefficients contain a wealth of information, for example, about the number of points over the finite field of prime order of elliptic curves, K3 surfaces and Calabi-Yau threefolds. Most importantly, they were the key players in Wiles' spectacular proof in 1994 of Fermat's Last Theorem. Quantum knot invariants have their origin in the seminal work of two Fields medalists, Vaughn Jones in 1984 on von Neumann algebras and Edward Witten in 1988 on topological quantum field theory. The equivalence between vacuum expectation values of Wilson loops (in Chern-Simons gauge theory) and knot polynomial invariants (for example, the Jones polynomial, HOMFLY polynomial and Kauffman polynomial) is a major source of inspiration for the development of new knot invariants via quantum groups.

Over the past two decades, there have been many tantalizing interactions between quantum knot invariants and modular forms. For example, quantum invariants of 3-manifolds are typically functions that are defined only at roots of unity and one can ask whether they extend to holomorphic functions on the complex disk with interesting arithmetic properties. A first result in this direction was found in 1999 by Lawrence and Zagier [17] who showed that Ramanujan's 5th order mock theta functions coincide asymptotically with Witten-Reshetikhin-Turaev (WRT) invariants of Poincaré homology spheres. More recently, Zagier has found experimental evidence of modularity properties of a new type for the Kashaev invariants of knots. This "modularity conjecture" implies one of the major outstanding open problems in this field, namely the Volume conjecture. This latter conjecture relates the value at $e^{2\pi i/N}$ of the Nth Kashaev invariant of a knot, or equivalently the Nth colored Jones polynomial, to its hyperbolic volume and, if true, would give striking relations between hyperbolic geometry, quantum topology and modular forms. Other examples of such intriguing interactions can be found in the construction of new mock theta functions from WRT invariants [3], [14], the stability of the coefficients of the colored Jones polynomial [1], [6], [9] and generalized quantum modular q-hypergeometric series [13].

Due to recent rapid developments on new theories of modular forms including mock modular forms, vector-valued modular forms and quantum modular forms and their appearance in quantum topology and physics, there was a strong desire amongst researchers with diverse backgrounds to hold a workshop in order to build further connections between previously believed disparate areas.

In addition to enhancing our knowledge of recent scientific progress, our focus was to create opportunities for junior participants and to ensure appropriate representation of women. For example, 8 of the 35 participants (and 5 of the 19 speakers) were women.

Scientific content of the meeting

This workshop showcased recent developments and open problems concerning modular forms and quantum knot invariants. All speakers were encouraged to have their talk videotaped and notes or slides posted online. In the following, we briefly summarize some highlights of each talk. Junior speakers are indicated with a bullet (•). Speakers from under-represented groups are designated with a star (⋆).

Abhijit Champanerkar (⋆) (College of Staten Island and the CUNY Graduate Center) spoke on *Mahler measure and the Vol-Det conjecture*. For a hyperbolic link in the 3-sphere, the hyperbolic volume of its complement is an interesting and well-studied geometric link invariant. Similarly, the determinant of a link is one of the oldest diagrammatic link invariants. Previously, the speaker studied the asymptotic behavior of volume and determinant densities for alternating links, which led to conjecturing a surprisingly simple relationship between the volume and determinant of an alternating link, called the Vol-Det Conjecture. This talk outlined an interesting method to prove the Vol-Det Conjecture for infinite families of alternating links using a variety of techniques from the theory of dimer models, Mahler measures of 2-variable polynomials and the hyperbolic geometry of link complements in the thickened torus.

Thomas Creutzig (University of Alberta) spoke on *Modularity and tensor categories for affine vertex algebras at admissible level*. A well-known result is that modules of a rational vertex algebra form a modular tensor category and that the modular group action on graded traces coincides with the categorical one. Prime examples are affine vertex algebras at positive integer level. This talk explained the state of the art for affine vertex algebras at admissible level and mainly restricted to the case of $sl(2)$. From the character point of view three types of traces arise: vector-valued modular forms, meromorphic Jacobi forms and formal distributions. There are also three types of categories one can associate to the affine vertex algebra and categorical action of the modular group seems to coincide with the one on characters.

Renaud Detcherry (•) (Michigan State University) spoke on *Quantum representations and monodromies of fibered links*. According to a conjecture of Andersen, Masbaum and Ueno, the Witten-Reshetikhin-Turaev quantum representations of mapping class groups send pseudo-Anosov mapping classes to infinite order elements, when the level is big enough. This talk discussed how to relate this conjecture to a properties about the growth rate of Turaev-Viro invariants, and derive infinite families of pseudo-Anosov mapping classes that satisfy the conjecture, in all surfaces with n boundary components and genus $g > n \geq 2$. These families are obtained as monodromies of fibered links containing some specific sublinks. For further details, see [7].

Amanda Folsom (⋆) (Amherst College) spoke on *Quantum Jacobi forms*. This talk introduced the notion of a quantum Jacobi form, marrying Zagier's notion of a quantum modular form with that of a Jacobi form. The speaker also offered a number of two-variable combinatorial generating functions as first examples of quantum Jacobi forms, including certain rank generating functions studied by Bryson-Ono-Pitman-Rhoades, Hikami-Lovejoy, and Kim-Lim-Lovejoy. These combinatorial functions are also duals to partial theta functions studied by Ramanujan. Additionally, it was shown that all of these examples satisfy the stronger property that they exhibit mock Jacobi transformations in $\mathbb{C} \times \mathbb{H}$ as well as quantum Jacobi transformations in $\mathbb{Q} \times \mathbb{Q}$. Finally, the talk discussed applications of these quantum Jacobi properties which yield new, simple expressions for the aforementioned combinatorial generating functions as two-variable polynomials when evaluated at pairs of rational numbers, and yield similarly simple evaluations of certain Eichler integrals. This is joint work with Bringmann. For further details, see [4].

Stavros Garoufalidis (Georgia Tech) spoke on *A meromorphic extension of the* $3D$*-index*. The 3D-index of Dimofte-Gaiotto-Gukov is a collection of q-series with integer coefficients which is defined for 1-efficient ideal triangulations, and gives topological invariants of hyperbolic manifolds, in particular counts the number of genus 2 incompressible and Heegaard surfaces. The talk discussed an extension of the 3D-index to a meromorphic function defined for all ideal triangulations, and invariant under all Pachner moves. This is joint work with Rinat Kashaev. For further details, see [10].

Frank Garvan (University of Florida) spoke on *Higher order Mock theta conjectures*. The Mock Theta Conjectures were identities stated by Ramanujan for his so called fifth order mock theta functions. Andrews and Garvan showed how two of these fifth order functions are related to rank differences mod 5. Hickerson was first to prove these identities and was also able to relate the three Ramanujan seventh order mock theta functions to rank differences mod 7. Based on work of Zwegers, Zagier observed that the two fifth order functions and the three seventh order functions are holomorphic parts of real analytic vector modular forms on $\mathrm{SL}_2(\mathbb{Z})$. Zagier gave an indication how these functions could be generalized. This talk detailed these generalizations and showed how Zagier's 11th order functions are related to rank differences mod 11.

Sergei Gukov (California Institute of Technology) spoke on $\hat{Z}_a(q)$. This talk discussed various ways to define and compute new q-series invariants that have integer powers and integer coefficients. After a quick review of the physical framework, the talk showed how it explains and generalizes the observations of Lawrence-Zagier and Hikami et. al. to arbitrary 3-manifolds. The talk also discussed a modular tensor category which is responsible for the modularity properties of $\hat{Z}_a(q)$. There are many unexpected and intriguing connections with various counting problems as well as with the works of Beliakova-Blanchet-Le and Garoufalidis-Le. For further details, see [11].

Shashank Kanade (•, ⋆) (University of Denver) spoke on *Some new* q*-series conjectures*. Representation theory of affine Lie algebras and more generally, vertex operator algebras, leads to interesting q-series identities. The q-series related to VOAs often exhibit deep modularity properties. Some of these q-series may also be of interest to the knot theorists. This talk presented some new q-series conjectures and is joint work with Matthew Russell and Debajyoti Nandi. For further details, see [15].

Rinat Kashaev (Université de Genève) spoke on *Quantum dilogarithms over gaussian groups and punctured surface mapping class group representations*. A gaussian group is a Pontryagin self-dual locally compact abelian group together with a fixed gaussian exponential that is a symmetric second order character associated with a non-degenerate self-pairing. This talk explained how a quantum dilogarithm can be used for construction of projective unitary representations of the mapping class groups of punctured surfaces of negative Euler characteristic.

Ruth Lawrence (⋆) (Hebrew University) spoke on *Higher depth quantum modular forms from* sl_3 *quantum invariants*. This talk presented work-in-progress on higher depth quantum modular forms arising from sl_3 WRT invariants of the Poincare homology sphere, following the work of Bringmann.

Christine Lee (•, ⋆) (University of Texas at Austin) spoke on *Understanding the colored Jones polynomial via surfaces in* 3*-manifolds*. Quantum link invariants lie at the intersection of hyperbolic geometry, 3- dimensional manifolds, quantum physics, and representation theory, where a central goal is to understand its connection to other invariants of links and 3-manifolds. This lecture introduced the colored Jones polynomial, an important quantum link invariant and discussed how studying properly embedded surfaces in a 3-manifold provides insight into the topological and geometric content of the colored Jones polynomial in view of the Slope Conjectures by Garoufalidis and Kalfagianni-Tran and the Coarse Volume Conjecture by Futer-Kalfagianni-Purcell, and we will explore the potential connection to the number-theoretic properties of the polynomial. In particular, the speaker indicated how their recent joint work with Garoufalidis and van der Veen on the Slope Conjectures for Montesinos knots is related to the existence of multiple tails of the polynomial for Montesinos knots.

Antun Milas (SUNY Albany) spoke on *False/Mock/Quantum modular forms and Vertex algebras*. An important problem in conformal field theory is to describe modular transformation properties of characters of representations of a vertex algebra. By now this is well-understand for "nice" vertex algebras (e.g., if the category of modules is semisimple). But most vertex algebras have non-semisimple category of representations so modular properties of their characters is difficult to formulate. This talk focused on a family of W-algebras coming from certain extensions of affine W-algebras. Their irreducible characters have recently been proposed and studied. The speaker explained two approaches to modular invariance and Verlinde formula for their modules, both based on iterated integrals of modular forms. In the first approach, modular invariance is formulated with the help of regularized variables. In the second approach, one replaces the characters with better behaved non-holomorphic integrals. This approach is intimately linked to mock and quantum modular forms. Finally, it was discussed how the two approaches can be understood from a unified viewpoint. For further details, see [5].

Jun Murakami (Waseda University) spoke on *Presentation of knots by a braided Hopf algebra*. The fundamental group of a knot complement is called a knot group. A way to present a knot groups is the Wirtinger presentation, which is given by a conjugation action at each crossing of the knot. This presentation is also given by a conjugate quandle, which matches well to the Hopf algebra structure of the group ring of the knot group. This talk introduced the braided conjugate quandle corresponding to the braided Hopf algebra, which is a deformation of a Hopf algebra. A typical example of the braided Hopf algebra is the braided $SL(2)$ introduced by S. Majid, and so it may give a q-deformation of a $SL(2)$ representation of the knot group. This is joint work with Roland van der Veen.

Satoshi Nawata (•) (Fudan University) spoke on *Large N duality of refined Chern-Simons invariants*. Refined Chern-Simons invariants of torus knots can be defined by using modular matrices associated to Macdonald polynomials or DAHA, generalizing colored quantum invariants. The theory was originally defined in string theory, and conifold transition in string theory leads to a positivity conjecture of refined Chern-Simons invariants of torus knots. This conjecture connects refined Chern-Simons theory to enumerative geometry.

Toshie Takata (⋆) (Kyushu University) spoke on *The strong slope conjecture for twisted generalized Whitehead doubles*. The slope conjecture proposed by Garoufalidis asserts that the degree of the colored Jones polynomial determines a boundary slope, and its refinement, the Strong Slope Conjecture proposed by Kalfagianni and Tran asserts that the linear term in the degree determines the topology of an essential surface that satisfies the Slope Conjecture. This talk presented a proof of the strong Slope Conjecture for a twisted, generalized Whitehead double of a knot K whenever K satisfies the strong Slope Conjecture and certain extra conditions. This is joint work with Kenneth L. Baker and Kimihiko Motegi.

Roland van der Veen (•) (Universiteit Leiden) spoke on *q-series coming from extending Turaev-Viro into the unit disk*. The Turaev-Viro invariant is a 3-manifold invariant (TQFT) defined at roots of unity q using a handle decomposition. Following Frohman and Kania Bartoszynska, this talk considered extending the variable q into the unit disk and discussed under what conditions one still gets an invariant and give some explicit examples of the ensuing q-series.

Katherine Walsh (•, ⋆) (University of Connecticut) spoke on *Patterns and higher order stability in the colored Jones polynomial*. This talk discussed the patterns and stability in the coefficients of colored Jones polynomial. While much work has been done looking at the leading sequence of coefficients, the speaker emphasized work moving towards understanding the middle coefficients. This included small steps like looking at the second N coefficients of the Nth colored Jones polynomial and larger steps like looking at the growth rate of the coefficients and looking at the patterns present in the coefficients under various re-normalizations. For further details, see [20].

Paul Wedrich (•) (Australian National University) spoke on *Knots and quivers, HOMFLY and DT*. Physicists have long been arguing that gauge theories at large rank are related to topological string theories. As a concrete example, this talk described a correspondence between the colored HOMFLY-PT polynomials of knots and the motivic DT invariants of certain symmetric quivers, which was recently proposed by Kucharski-Reineke-Stosic-

Sulkowski. The speaker outlined a proof of this correspondence for 2-bridge knots and then speculated about how much of the HOMFLY-PT skein theory might carry over to the realm of DT quiver invariants. This is joint work with Marko Stosic. For further details, see [19].

Tian Yang (•) (Texas A&M) spoke on *Volume conjectures for Reshetikhin-Turaev and Turaev-Viro invariants*. Supported by numerical evidence, Chen and the speaker conjectured that at the root of unity $e^{2\pi\sqrt{-1}/r}$, instead of the usually considered root $e^{\pi\sqrt{-1}/r}$, the Turaev-Viro and the Reshetikhin-Turaev invariants of a hyperbolic 3-manifold grow exponentially with growth rates respectively the hyperbolic and the complex volume of the manifold. This revealed a different asymptotic behavior of the relevant quantum invariants than that of Witten's invariants (that grow polynomially by the Asymptotic Expansion Conjecture), which may indicate a different geometric interpretation of those invariants than the $SU(2)$ Chern-Simons gauge theory. This talk introduced the conjecture and showed further supporting evidence, including recent joint work with Detcherry-Kalfagianni. For further details, see [8].

Outcome of the Meeting

The workshop was well-attended by researchers at different career levels and from a variety of countries: Canada, USA, Australia, China, Japan, Ireland, Switzerland, Israel, Germany, the Netherlands and France. After the workshop, we received extremely positive feedback, like

"Thank you for a wonderful workshop!"

or

"It was an excellent line-up of speakers."

Regarding the interdiscplinary nature of the workshop, one participant wrote,

"This was a wonderful workshop which brought together number theorists and knot theorists studying various forms of q-series. It was very helpful to get the other perspective on research and talk to many experts in both fields. These conversations gave me a good idea of what people in both areas are interested in and which directions I should extend my research."

The workshop also led to a number of new results, some of which were even announced before the end of the week! For example, it was generally expected that for every knot there exists a p such that for sufficiently large N, the first N coefficients of the N-colored Jones polynomial only depend on the class of N mod p. These stabilized coefficients are known as the "tail" of the colored Jones polynomial and much work has gone into studying such tails. During the workshop, Lee and van der Veen announced the surprising result that there is an infinite family of knots that does not have this property; instead the first few coefficients grow linearly in N. They proposed calling these knots Manx knots after a breed of tailless cats. The simplest known Manx knot is the pretzel knot $P(-3, 5, 5)$.

Other new results established during the workshop were reported by Detcherry, Kalfagianni, and Yang. They proved that at appropriate roots of unity, the Turaev-Viro invariants of an infinite family of links, including the "fundamental shadow links," grow exponentially with growth rate the hyperbolic volume of the link complement. This verifies the Volume Conjecture by Chen and Yang of the Turaev-Viro invariants for these links.

Finally, the workshop perfectly complemented recent activities such as the Workshop on "Low-dimensional topology and number theory" at the Mathematisches Forschungsinstitut Oberwolfach, August 20–26, 2017. We are very grateful for the opportunity to organize such a workshop and hope to continue its success with another 5-day workshop at Banff in 2020 or 2021.

Future Directions

The goal of this intense five-day workshop was to bring together international experts and young researchers in low-dimensional topology, number theory, string theory, quantum physics, algebraic geometry, conformal field theory, special functions and automorphic forms to discuss new developments and investigate potential directions for future research at the crossroads of modular forms and quantum knot invariants. A brief description of some future directions are as follows:

The Quantum Modularity and Volume conjectures: Quantum invariants of knots and 3-manifolds have been constructed rather combinatorially based on quantum groups, and their geometrical meanings are still unclear. The key is the Volume Conjecture, proposed by Kashaev and Murakami–Murakami, which states that, as $N \to \infty$, the N-th colored Jones polynomial $J_N(K;q)$ for a knot K at the N-th root of unity $q = e^{2\pi i/N}$ is dominated by the hyperbolic volume of the knot complement. The Volume Conjecture was proved for some knots such as the figure-eight knot and torus knots, but is still open for arbitrary K.

The relationship between quantum invariants and the hyperbolic volume motivated Zagier [21] to propose the notion of a "quantum modular form" as a function having nice properties at a root of unity. A typical example is the Kontsevich–Zagier series; it coincides, at a root of unity, with the Kashaev invariant for the trefoil, and furthermore can be written in terms of the Eichler integral of the Dedekind η-function. One goal would be to analyze the asymptotic behavior of the Kashaev invariants for hyperbolic knots and to clarify their quantum modularity. These are important problems from the viewpoint of quantum topology and modular forms.

Modularity of WRT invariants: A unified WRT invariant for integral homology spheres was recently proposed by Habiro. Interestingly, the computation of this unified WRT invariant for certain manifolds leads to new mock theta functions. For example, a result of Bringmann, Hikami and Lovejoy [3] says that a certain q-series $\phi(q)$ is a mock theta function and $\phi(-q^{1/2})$ is (up to an explicit factor) the unified WRT invariant of the Seifert manifold $\Sigma(2,3,8)$ which arises from $+2$ surgery on the trefoil knot.

One goal would be to study the unified WRT invariants of manifolds which arise from rational surgeries on other kinds of knots. These are typically quantum modular forms when viewed as functions at roots of unity, but when they converge inside the unit circle their behavior can vary. In some cases one obtains the usual indefinite binary theta functions related to mock theta functions, but in other cases one has less familiar expressions involving indefinite ternary quadratic forms or "partial" positive definite forms. An important task is to make the modularity properties of these unified WRT invariants explicit.

Stability: In 2006, Dasbach and Lin [6] observed stability in the coefficients of the colored Jones polynomial $J_N(K;q)$ for an alternating knot K. Precisely, they proved that the three leading coefficients of $J_N(K;q)$ are (up to a common sign) independent of N for $N \geq 3$. They then conjectured that for every N, the N leading coefficients of $J_N(K;q)$ are (up to sign) equal to the N leading coefficients of $J_{N+1}(K;q)$. This conjecture and its consequences have sparked a flurry of activity in both number theory and quantum topology. A few highlights are a resolution of this conjecture due to Armond [1] and (independently) Garoufalidis and Lê [9], the study of Rogers-Ramanujan type identities for "tails" of $J_N(K;q)$ from the perspectives of skein theory [12] and q-series [2], [16] and the study of potential stability of coefficients for generalizations of $J_N(K;q)$, namely for colored HOMFLY polynomials and colored superpolynomials.

Explicit methods for q-hypergeometric series: Quantum knot invariants are often expressible in terms of q-hypergeometric series, and explicit methods for these series are crucial. To give just two examples, the recent computation of the cyclotomic expansion of the colored Jones polynomial for the torus knots $(2, 2t+1)$ depended on key advances in the method of Bailey pairs [13], while the proofs of conjectures of Garoufalidis, Lê and Zagier on the tails of alternating knots [16] relied heavily on the Andrews-Bowman generalization of Sears' identity. Further development of these techniques is still needed, especially with a view toward applications to properties of knot invariants.

Participants

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Chapter 6

Physical, Geometrical and Analytical aspects of Mean Field Systems of Liouville type (18w5209)

April 2 - 6, 2018

Organizer(s): Daniele Castorina (University of Rome ÒTor VergataÓ), Changfeng Gui (University of Texas at San Antonio), Gabriella Tarantello (University of Rome ÒTor VergataÓ)

Overview of mean field systems of Liouville type

The study of mean field systems of Liouville type, in particular of the Chern–Simons vortices, has received a great interest in recent years, especially in the critical coupling of the self-dual regime, where the theory can be embedded into a supersymmetric field theory. In this way, a new and unexpected role of non-abelian vortices has emerged also in connection with the delicate issue of quark confinement, see [18, 21, 63].

In this workshop we have discussed some rigorous mathematical results concerning the existence of such vortex configurations and their asymptotic behaviour, as relevant physical parameters approach their limiting values.

To motivate the nature of the mathematical questions we need to address in the study of gauge field vortices, we start to discuss the "pure" abelian Chern–Simons model introduced by Jackiw–Weinberg [31] and Hong–Kim–Pac [29]. It provides a simple yet non-trivial theory, which captures the most interesting features about self-dual Chern–Simons (CS) vortices.

The model in [31] and [29] proposes a 2D theory governed only by the CS-electromagnetism which supports charged vortices (both electrically and magnetically). For this reason, such model is particularly appropriate to describe phenomena such as Superconductivity and the Quantum Hall effect [19].

In comparison, we recall that the more familiar Ginzburg–Landau theory can support only magnetically charged but electrically neutral vortices.

More precisely, the electromagnetic theory in [31, 29] is formulated within an abelian $U(1)$-gauge field theory in terms of the complex valued Higgs field ϕ and the electromagnetic potential: $\mathbf{A} = (A_0, A_1, A_2)$, which are weakly coupled through the covariant derivative:

$$D_\alpha \phi = \partial_\alpha \phi - \mathrm{i} A_\alpha \phi, \quad \alpha = 0, 1, 2.$$

As usual the value of the parameter $\alpha = 0$ refers to the time-variable, while $\alpha = 1, 2$ are used for the space variables.

The self-dual equations (formulated in the temporal gauge) for the Abelian CS- model with a 6th order potential [31, 29] are given as follows:

$$\begin{cases} D_1\phi \pm \mathrm{i}D_2\phi = 0 \\ F_{12} = \pm \dfrac{2}{\kappa^2}|\phi|^2(1-|\phi|^2) \end{cases} \tag{6.0.1}$$

supplemented by the following Gauss-law constraint governing the system:

$$\kappa F_{12} = \mathrm{i}(\overline{\phi}D_0\phi - \phi\overline{D_0\phi}), \tag{6.0.2}$$

with $\rho = \mathrm{i}(\overline{\phi}D_0\phi - \phi\overline{D_0\phi})$ the charge density, $\mathbf{F} = (F_{12}, -F_{02}, F_{01}) = \mathrm{curl}\mathbf{A}$ the electromagnetic field, $\kappa > 0$ the Chern–Simons coupling parameter.

In particular, $F_{12} = \partial_1 A_2 - \partial_2 A_1$ defines the (time-independent) magnetic field (a scalar in 2D), while ϕ is the (time independent) complex wave function.

To obtain a self-dual CS vortex, we need to provide a complex function $\phi : \mathbb{C} \to \mathbb{C}$ and real functions $A_\alpha : \mathbb{R}^2 \to \mathbb{R}, \quad \alpha = 0, 1, 2$; such that $(\phi; A_1, A_2)$ solves (6.0.1), while A_0 is determined by (6.0.1) and (6.0.2), so that (away from zero set of of ϕ) we have :

$$A_0 = \pm\frac{2}{\kappa^2}(1-|\phi|^2). \tag{6.0.3}$$

We can focus only to the vortex equation with "plus" sign, since the opposite sign is obtained simply by complex conjugation. In the self-dual regime, the following relation holds between the total energy E, the magnetic flux Φ and the electric charge Q :

$$E = \int F_{12}\mathrm{d}x = \Phi \quad \text{and} \quad Q = \kappa\Phi, \tag{6.0.4}$$

(see [29, 31] for details) so to ensure finite total energy and fluxes we need to supplement (6.0.1) with the condition:

$$\int F_{12}\mathrm{d}x < +\infty, \tag{6.0.5}$$

Although (6.0.1) provide a first-order reduction of the more involved second-order field equations, still they are analytically delicate to handle for their invariance with respect to the following gauge transformations:

$$\phi \to \mathrm{e}^{\mathrm{i}\omega\phi}, \quad A_\alpha \to A_\alpha + \partial_\alpha\omega, \quad \alpha = 0, 1, 2$$

$\omega : \mathbb{R}^2 \to \mathbb{R}$ a smooth (gauge) function.

Thus analytically, we are able to express explicitly the wave function ϕ only in terms of a (suitably) fixed gauge. An appropriate choice of gauge function was introduced by Taubes for the Maxwell–Higgs model (see [32]) based on the observation that the equation:

$$D_1\phi + \mathrm{i}D_2\phi = 0 \tag{6.0.6}$$

provides a gauge invariant version of the Cauchy–Riemann equation. Therefore, by the Poincaré $\overline{\partial}$ lemma, for a suitable choice of the gauge function η, we have that $\mathrm{e}^{\mathrm{i}\eta}\phi$ is holomorphic (see [32] for details). Hence, ϕ admits isolated zeros (vortex points), say at $\{p_1, \cdots, p_N\}$, with integral multiplicity ("quantized " local flux). The vortex points and their multiplicities are "observable" quantities, (i.e. gauge independent) together with F_{12} (magnetic field) and $|\phi|^2$ (density).

Hence, to obtain an analytical expression for solutions, we need to formulate problem (6.0.1) only in terms of such "observable" quantities. To this purpose, we express ϕ in polar (complex) coordinates, according to the following ansatz:

$$\phi(x) = \mathrm{e}^{\frac{u(x)}{2} + \mathrm{i}\left(\sum_{j=1}^{N} \mathrm{Arg}(x-p_j)\right)}. \tag{6.0.7}$$

So that,

$$|\phi|^2 = \mathrm{e}^u \quad \text{with} \quad u(x) = \ln|x-p_j|^{2n_j} + \mathrm{O}(1), \quad \text{as} \quad x \to p_j \tag{6.0.8}$$

(with n_j the multiplicity of $p_j,\ j \in \{1, \dots, N\}$), and by (6.0.1), we find that u must satisfy:

$$-\Delta u = \frac{4}{\kappa^2} \mathrm{e}^u (1 - \mathrm{e}^u) - 4\pi \sum_{j=1}^{N} \delta_{p_j}. \tag{6.0.9}$$

Conversely, from any solution u of (6.0.9) we can reconstruct a full vortex solution $(\phi, (A_\alpha)_{\alpha=0,1,2})$, with ϕ vanishing exactly at $p_1, \dots, p_N$, by means of (6.0.7) and (6.0.3).

Therefore, if we search for periodic CS vortices in the style of Abrikosov's mixed states [1] then it suffices to solve (6.0.9) over the torus, while to obtain planar vortices we need to to solve (6.0.9) over $\mathbb{R}^2$ supplemented by the appropriate boundary conditions that ensure the finite energy condition:

$$\int_{\mathbb{R}^2} \mathrm{e}^u (1 - \mathrm{e}^u) \mathrm{d}x < +\infty. \tag{6.0.10}$$

Based on physically consistent ansatz, a similar procedure can be adopted in the search of non-abelian CS vortices. In this way, we reduce their construction to the search of solutions of elliptic problems involving exponential nonlinearities in system form. More precisely, the corresponding system of PDE's governing self-dual non-abelian CS vortices takes the following form:

$$-\Delta u_i = \lambda_i \left(\sum_{j=1}^{n} K_{ji} \mathrm{e}^{u_j} - \sum_{j=1}^{n} \sum_{k=1}^{n} K_{kj} K_{ji} \mathrm{e}^{u_j} \mathrm{e}^{u_k} \right) - 4\pi \sum_{s=1}^{N_i} \delta_{p_{i,s}}(x), \quad i = 1, \dots, n, \tag{6.0.11}$$

with respect to the unknown functions $(u_1, \dots, u_n)$; where $\lambda_i > 0$, $\{p_{i,s}, s = 1, \dots, N_i\}$ are the vortex points of the ith-component with total multiplicity $N_i \in \mathbb{N}$, $i = 1, \dots, n$ and the coupling matrix:

$$K = (K_{ij})_{i,j=1,\dots,n}$$

is fixed by the gauge group G specified by the physical model under exam, since a unified theory including all fundamental particle interaction is not available yet. To give some examples, we recall that the abelian group $U(1)$ describe eletro-magnetic interactions, the gauge group $G = SU(2)$ allows for weak particle interactions, $G = SU(3)$ for strong particle interactions, and $G = U(1) \times SU(2)$ describe electroweak particle interactions. While we refer to [11, 24, 25, 26, 28, 27, 71] for more details, we mention that for the "pure" non-abelian CS model introduced by Dunne [17], the matrix K corresponds to the Cartan matrix of the group G. So for example, if $G = SU(n+1)$ then K is given by the following $n \times n$ matrix:

$$K = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & -1 & 2 & -1 \\ 0 & \dots & 0 & -1 & 2 \end{pmatrix} \tag{6.0.12}$$

related to the integrable Toda system, see [54, 26, 72]

Furthermore, if G is a semi-simple Lie group with rank 2, then besides $G = SU(3)$, we have the choices of a group G of the type $B_2 (= C_2)$ with corresponding 2×2 corresponding Cartan matrix:

$$K = \begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix} \tag{6.0.13}$$

or $G = G_2$ with Cartan matrix:

$$K = \begin{pmatrix} 2 & -1 \\ -3 & 2 \end{pmatrix}. \tag{6.0.14}$$

More recently, self-duality for Chern–Simons gauge field theories has been attained by exploiting the general framework of Supersymmetry. Under this point of view, several classes of new genuinely non-abelian vortices (or supersymmtric monopoles) have been identified, see [22, 23, 46] and references therein. For example the model in [46] unifies some of the previous models by proposing a theory over the gauge group $G = U(1) \times SU(N)$, $N \geq 2$, whose vortex configurations can be obtained by solving a 2×2 system of the type (6.0.11) with coupling matrix given as follows:

$$K = \frac{1}{N}\begin{pmatrix} N-1+\kappa & 1-\kappa \\ (N-1)(1-\kappa) & 1+(N-1)\kappa \end{pmatrix}, \tag{6.0.15}$$

where $\kappa = \frac{\kappa_1}{\kappa_2} > 0$, and κ_1 and κ_2 are the coupling parameters respectively of the $U(1)$-fields and $SU(N)$-fields, see [22, 23, 46] and [24, 11] for details.

Notice that, for $N = 2$ and $\kappa = 3$, then K in (6.0.15) coincides with the 2×2-Toda matrix in (6.0.12).

Another interesting example can be found in [52, 53]. There the authors propose an abelian truncation of the Aharony–Bergman–Jafferis–Maldacena (ABJM) model [2], for which it is possible to introduce a suitable vortex ansatz, and obtain a system of the type (6.0.11) with an off-diagonal 2×2 coupling matrix $K = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, (in normalized units). This model has been analyzed in [27].

Again, for the physical applications, it is relevant to consider solutions of the system (6.0.11) over a compact surface (e.g. the flat 2-torus) or over $\mathbb{R}^2$ supplemented by suitable integrability conditions of type (6.0.10), which guarantee finite energy and fluxes.

As discussed during the workshop the analysis of the governing CS-vortex equations (6.0.9) and (6.0.11) (also referred to as the Master equations), touch upon many analytical issues concerning singular Mean Field equations of Liouville-type, see e.g. [66, 67], surfaces with conical singularities, see e.g. [69], sharp Moser–Trudinger or log(HLS)-inequalities, see e.g. [61, 62, 70], bubbling phenomena, see e.g. [5, 13, 14] etc.

In this respect, we have learnt that, while for the single equation (6.0.9) the understanding of the (abelian) vortex-equation is rather satisfactory, in the system case the results available are only partial, as pointed out by the talks of L. Battaglia, Z. Nie and A. Poliakovsky.

To be more specific, for simplicity we shall focus on 2×2 systems and assume (as in the physical applications) that in (6.0.11) the 2×2 coupling matrix $K = (K_{ij})_{i,j=1,2}$ satisfies:

$$\det K \neq 0 \quad \text{and} \quad K_{ii} > 0, \quad i = 1, 2. \tag{6.0.16}$$

Furthermore, via the transformation: $u_i \to u_i + \ln(K_{ii})$, and by setting:

$$\tau_i = \frac{K_{ji}}{K_{jj}} \quad i \neq j \in \{1, 2\}, \tag{6.0.17}$$

we arrive at the following normalized expression of (6.0.11):

$$\begin{cases} -\Delta u_1 = \lambda_1 \left(\mathrm{e}^{u_1} + \tau_1 \mathrm{e}^{u_2} - \mathrm{e}^{2u_1} - \tau_1 \mathrm{e}^{2u_2} - \tau_1(1+\tau_2)\mathrm{e}^{u_1+u_2}\right) - 4\pi \sum_{j=1}^{N_1} \delta_{p_{1,j}} \\ -\Delta u_2 = \lambda_2 \left(\mathrm{e}^{u_2} + \tau_2 \mathrm{e}^{u_1} - \mathrm{e}^{2u_2} - \tau_2 \mathrm{e}^{2u_1} - \tau_2(1+\tau_1)\mathrm{e}^{u_1+u_2}\right) - 4\pi \sum_{j=1}^{N_2} \delta_{p_{2,j}} \end{cases} \tag{6.0.18}$$

with $\lambda_i > 0$, $i = 1, 2$.

As in the abelian case, in the search of planar non-abelian vortices, we need to solve (6.0.18) over $\mathbb{R}^2$, under appropriate boundary conditions which guarantee the integrability of the right hand side of the equations in (6.0.18), in order to ensure finite energy for the corresponding vortex.

Therefore, we recognize the topological boundary condition to be given as follows:

$$u_i(x) \to \ln\left(\frac{1-\tau_i}{1-\tau_1\tau_2}\right) \quad \text{as} \quad |x| \to +\infty, \quad i = 1, 2; \tag{6.0.19}$$

whenever the right hand side of (6.0.19) is well defined. Indeed, we easily check that (6.0.19) is always well defined for the physical examples (6.0.12)–(6.0.15).

The existence of such class of solutions has been established under rather general assumptions for the coupling matrix K, which cover all the interesting physical models. We refer to [11, 24, 25, 26, 71] for more details about non-abelian topological vortices and their "quantization" property.

On the contrary, much less is understood about the presence of "non-topological vortices" satisfying:

$$u_i(x) \to -\infty \quad \text{as} \quad |x| \to +\infty, \quad i = 1, 2, \tag{6.0.20}$$

Also it is of interest the existence of the so-called "mixed" vortices where the topological and non-topological boundary conditions are each satisfied by either one of the two components available. Unfortunately, mixed vortices have been constructed only in some special situation, see [54, 20], and are difficult to grasp also in the radial case, see [30]; so that much of their study remains open to future investigation.

Concerning the construction of non-topological vortices, we mention a "perturbation" approach where we introduce the following scaled version of the solutions:

$$u_{i,\varepsilon}(x) = u_i\left(\frac{\sqrt{\lambda}x}{\varepsilon}\right) + 2\ln\frac{1}{\varepsilon}, \quad \varepsilon > 0 \tag{6.0.21}$$

so that planar solutions of (6.0.18) satisfying:

$$\int_{\mathbb{R}^2} \mathrm{e}^{u_i}\mathrm{d}x < +\infty, \quad i = 1, 2 \tag{6.0.22}$$

can be sought (for $\varepsilon \to 0$) as "bifurcating" from solutions of the following system of Liouville type:

$$\begin{cases} -\Delta u_1 = \mathrm{e}^{u_1} + \tau_1 \mathrm{e}^{u_2} - 4\pi N_1 \delta_0 & \text{in} \quad \mathbb{R}^2 \\ -\Delta u_2 = \mathrm{e}^{u_2} + \tau_2 \mathrm{e}^{u_1} - 4\pi N_2 \delta_0 & \text{in} \quad \mathbb{R}^2 \\ \displaystyle\int_{\mathbb{R}^2} \mathrm{e}^{u_i}\mathrm{d}x < +\infty, \quad i = 1, 2. \end{cases} \tag{6.0.23}$$

Unlike the single-(singular) Liouville equation, (corresponding to the decoupled case: $\tau_1 = \tau_2 = 0$), in general the solvability of (6.0.23) is far from understood, except for the integrable and fully conformal case of the Toda-system (6.0.12), which according to our normalization corresponds to the case where, $\tau_1 = \tau_2 = -\frac{1}{2}$. In fact, for (6.0.23), a full characterization of solutions (analogous to single Liouville equation [60]) has been obtained by Lin–Wei–Ye in [40], which extends and completes the previous characterization result of Jost–Wang [36] concerning the "regular" case, where $N_1 = N_2 = 0$.

In particular from [40] and [31] we know that all solutions of (6.0.23) with $\tau_1 = \tau_2 = -\frac{1}{2}$ satisfy:

$$\frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{e}^{u_1}\mathrm{d}x = \frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{e}^{u_2}\mathrm{d}x = 4(N_1 + N_2 + 2). \tag{6.0.24}$$

Furthermore, the explicit expression of the solutions of (6.0.23) as provided in [40, 31] together with their non-degeneracy properties (see [40]) have been exploited by Ao–Lin–Wei in [3] to carry out a "perturbation" approach in the same spirit of Chae–Imanuvilov [9] . In this way the authors in [3] obtained a class of non-topological solutions for the $SU(3)$-model [17]. Such construction was extended by the same authors in [4] for the gauge group G of the type B_2 and G_2. Moreover, we mention the recent work of Lin–Nie–Wei [38] which uses more algebraic tools to fully characterize solutions and their total integrals, for any $n \times n$ Liouville system of the type (6.0.23) with coupling matrix corresponding to a Cartan matrix.

However, in view of the physical applications, we need to treat with the same accuracy, also the case where the coupling matrix admits a structure other than a Cartan matrix, as for example (6.0.15). In particular, for the normalized system (6.0.23), we need to identify the sharp range of admissible pairs (β_1, β_2) such that problem (6.0.23) with $(\tau_1, \tau_2) \neq (-\frac{1}{2}, -\frac{1}{2})$ admits a solution satisfying:

$$\beta_i = \frac{1}{2\pi}\int_{\mathbb{R}^2} \mathrm{e}^{u_i}\mathrm{d}x, \quad i = 1, 2. \tag{6.0.25}$$

This task was carried out by Poliakovsky-Tarantello [59] with respect to the radial solvability of (6.0.23)–(6.0.25), see also [57, 58, 10, 15, 61, 62] for related results. Notice that, as in the analysis of the single Liouville equations, [60, 12], we expect the radial problem to furnish a full description about the pairs (β_1, β_2) admissible for the solvability of (6.0.23), (6.0.25), in the sense that, non-radial solutions can only occur as "bifurcation" from radial ones while keeping the same integral pair (β_1, β_2).

In addition the role of (6.0.23) and (6.0.25) is relevant also in the analysis of the "bubbling" phenomenon in the context of systems, which is a very delicate task (see [55, 41, 44, 43, 45, 34]) but crucial to obtain solutions via topological, variational and perturbative methods, as e.g. [8, 14, 33, 7, 49, 50, 51].

Even more involved is the blow-up analysis when the different components blow-up at the same point but with a different rate. Here a new phenomenon occurs, namely the possibility of blow-up without an associated "concentration" phenomenon and a "quantization" property, as recently shown in [39]. Similar blow-up phenomena with "residual mass" (in the terminology of [56]) have been shown to occur when different vortex points collapse into each other (see to [39, 37] for details), a situation of great interest from the physical point of view.

All such new, interesting and delicate aspects have been discussed during the meeting and we expect to see some further developments and progress in the near future as an outcome of the workshop.

Scientific activities of the workshop

The workshop has brought together a group of expert mathematicians as well as junior researchers studying different aspects of Mean Field Equations of Liouville type, as they arise from physical and geometrical problems. The topics discussed during the workshop have concerned the analysis of self-dual gauge field vortices, including the Abrikosov's configurations for the celebrated Electroweak theory of Glashow-Salam-Weinberg, and the "uniformization" problem in differential geometry for Riemann surfaces with conical singularities and various other generalizations concerning the assigned (also sign-changing) Gauss curvature problem.

A first successful outcome of the workshop was stimulated by the new "sphere covering inequality " of C. Gui and A. Moradifam and its application towards uniqueness results. Already, other applications of Gui- Moradifam's sharp inequality were presented during the workshop by D. Bartolucci and A. Jevnikar in the setting of the Riemann sphere with conical singularities. But during the discussionÕs section many of the participants have remarked about the strength of such inequality and have proposed several other applications, in the form of future projects and collaborations. For example, the "Sphere covering inequality" seems flexible enough to yield new non-existence results in the supercritical and in the non-radial setting, in the presence of more than three conical singularities.

Another important problem discussed during the workshop has concerned traveling waves of the Gross-Pitaevskii equation, for which ground state solutions have been already established. The results presented by J. Wei show the asymptotic behaviour of a new class of solutions for small values of the velocity. This however leaves open the existence of excited state for fixed values of the velocity. During the workshop D. Ruiz and J. Wei discussed about a possible approach to handle such problem, and on this basis formulated a future project in collaboration.

The recent developments about the spectral gap conjecture, as reported in D. Hauer's talk got also a lot of attention. For example, it was observed by D. Bartolucci that in order to describe the global bifurcation diagram for solutions of mean field equations, so far it has been possible under a spectral gap assumption about entropy maximizers. It was suggested that (by further investigation) HauerÕs result may be helpful in the understanding of the above mentioned bifurcation diagram. Furthermore, J. Dolbeault and D. Hauer have been discussing an issue related with stability in functional inequalities, based on hyper-contractivity. For the fast diffusion equation in the subcritical range, one can get explicit rates of regularization. A more or less explicit control of the relative uniform norm in terms of the initial data has recently been obtained by M. Bonforte and N. Simonov (arXiv:1804.03537v1). Then using the improved spectral gap and an improved entropy (i.e. entropy production inequality), one should be in position to get an explicit stability result for the Gagliardo-Nirenberg inequality. In the subcritical case, this is a project of M. Bonforte, J. Dolbeault, B. Nazaret and N. Simonov. The major issue is the critical case (Sobolev inequality). Techniques based on hyper-contractivity (using the framework of the book of T. Coulhon and D. Hauer, in preparation) could provide at least a partial answer.

Finally, another important topic widely discussed during the meeting concerned systems of Liouville type, which arise in the construction of non-abelian vortices. Indeed, the most natural extension of the Mean Field

Equations into a system form is given by the Toda-system, whose solutions describe the asymptotic profile of non-abelian vortices for the $SU(n+1)$-Chern-Simons model. More generally in this context mean field equations of Liouville type are coupled together via the Cartan matrix associated to the gauge group. After the talks of L. Battaglia, Z. Nie and A. Poliakovsky we have seen that many interesting questions still need to be answered. Especially concerning the blow-up analysis for systems we still need a complete classification of solutions for the ”limiting” problem in the plane (describing the blow-up profile) away from the conformal case.

According to D. Hauer, who recently started a new collaboration on Mean Field Systems with C. Gui, this workshop provided many backgrounds, geometrical and mathematical motivations and new knowledge about this topic, and helped to push forward his current research project. All the participants have remarked that: the workshop was very central to their research interest about a field in great development in recent years, with exciting novelties in unexpected directions. There were people from different backgrounds so that fruitful exchanges of ideas were encouraged. The intellectual environment during the workshop was notably vibrant.

The discussions during question sessions were remarkably interesting, and served as further motivation to encourage and enhance the participantsÕ interactions. Also they took a great advantage of the breaks to actively interact clarifying doubts and intellectual curiosities raised by the talks.The BIRS center offered a very warm and cozy atmosphere, (despite the unusual winter temperatures of -10 to -15 centi-grades). To have a scientific workshop in an environment of arts, dance and drama certainly provided an inspiring atmosphere and contributed to the success of the meeting.

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Chapter 7

Entropies, the Geometry of Nonlinear Flows, and their Applications (18w5069)

April 8 - 13, 2018

Organizer(s): Eric A. Carlen (Rutgers), José A. Carrillo (Imperial College), Jean Dolbeault (Paris-Dauphine), Daniel Matthes (TU München), Dejan Slepčev (Carnegie Mellon)

A Brief Introduction to the Field

Many natural processes involving the interaction of a very large number of particles, such as conduction of heat, fluid flows and chemical reactions, possess an entropy, a quantity that increases during the evolution. A powerful strategy for quantitatively understanding the properties of such systems is to establish mathematical relations between entropies and other quantities characterizing the state of the system. The investigation of these relations has been extremely successful in explaining and predicting the properties of the dynamics of such large and complicated systems. In order to draw the precise conclusions it is important to establish the optimal relations between relevant quantities.

There is also an important geometric aspect to the evolutions of such systems. Mathematically, many nonlinear evolution equations can be interpreted as gradient flows of entropy/energy functionals, i.e., steepest ascent (or descent) over the entropy/energy landscape with respect to an appropriate notion of distance. This interpretation is useful not only to understand the abstract geometric framework of the nonlinear equations, but also to deal, for instance, with particle approximations and handle mass conservative models in connection with mass transport theory.

A large scientific community has been involved in this area since the first meeting held in Banff in 2006. This meeting played an important role in the development of the topic, and entropy methods have now reached a certain maturity through the geometric interpretation of nonlinear flows. The area is now more vibrant than ever involving a growing network of interactions between branches of mathematics, physics, biology and social sciences. This meeting has been intended to consolidate this progress and set the stage for new advances.

Recent Developments and Open Problems

State of the Art

Entropy estimates for nonlinear evolution equations have proved to be the basis of extremely successful methods for the investigation of many quantitative issues such as rates of convergence and sharp constants in functional inequalities. These methods are well-suited to marry with multi-scale analysis and useful to understand physical systems that are described by systems of evolution equations on different scales, for instance a rarefied gas on the microscopic individual particle scale, the mesoscopic kinetic many-particle scale and the continuum scale of hydrodynamics. The existence of entropies at all these levels is a crucial property underpinning the physical/biological derivation of systems of equations, allowing for the understanding of qualitative properties as diverse as stability of steady states, asymptotic behavior and convergence of numerical schemes.

A major break-through in the theory was the observation that many nonlinear evolution equations constitute gradient flows of entropy functionals with respect to the Wasserstein or related transport metrics. Understanding the connection between nonlinear flows and the geometry of optimal transportation has paved the road towards a broad variety of profound results on large-time asymptotics of diffusion, towards novel proofs of sharp functional inequalities, and towards structure preserving discretizations of evolution equations and manifolds, just to name a few. Generalizing the ideas of optimal mass transport to coupled systems of evolution equations is not straightforward at all. Finding sharp conditions under which, e.g., a given reaction-diffusion system has a good entropy or gradient flow structure is still an open problem, although some recent advances have been done.

Another very novel direction is the application to the "discrete world". There has been a surge of activity around using entropy like ideas in Markov chains considered by themselves or as numerical schemes for some of the standard Fokker-Planck equations related to linear/nonlinear diffusion equations, as well as the extension of these methods to the quantum setting. Understanding the different notions of steepest descent in these methods, their interconnections and their potential in other applications such as clustering in machine-learning applications is another topic of current interest.

Another important theme to emerge from the work discussed at the previous meetings is the role of stability theorems for sharp functional inequalities in the study of nonlinear evolution equations. The use of nonlinear flows for proving functional inequalities has developed into a powerful method for establishing new remainder terms for classical inequalities – which have then been applied to study other nonlinear laws. It will certainly be fruitful to continue this development in the context of further problems arising in mathematical biology and physics. Interesting variational arguments involving the use of entropies have been proposed in order to show symmetry of optimizers in the Caffarelli-Kohn-Nirenberg inequalities or in stationary states of nonlinear diffusion variants of the Keller-Segel system. Finding an analytical framework to attack the symmetry breaking in some problems of this type would be an excellent tool in various problems such as questions related to interaction potential functionals.

The extension of gradient flow methods into the domain of non-convex functionals has been another source of recent progresses. Non-convex functionals appear naturally in many physical/biological problems related to phase transitions. These free energies have several stationary states and finding good mathematical approaches to understand the basin of attraction for these cases is an interesting topic. Isotropy or not in the long-time asymptotics is observed or not depending on the presence and intensity of noise/diffusion. This has been realized only in few cases in one spatial dimension, and therefore its generalization to more physical dimensions would be a large push to the theory. Hypocoercivity tools might be a good track for this question.

Nonlocal diffusion equations have been so far elusive to the use of entropy methods except when the interaction potential is defined as the inverse nonlocal Laplacian of the density or in one dimensional settings. In these cases the connection to obstacle problems recently found is an excellent tool bridging to the world of nonlocal elliptic equations. The potential use of these ideas for nonlocal versions of nonlinear diffusion equations is to be explored.

And finally, since these entropy methods are now used not only as tools to solve problems of pure functional analysis but also as techniques in various applied and even computational areas, it was important to bring together a group of researchers who can profitably interact, but who might not meet at other meetings.

Topics of Current Interest

Here are some emerging topics in entropy methods in PDEs and the study of their associated flows which will probably play an important role in the development of the field in the near future:

- Reaction-Diffusion equations & systems as gradient flows.
- Advances on gradient flows of non-geodesically convex functionals.
- Symmetries of critical points which are not necessarily global minimizers of entropies.
- Stability inequalities for remainder terms involving entropies and rates of decay.
- Hypocoercivity & multiplicity of stationary states.
- Discrete Entropies: Markov chains & clustering in machine learning.
- Non-equilibrium steady states.
- Non-locality and non-isotropy in diffusions and mean-field interactions.

Identification of Relevant Topics for the Workshop

The workshop has been in part intended as a follow-up to the workshops "Nonlinear diffusions: entropies, asymptotic behavior and applications", "Nonlinear Diffusions and Entropy Dissipation: From Geometry to Biology" and "Entropy Methods, PDEs, Functional Inequalities, and Applications", held at BIRS in April 2006, in May 2010 and in June 2014, respectively. Ideas emanating from stimulating exchanges at these events have led to important advances in optimality issues in the theory of functional inequalities, in problems of mathematical biology and geometric flows, with seemingly far-apart applications such as quantum Markov semigroups and collective behavior models. All in all there is an outstanding track record of this series of workshops as effective catalyzers for far-reaching consequences outside the comfort zone of mathematical applications of these tools. The organizers took care to bring together different researchers of the "core communities" involved: PDE analysts, differential geometers and probabilists; and potential users of these techniques in pure and applied mathematics.

The organizers had given the participants complete freedom in the choice of topic they want to present, as long as it fits with the general scope of the conference. The portfolio of proposed talks is therefore a good indicator for general directions and specific problems that are currently topical in the various branches of the community. In comparison to the previous edition of this workshop in 2014, there was a stronger focus on the further development of various aspects of the theory, while the adaptation of existing theory to study specific PDEs played a less prominent role. The new theoretical developments that have been presented were rich and profound.

Already in the past, we could observe that gradient flow dynamics on metric spaces, specifically flows in the Wasserstein distance, played a role of continuously increasing significance. The current event has been no exception to that trend: two morning sessions have been devoted exclusively to applications of optimal transport in the context of entropy methods, and many further talks featured Wasserstein gradient flows as an essential element. A recurrent theme in that context was that of mean field games, a class of equations and models with surprising, but yet not fully understood relations to smoothed optimal transport.

For the more classical aspects of the theory, the organizers could observe a shift of interest from fully dissipating to hypocoercive systems. The first general characteristic of the latter is that there is a part of phase space in which entropy is dissipated at exponential rates, while in other parts, the flow is almost entropy conserving. However, the second key feature of hypocoercivity is the existence of a global, possibly slow dynamics that forces any solution to pass through the rapidly dissipating region at a quantifiable frequency, and thus leads to a continuous decay of the entropy in the end.

Presentation Highlights

The organizers were extremely pleased both with the wide range of topics that had been proposed by the participants and the quality of each individual presentation. The speakers took great care to make their results understandable to the audience.

Nonlinear diffusion

Nonlinear diffusion equations of the form $\partial_t u = \Delta u^m$ constitute one of the classical playgrounds for the entropy method, and possibly the field where the method had its most significant achievements in the past twenty years. The field is still remarkably lively.

One of the highlights of the conference was the impressive talk by **Esteban** in which she gave a precise characterization of the symmetry breaking in the Caffarelli-Kohn-Nirenberg inequality [28]. It has been relatively easy to conjecture the line of transition between radial symmetry and non-symmetry of minimizers by a linear stability analysis of the Euler-Lagrange equations and then to identify a region where symmetry breaking must occur. On the contrary, the rigorous proof for radial symmetry in the complement of that region is highly demanding both on the conceptual and the technical level. The application of entropy method to nonlinear diffusion equations on particular manifolds plays a key role in the proof.

Figalli gave the first results ever on qualitative properties of the equation $\partial_t u + (-\Delta)^s\, u^m = 0$ on a bounded domain involving the fractional Laplacian, in the porous medium case $m > 1$. One of the first difficulties lies in the appropriate definition of the fractional Laplacian in that context. Three alternative definitions were given, and for two of them, uniform relative convergence to a self-similar profile could be proven. The key key tool is a comparison principle. These results are explained in the works [5, 4].

Not far from that is the singular diffusion equation considered by **Iacobelli**, which is of the form $\partial_t u = -(u^p(u/u_\infty)_x)_x$, where the target density u_∞ is given, and p is a negative power. Under positivity conditions on u_∞ and the initial datum, it has been shown that solutions converge exponentially fast to u_∞. As before, the key element of the proof is a comparison principle. The main objective of her talk was to apply these ideas to the quantization of measures problem [7, 36].

The very general class of coupled systems of reaction-diffusion equations presented by **Fellner** bears a problem that is similar to hypocoercivity. He applies the entropy method to the sum of the physical entropies of the individual components and uses it as Lyapunov functional. There is no uniform exponential rate of decay for that quantity: the dissipation vanishes if one of the components is depleted, and becomes arbitrarily slow close to such solutions.

Nonlinear aggregation/diffusion

More recent than the studies of pure nonlinear diffusion is the combination of diffusion with binary particle interactions moderated by a (typically singular) interaction kernel K. This leads aggregation-diffusion equations of the type $\partial_t u = \Delta u^m + \nabla \cdot (u \nabla K * u)$. Several speakers presented novel results on the long time asymptotics of solutions. Their general line of approach was to exploit the equation's gradient flow structure in the Wasserstein distance.

Craig introduced a method to approximate optimizers for the generalizations of Poincaré 's problem, that is, one wants to find a set of given measure on which the integral of a given kernel K is minimized. By means of Γ-convergence, she could show that the associated aggregation-diffusion equation with exponent $m > 1$ converges as $m \to \infty$ to a flow on the space of functions with $0 \leq u \leq 1$, and that it approximates in the long time limit a solution to a relaxation of the Poincaré problem. The results are related to several recent works [24, 22, 23, 13] and a work in preparation with Topaloglu.

Yao considered a model for the reproduction of coral, which leads to a aggregation-diffusion equation with an additional harvesting term. The main question, namely if the combination of diffusion and interaction leads to a faster rate of convergence to the trivial equilibrium than diffusion alone, boils down to understanding the long time asymptotics in a linear Fokker-Planck equation with an attractive, but slowly growing potential. The general answer to the question is quite subtle, as she demonstrated on a particular example where the interactions even leads to a slow-down. The results are based on a work in preparation.

Volzone gave an overview over new conditions for existence, uniqueness and radial symmetry of the stationary solutions to the Keller-Segel equation in the diffusion dominated regime, i.e., $m > 2 - 1/n$. The dynamical stability of these states was also discussed. He showed an impressive result of radial symmetry of stationary states in the degenerate case that leads to uniqueness of steady states in the Newtonian kernel in two dimensions [12, 16, 17]. A result sought for a long time. Convergence results were obtained without rate of convergence in the two dimensional Keller-Segel model with nonlinear diffusion $m > 1$.

The first goal of **Patacchini**'s presentation was essentially opposite: for a general class of aggregation/diffusion equations, he derived conditions for the non-existence of stationary solutions. He also derived conditions in order to have ground states which are sharp for the case of linear diffusion [14].

Schlichting talked about phase transitions in McKean-Vlasov equations (aggregation equation with diffusion) with periodic boundary conditions. Together with Carrillo, Gvalani and Pavliotis in [15], he has shown that in the H-stable regime the relative entropy to the minimizer is decaying exponentially fast, while for H-unstable systems the asymptotic dynamics can be substantially richer. In particular they consider the bifurcation of nontrivial steady states as the parameter controlling the strength of the nonlocal term (aggregation) increases. Continous and discontinuous phase transtions can exist depending on assumptions on the Fourier coefficients of the interaction potential.

Linear kinetic equations

Several talks have been devoted to novel estimates on the rate of equilibration in linear BGK models, or even more general linear kinetic equations. The main difficulty that was present in each talk was the hypocoercive nature of the dynamics, which is highly entropy dissipative but only with respect to the velocity variable. To measure global convergence rates, one has to understand how the transport operator transfers the relaxation to the spatial variable.

Arnold started by showing a seemingly easy way to prove exponential decay of a suitable norm for general linear systems $\dot{x} = Cx$, where the matrix C is positive definite but not symmetric. The applicability of his strategy to linear BGK equations, however, requires to a find a suitable adapted norm, with a choice that is independent of the Fourier mode under consideration, and this is a challenging task, that could only be undertaken by sophisticated trial and error so far. Beyond the systematic method he developed with his collaborators, a significant achievement compared to standard approaches based on hypo-elliptic methods is that norms can be explicitly constructed and rates are optimal. The results presented were based on [1, 2]. **Evans** in [32] was also using a relatively algebraic approach, but took a different angle of attack: she studied the dissipation of Φ-entropies and related functional inequalities. Φ-entropies are a natural interpolation between the logarithmic Boltzmann entropy functional and the quadratic norms considered by Arnold.

A different approach to linear BGK models has been presented by **Canizo**. His ideas originated from Harris' ergodic theorem, which states that if a markovian semi-group admits a uniform lower bound after a transition time $t_0 > 0$, then solutions converge exponentially fast in total variation. Canizo showed how to massage the technique to be applicable to BGK equations, using geometric and probabilistic arguments. In contrast to the aforementioned speakers, **Guillin** did not study the BGK approximation, but a more general linear kinetic equation with diffusion in the velocity variable and a non-quadratic external potential, see [**?**]. Previous approaches like those by Villani were relying on log-Sobolev inequalities and thus induced demanding convexity assumptions on the potential. Guillin showed a strategy how to make the proof work under essentially weaker hypotheses.

Kac master equation

In two related talks, **Carvalho** and **Loss** discussed new results on the old problem of propagation of chaos in the Boltzmann equation [8]. Specifically, they were looking at the Kac walk on the sphere and gave novel estimates on the rate of convergence to equilibrium. For the Kac equation (for infinitely many particles), Cercignani's conjecture states that the entropy production $D(f)$ dominates the entropy $H(f)$ in a linear way, yielding exponential convergence to the steady state. It was shown by Villani that this conjecture is wrong in general, but one can at least expect $D(f) \geq c_\varepsilon H(f)^{1+\varepsilon}$ for every $\varepsilon > 0$. Carvalho showed that a similar inequality is still true for the

Kac walk, with a c_ε independent of the number of particles. Her proof, however, uses a strong assumption on the disorder of the distribution, for which propagation along solutions is unclear. Loss instead verifies the linear dependence $D(f) \geq cH(f)$ originally conjectured by Cercignani, however for a variant of the Kac model, where the particles are coupled to a huge (but still finite) heat bath, and in a regime which is away from equilibrium.

Entropy methods on discrete structures

One of the goals of the entropy method is to provide guidelines for the definition of structure preserving discretizations. Currently, the main interest is to build a consistent discrete theory that reproduces key elements of the original continuous one, but many of the concepts that have been developed so far are directly applicable in the design of numerical methods that preserve features like entropy dissipation.

One of the forerunners in the field of discretizing the theory of optimal transport is **Maas**. He had already developed a successful strategy to define analogues of the Wasserstein metric, associated gradient flows, and curvature properties on graphs [31, 30, 35]. In his presentation, he showed a surprising limitation of his concepts for the passage the continuum limit: in general, one cannot expect Gromov-Hausdorff convergence of his transport distance on the dual graph of a finite-element decomposition of a domain unless rather restrictive geometric conditions are met. A remarkable fact is that the associated heat equation converges under much more general hypotheses. On the basis of Maas' discretized transport distance, **Erbar** has developed a notion of super-Ricci flow on graphs. The main quantities of interest are lengths associated to the edges of the graph, and these change according to an evolution inequality. Moreover, at certain instances of time, the graph itself changes as well, when either an edge collapses because its length becomes zero, or a new edge is born out of a point. Erbar justifies his ansatz by proving discrete analogues of various equivalent characterizations of the continuous super-Ricci flow, like estimates on the heat kernel or the modulus of convexity of the entropy, see [29].

A complementary approach was taken in the discretization of a model for traffic flow considered by **Di Francesco**, who did not use a graph structure but instead a moving mesh, define by the Lagrangian map. The underlying evolution equation is of aggregation type, but with a nonlinear mobility function that saturates, corresponding to a maximal admissible density of cars on the road. Albeit the PDE has been introduced in arbitrary dimensions, the traffic flow model is naturally one-dimensional, and that is where most of the analysis has been carried out. The main result is the convergence of the discrete solutions to an entropy solution, in total variation, see [27]. Finally, **Plazotta** discussed a spatially continuous but time discrete approximation to Wasserstein gradient flows. The scheme, which is formally of second order in time, mimicks the JKO method, but the variational functional contains the difference of two distances (instead of one distance). He has shown that discrete solutions converge strongly in L^p to a weak solution in the continuous limit [38]. However, second order convergence could not be verified due to the roughness of the Wasserstein space.

Derivation of models

Principles like monotonicity of the entropy have always been of great importance in the derivation of PDEs for models in physics, and — more recently and possibly surprisingly — biology. This was illustrated in the talks of Degond, Filbet and Raoul, all of which studied micro-to-macro-limits of biological models.

Degond considered swelling materials (like gels and tumors) and explained why Darcy's law alone is not sufficient to derive a closed system of evolution equations [26]. He henceforth proposes as an alternative first principle simple rules on the microscopic scale: essentially maximal packing density and minimal motion. These indeed lead to a consistent macroscopic model. **Filbet** started from an spatially extended version of the FitzHugh-Nagumo model, with forced local interactions. The resulting equation is of kinetic type. The dynamics of appropriate "macroscopic" quantities, i.e., suitable moments of the kinetic solution, converges to the classical non-local reaction-diffusion model in the hydrodynamic limit, see [25]. For **Raoul**, who considered a model for sexual reproduction, the initial equation was of collisional Boltzmann type, and his goal was to obtain the macroscopic Kirkpatrick-Barton model from population genetics, which is of reaction-diffusion system, as a limit in suitable parameter ranges. The key tool in his derivation were Tanaka-like contraction estimates in the Wasserstein distance. The derivation of such models is of crucial importance for the understanding of ecological problems like the ones induced by climate change, see [39].

A very different set of problems was considered by **Kinderlehrer**. He studied structure of grain-boundary networks in polycrystaline materials, as well as their evolution. He discussed the observation that during the evolution the grain boundary network quickly achieves a stable distribution of grain boundaries with the average length of boundaries of a certain energy characteristics. This distribution is known as the grain boundary character. The talk focused on ode-based models to explain and predict the grain boundary character distribution. The models were derived following ideas of entropy and gradient flows in appropriate metrics. At this point it is worth to be mentioned that Kinderlehrer's ideas have been extraordinarily influential in the mathematical community targeted by the workshop and once more he has challenged the participants by proposing a new area of investigation in [3].

Optimal transportation

Optimal transport has played a key role in understanding nonlinear flows. Primarily by being the metric on the space of configurations with respect to which many nonlinear flows are gradient flows of an appropriate free energy. Studying the geometry of optimal transportation, its properties and role in functional inequalities has led to remarkable progress. Several speakers have focused on new variants of optimal transportation and their connections to dissipative systems.

Carlier gave a talk on entropy regularized optimal transport and connections to mean-field games. Entropic regularization of optimal transport was independently introduced by Galichon and Cuturi. In particular the associated Sinkhorn numerical algorithm by Cuturi has become one of the most popular approaches to computational optimal transport. Optimal transport is recovered as the regularization parameter $\varepsilon \to 0$. In contrast, Carlier focused on fixed entropic regularization, $\varepsilon = 1$, and developed the connections with variational descriptions of mean-field games. In particular he discussed the connections between mean-filed games of Lasry and Lions [37] with the dynamic description of the entropy regularized optimal transport studied by Chen, Georgiu, and Pavon, [19], and by Gentil, Léonard, and Ripani. [33]. Carlier also introduces the time discretized dynamical version as a new and useful tool.

Savaré spoke about dynamic formulation for the entropic regularization of the optimal transportation and connections to mean-field games. In particular he studied the dual formulation of the dynamic description of optimal transportation, due to Benamou and Brenier. The dual formulation leads to a Hamilton-Jacobi equation and connections to mean-field games. Savaré carefully discussed the notions of solutions, hence building the setup that would allow to study the limit of viscous regularizations of the equations and consequently the limits of the entropic regularizations of optimal transport.

Ghoussoub gave a presentation on the Theory of Transfers that he recently introduced with Bowles [6]. Namely using notions of convex duality they introduced the notion of (forward and backward) linear transfer which encompasses all of the classical optimal transportation, martingale optimal transport, entropy regularized optimal transport (Schrödinger bridges), as well as weak mass transports. For the classical optimal transport the notion is closely related to the dual formulation of Kantorovich. Ghoussoub also introduced the notion of convex transfers with particular focus on its subset of entropic transfers. In particular he showed that Donsker-Varadhan entropy can be described as an entropic transfer.

Palmer talked about a generalization of the dynamic description of optimal transportation where the end time when a mass reaches its destination is not fixed but can vary over the mass being transferred. Furthermore he considered general Lagrangian terms in the dynamical description and introduced density processes to be able to present an eulerian description of the problem. Using Hamilton-Jacobi-Bellman variational inequalities he gave a characterization of the new transportation distance [34]. Moreover Palmer talked about the extension of the transportation distances with free end times to a stochastic setting. These have important applications in mathematical finance and have strong connections to stochastic optimal control. Again he was able to obtain an eulerian characterization of the optimal stochastic transport with free end times.

Other

There were several talks that did not fall in any of the categories above. In his talk **McCann** explored possible geometric explanations for the second law of thermodynamics. Namely just as Einstein's theory of general relativity provides a geometric explanation for gravity, one is wondering if geometric explanations can be given for entropy in statistical mechanics. As a step in that direction McCann investigated the relation between entropy and curvature on Lorentzian manifolds. **Gangbo** spoke about stochastic processes on the space of probability measures. Developing a theory of stochastic processes in the infinite dimensional space of probability measures is a topic of substantial current interest which has applications in mean-field games. Chow and Gangbo [20] introduce the notion of partial Laplacian which allows for only a certain family of stochastic paths. Gangbo explained its well posedness, basic properties and relevance to the field.

Fathi discussed a new approach to proving rates in Central Limit Theorems (CLT) by proving regularity estimates for the Monge-Ampère equation. Namely, in order to compare probability measures one often uses the Stein method, by proving the existence of a Stein kernel. In their very interesting work, Fathi and collaborators use a type of Monge-Ampère equation studied by Cordero-Erausquin and Klartag, [21] to show the existence of Stein Kernels. Fathi also discussed the consequences of the existence of the new Stein Kernels to CLT rates for the Wasserstein metric.

Outcome of the Meeting

This 5-day workshop at BIRS had been a perfect venue for an event like this. The group size of around 40 people has been large enough for bringing together a representative cross section of the different involved communities, in the whole range from the established leaders like Robert McCann (differential geometry), Wilfried Gangbo (optimal transport), Michael Loss (kinetic equations), and Guiseppe Savaré (gradient flows), to young faculty like Katy Craig (nonlinear diffusions, aggregation), Mikaela Iacobelli (nonlinear diffusions, kinetic equations), and Yao Yao (aggregation models), to PhD students and Post-Docs, like Josephine Evans (kinetic equations), Aaron Palmer (optimal transport), Francesco Patacchini (diffusion, aggregation models), and Simon Plazotta (gradient flows). And on the other hand, the group was compact enough for the exchange of ideas in a relaxed and friendly atmosphere. According to the feedback that we received from young researchers, they enjoyed the workshop, got a broad overview of the field, and benefitted from interactions with prominent researchers in the field.

Although we gave essentially everybody the opportunity to present his or her results, we had a strict time limit of thirty minutes for most of the talks, including questions. The longer slots of forty-five minute were reserved for a few selected speakers presenting overview talks. This format gave the participants enough freedom for individual discussions and collaboration in small groups.

Overall there was a sense that the range of applications of entropy methods and related functional inequalities has significantly broadened over the last five years and that there are subfields and connections with other fields that are advancing at rapid pace. Among these we noted analysis on discrete spaces, applications to statistics, numerical computation, highly non-trivial mathematical modeling with applications in particular in mathematical biology, connections with new forms of optimal transport (martingale, unbalanced, etc.). In addition substantial progress on some classical problems, as highlighted by the talks of Esteban, Volzone and Loss, has been made.

Appendix A. Abstracts of the lectures

• LARGE-TIME BEHAVIOR IN HYPOCOERCIVE BGK-MODELS. **Arnold, Anton**. BGK equations are kinetic transport equations with a relaxation operator that drives the phase space distribution towards the spatially local equilibrium, a Gaussian with the same macroscopic parameters. Due to the absence of dissipation w.r.t. the spatial direction, convergence to the global equilibrium is only possible thanks to the transport term that mixes various positions. Hence, such models are hypocoercive.

We shall prove exponential convergence towards the equilibrium with explicit rates for several linear, space periodic BGK-models in dimension 1 and 2. Their BGK-operators differ by the number of conserved macroscopic quantities (like mass, momentum, energy), and hence their hypocoercivity index. Our discussion includes also discrete velocity models, and the local exponential stability of a nonlinear BGK-model.

The proof is based, first, on a Fourier decomposition in space and Hermite function decomposition in velocity. Then, the crucial step is to construct a problem adapted Lyapunov functional, by introducing equivalent norms for each mode.

• ON A NEW PROOF OF THE HARRIS ERGODIC THEOREM AND RELATED SUB-EXPONENTIAL CONVERGENCE RESULTS. **Cañizo, José A.** We revisit a result in probability known as the Harris theorem and give a simple proof which is well-suited for some applications in PDE. The proof is not far from the ideas of Hairer & Mattingly (2011) but avoids the use of mass transport metrics and can be readily extended to cases where there is no spectral gap and exponential relaxation to equilibrium does not hold. We will also discuss some contexts where this result can be useful, particularly in a model for neuron populations structured by the elapsed time since the last discharge. This talk is based on joint works with Stéphane Mischler and Havva Yolda.

• ENTROPIC REGULARIZATION OF OPTIMAL TRANSPORT AND APPLICATIONS. **Carlier, Guillaume**. Entropic regularization of optimal transport is appealing both from a numerical and theoretical perspective. In this talk we will discuss two applications, one from incompressible fluid dynamics and the other from mean-field games theory.

• ENTROPY PRODUCTION INEQUALITIES FOR THE KAC WALK. **Carvalho, Maria C.** We investigate new functional inequalities for the well-known Kac's Walk, and largely resolve the 'Almost' Cercignani Conjecture on the sphere. A new notion of chaoticity plays an essential role. The results we obtain validate Kac's suggestion that functional inequalities for the Kac walk could be used to quantify the rate of approach to equilibrium for the Kac-Boltzmann equation. This is joint work with E. Carlen and A. Einav.

• FROM SLOW DIFFUSION TO A HARD HEIGHT CONSTRAINT: A SINGULAR LIMIT OF KELLER-SEGEL. **Craig, Katy**. For a range of physical and biological processes from dynamics of granular media to biological swarming the evolution of a large number of interacting agents is modeled according to the competing effects of pairwise attraction and (possibly degenerate) diffusion. We prove that, in the slow diffusion limit, the degenerate diffusion becomes a hard height constraint on the density of the population, as arises in models of pedestrian crown motion. We then apply this to develop numerical insight for open conjectures in geometric optimization.

• A NEW CONTINUUM THEORY FOR INCOMPRESSIBLE SWELLING MATERIALS. **Degond, Pierre**. Swelling media (e.g. gels, tumors) are usually described by mechanical constitutive laws (e.g. Hooke or Darcy laws). However, constitutive relations of real swelling media are not well-known. Here, we take an opposite route and consider a simple heuristics relying on the following rule: (i) particles are at packing density; (ii) any two particles cannot swap their position; (iii) motion should be as slow as possible. These heuristics determine the medium velocity uniquely. In general, this velocity cannot be retrieved by a simple Darcy law.

• DETERMINISTIC PARTICLE APPROXIMATIONS OF LOCAL AND NONLOCAL TRANSPORT EQUATIONS. **Di Francesco, Marco**. Nonlinear convection and nonlocal aggregation equations are known to feature a "formal" gradient flow structure in presence of a "nonlinear mobility", in terms of the generalized Wasserstein distance "à la" Dolbeault-Nazaret-Savaré. Such a structure is inherited by the discrete Lagrangian approximations of those equations in a quite natural way in one space dimension, and this simple remark allows to formulate a discrete-to-continuum "many particle" approximation. I will describe some recent results in this direction, which include the discrete (deterministic) particle approximation for scalar conservation laws and (more recently) a large class of nonlocal aggregation equations as main examples. The results are in collaboration with M. D. Rosini (Ferrara), S. Fagioli and E. Radici (L'Aquila).

• SUPER RICCI FLOWS FOR MARKOV CHAINS. **Erbar, Matthias**. I will present a discrete notion of super Ricci flow that applies to time dependent Markov chains or weighted graphs. This notion can be characterized equivalently in terms of a discrete time-dependent Bochner inequality, gradient estimates for the heat propagator on the evolving graph, contraction estimates in discrete transport distances, or dynamic convexity of the entropy. I will also discuss several examples. This is joint work with Eva Kopfer.

• WHY IN SOME CASES THE ASYMPTOTIC LINEARIZED PROBLEM YIELDS OPTIMAL RESULTS FOR A NONLINEAR VERSION OF THE CARRÉ DU CHAMP. **Esteban, Maria J.** Using a nonlinear parabolic flow, in this talk I will explain why the optimal regions of symmetry and symmetry breaking for the extremals of critical and subcritical Caffarelli-Kohn-Nirenberg inequalities are related to the spectral gap of the linearized problem around the asymptotic Barenblatt solutions. This is a surprising result since it means that a global test yields a global result. The use of the parabolic flow also allows to get improved inequalities with explicit remainder terms.

• HYPOCOERCIVITY IN PHI-ENTROPY FOR LINEAR RELAXATION BOLTZMANN EQUATION. **Evans, Josephine**. As well as results in Hilbert spaces, Villani's memoire on hypocoercivity contains convergence to equilibrium results measured in relative entropy. Since then hypocoercivity in more general Phi entropies has been studied by several authors. These works have mainly been for diffusion equations which can be put in a "Hörmander sum of squares form". The linear relaxation Boltzmann equation is a simple equation not of this form for which hypocoercivity in Phi entropies can still be shown but with extra terms added to the functional which would not be needed for a diffusion.

• STEIN KERNELS, OPTIMAL TRANSPORT AND THE CLT. **Fathi, Max**. Stein kernels are a way of measuring distance between probability measures, defined via integration by parts formulas. I will present a connection between these kernels and optimal transport. The main result is a way of deriving rates of convergence in the classical central limit theorem using regularity estimates for a variant of the Monge-Ampère PDE. As an application, we obtain new rates of convergence for the multi-dimensional CLT, with explicit dependence on the dimension.

• EQUILIBRATION OF RENORMALISED SOLUTIONS TO NONLINEAR CHEMICAL REACTION-DIFFUSION SYSTEMS. **Fellner, Klemens**. We prove exponential convergence to equilibrium for renormalised solutions to general complex balanced reaction-diffusion systems without boundary equilibria and even for systems with boundary equilibria provided a finite dimensional inequality holds along solutions trajectories. Our proofs are based on the entropy method and represent the most general results on the convergence to equilibrium for complex balanced RD systems currently available. (joint works with Bao Quoc Tang)

• GLOBAL ESTIMATES FOR LOCAL AND NONLOCAL POROUS MEDIUM TYPE EQUATIONS ON BOUNDED DOMAINS. **Figalli, Alessio**. The behavior of solutions to the classical porous medium equation is by now well understood: the support of the solution expands at finite speed, and for large times it behaves as the separate-variable solution. When the Laplacian is replaced by a nonlocal diffusion, completely new and surprising phenomena arise depending on the power of the nonlinearity and the one of the diffusion. The aim of the talk is to give an overview of this theory.

• RIGOROUS DERIVATION OF THE NONLOCAL REACTION-DIFFUSION FITZHUGH-NAGUMO SYSTEM. **Filbet, Francis**. We introduce a spatially extended transport kinetic FitzHugh-Nagumo model with forced local interactions and prove that its hydrodynamic limit converges towards the classical nonlocal reaction-diffusion FitzHugh-Nagumo system. Our approach is based on a relative entropy method, where the macroscopic quantities of the kinetic model are compared with the solution to the nonlocal reaction-diffusion system. This approach allows to make the rigourous link between kinetic and reaction-diffusion models

• A PARTIAL LAPLACIAN AS AN INFINITESIMAL GENERATOR ON THE WASSERSTEIN SPACE. **Gangbo, Wilfrid**. We study stochastic processes on the Wasserstein space, together with their infinitesimal generators. One of these processes plays a central role in our work. Its infinitesimal generator defines a partial Laplacian on the space of Borel probability measures, and we use it to define heat flow on the Wasserstein space. We verify a distinctive smoothing effect of this flow for a particular class of initial conditions. To this end, we will develop a theory of Fourier analysis and conic surfaces in metric spaces. We note that the use of the infinitesimal generators has been instrumental in proving various theorems for Mean Field Games, and we anticipate they will play a key role in future studies of viscosity solutions of PDEs in the Wasserstein space (Joint work with Y. T. Chow).

• WHEN OTTO MEETS NEWTON AND SCHRÖDINGER, AN HEURISTIC POINT OF VIEW. **Gentil, Ivan**. We propose a generalization of the Schrödinger problem by replacing the usual entropy with a functional $\mathcal{F}$ which approaches the Wasserstein distance along the gradient of $\mathcal{F}$. From an heuristic point of view by using Otto calculus, we show that interpolations satisfy a Newton equation, extending the recent result of Giovani Conforti. Various inequalities as Evolutional-Variational-inequalities are also established from a heuristic point of view. As a rigorous result we prove a new and general contraction inequality for the usual Schrödinger problem under Ricci bound on a smooth and compact Riemannian manifold. This is a joint work with L. Ripani and C. Léonard.

• A THEORY OF TRANSFERS. **Ghoussoub, Nassif**. I introduce and study the class of "linear transfers" between probability measures. This class contains all cost minimizing mass transports, including "equivariant mass transports" and "martingale mass transports". It also contain the "Schrödinger bridge" associated to a reversible Markov process, and the "weak mass transports" of Talagrand, Marton, Gozlan and others. However, what motivated us to develop the concept are the stochastic mass transports in their various forms. We also introduce the cone of "convex transfers," which in addition to linear transfers, include any p-power of a linear transfer, but also the logarithmic entropy, other energy functionals, as well as the Donsker-Varadhan information. The ultimate goal: Stochastic Weak KAM theory.

• LONG TIME BEHAVIOR OF KINETIC LANGEVIN EQUATION. **Guillin, Arnaud**. We will present here two different approaches to study the long time behavior of the kinetic Langevin equation : 1) hypocoercivity technique for entropic convergence via a new weighted logarithmic Sobolev inequality ; 2) Wasserstein convergence via a particular reflection coupling.

• EQUILIBRIA IN THE DIFFUSION-DOMINATED REGIME AND RELATED FUNCTIONAL INEQUALITIES. **Hoffmann, Franca**. We study interacting particles behaving according to a reaction-diffusion equation with nonlinear diffusion and nonlocal attractive interaction. This class of partial differential equations has a very nice gradient flow structure that allows us to make links to different families of functional inequalities. Depending on the nonlinearity of the diffusion, the choice of interaction potential and the space dimensionality, we obtain different regimes. Understanding the asymptotic profiles of this model is related to the minimization problem of the corresponding energy functional. We will provide an overview of recent advances. These are joint works with José A. Carrillo, Vincent Calvez, Jean Dolbeault, Rupert Frank, Edoardo Mainini and Bruno Volzone.

• ASYMPTOTICAL ANALYSIS OF A WEIGHTED VERY FAST DIFFUSION EQUATION ARISING IN QUANTIZATION OF MEASURES VIA THE JKO SCHEME. **Iacobelli, Mikaela**. In this talk I would like to present some recent results on the asymptotic behavior of a very fast diffusion PDE with periodic boundary conditions. This equation is motivated by the gradient flow approach to the problem of quantization of measures. I prove exponential convergence to equilibrium under minimal assumptions on the data, and I also provide sufficient conditions for W2-stability of solutions. Moreover, I will present a work in progress with Filippo Santambrogio and Francesco Saverio Patacchini where we use the JKO scheme to relax the hypotheses of my previous convergence result.

• TOWARDS A GRADIENT FLOW FOR MICROSTRUCTURE. **Kinderlehrer, David**. A central problem of microstructure is to develop technologies capable of producing an arrangement, or ordering, of the material, in terms of mesoscopic parameters like geometry and crystallography, appropriate for a given application. Is there such an order in the first place? We describe very briefly the emergence of the grain boundary character distribution (GBCD), a statistic that details texture evolution, and illustrate why it should be considered a material property. Its identification as a gradient flow by our method is tantamount to exhibiting the harvested statistic as the iterates in a mass transport JKO implicit scheme, which we found astonishing. Consequently the GBCD is the solution, in some sense, of a Fokker-Planck Equation. The development exposes the question of how to understand the circumstances under which a harvested empirical statistic is a property of the underlying process (joint work with P. Bardsley, K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, X.-Y. Lu and S. Ta'asan)

• ENTROPY DECAY FOR THE KAC MASTER EQUATION. **Loss, Michael**. The Kac master equation models the behavior of a large number of randomly colliding particles. Due to its simplicity it allows, without too much pain, to investigate a number of issues. E.g., Mark Kac, who invented this model in 1956, used it to give a simple derivation of the spatially inhomogeneous Boltzmann equation. One important issue is the rate of approach to equilibrium, which can be analyzed in various ways, using, e.g., the gap or the entropy. Explicit entropy estimates will be discussed for a Kac type master equation modeling the interaction of a finite system with a large but finite reservoir. This is joint work with Federico Bonetto, Alissa Geisinger and Tobias Ried.

• GROMOV-HAUSDORFF CONVERGENCE OF DISCRETE OPTIMAL TRANSPORT. **Maas, Jan**. For a natural class of discretisations of a convex domain in R^n, we consider the dynamical optimal transport metric for probability measures on the discrete mesh. Although the associated discrete heat flow converges to the continuous heat flow, we show that the transport metric may fail to converge to the 2-Kantorovich metric. Under an additional symmetry condition on the mesh, we show that Gromov-Hausdorff convergence to the 2-Kantorovich metric holds. This is joint work with Peter Gladbach and Eva Kopfer.

• ENTROPIC CONCAVITY AND POSITIVE ENERGY. **McCann, Robert**. On a Riemannian manifold, lower Ricci curvature bounds are known to be characterized by geodesic convexity properties of various entropies with respect to the Kantorovich-Rubinstein-Wasserstein square distance from optimal transportation. These notions also make sense in a (nonsmooth) metric measure setting, where they have found powerful applications. In this talk I describe the development of an analogous theory for lower Ricci curvature bounds in time-like directions on a Lorentzian manifold. In particular, by lifting fractional powers of the Lorentz distance (a.k.a. time separation function) to probability measures on spacetime, I show the strong energy condition of Penrose is equivalent to geodesic concavity of the Boltzmann-Shannon entropy there.

• GRADIENT FLOWS IN ABSTRACT METRIC SPACES: EVOLUTION VARIATIONAL INEQUALITIES AND STABILITY. **Muratori, Matteo**. We study the main consequences of the existence of a Gradient Flow (GF for short), in the form of Evolution Variational Inequalities (EVI), in the very general framework of an abstract metric space. In particular, no volume measure is needed. The hypotheses on the functional associated with the GF are also very mild: we shall require at most completeness of the sublevels (no compactness assumption is made) and, for some convergence and stability results, approximate λ-convexity. The main results include: quantitative regularization properties of the flow (in terms e.g. of slope estimates and energy identities), discrete-approximation estimates of a minimizing-movement scheme and a stability theorem for the GF under suitable gamma-convergence-type hypotheses on a sequence of functionals approaching the limit functional. Existence of the GF itself is a quite delicate issue which requires some concavity-type assumptions on the metric, and will be addressed in a future project. This is a joint work with G. Savaré.

• OPTIMAL TRANSPORTATION WITH FREE END-TIMES. **Palmer, Aaron**. We explore a dynamic formulation of the optimal transportation problem with the additional freedom to choose the end-time of each trajectory. The dual problem is then posed with a Hamilton-Jacobi variational inequality, which we analyze with the method of viscosity solutions. We find properties that imply the optimal stopping-time is the hitting-time of the free boundary to the variational inequality. Joint work with N. Ghoussoub and Y.H. Kim.

• EXISTENCE OF GROUND STATES FOR AGGREGATION-DIFFUSION EQUATIONS. **Patacchini, Francesco Saverio**. We analyze free energy functionals for macroscopic models of multi-agent systems interacting via pairwise attractive forces and localized repulsion. The repulsion at the level of the continuous description is modeled by pressure-related terms in the functional making it energetically favorable to spread, while the attraction is modeled through nonlocal forces. We give conditions on general entropies and interaction potentials for which neither ground states nor local minimizers exist. We show that these results are sharp for homogeneous functionals with entropies leading to degenerate diffusions while they are not sharp for fast diffusions. The particular relevant case of linear diffusion is totally clarified giving a sharp condition on the interaction potential under which the corresponding free energy functional has ground states or not. This is joint work with J. A. Carrillo and M. G. Delgadino.

• A BDF2-APPROACH FOR THE NON-LINEAR FOKKER-PLANCK EQUATION. **Plazotta, Simon**. In this talk I will discuss the construction of approximate solutions for the Non-linear Fokker-Planck equation. We utilize the L^2-Wasserstein gradient flow structure of this PDEs to perform a semi discretization in time by means of the variational BDF2 method. Our approach can be considered as the natural second order analogue of the Minimizing Movement or JKO scheme. In comparison to our own recent work on constructing solutions to λ-contractive gradient flows in abstract metric spaces, the technique presented here exploits the differential structure of the underlying L^2-Wasserstein space. We directly prove that the obtained limit curve is a weak solution of the non-linear Fokker-Planck equation without using the abstract theory of curves of maximal slope. Additionally, we provide strong L^m convergence instead of merely weak convergence in the L^2-Wasserstein topology of the time-discrete approximations.

• WASSERSTEIN ESTIMATES AND MACROSCOPIC LIMITS IN A MODEL FROM ECOLOGY. **Raoul, Gaël**. We are interested in evolutionary biology models for sexual populations. The sexual reproductions are modeled through the so-called Infinitesimal Model, which is similar to an inelastic Boltzmann operator. This kinetic operator is then combined to selection and spatial dispersion operators. In this talk, we will show how the Wasserstein estimates that appear naturally for the kinetic operator can be combined to estimates on the other operators to study the qualitative properties of the solutions. In particular, this approach allows us to recover a well-known (in populations genetics) macroscopic model.

• ENTROPIC OPTIMAL TRANSPORT AND NONLINEAR PDE'S. **Savaré, Giuseppe**. We discuss two examples of "dynamical optimal transport problems", whose formulations involve a relative entropy functional. The first case is related to the Hellinger-Kantorovich distance and induces an interesting geometric structure on the space of positive measures with finite (but possibly different) mass. In particular, contraction estimates of nonlinear flows are strongly related to geodesic convexity of the generating entropy functionals.

In the second example an entropy functional penalizes the density of the connecting measures with respect to a given reference measure (typically the Lebesgue one) and leads to a first order "mean field planning" problem, which is classically formulated by a continuity equation and a Hamilton Jacobi equation with a nonlinear coupling. In this case, the variational approach and the displacement convexity of the entropy functionals (in the usual sense of optimal transport) provide crucial tools to give a precise meaning to the PDE system and to prove the existence of a solution.

• PHASE TRANSITIONS FOR THE MCKEAN-VLASOV EQUATION ON THE TORUS. **Schlichting, André**. In the talk, the McKean-Vlasov equation on the flat torus is studied. The model is obtained as the mean field limit of a system of interacting diffusion processes enclosed in a periodic box. The system acts as a model for several real-world phenomena from statistical physics, opinion dynamics, collective behavior, and stellar dynamics.

This work provides a systematic approach to the qualitative and quantitative analysis of the McKean-Vlasov equation. We comment on the longtime behavior and convergence to equilibrium, for which we introduce a notion of H-stability.

The main part of the talk considers the stationary problem. We show that the system exhibits multiple equilibria which arise from the uniform state through continuous bifurcations, under certain assumptions on the interaction potential. Finally, criteria for the classification of continuous and discontinuous transitions of this system are provided. This classification is based on a fine analysis of the free energy.

The results are illustrated by proving and extending results for a wide range of models, including the noisy Kuramoto model, Hegselmann-Krause model, and Keller-Segel model (joint work with José Carrillo, Rishabh Gvalani, and Greg Pavliotis).

• PATTERN FORMATION DRIVEN BY TRANSPORT, DRIFT, AND LOCALIZED INTERACTIONS. **Stevens, Angela**. An exemplary drift-reaction system with mass conservation is studied w.r.t. pattern formation. The occurrence of rippling patterns in this system relates to an aggregation equation, whose qualitative behavior will also be discussed.

If time permits, aggregation equations with local interactions will be presented, respectively Chemotaxis-models with a non-diffusive chemical.

All models have in common that their qualitative features are more of "hyperbolic type". Thus pattern formation and the analysis of these systems is different from the one of their "parabolic counterparts".

• RECENT RESULTS ON NONLINEAR AGGREGATION-DIFFUSION EQUATIONS: RADIAL SYMMETRY AND LONG TIME ASYMPTOTICS. **Volzone, Bruno**. One of the archetypical aggregation-diffusion models is the so-called classical parabolic-elliptic Patlak-Keller-Segel (PKS for short) model. This model was classically introduced as the simplest description for chemotatic bacteria movement in which linear diffusion tendency to spread fights the attraction due to the logarithmic kernel interaction in two dimensions. For this model there is a well-defined critical mass. In fact, here a clear dichotomy arises: if the total mass of the system is less than the critical mass, then the long time asymptotics are described by a self-similar solution, while for a mass larger than the critical one, there is finite time blow-up. In this talk we will show some recent results concerning the symmetry of the stationary states for a nonlinear variant of the PKS model, of the form

$$\partial_t \rho = \Delta \rho^m + \nabla \cdot (\rho \nabla (W * \rho)), \tag{7.0.1}$$

being $W \in C^1(\mathbb{R}^d \setminus \{0\})$, $d \geq 2$, a suitable aggregation kernel, in the assumptions of dominated diffusion, i.e. when $m > 2 - 2/d$. In particular, if W represents the classical logarithmic kernel in the bidimensional case, we will show that there exists a unique stationary state for the model (7.0.1) and it coincides, according to one of the main results in the work [**?**], with the global minimizer of the free energy functional associated to (7.0.1). In the case $d = 2$ we will also show how such steady state coincides with the aymptotic profile of (7.0.1). Finally, we will also discuss some recent results concerning the model (7.0.1) with a Riesz potential aggregation, namely when $W(x) = c_{d,s}|x|^{2s-d}$ for $s \in (0, d/2)$, again in the diffusion dominated regime, i.e. for $m > 2 - (2s)/d$. In particular, all stationary states of the model are shown to be radially symmetric decreasing and that global minimizers of the associated free energy are compactly supported, uniformly bounded, Hölder regular, and smooth inside their support. These results are objects of the joint works [**?**], [**?**].

• ENHANCEMENT OF BIOLOGICAL REACTION BY CHEMOTAXIS. **Yao, Yao**. In this talk, we consider a system of equations arising from reproduction processes in biology, where two densities evolve under diffusion, absorbing reaction and chemotaxis. We prove that chemotaxis plays a crucial role to ensure the efficiency of reaction: Namely, the reaction between the two densities is very slow in the pure diffusion case, while adding a chemotaxis term greatly enhances reaction. While proving our main results we also obtain a weighted Poincare's inequality for the Fokker-Planck equation, which might be of independent interest.

Appendix B. Schedule

• Monday, April 9
09:00 - 09:30 : David Kinderlehrer: Towards a gradient flow for microstructure
09:30 - 10:00 : Gaël Raoul: Wasserstein estimates and macroscopic limits in a model from ecology
10:30 - 11:00 : Pierre Degond: A new continuum theory for incompressible swelling materials
11:00 - 11:30 : Francis Filbet: Rigorous derivation of the nonlocal reaction-diffusion FitzHugh-Nagumo system
14:20 - 15:05 Angela Stevens: Pattern formation driven by transport, drift, and localized interactions
15:30 - 16:00 : Yao Yao: Enhancement of biological reaction by chemotaxis
16:00 - 16:30 : Katy Craig: From slow diffusion to a hard height constraint: a singular limit of Keller-Segel
16:30 - 17:15 : Nassif Ghoussoub: A Theory of Transfers

• Tuesday, April 10
08:45 - 09:15 : Guillaume Carlier: Entropic regularization of optimal transport and applications
09:15 - 10:00 : Robert McCann: Entropic concavity and positive energy
10:30 - 11:15 : Wilfrid Gangbo: A partial Laplacian as an infinitesimal generator on the Wasserstein space
11:15 - 12:00 : Aaron Palmer: Optimal transportation with free end-times
14:00 - 14:30 : Anton Arnold: Large-time behavior in hypocoercive BGK-models
14:30 - 15:00 : Arnaud Guillin: Long time behavior of kinetic Langevin equation
15:30 - 16:15 : Michael Loss: Entropy decay for the Kac master equation
16:15 - 16:45 : Maria C Carvalho: Entropy production inequalities for the Kac Walk
16:45 - 17:30 : Josephine Evans: Hypocoercivity in Phi-entropy for linear relaxation Boltzmann equation

• Wednesday, April 11
08:45 - 09:15 : Klemens Fellner: Equilibration of renormalised solutions to nonlinear chemical reaction-diffusion systems
09:15 - 10:00 : Alessio Figalli: Global estimates for local and nonlocal porous medium type equations on bounded domains
10:30 - 11:00 : Maria J. Esteban: Why in some cases the asymptotic linearized problem yields optimal results for a nonlinear version of the carré du champ
11:00 - 11:30 : Mikaela Iacobelli: Asymptotical analysis of a weighted very fast diffusion equation arising in quantization of measures via the JKO scheme

• Thursday, April 12
08:45 - 09:15 : Simon Plazotta: A BDF2-Approach for the Nonlinear Fokker-Planck Equation
09:15 - 10:00 : Giuseppe Savaré: Entropic optimal transport and nonlinear PDE's
10:30 - 11:00 : Jan Maas: Gradient flows and quantum entropy inequalities via matrix optimal transport
11:00 - 11:30 Matteo Muratori: Gradient flows in abstract metric spaces: evolution variational inequalities and stability
14:00 - 14:30 : Marco Di Francesco: Deterministic particle approximations of local and nonlocal transport equations
14:30 - 15:00 : Bruno Volzone: Recent results on nonlinear aggregation-diffusion equations: radial symmetry and long time asymptotics
15:30 - 16:00 : Francesco Patacchini: Existence of ground states for aggregation-diffusion equations
16:00 - 16:30 Ivan Gentil: When Otto meets Newton and Schrödinger, an heuristic point of view
16:30 - 17:15 : Max Fathi: Stein kernels, optimal transport and the CLT

• Friday, April 13
08:45 - 09:15 : Matthias Erbar: Super Ricci flows for Markov chains
09:15 - 10:00 : José Alfredo Cañizo: On a new proof of the Harris ergodic theorem and related sub-exponential convergence results

10:30 - 11:00 : André Schlichting: Phase transitions for the McKean-Vlasov equation on the torus

Participants

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Blanchet, Adrien (Université de Toulouse)
Bowles, Malcolm (University of British Columbia)
Cañizo, José Alfredo (Universidad de Granada)
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Carlier, Guillaume (Université Paris Dauphine)
Carrillo, Jose (Imperial College London)
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Craig, Katy (University of California Santa Barbara)
Degond, Pierre (Imperial College London)
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Di Francesco, Marco (University of L'Aquila)
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Fellner, Klemens (University of Graz)
Figalli, Alessio (ETH Zurich)
Filbet, Francis (Université de Toulouse)
Gangbo, Wilfrid (UCLA)
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Loss, Michael (Georgia Institute of Technology)
Maas, Jan (IST Austria)
Matthes, Daniel (TU-Munich)
McCann, Robert (University of Toronto)
Muratori, Matteo (Politecnico di Milano)
Palmer, Aaron (University of British Columbia)
Patacchini, Francesco (Carnegie Mellon University)
Plazotta, Simon (Technical University of Munich)
Raoul, Gaël (Ecole polytechnique)
Savaré, Giuseppe (University of Pavia)
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Chapter 8

Geometric Quantization (18w5182)

April 15 - 20, 2018

Organizer(s): Xiaonan Ma (Université Paris Diderot), Eckhard Meinrenken (University of Toronto), Paul-Emile Paradan (Université de Montpellier)

Overview

Quantization is an important theme in many areas of mathematics and physics. Geometric quantization aims to associate to any classical phase space, modeled by a symplectic manifold, a corresponding quantum space, modeled by a Hilbert space. Classical observables, given by smooth functions (Hamiltonians), should be quantized to quantum observables.

The original concept of quantization, nowadays usually referred to as canonical quantization, goes back to the work of H. Weyl, J. von Neumann, P. Dirac and I.E. Segal. Nevertheless, canonical quantization encountered several problems, and among other things failed to provide a unified framework for the Schrödinger and Bargmann-Fock representation.

In the 1960s, a theory called geometric quantization emerged. Its main goal is to set a relation between classical and quantum mechanics from a geometrical point of view, taking as a model the canonical quantization method, but removing some ambiguities involved in the canonical quantization procedure.

The pioneering works on geometric quantization are due to J.M. Souriau [24], B. Kostant [12], although many of their ideas were based on previous works by A.A. Kirillov [13]. In this theory the Hilbert space of quantum states of a mechanical system is constructed of some sections of a complex line bundle over a symplectic manifold. The foundation of geometric quantization is the fact, discovered independently by Kirillov, Souriau and Kostant, that every coadjoint orbit of a Lie group is endowed with a symplectic structure, and for the integrable one the symplectic structure is pre-quantized by a line bundle.

A relevant feature of geometric quantization is its close relationship with the theory of irreducible unitary representations of Lie groups. Kirillov [13] proposed a program of realizing irreducible unitary representations of a Lie group G by geometric quantization of its coadjoint orbits. This program, which became known as the orbit method, has been highly successful, with contributions from many mathematicians such as Auslander-Kostant, Duflo, Rossmann, Schmid, Vogan, and others.

In the 1980s, Guillemin and Sternberg [10] studied the geometric quantization of more general G-equivariant Kähler manifolds M. The resulting G-representations are reducible in general. Guillemin and Sternberg proved the ground-breaking result that the multiplicities of this G-representation are calculated in terms of geometric quantizations of the symplectic quotients of M. They conjectures that the phenomenon of "quantization commutes with reduction" (in short, "[Q,R]=0") holds in much greater generality, for the quantization of arbitrary prequantized symplectic manifolds by Dirac operators.

In the 1990s, following Witten's idea of non-abelian localization, there was considerable progress on the "[Q,R]=0" problem, through work of Meinrenken, Vergne, Jeffrey-Kirwan, Guillemin, Duistermaat and Wu. The conjecture was finally solved by Meinrenken (1996) [18] using Lerman's technique of symplectic cutting. Subsequently, Tian and Zhang (1997) gave an analytic proof of the Guillemin-Sternberg conjecture using a deformation of the Dirac operator, and Paradan developed a K-theoretic approach using the theory of transversally elliptic operators (2001).

Recent Developments

Today, geometric quantization continues to be a highly active area, with links to physics, symplectic geometry, representation theory, index theory, differential geometry and geometric analysis. One purpose of the workshop was to present different facets of the "geometric quantization" theme, including topics such as

– quantization of Hamiltonian manifolds,
– group valued momentum maps,
– moduli space problems,
– branching rules in representation theory,
– semiclassical asymptotics,
– index theory (Atiyah-Singer and Connes-Kasparov).

There are many open problems and active developments surrounding geometric quantization, many of which were addressed during the workshop. For example, the recent generalization of the Verlinde formulas to equivariant Verlinde formula opens a wide range of question. The application of simplicial techniques to the geometric realization of higher cohomology groups is a new direction; for instance, there still is no good finite-dimensional realization of the multiplicative gerbe on compact Lie groups. Also quite recently, there have been exciting new developments on the application of C^*-algebras to problems in representation theory. These and other directions were all presented in workshop talks.

Presentation Highlights

The workshop featured researchers with distinct backgrounds and research interests, as well as PhD students and postdoctoral fellows. We made an effort to organize each day of the workshop around a different theme, starting with one or two one-hour survey lectures. This was followed by more specialized 45-minute talks in the afternoon.

Below, we describe some of the highlights in each of these themes.

Foundational aspects of geometric quantization

Yael Karshon: Geometric quantization with metaplectic-c structures

The classical geometric quantization procedure with the "half-form correction", as developed in the 1960s and 1970s, has a number of deficiencies. For example, this approach does not provide a quantization of complex projective space of even complex dimension, due to the absence of a "half form bundle", and one cannot equivariantly quantize any symplectic toric manifold, due to the absence of an "equivariant half form bundle". In her talk, Yael Karshon reported on work with Jennifer Vaughan (expanding on earlier work of Harald Hess), of a new type of geometric quantization procedure. The new approach uses metaplectic-c structures to incorporate the "half form correction" into the prequantization stage, and it does apply to the examples mentioned above.

Michèle Vergne: Semi-classical limits of geometric quantization and the graded equivariant Todd class

Let T be a torus with Lie algebra $\mathfrak{t}$ and let M be a compact Hamiltonian T-manifold with Kostant prequantum line bundle L, and with a proper moment map. The quantization $RR(M, L)$ of these data is a virtual representation of T, defined as the index of the T-equivariant Spin-c Dirac operator with coefficients in L. Replacing L with its tensor powers, one obtains a sequence $RR(M, L^k)$ of such representations. Let $Q \subset \mathfrak{t}^*$ be the weight lattice, and

$$m(\lambda, k)$$

the multiplicity of the irreducible representation of highest weight $\lambda \in Q$ in $RR(M, L^k)$. The distribution

$$\mathfrak{m} = k^{-\dim M/2} \sum_{\lambda \in Q} m(\lambda, k)\delta_{\frac{1}{k}\lambda}$$

has been much-studied in the literature; its limit for $k \to \infty$ is the Duistermaat-Heckman measure of the Hamiltonian T-space. In her lecture, Michèle Vergne explained that this distribution has a complete asymptotic expansion

$$\mathfrak{m} \sim \sum_{i=0}^{\infty} k^{-i}\,\mathrm{Td}_i$$

where the coefficients are the twisted Duistermaat–Heckman distributions associated with the graded equivariant Todd class of M. When f polynomial, the resulting asymptotic series for the pairing $\langle \mathfrak{m},\ f\rangle$ is finite and exact.

Mathai Varghese: Equivariant index theory in the noncompact context, and the relation to quantisation, reduction and PSC metrics

Mathai Varghese gave a survey lecture on aspects of index theory and quantization, in situations where the group or the manifold (or both) are non-compact. For compact spin manifolds, the non-vanishing of the index gives a topological obstruction to the existence of positive scalar-curvature metrics (PSC's). Mathai explained his lecture how to generalize Lichnerowicz' theorem, to the setting where M is a noncompact spin manifold with a proper cocompact action of a Lie group G. To define the equivariant index, he works with a group C^*-algebra, whose K-theory $K_0(C^*(G))$ is a recipient of the equivariant index map. In recent joint work with Hao Guo and Hang Wang, he thus obtains an obstruction to the existence of G-invariant positive scalar-curvature metrics as an element of this K_0-group. Mathai also described some existence results, for the case of 'almost connected Lie groups' whose maximal compact subgroup has nonabelian identity component. For instance, if the G-action is cocompact and proper, and if the action has a global slice with a proper K-action, then a G-invariant PSC metric exists. He discussed many applications of these results, as well as further generalizations. He furthermore explained various results of Mathai-Zhang and Mathai-Hochs on the 'quantization commutes with reduction' conjecture, again for situations where the group or the manifold are non-compact.

Applications of geometric quantization

Martin Puchol: G-invariant holomorphic Morse inequalities

Let G be a connected compact Lie group, acting on a manifold M, and let $L \to M$ be a holomorphic line bundle. Suppose $E \to M$ is a G-equivariant holomorphic vector bundle, and consider the sequence of vector bundles $E \otimes L^k$. In his talk, Martin Puchol described an extension of Demailly's holomorphic Morse inequalities to this equivariant context, computing the invariant part of the Dolbeault cohomology of $E \otimes L^k$. The formula is an instance of the "quantization commutes with reduction", relating the invariant part of the Dolbeault cohomology of M to the Dolbeault cohomology of the symplectic quotient $M/\!\!/G = \mu^{-1}(0)/G$, where $\mu\colon M \to \mathfrak{g}^*$ is Kostant's momentum map for the line bundle L, and using a regularity assumption to guarantee that the quotient is smooth. The inequalities are expressed in terms of the curvature of the bundle induced by $E \otimes L^k$ on this reduction.

Laurent Charles: Toeplitz operators and entanglement entropy

The first part of Laurent Charles' talk was an expository introduction to the Berezin-Toeplitz quantization of Kähler manifolds. The second part described his work with B. Estienne, focussing on a particular class of Berezin-Toeplitz operators whose symbols are characteristic functions. He described their spectral distribution, and presented a two-terms Weyl law. As an application, he obtained the so-called area law for the entanglement entropy in the Quantum Hall Effect.

George Marinescu: Berezin-Toeplitz quantization for eigenstates of the Bochner-Laplacian on symplectic manifolds

George Marinescu's talk continued the theme of Berezin-Toeplitz quantization, describing joint work with L. Ioos, W. Lu and X. Ma. In this context, he regarded as the quantum space the space of eigenstates of the renormalized Bochner Laplacian on a symplectic manifold, corresponding to eigenvalues localized near the origin. He showed that this quantization has the correct semiclassical behavior, and constructed the corresponding star-product.

Geometric quantization and mathematical physics

Sergei Gukov: Geometric quantization and the equivariant Verlinde formula

Sergei Gukov reported on his work, with Andersen and Pei, on the Verlinde formula for the quantization of the Higgs bundle moduli spaces and stacks for any simple and simply-connected reductive group G. This was generalized to a Verlinde formula for the quantization of parabolic Higgs bundle moduli spaces and stacks. These authors also proved that these dimensions form a one-parameter family of 1 + 1-dimensional TQFT, uniquely classified by the complex Verlinde algebra. It is a one-parameter family of Frobenius algebras obtained as a deformation of the classical Verlinde algebra for G.

Daniel Freed: Eta-invariants on pin manifolds and time-reversal symmetry

Daniel Freed described some recent joint work with Mike Hopkins. As he explained, this work may be seen as a consistency check for M-theory, specifically its invariance property under time reversal. This consistency check leads to concrete calculations, involving eta-invariants for odd-dimensional pin manifolds.

Stephan Stolz: From factorization algebras to functorial field theories

The concept of functorial field theories was introduced by Atiyah-Segal in the 1980s, while factorization algebras were pioneered by Beilinson and Drinfeld (2004) and further developed in the recent work by Costello and Guilliam. Stefan Stolz decribed a further understanding of the relationship between these two approaches, based on his joint work with Gwyer and Teichner. In broad terms, their result states that any $\mathcal{G}$-factorization algebra determines a twisted $\mathcal{G}$-field theory. Here $\mathcal{G}$ is additional structure, and a $\mathcal{G}$-factorization algebra is a functor from manifolds M with a $\mathcal{G}$-structure, with morphisms the embeddings, into the category of cochain complexes, the latter playing the role of observables. One advantage of this approach is that concrete examples factorization algebra are rather easy to describe in practice.

Nikhil Savale: A Gutzwiller type trace formula for the magnetic Dirac operator

The usual Gutzwiller trace formula gives a semi-classical approximation to the spectrum of a Schrödinger operator, in terms of data (periods, Maslov indices and so on) of the periodic orbits of the associated classical mechanical system. For a suitable class of manifolds, including metric contact manifolds with non-resonant Reeb flow, Nikhil Savale proved a Gutzwiller type trace formula for the associated magnetic Dirac operator involving contributions from Reeb orbits on the base. As an application, he obtained a semiclassical limit formula for the eta invariant.

Geometric quantization in representation theory

Nigel Higson: Discrete series representations, the Dirac operator and C^*-algebra K-theory

Nigel Higson gave an expository talk on the subject of C^*-algebra K-theory for reductive groups. Following an explanation of the foundations of operator K-theory, he explained how some of the known results of the representation theory of Lie groups can be formulated in K-theoretic, and described some of the new results suggested by this viewpoint. A central theme in this story is Harish-Chandra's parametrization of the discrete series representations, and the realization of discrete series representations using the Dirac operator. Higson also touched on other parts of Harish-Chandra's theory of tempered representations that are relevant from the K-theoretic point of view, as well as the the philosophy of Mackey's machine.

Yanli Song: Fourier transform, orbital integral and character of representations

In the 1980s, Connes and Moscovici studied the equivariant index theory of G-invariant elliptic pseudo-differential operators, acting on non-compact homogeneous spaces. They proved an L^2-index formula using the heat kernel method, which is related to the discrete series representation of Lie groups. In his talk, Yanli Song, following his joint work with Xiang Tang, discussed the orbital integral of the heat kernel, and its relation with the Plancherel formula. One result in this context is a generalization of Connes-Moscovici's analytic index to the limit of discrete series case. Song's talk also touched on recent work by Hochs and Wang, who had obtained a fixed point theorem for the topological side of the index.

Hang Wang: K-theory, fixed point theorem and representation of semisimple Lie groups

The approach to representation theory of Lie groups through the K-theory of C^*-algebras was continued in the talk of Hang Wang, who reported on her work with Peter Hochs. More specifically, their work used the K-theory of reduced group C^*-algebras and their trace maps, in order to study tempered representations of semisimple Lie groups from the viewpoint of index theory. She explained how for a semisimple Lie group G, every K-theory generator can be viewed not only as the equivariant index of some Dirac operator, but also as a family of representations, parametrised by the A-factor of the Levi component of a cuspidal parabolic subgroup. In particular, if the Lie group G admits discrete series representations, then the corresponding K-theory classes are realized as equivariant geometric quantizations of the associated coadjoint orbits. Applying orbital traces to the K-theory group, Hochs and Wang obtained a fixed point formula; its application to the realization of discrete series representations, recovered the Harish-Chandra character formula. The result may be regarded as a noncompact analogue of the Atiyah-Segal-Singer fixed point theorem, in relation to the Weyl character formula.

Peter Hochs: K-types of tempered representations

Peter Hochs desribed his joint work with Song and Yu, as well as with Higson and Song. Let G be a real semisimple Lie group, and $K \subset G$ a maximal compact subgroup. A tempered representation π of G is an irreducible representation that occurs in the Plancherel decomposition of $L^2(G)$. Similar to the fact that an irreducible representation of a compact Lie group is determined by its restriction to the maximal torus, a substantial amount of information about π is captured by the restriction $\pi|_K$ of π to the maximal compact subgroup K. By realizing this restriction as the geometric quantization of a suitable space, which (under a regularity assumption on π) is a coadjoint orbit, a suitable version of the quantization commutes with reduction principle leads to geometric expressions for the multiplicities of the irreducible representations of K in $\pi|_K$, that is, the K-types of π. This was done for the discrete series representations in work of Paradan in 2003. Hochs' joint work with Song and Yu extended this result to arbitrary tempered representation. The resulting multiplicity formula was obtained in a different way, for tempered representations with regular parameters, by Duflo and Vergne in 2011. In joint work with Higson and Song, Hochs also gave a new proof of Blattner's formula for multiplicities of K-types of discrete series representations, using the ideas of geometric quantization. This formula was first proved by Hecht and Schmid in 1975, and later by Duflo, Heckman and Vergne in 1984.

Loop groups, Higher structures

Konrad Waldorf: Fusion in loop spaces

In his lecture, Konrad Waldorf gave a general overview of fusion operations in loop spaces, based on his work since around 2010. The notion of a fusion structure on objects over the loop space was emphasized by Stolz and Teichner in their 2005 article "The spinor bundle on loop spaces". Specifically, these authors had developed the notion of an orientation on loop spaces, giving precise definitions and proofs for the fact that orientations of the loop space LM are in canonical 1-1 correspondence with spin structures on M. Waldorf proved that the category of abelian gerbes with connection over a smooth manifold is equivalent to a category of principal bundles over the free loop space, equipped with a connection and with a "fusion" product with respect to triples of paths.

Chris Kottke: A new theory of higher gerbes

Complex line bundles on a manifold M are classified naturally up to isomorphism by degree two integer cohomology $H^2(M, \mathbb{Z})$, and it is of interest to find finite-dimensional geometric objects which are similarly associated to higher degree cohomology, and which would allow for a similar theory of connections, curvature and so on. For degree 3 cohomology $H^3(M, \mathbb{Z})$, such geometric realizations are known as gerbes. There are various models for gerbes, due respectively to Giraud, Brylinski, Hitchin and Chatterjee, and Murray. Various notions of"higher gerbes" have also been defined, though these tend to run into technicalities and complicted bookkeeping associated with higher categories.

Chris Kottke's talk, based on his joint work with Melrose, proposed a new geometric version of higher gerbes in the form of "multi simplicial line bundles". The basic idea is to replace the simplicial manifolds, as used for example in Murray's notion of bundle gerbes, by multi-simplicial manifolds, and to study line bundles with connections on such spaces. The theory avoids many of the higher categorical difficulties, yet still captures key examples including the string obstruction associated to the first Pontrjagin class

$$\frac{1}{2}p_1(M) \in H^4(M, \mathbb{Z}).$$

The authors found that every integral cohomology class is represented by one of these objects, in the guise of a line bundle on the iterated free loop space equipped with a "fusion product" (as defined by Stolz and Teichner and further developed by Waldorf) for each loop factor.

Richard Melrose: Generalized products and quantization

The 'generalized products' in Richard Melroses lecture are simplicial manifolds, for example a sequence of manifolds

$$M,\ M \times M,\ M \times M \times M, \dots$$

with the usual face and degeneracy maps. He explained how any simplicial manifold $M(1), M(2), \dots$ generates an algebra of pseudo-differential operators on $M(1)$, using conormal distributions relative to the degeneracy map $M(1) \to M(2)$ as integral kernels. The fact that these form an algebra is encoded in the properties of a simplicial manifold. Instead of manifolds, one can also consider other categories, and Melrose's talk focused on the category of manifolds with corners. He then applied these ideas to various examples, including compactifications of Lie groups.

Yiannis Loizides: Quantization of Hamiltonian loop group spaces

A theorem of Freed, Hopkins and Teleman relates the representation theory of the loop group LG of a compact Lie group G to the equivariant twisted K-theory of G. In the special case of a connected, simply connected and simple Lie group, the theorem states that there is an isomorphism of rings

$$R_k(G) \cong K_0^G(G, \mathcal{A}^{k+h^\vee})$$

where the left hand side is the level k Verlinde ring, and the right hand side the equivariant K-homology of G with twisting (Dixmier-Douady class) at the shifted level $k + h^\vee$, where $h^\vee$ is the dual Coxeter number. (Freed-Hopkins-Teleman work with twisted equivariant K-cohomology, which is related by a Poincare duality isomorphism.) In his talk, explained how to realize classes in $K_0^G(G, \mathcal{A}^{k+h^\vee})$ in terms of D-cycles, thereby defining an explicit inverse to the Freed-Hopkins-Teleman map on the chain level. One idea in this construction is an abelianization procedure, working with a tubular neighborhood of the maximal torus T in G. One application of this result, relating it to earlier work of Loizides with Meinrenken and Song, provides the equivalence of two methods for quantizing Hamiltonian loop group spaces.

Index theory

Jean-Michel Bismut: Hypoelliptic Laplacian and the trace formula

The hypoelliptic Laplacian gives a natural interpolation between the Laplacian and the geodesic flow. This interpolation preserves important spectral quantities. In his talk, Jean-Michel Bismut explained the construction of the hypoelliptic Laplacian in the context of compact Lie groups. In this case, the hypoelliptic Laplacian is the analytic counterpart to localization in equivariant cohomology on the coadjoint orbits of loop groups. The construction for noncompact reductive groups ultimately produces a geometric formula for the semisimple orbital integrals, which are the key ingredient in Selberg trace formula. In both cases, the construction of the hypoelliptic Laplacian involves the Dirac operator of Kostant.

Xiang Tang: Hochschild Homology of Proper Lie Groupoids

Xiang Tang reported on his ongoing work with Pflaum and Posthuma. For a compact Lie group acting on a smooth manifold, this work studies the complex of basic relative forms on the inertia space of a proper Lie groupoid, as originally constructed by Brylinski. In his talk, Xiang Tang explained how basic relative forms can be used to study the Hochschild homology of the convolution algebra.

Rudy Rodspohn: Diff-equivariant index theory

Since the early 1980s, Alain Connes had developed his Noncommutative Geometry program. One of the primary goals of this program was to extend index theory to singular situations, where the usual tools of differential geometry are no longer available. A typical instance of such a setting are regulations foliations on manifolds for which there does not exist a transverse measure invariant under the action of the holonomy group. In the late 1990s, Connes and Moscovici proved an equivariant index theorem for this these context, and formulated a conjecture concerning the calculation of this index in terms of characteristic classes. In his talk, Rudy Rodspohn gave an account of the history and motivation of the index problem. And explained his solution, together with Denis Perrot, of the Connes-Moscovici conjecture, with special emphasis on aspects relating to quantization.

Frédéric Rochon: Torsion on hyperbolic manifolds of finite volume

Frédéric Rochon described joint work with Werner Mueller. Let X be any finite volume hyperbolic manifold of dimension d. Given a finite dimensional irreducible complex representation of the group $G = \mathrm{SO}_0(d, 1)$, one can associate a canonical flat vector bundle E over X, together with a canonical bundle metric h. For d odd and under some mild hypotheses on the manifold X, Rochon explained how to obtain a formula relating the analytic torsion of (X, E, h) with the Reidemeister torsion of an associated manifold with boundary. The argument involves a family of compact manifolds degenerating to X in a suitable sense. In the arithmetic setting, this formula can be used to derive exponential growth of torsion in cohomology for various sequences of congruence subgroups.

Thomas Schick: Index theory and secondary spectral invariants to understand moduli spaces of Riemannian metrics

Thomas Schick presented an overview of applications of index theory to the existence of positive scalar curvature metrics. Given a manifold X, his talk considered the moduli space of positive scalar curvature metrics by the action of the diffeomorphism group of X, fixing some base point x_0 and also having differential at x_0 equal to the identity:

$$\mathrm{Riem}^+(X)/\,\mathrm{Diff}_{x_0}(X)$$

There are many questions about this space – for example, whether it is empty, if non-empty what the number of connected components would be. Another interesting quotient to consider is the the set of concordance equivalence classes

$$\mathrm{Riem}^+(X)/\,\mathrm{concordance}\,.$$

To investigate the relationship, one considers more general bordisms, and introduces a space $\mathrm{Pos}(X)$ of cycles (M, g, f) (where g is a PSC metric and $f\colon M \to X$ is a map) modulo an equivalence relation. A deep theorem of Stolz fits $\mathrm{Pos}_m(X)$ into an exact sequence gives an exact sequence involving the spin bordism group $\Omega^m(X)$. Schick's lecture described the many unknown questions about this exact sequence, and some recent progress. The second part of the lecture explained the relationship of these ideas to the Lichnerowicz-Schrödinger formula for the square of a Dirac operator.

Outcome of the Meeting

The workshop at BIRS brought together mathematicians whose work involves quantization in rather different forms and with many different techniques: loop groups, topological K-theory, analytic estimates, C^*-algebras, representation theory. The philosophy of geometric quantization served as a focal point for the interaction between all of these areas. The workshop provided an opportunity for experts working on different aspects of the theory to exchange ideas, leading to fresh insights and new developments.

Participants

Barron, Tatyana (University of Western Ontario)
Blacker, Casey (University of California Santa Barbara)
Charles, Laurent (University Pierre et Marie Curie)
Dai, Xianzhe (University of California Santa Barbara)
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Hawkins, Eli (University of York)
Hekmati, Pedram (The University of Auckland)
Higson, Nigel (Pennsylvania State University)
Hochs, Peter (University of Adelaide)
Ioos, Louis (Pierre and Marie Curie University - Paris 6)
Karshon, Yael (University of Toronto)
Kottke, Chris (New College of Florida)
Krepski, Derek (University of Manitoba)
Lackman, Joshua (University of Toronto)
Lerman, Eugene (Uniiversity of Illinois)
Loizides, Yiannis (Pennsylvania State University)
Ma, Xiaonan (Université Paris Diderot - Paris 7)
Marinescu, George (Köln University)
Meinrenken, Eckhard (University of Toronto)

Melrose, Richard (Massachusetts Institute of Technology)
Paradan, Paul-Emile (Université de Montpellier)
Puchol, Martin (University of Lyon)
Rochon, Frédéric (Université du Québec à Montréal)
Rodsphon, Rudy (Vanderbilt University)
Savale, Nikhil (Universität zu Köln)
Schick, Thomas (Universität Göttingen)
Sniatycki, Jedrzej (University of Calgary)
Song, Yanli (Washington University at St.Louis)
Stolz, Stephan (University of Notre Dame)
Tang, Xiang (Washington University)
Uribe, Alejandro (University of Michigan)
Valiveti, Kaavya (Massachusetts Institute of Technology)
Varghese, Mathai (University of Adelaide)
Vergne, Michèle (University Paris Diderot)
Waldorf, Konrad (Universität Greifswald)
Wang, Hang (East China Normal University)
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Chapter 9

An Algebraic Approach to Multilinear Maps for Cryptography (18w5118)

May 6 - 11, 2018

Organizer(s): Alice Silverberg (University of California, Irvine), Dan Boneh (Stanford University), Ted Chinburg (University of Pennsylvania)

Objectives

A main goal of the BIRS workshop "An Algebraic Approach to Multilinear Maps for Cryptography" was to bring together cryptographers, number theorists and arithmetic geometers to discuss problems of central importance in electronic communication. The focus of the workshop was on cryptographic multilinear maps. It is an open problem to construct secure cryptographic multilinear maps with more than two arguments in their domain [1]. A solution to this problem would have many applications. These include allowing groups of people to share a common secret securely and the ability to obfuscate computer programs in order to protect the intellectual property they represent. The workshop also dealt with other problems in cryptography such as quantum computation, pseudo-random number generators and applications of isogenies of abelian varieties to cryptography.

Two specific objectives of the workshop were to

(i) analyze various proposed constructions of cryptographic multilinear maps, and

(ii) familiarize the participants with open problems in number theory and arithmetic geometry arising from cryptography.

The workshop brought together researchers and advanced Ph.D. students working on cryptography and related topics in number theory and arithmetic geometry.

The workshop was timely in view of recent research activity in this area. It built on progress resulting from an AIM workshop organized by the same organizers in October of 2017.

Besides the generous support from the Banff International Research Station, this workshop was also supported by an SaTC award from the National Science Foundation titled "An algebraic approach to secure multilinear maps for cryptography." The P.I.'s on this NSF SATC award were the organizers (Silverberg, Boneh and Chinburg) and A. Venkatesh.

The workshop had 29 participants and ten scheduled 50-minute talks. In between these talks, the participants broke into working groups to discuss particular questions arising from the talks as well as new ideas related to the subject of the workshop.

Talks

In the following we give a description of each talk, in the order in which the talks were given.

Alice Silverberg, Introduction to cryptographic multilinear maps.

The talk introduced the concept of a cryptographic multilinear map as in [1], starting from basic concepts familiar to the diverse audience of the workshop, who consisted of both mathematicians and computer scientists. In addition to presenting some open problems to be considered during the workshop, a goal was to give the participants a common language and background on which to build. The talk began with Diffie-Hellman key exchange [4], and went on to present the one-round tripartite Diffie-Hellman protocol of Joux [12], and an identity-based key agreement scheme of Sakai, Ohgishi, and Kasahara [17]. We also mentioned a destructive use of pairings due to Menezes, Okamoto, and Vanstone [14].

Dan Boneh: Background on multilinear maps, and applications.

The talk defined the notion of a cryptographic multilinear map and explored applications of such maps in cryptography. Applications include digital signatures, broadcast encryption, indistinguishability obfuscation (iO), and many others. It has been shown that a cryptographic trilinear map is sufficient for the application to iO. Dan posed the construction of such a map as a key challenge for the participants.

Ming-Deh Huang: Trilinear maps for cryptography.

The talk presented the approach discussed in [11] to constructing a cryptographic trilinear map using principally polarized abelian surfaces A over the algebraic closure of a finite field. The map has the form

$$A[\ell] \times A[\ell] \times NS(A)/\ell NS(A) \to \mu_\ell$$

where $A[\ell]$ is the ℓ-torsion of A for a large prime ℓ and $NS(A)$ is the Neron Severi group of A. This map can be interpreted as a cup product in étale cohomology, and it can be quickly computed given enough data on the arguments. The main challenge discussed at the meeting was to represent elements in $NS(A)$ in a way that makes the discrete-log problem difficult.

Peter Stevenhagen: A reciprocity law for Redei symbols.

This talk concerned the possibility of constructing cryptographically useful trilinear maps using generalizations of the Redei symbol [16]. The Redei symbol is a concrete trilinear map defined on suitable triples (a, b, c) of elements of $\mathbb{Q}^*/(\mathbb{Q}^*)^2$. The talk focused on formulas for this symbol and its properties and applications. One property is that the value of the symbol does not change if one permutes the arguments a, b and c. An application is to understanding the Galois group of the maximal pro-2 extension of $\mathbb{Q}$ that is unramified outside a given set of primes. The participants of the workshop focused after the talk on connections between the Redei symbol and Massey products (see [9], for example).

David Jao: Isogeny based crypto.

The talk surveyed the burgeoning area of isogeny-based cryptography. David explained the different flavors of the available schemes, using ordinary and supersingular elliptic curves. David also described the sub-exponential time quantum attack on the isogeny problem on ordinary curves.

Ted Chinburg: Background on the cohomological point of view.

This talk focused on two potential constructions of cryptographic trilinear maps via étale cohomology. The first involved using work of Skorobogatov and Zarhin in [18] to replace the group $NS(A)/\ell NS(A)$ in Huang's talk by the larger group $H^2(A, \mu_\ell)$. The main open question is to specify elements of $H^2(A, \mu_\ell)$ without encountering discrete log problems of the kind associated to $NS(A)/\ell NS(A)$. The other construction discussed in the talk was the trilinear cup product map

$$H^1(C, \mathbb{Z}/\ell) \times H^1(C, \mu_\ell) \times H^1(C, \mu_\ell) \to H^3(C, \mu_\ell^{\otimes 2}) = \mu_\ell$$

associated to a curve C over a finite field. Work of McCallum and Sharifi [MS] leads to an inefficient algorithm for computing this map. The possibility of using modular forms to compute it efficiently was discussed.

Amit Sahai: Multilinear maps and obfuscation.

The talk explained why indistinguishability obfuscation (iO) is such a useful mechanism in cryptography. It also described at a high level why multilinear maps are useful for constructing an iO obfuscator.

Dan Boneh: Candidate multilinear maps from ideal lattices, and attacks.

The talk looked at current proposals for multilinear maps based on hard problems on lattices. The GGH13 and CLT13 constructions fall in this category. The talk also explained why these constructions, in their basic form, are insecure.

Working groups

In addition to formal lectures, we had moderated Open Problems sessions in which the participants suggested problems that might be of interest, including some to be worked on during the week. The participants then split up into working groups to work on some of these problems. We also had sessions in which representatives of the working groups gave progress reports on the results obtained to that point. Moderators for the Open Problems and Interim Reports sessions included Kiran Kedlaya and Steven Galbraith.

The working group topics included:

- Multiparty key agreement based on isogenies on abelian varieties.
- Trilinear maps via Neron-Severi groups and abelian surfaces.
- Trilinear maps via curves over finite fields, Brauer groups, and Massey and Redei symbols.
- Quantum algorithms to solve isogeny problems.
- Hilbert's 10th problem over the rational numbers.
- The local pseudo-random number generator problem.

Extracurricular activities

The participants also attended a public lecture on Escher and the Droste Effect by Hendrik W. Lenstra, Jr. on Tuesday evening, and a piano performance "88 Public Keys" on mathematical themes related to the workshop topic by Noam D. Elkies on Thursday evening.

Schedule

The schedule of the workshop allowed for ample discussions among the participants. This was appreciated by everyone.

Sunday, May 6

16:00	Check-in begins
	(Front Desk - Professional Development Center - open 24 hours)
17:30 - 19:30	Buffet Dinner, Sally Borden Building
20:00	Informal gathering (Corbett Hall, 2nd floor lounge)

Monday, May 7

7:00 - 9:00	Breakfast
9:05 - 9:20	Introduction and welcome by BIRS station manager
9:20 - 9:30	A. Silverberg: *Welcome by workshop organizers.*
9:30 - 10:00	A. Silverberg: *Introduction to cryptographic multlinear maps.*
10:00 - 10:30	Coffee break
10:30 - 12:00	D. Boneh: *Background on multilinear maps, and applications.*
12:00 - 13:00	Lunch
13:00 - 14:00	Guided Tour of The Banff Centre
	(meet in the 2nd floor lounge, Corbett Hall)
14:00 - 14:20	Group Photo
14:20 - 15:20	M-D. Huang: *Trilinear maps for cryptography.*
15:20 - 16:00	Coffee break
16:00 - 18:00	Open problems session
18:00 - 19:30	Dinner

Tuesday, May 8

7:00 - 9:30	Breakfast
9:00 - 9:50	P. Stevenhagen: *A reciprocity law for Redei symbols.*
10:30 - 11:00	Coffee break
11:00 - 12:00	*Discussion about splitting into working groups.*
12:00 - 13:30	Lunch
13:30 - 14:30	D. Jao: *Isogeny based crypto.*
14:30 - 15:00	Coffee break
15:00 - 17:30	Working groups
17:30 - 19:30	Dinner

Wednesday, May 9

7:00 - 9:00	Breakfast
9:00 - 10:00	T. Chinburg: *Background on cohomological point of view.*
10:00 - 10:30	Coffee break
10:30 - 11:30	A. Sahai *Multilinear maps and obfuscation.*
11:30 - 13:30	Lunch
	Free Afternoon
17:30 - 19:30	Dinner

Thursday, May 10

7:00 - 9:00	Breakfast
9:30 - 10:30	Working groups
10:30 - 11:00	Coffee break
11:00 - 12:00	Open problems Session II
12:00 - 13:30	Lunch
13:30 - 14:00	Woirking groups
14:00 - 14:30	D. Boneh: *Candidate multilinear maps from ideal lattices, and attacks.*
14:30 - 15:00	Coffee break
15:00 - 18:00	Working groups
17:30 - 19:30	Dinner

Friday, May 11

7:00 - 9:00	Breakfast
9:00 - 10:00	Working groups
10:00 - 10:30	Coffee break
10:30 - 11:45	Reports of working groups
11:30 - 12:00	Checkout by Noon (Front Desk - Professional Development Centre)
12:00 - 13:30	Lunch
13:00 - 14:00	T. Chinburg: *Redone video of the talk given on May 9. The video of the May 9 talk did not record.*

Participants

The participants of the workshop and their affiliations at the time of the workshop were as follows.

Bleher, Frauke	University of Iowa
Boneh, Dan	Stanford University
Bright, Martin	Universiteit Leiden
Chinburg, Ted	University of Pennsylvania
Elkies, Noam D.	Harvard University
Galbraith, Steven	University of Auckland
Gangl, Herbert	Durham University
Glass, Darren	Gettysburg College
Guy, Richard	The University of Calgary
Heninger, Nadia	University of Pennsylvania
Huang, Ming-Deh	USC
Jao, David	University of Waterloo
Kedlaya, Kiran	University of California, San Diego
Lee, Changmin	Seoul National University
Lenstra, Hendrik	Universiteit Leiden
Pellet–Mary, Alice	LIP, ENS de Lyon
Rubin, Karl	University of California, Irvine
Sahai, Amit	UCLA
Scheidler, Renate	University of Calgary
Scherr, Zach	Bucknell University
Shani, Barak	University of Pennsylvania
Sharif, Shahed	CSU San Marcos
Silverberg, Alice	University of California, Irvine
Stange, Katherine	University of Colorado Boulder
Stevenhagen, Peter	Universiteit Leiden
Takashima, Katsuyuki	Mitsubishi Electric / Kyushu University

Tibouchi, Mehdi	NTT Corporation
Tran, Ha	University of Calgary
Zobernig, Lukas	The University of Auckland

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Chapter 10

Topics in the Calculus of Variations: Recent Advances and New Trends (18w5094)

May 20 - 25, 2018

Organizer(s): Giovanni Leoni (Carnegie Mellon University), Maria Giovanna Mora (University of Pavia)

Overview and Outcome of the Meeting

The calculus of variations is at the same time a classical area of mathematical analysis with longstanding open problems and a very active subject of modern mathematics, that has important applications in a variety of different fields, such as materials science, mathematical physics, and treatment of digitalized images, just to name a few examples. In the last decades this subject has enjoyed a flourishing development worldwide, driven both by mathematical developments and emergent applications.

In this workshop a special emphasis was given to young researchers. Indeed, out of the 31 talks, 2 were given by graduate students (Hagerty and Gravina), 12 by postdoctoral fellows (Carroccia, Cristoferi, Davoli, Ginster, Gladbach, Maor, Morandotti, Murray, O'Brien, Piovano, Tobasco, Wojtowytsch) and 3 by junior faculty (Friedrich, Iurlano, Rüland). These were complemented by talks from worldwide experts in different areas of calculus of variations and partial differential equations including Gianni Dal Maso (Gamma-convergence, fracture mechanics), Georg Dolzmann (elasticity, plasticity, microstructure), Nicola Fusco (regularity of partial differential equations, geometric measure theory), and Giuseppe Savaré (abstract evolution equations, optimal transport, analysis in metric-measure spaces). The presence of so many young participants and the wonderful environment of the Banff International Research Center contributed to a very informal, friendly, and unique atmosphere. We kept the talks to 35 minutes. This gave plenty of time for informal discussions and networking. New friendships were formed and collaborations were initiated during the meeting. There were several social activities, including an official hike along the Hoodoos Trail, as well as a 7 hours hike to Mount Rundle by some of the more adventurous participants. From the feedback we received, the workshop was very successful and many participants expressed the desire to have another one in the next few years.

Participants and especially young people were exposed to a wide range of topics at the cutting edge in nonlinear and applied analysis. Below we highlight some of them.

Epitaxial Growth

Four of the talks (Cristoferi, Lu, Piovano, and partially Fusco) were on epitaxial growth, which is the deposition of a crystalline film onto a substrate, in which the atoms of the film occupy natural lattice positions of the substrate. If the film and the substrate are of the same material, the epitaxial deposition is called homoepitaxy, while if they are of different material, it is called eteroepitaxy. In eteroepitaxial growth if the mismatch in lattice parameter of the film crystal and the substrate crystal is large, then the film tends to gather into islands on the surface and the substrate is exposed between islands. This is called the Volmer-Weber (VW) growth mode. On the other hand, if the mismatch in lattice parameter is small the atoms of the film tend to align themselves with those of the substrate, continuing its atomic structure. This is due to the fact that the energy gain associated with the chemical bonding effect is greater than the strain in the film. This layer-by-layer film growth mode is called the Frank–van der Merwe (FM) growth mode. However, as the film continues to grow, the stored strain energy per unit area of interface increases linearly with the film thickness. Eventually, the presence of such a strain renders a flat layer of the film morphologically unstable or metastable, after a critical value of the thickness is reached. To release some of the elastic energy due to the strain, the atoms on the free surface of the film tend to rearrange into a more favorable configuration. Typically, after entering the instability regime, the film surface becomes wavy or the material agglomerates into clusters or isolated islands on the substrate surface. Island formation in systems such as In-GaAs/GaAs or SiGe/Si turns out to be useful in the fabrication of modern semiconductor electronic and optoelectronic devices such as quantum dots laser.

This growth mode in which islands are separated by a thin wetting layer is known as the Stranski-Krastanow (SK) growth mode.

In the literature several atomistic and continuum theories for the growth of epitaxially strained solid films are available. In [30] Spencer proposed the following variational approach in which the film and the substrate are modeled as linearly elastic solids. Consider an epitaxial layer (with variable thickness h) grown on a flat semi-infinite substrate. Restricting attention to two-dimensional morphologies which correspond to three-dimensional configurations with planar symmetry, assume that the material occupies the infinite strip

$$\Omega_h := \{\boldsymbol{x} = (x, y) : \, 0 < x < b, \, y < h\,(x)\} \tag{10.0.1}$$

where $h : [0, b] \to [0, \infty)$ is a Lipschitz function. Thus the graph of h represents the free profile of the film, the open set and the line $y = 0$ corresponds to the film/substrate interface. We work within the theory of small deformations, so that $\boldsymbol{E}\,(\boldsymbol{u}) := \frac{1}{2}\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T\right)$ represents the strain, with $\boldsymbol{u} : \Omega_h \to \mathbb{R}^2$ the planar displacement. The displacement is measured from a configuration of the layer in which the lattices of the film and the layer are perfectly matched; this configuration, in which $\boldsymbol{E} \equiv \boldsymbol{0}$, will not correspond to a minimum energy state of the film, which we assume to occur at a strain $\boldsymbol{E}_0 = \boldsymbol{E}_0\,(y)$. If the film and the substrate have similar material properties, then they share the same homogeneous elasticity tensor C. Hence, bearing in mind the mismatch, the elastic energy per unit area is given by $W\,(\boldsymbol{E} - \boldsymbol{E}_0\,(y))$, where

$$W\,(\boldsymbol{E}) := \frac{1}{2}\boldsymbol{E} \cdot C\,[\boldsymbol{E}] \tag{10.0.2}$$

with C a positive definite fourth-order tensor.

In the sharp interface model the interfacial energy density ψ has a step discontinuity at $y = 0$: It is $\gamma_{\text{film}} > 0$ if the film has positive thickness and $\gamma_{\text{sub}} > 0$ if the substrate is exposed, to be precise,

$$\psi\,(y) := \begin{cases} \gamma_{\text{film}} & \text{if } y > 0, \\ \gamma_{\text{sub}} & \text{if } y = 0. \end{cases} \tag{10.0.3}$$

Hence the total energy of the system is given by

$$\mathcal{F}\,(\boldsymbol{u}, h) := \int_{\Omega_h} W\,(\boldsymbol{E}\,(\boldsymbol{u}) - \boldsymbol{E}_0)\; d\boldsymbol{x} + \int_{\Gamma_h} \psi\, ds, \tag{10.0.4}$$

where Γ_h represents the free surface of the film, that is,

$$\Gamma_h := \partial\Omega_h \cap ((0, b) \times \mathbb{R})\,. \tag{10.0.5}$$

Most of the recent literature (see [24] and the references therein) deals with the Stranski-Krastanow (SK) growth mode, which corresponds to the case $\gamma_{\text{film}} < \gamma_{\text{sub}}$. In his talk, Paolo Piovano (University of Vienna) presented some recent work [8] in collaboration with Elisa Davoli (University of Vienna), another of the workshop speakers, in the Volmer-Weber (VW) growth mode $\gamma_{\text{film}} > \gamma_{\text{sub}}$ and in the case in which the film and the substrate have different homogeneous elasticity tensor C. The Young-Dupré law is shown to be satisfied by the angle that energetically-optimal profiles form at contact points with the substrate. This is one of the first analytical validations of such relation, which was originally formulated in Fluid Mechanics, in the context of Continuum Mechanics for a thin-film model.

Riccardo Cristoferi (Carnegie Mellon University) and Xin Yang Lu (Lakehead University) in their talks considered modified variational models that take into consideration the effect of the free atoms moving on the surface (adatoms).

Ferromagnetism

Ferromagnetic materials have the physical property of exhibiting spatially ordered magnetization patterns (magnetic domains) under a variety of conditions. This property is at the basis of the large use of ferromagnets in technological applications. The mechanisms behind the magnetic domain formation can be quite complex, but usually domain patterns may be understood from energetic considerations based on the micromagnetic modeling framework. Ground states of various ferromagnetic systems have been widely studied in the physics community and more recently in the mathematical literature (see the review [11]). In particular, within the micromagnetic framework the ground state domain structure of macroscopically thick uniaxial ferromagnetic films is by now fairly well understood mathematically. In contrast, most mathematical treatments of microscopically thin ferromagnetic films deal with the case where the magnetization prefers to lie in the film plane. Thus, one of the main open questions in the theory of uniaxial ferromagnets is to rigorously characterize their ground states in the case of films of vanishing thickness where the magnetization prefers to align normally to the film plane. This was the subject of Hans Knüpfer's talk, who reported on a joint work [21] with C. Muratov (another of the workshop speakers) and F. Nolte. Experimental observations show the formation of bubble and stripe domain patterns in thin ferromagnetic films with strong perpendicular anisotropy. Using rigorous analysis, Knüpfer and collaborators identified the critical scaling at which the phase transition from a single domain state to multi-domain states occurs. Moreover, they derived a two-dimensional effective model in the single domain regime and a scaling law for the minimal energy in the multidomain regime.

Free Boundary and Obstacle Problems

Cagnetti, Gravina, and Rüland talked about free boundary and thin obstacle problems. Many problems in imaging, materials science, physics, and other areas can be described by partial differential equations that exhibit apriori unknown sets, called free boundaries, such as interfaces and moving boundaries. The study of such sets occupies a central position in such problems. A classical example is the one-phase free boundary problem studied by Alt and Caffarelli in [2], to be precise,

$$\begin{cases} \Delta u = 0 & \text{in } \Omega \cap \{u > 0\}, \\ u = 0 & \text{on } \Omega \cap \partial\{u > 0\}, \\ |\nabla u| = Q & \text{on } \Omega \cap \partial\{u > 0\}, \\ u = u_0 & \text{on } \Gamma. \end{cases} \tag{10.0.6}$$

Here Ω is an open connected subset of $\mathbb{R}^N$ with locally Lipschitz continuous boundary and Q is a nonnegative measurable function. Solutions to (10.0.6) are critical points for the functional

$$J(u) := \int_\Omega \left(|\nabla u|^2 + \chi_{\{u>0\}} Q^2\right) dx, \quad u \in \mathcal{K}, \tag{10.0.7}$$

where $\mathcal{K} := \{u \in H^1_{\text{loc}}(\Omega) : u = u_0 \text{ on } \Gamma\}$, with $\Gamma \subset \partial\Omega$ a measurable set with $\mathcal{H}^{N-1}(\Gamma) > 0$ and $u_0 \in H^1_{\text{loc}}(\Omega)$ a nonnegative function satisfying $J(u_0) < \infty$. The equality $u = u_0$ on Γ is in the sense of traces. Under the assumption that Q is a Hölder continuous function satisfying

$$0 < Q_{\min} \leq Q(x) \leq Q_{\max} < \infty, \tag{10.0.8}$$

Alt and Caffarelli proved local Lipschitz regularity of local minima and showed that the free boundary $\partial\{u > 0\}$ is a $C^{1,\alpha}_{\text{loc}}$ regular curve in Ω if $N = 2$, while if $N \geq 3$ they proved that the reduced free boundary is a hypersurface of class $C^{1,\alpha}_{\text{loc}}$ in Ω, for some $0 < \alpha < 1$. The regularity of the free boundary is strongly related to the assumption $0 < Q_{\min} \leq Q(x)$. Indeed, in the special case in which $\Omega = R \times (0, \infty)$, with $R \subset \mathbb{R}^{N-1}$ a cube, $Q(x) = (h - x_N)_+$, $u_0(x) = (m - x_N)_+$, and $Q \times \{0\} \subset \Gamma$, the free boundary problem (10.0.6) is related to water waves and to Stokes' conjecture of water waves of greatest height (see [29] and the references therein). In his talk, Ph.D. student Giovanni Gravina (Carnegie Mellon University) showed that by taking $\Gamma = (Q \times \{0\}) \cup (\partial Q \times (\gamma, \infty))$ minimizers of (10.0.2) are not one-dimensional for a suitable choice of the parameters m and γ. This is a first crucial step towards a variational proof of Stokes' conjecture (see [20], see also [13]).

The speaker Angkana Rüland (Max Planck Institute for Mathematics, Leipzig) discussed higher regularity of the free boundary for the thin obstacle problem with variable coefficients, to be precise

$$\sum_{i,j=1}^{N} \int_{B^+} a_{ij} \partial_i u \partial_j u \, dx$$

in $\mathcal{K} := \{u \in H^1(B^+) : u \geq 0 \text{ on } B' \times \{0\}\}$, where $B^+ := B(0,1) \cap \{x_N > 0\}$ and $B' := \{x' \in \mathbb{R}^{N-1} : |x'| < 1\}$, and the coefficients a_{ij} are symmetric, satisfy standard uniform ellipticity conditions, and are sufficiently regular. Together with her collaborators in [22] she proved that if the coefficients a_{ij} belong to $W^{1,p}$ for $p > N$, then the regular free boundary is of class $C^{1,1-N/p}$, while if the coefficients a_{ij} belong to $C^{k,\alpha}$ for $k \in \mathbb{N}$ and $\alpha \in (0,1)$, then the regular free boundary is of class $C^{k,\alpha}$, and, finally, that if the coefficients a_{ij} are analytic, then so is the regular free boundary.

Gradient Flows and Abstract Evolution Equations

The speakers Dal Maso, Fusco, Lu, Morini, Savaré discussed about gradient flows and abstract evolution equations with applications to crystalline mean curvature flows, epitaxial growth, and wave equations in time-dependent domains.

The variational notion of minimizing movements was introduced by De Giorgi in [9] to present a general and unifying approach to a large class of evolution problems. Given a topological space X, a functional $\Phi : (0,\infty) \times X \times X \to \mathbb{R}$, an initial datum $u_0 \in X$, and a discrete time step $\tau > 0$, one looks for sequences $\{u_\tau^n\}_n$ such that $u_\tau^0 = u_0$ and u_τ^n is defined recursively as the minimizer of the functional

$$x \in X \mapsto \Phi(\tau, x, u_\tau^{n-1}),$$

if it exists. Setting

$$u_\tau(t) := \begin{cases} u_\tau^0 & \text{if } t = 0, \\ u_\tau^{n-1} & \text{if } (n-1)\tau < t \leq n\tau,\ n \in \mathbb{N}, \end{cases}$$

a function $u : (0,\infty) \to X$ is called generalized minimizing movement associated to Φ and u_0 if there exist a subsequence $\{\tau_k\}_k$ such that $\tau_k \to 0^+$ and corresponding functions $u_{\tau_k} : (0,\infty) \to X$ such that $u_{\tau_k} \to u$ pointwise in $(0,\infty)$.

In [9] De Giorgi conjectured that if $X = \mathbb{R}^N$, $\phi : \mathbb{R}^N \to \mathbb{R}$ is a continuously differentiable and Lipschitz function, and $u_0 \in \mathbb{R}^N$, a function $u \in C^1([0,\infty); \mathbb{R}^N)$ is a solution of the Cauchy problem for the gradient flow

$$\begin{cases} u'(t) = -\nabla\phi(u(t)), \\ u(0) = u_0, \end{cases}$$

if and only if there exist a family of Lipschitz continuous functions $\phi_\tau : \mathbb{R}^N \to \mathbb{R}$, $\tau > 0$, such that $\mathrm{Lip}(\phi_\tau - \phi) \to 0$ as $\tau \to 0^+$ and u is the generalized minimizing movement associated to the function

$$\Phi(\tau, x, y) := \frac{1}{2\tau}|x-y|^2 + \phi_\tau(x), \quad \tau > 0, \quad x, y \in \mathbb{R}^N.$$

In his blackboard talk Giuseppe Savaré (University of Pavia) described how he solved this conjecture in [12].

The speaker Gianni Dal Maso (SISSA, Italy) discussed second order abstract evolution equations in moving domains of the form

$$\begin{cases} u''(t) + Au(t) = 0 & \text{for a.e. } t > 0, \\ u(t) \in V_t & \text{for a.e. } t > 0, \\ u(0) = u_0,\ u'(0) = u_1. \end{cases}$$

Here $\{V_t\}_t$ is an increasing sequence of spaces contained in a common Hilbert space H, $u_0 \in V_0$, $u_1 \in H$, and A is a linear continuous and coercive operator mapping V_t into its dual V_t'. In applications to fracture mechanics, $H = L^2(\Omega)$ with $\Omega \subset \mathbb{R}^N$ and $V_t = H^1(\Omega \setminus \Gamma_t)$, where Γ_t is an $(N-1)$-dimensional closed set representing the crack at time t. Existence of weak solutions is obtained in [7] using an approach suggested by De Giorgi and developed by Serra and Tilli for the wave equation. Weak solutions are obtained as limits of minimizers of the family of functionals

$$\mathcal{F}_\varepsilon(u) = \frac{1}{2}\int_0^\infty e^{-t/\varepsilon}(\varepsilon^2\|u''(t)\|_H^2 + a(u(t), u(t)))\,dt$$

defined on an appropriate space.

The speaker Nicola Fusco (University of Naples) discussed a surface diffusion problem of the type

$$V_t = \kappa\Delta_{\Gamma_t}(\mathrm{div}_{\Gamma_t}\nabla\varphi(\nu_t) - W(E(u_t))),$$

which describes the evolution of voids in a crystalline material. Here φ is the anisotropic surface density, Γ_t is the evolving surface, $E(u_t)$ is the trace of the infinitesimal strain at time t, and Δ_{Γ_t} and div_{Γ_t} are the tangential Laplacian and divergence. This evolution equation is the gradient flow with respect to H^{-1} of the energy

$$F \mapsto \int_{\Omega\setminus F} W(E(u))\,dx + \int_{\partial F}\varphi(\nu_F)\,ds,$$

where F is the void. In the recent paper [18] it was proved that if the initial configuration is stable then the solution exists for all time. This is the first existence result for this type of geometric motion without the presence of a higher order regularizing term involving the curvature in the energy.

The speaker Morini (University of Parma) considered the gradient flow of the same anisotropic surface energy $F \mapsto \int_{\partial F} \varphi(\nu_F)\, ds$ with respect to L^2. This gives rise to the motion by mean curvature

$$V_t = -m(\nu_t)\kappa_{F_t},$$

where $m(\nu_t)$ is the mobility and k_{F_t} is the mean curvature, which can be written as $\kappa_{F_t} = \operatorname{div}_{\Gamma_t} \nabla\varphi(\nu_t)$, when F_t is smooth. The well-posedness and the validity of the maximum principle for this type of evolution equations had been a long standing open problem, which was finally solved in [5].

Phase Transitions Problems

The speakers Davoli, Hagerty, and Murray addressed various problems in liquid-liquid and solid-solid phase transitions. The prototype for these kind of singularly perturbed problems is the van der Walls–Cahn–Hilliard theory of phase transitions. Consider a fluid confined into a container $\Omega \subset \mathbb{R}^N$. Assume that the total mass of the fluid is m, so that admissible density distributions $u : \Omega \to \mathbb{R}$ satisfy the constraint $\int_\Omega u(x)\, dx = m$. The total energy is given by the functional $u \mapsto \int_\Omega W(u(x))\, dx$, where $W : \mathbb{R} \to [0, \infty)$ is the energy per unit volume. Assume that W supports two phases $a < b$, that is, W is a double-well potential, with

$$\{z \in \mathbb{R} : W(z) = 0\} = \{a, b\}. \tag{10.0.9}$$

Then any density distribution u that renders the body stable in the sense of Gibbs is a minimizer of the following problem

$$\min\left\{ \int_\Omega W(u(x))\, dx : \int_\Omega u(x)\, dx = m\right\}. \tag{10.0.10}$$

If $a|\Omega| < m < b|\Omega|$, then given any measurable set $E \subset \Omega$ with

$$|E| = \frac{m - a|\Omega|}{b - a}, \tag{10.0.11}$$

the function $u = b\chi_E + a\chi_{\Omega\setminus E}$ is a solution of problem (10.0.10). This lack of uniqueness is due the fact that interfaces between the two phases a and b are not penalized by the total energy. The physically preferred solutions should be the ones that arise as limiting cases of a theory that penalizes interfacial energy, so it is expected that these solutions should minimize the surface area of $\partial E \cap \Omega$.

In the van der Walls–Cahn–Hilliard theory of phase transitions, the energy depends not only on the density u but also on its gradient, precisely,

$$G_\varepsilon(u) := \int_\Omega (W(u) + \varepsilon^2|\nabla u|^2)\, dx, \quad u \in H^1(\Omega). \tag{10.0.12}$$

Note that the gradient term penalizes rapid changes of the density u, and thus it plays the role of an interfacial energy. Stable density distributions u are now solutions of the minimization problem

$$\min\left\{\int_\Omega (W(u) + \varepsilon^2|\nabla u|^2)\, dx\right\}, \tag{10.0.13}$$

where the minimum is taken over all smooth functions u satisfying $\int_\Omega u(x)\, dx = m$. In 1985 Gurtin conjectured that the limits, as $\varepsilon \to 0$, of solutions u_ε of (10.0.13) are solutions u_0 of (10.0.10) with minimal surface area, that is, if $u_0 = a\chi_{E_0} + b\chi_{\Omega\setminus E_0}$, then

$$\text{surface area of } E_0 \le \text{surface area of } E \tag{10.0.14}$$

for every measurable set with $|E| = \frac{m-a|\Omega|}{b-a}$. Moreover, he also conjectured that

$$G_\varepsilon(u_\varepsilon) \sim \varepsilon \text{ surface area of } E_0. \tag{10.0.15}$$

Using results of Modica and Mortola this conjecture was proved independently for $N \ge 2$ by Modica [27] and by Sternberg [31] using Gamma-convergence.

In his talk Ryan Murray (Penn State) presented the solution of a long standing open problem, the asymptotic development of order 2 by Gamma-convergence of the mass-constrained Cahn–Hilliard functional (10.0.12) (see [25]) and its applications to the slow motion of interfaces for the mass preserving Allen–Cahn equation and the Cahn–Hilliard equations in higher dimension.

The corresponding problem for gradient vector fields, where in place of G_ε we introduce

$$I_\varepsilon(\boldsymbol{u}) := \int_\Omega \left(W(\nabla \boldsymbol{u}) + \varepsilon^4 |\nabla^2 \boldsymbol{u}|^2\right) \, d\boldsymbol{x}, \quad \boldsymbol{u} \in W^{2,2}\left(\Omega; \mathbb{R}^d\right),$$

arises naturally in the study of elastic solid-to-solid phase transitions. Here $\boldsymbol{u} : \Omega \to \mathbb{R}^d$ stands for the deformation. One of the main differences with the functional G_ε is that in the case of gradients, some geometrical compatibility conditions must exist between the wells. The speaker Elisa Davoli (University of Vienna), in collaboration with the speaker Manuel Friedrich (University of Münster) considered in dimension $N = 2$ the modified functional

$$J_\varepsilon(\boldsymbol{u}) := \int_\Omega \left(W(\nabla \boldsymbol{u}) + \varepsilon^4 |\nabla^2 \boldsymbol{u}|^2 + \varepsilon^2 \eta_\varepsilon^2 (|\partial^2_{11} \boldsymbol{u}|^2 + |\partial^2_{12} \boldsymbol{u}|^2)\right) \, d\boldsymbol{x}, \quad \boldsymbol{u} \in W^{2,2}\left(\Omega; \mathbb{R}^d\right),$$

where the new term $|\partial^2_{11} \boldsymbol{u}|^2 + |\partial^2_{12} \boldsymbol{u}|^2$ represents a penalization in the direction e_2 and $\eta_\varepsilon \to \infty$ as $\varepsilon \to 0^+$. The main result obtained were a two-well rigidity estimate, compactness of equibounded sequence, and the characterization of the effective limiting model, where the effective linearized energy involves elastic energy as well as two surface terms, one for the jumps of ∇u , which represent the energy associated to single phase transitions between the wells A and B. The second surface term corresponds to two consecutive phase transitions with a small intermediate layer. It enters the energy functional with double cost with respect to single phase transitions.

Plasticity and Fracture

One of the major subjects of the workshop was the study of failure phenomena in solids, such as plasticity, crack propagation, damage, and their microscopic mechanisms.

Plasticity is the property of a material that can undergo permanent deformations in response to an applied force. In the last decade the mathematical treatment of plasticity at the continuum scale has received a renewed interest, motivated by a change of perspective. While in the seminal work [52] quasistatic evolution was seen as the limit of viscoplastic evolutions when the viscosity parameter tends to zero, in [6] the classical theory of Prandtl-Reuss plasticity was revisited within the modern framework of rate-independent systems [26]. The advantage of this formulation is that quasistatic evolution is now viewed as a time-parameterized family of minimization problems, so that very mild regularity is needed in the definition of solutions and variational methods can be used to prove existence.

Dynamic evolution in plasticity was discussed in the talk by Jean-François Babadjian (Paris Orsay). On the one hand, using variational methods, one can show that the problem of dynamic perfect plasticity is well-posed in a suitable measure theoretic setting. On the other hand, the problem can be formulated as a constrained boundary value Friedrichs' system. He showed that the variational solution coincides with the unique entropic solution of the hyperbolic formulation and, owing to the finite speed propagation property, he established a new short time regularity result for the solution.

Plasticity in metals is considered to be the macroscopic consequence of the presence (and motion) of curve-like defects in the atomic structure, called dislocations: plastic deformation is the overall result of the relative slip of atomic layers, which is favored by the presence of dislocations. Any predictive theory of plasticity at the continuum scale should therefore take into account the presence and the motion of these defects. Although several models are available in the engineering literature to describe the dislocation behavior at the microscopic scale, it is not yet clear how to include the effect of their presence and motion in a model at the macroscopic level. In the last years this issue has been the object of intense research in the engineering and in the mathematical community. In particular, the approach by Gamma-convergence has led to rigorous upscaling results, both in the static and in the evolutionary setting, see, e.g., [1, GLP, 28]. However, these contributions, as well as the majority of the mathematical literature, only apply to an idealized setting, where dislocations are modeled as straight and parallel lines. Although the mathematical challenges are still numerous, this modeling assumption strongly reduces the complexity of the problem: in reality dislocations are curves in three dimensions, that typically form loops, entangle with one another, and get pinned at obstacles. Janusz Ginster (Carnegie Mellon University) presented a very recent work, where the equilibrium problem for a curved dislocation line in a three-dimensional domain is considered. Using a core radius regularization and sending the core radius to zero, he derived an asymptotic expression for the induced elastic energy. He then deduced the expression of the force acting on the dislocation line by computing the variation of the induced elastic energy. In his lecture Georg Dolzmann (University of Regensburg) discussed how to describe crystals with one active slip system in a continuum plasticity model.

Fracture processes have been widely studied in the last twenty years, starting from the pioneering work of Griffith and the variational approach of Francfort-Marigo [14], where crack evolution is determined through a competition between the surface energy spent to increase the crack and the corresponding release of the bulk elastic energy. Damage corresponds to the worsening of the elastic properties of a material as a consequence of applied stresses. There is an obvious connection between damage and fracture: on the one hand, a large number of microcracks may weaken the elastic properties of the material; on the other hand, concentration of damage may macroscopically results in a fracture. The classical phase-field approximation result of the Mumford-Shah functional by Ambrosio-Tortorelli [3] can be reinterpreted in this spirit, where the phase-field variable describes the local amount of damage. An overview on this topic was given in the talk by Marco Caroccia (Lisbon), who also reported on a new approximation result for a fluid-driven fracture model. The speaker Flaviana Iurlano (University of Paris 6) showed existence of strong minimizers for the Griffith model in the formulation by Francfort and Marigo, in the framework of linearized elasticity. A strong minimizer is a minimizer given by a function defined in an open set with a closed discontinuity set of codimension one. What makes this variational problem hard to tackle is that its natural formulation takes place in the space SBD of special functions with bounded deformation, where standard approximation methods based on truncation and on the coarea formula do not apply. In the recent paper [4] it was shown that SBD functions with small jump sets are close in energy to functions which are smooth in a slightly smaller domain. This result is a key ingredient in proving existence of strong minimizers for the Griffith's problem and may prove useful in several applications, including the study of quasistatic crack evolution.

Thin Structures and Pattern Formation

Since the beginning of research in elasticity a large body of work has been devoted to the justification of lower dimensional theories for thin structures in terms of the fully three-dimensional theory. A thin structure is a three-dimensional body, whose thickness in one or two directions is very small compared with the remaining dimensions, such as a rod, a membrane, a plate, or a shell. These kinds of structures are ubiquitous in the physical world. A precise understanding of the laws governing their equilibrium configurations is therefore crucial in a large number of applications, ranging from aerospace and civil engineering to biology.

In the classical approach lower dimensional theories are usually obtained by formal asymptotic expansions, and hence their range of validity is typically unclear. In the early 90's a rigorous approach based on Gamma-convergence has emerged and, starting from the seminal papers [16, 17], has led to the identification of a hierarchy of limit models for plates, rods, and shells. In his talk Marco Morandotti (Technical University Munich) discussed how to perform dimension reduction within the framework of structured deformations. Structured deformations [10] provide a rich geometrical setting that includes not only the smooth, classical deformations that underlie much of solid mechanics, but also the piecewise smooth deformations that describe macroscopic cracking in fracture mechanics, as well as the complex combination of macroscopic and microscopic changes relevant for the study of crystals with defects and granular materials.

Recently, there has been a growing interest in the study of prestrained elastic plates, that is, plates that do not have a stress-free configuration. These plates, also known as non-Euclidean plates, can be generated via growth, plastic deformation, or active swelling, which are nonuniform across the sheet. Within the formalism of incompatible elasticity such nonuniform deformations prescribe a non-Euclidean reference metric field on the plate. Because of this geometric incompatibility non-Euclidean plates assume non-trivial equilibrium configurations in the absence of exterior forces or imposed boundary conditions. This is a desired property in applications, for instance in the design of self-shaping bodies. Mathematically, minimizing the elastic energy for a non-Euclidean plate corresponds to the question of finding the "most isometric" immersion of a Riemannian manifold into another one of the same dimension. The speaker Cy Maor (University of Toronto) showed how this question relates to a generalization of Reshetnyak's rigidity theorem to Riemannian manifolds.

Another topic of the workshop was the study of energy-driven pattern formation in thin sheets. In the last years the wrinkling of thin elastic sheets has attracted a lot of attention in both the mathematics and the physics communities. A general feature of these problems is that wrinkling arises as an energetically preferable alternative to compression. In particular, a growing literature is developing on the scaling law of the elastic energy, i.e., its dependence on the sheet thickness h, for problems involving wrinkling. Wrinkled configurations can be viewed as (local) minimizers of a suitable elastic energy E^h, consisting of a non-convex membrane energy plus a higher order singular perturbation representing bending energy. It is intuitively clear that the bending energy is small in h: stretching a thin sheet ought to take much more energy than bending it. On the other hand, the membrane energy alone is non-convex, so, if the bending energy is ignored, then there might not exist a minimizer. Computing the relaxed energy gives partial information about the minimizers of E^h, but any feature that vanishes in the limit $h \to 0$ is invisible to the relaxed problem. This is where energy scaling laws may prove useful to have more quantitative bounds on the minimal energy and on fine properties of the wrinkles. In the talk by Ethan O'Brien (Carnegie Mellon University) a specific system in the mechanics of thin elastic sheets was explored [23], in which geometry and loading conspire to generate fine-scale wrinkling, and the optimal energy scaling was determined.

Pattern formation in graphene was the subject of the talk by Manuel Friedrich (University of Münster). Graphene is a one-atom thick layer of carbon atoms arranged in a regular hexagonal lattice. Despite the progressive growth of experimental, computational, and theoretical understanding of graphene, the accurate description of its fine geometry is still elusive. Observations on suspended samples seem to indicate that graphene is generally not exactly flat but gently rippled. On the other hand, free graphene samples in absence of support have the tendency to roll-up in tube-like structures. Friedrich reported on a recent work [15], where a complete classification of ground-state deformations of the hexagonal lattice with respect to configurational energies including two- and three-body terms was provided. He showed that all energy minimizers are either periodic in one direction, as in the case of ripples, or rolled up, as in the case of nanotubes. For suspended samples the analysis can be further refined and the emergence of wave patterning can be proved.

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Chapter 11

Adaptive Numerical Methods for PDEs with Applications (18w5148)

May 27 - June 1, 2018

Organizer(s): Christopher J. Budd (University of Bath), Ronald D. Haynes (Memorial University of Newfoundland), Weizhang Huang (University of Kansas)

Overview

Scientific computing is an increasingly important tool in many areas of science and engineering. By simulating models of physical phenomena on a computer we can, for example, gain insight into processes that are difficult or impossible to measure experimentally. Such computations can be used to verify or guide theoretical explorations. Here we are driven by physical solutions which would require prohibitive computational resources if implemented in a naive way. The solutions evolve on disparate space and time scales requiring techniques which self adapt and direct computational resources to the regions of interest.

Adaptive moving mesh methods have received increasing attention from researchers and practitioners over the last two decades. These methods, either used as stand-alone methods or combined with other adaptive mesh methods, are capable of producing meshes of good quality (smoothness and alignment), and meshes which resolve the features of interests in the physical solution with significant increases in accuracy whilst reducing the computational cost. Capitalizing on the recent progress, there is a continuing effort to improve the efficiency of existing methods and to implement these approaches in numerical solvers for application problems of interest.

Loosely speaking, there are three types of adaptive mesh methods, h-, p-, and r-adaptive methods. h-adaptive methods achieve adaptivity by adding and deleting mesh points and swapping mesh edges/faces while p-adaptive methods do so by adjusting the order of solution approximation over mesh elements. On the other hand, r-adaptive methods, also called adaptive moving mesh methods or more simply, moving mesh methods, achieve desired adaptivity by relocating or moving mesh points. The mesh connectivity is kept fixed during mesh movement; nevertheless, the mesh points can be reconnected between time steps or iterations. Adaptive moving mesh methods can be used alone or combined with h- and p-adaptive methods. It should be pointed out that Lagrangian methods and arbitrary Lagrangian-Eulerian (ALE) methods in computational fluid dynamics are special types of adaptive moving mesh methods. Moreover, mesh smoothing methods such as Laplacian smoothing and optimization-based smoothing methods employed in mesh generation and mesh refinement can be viewed as a type of moving mesh method although their goal is to improve mesh quality.

Whilst h-adaptive methods are now mature in their development, the newer r-adaptive methods show much promise, and have certain advantages in that they have much less complex data structures, can be easily coupled to legacy codes, they are well suited to problems with moving boundaries and/or Lagrangian structures, and often result in much more regular meshes. However, they have yet to realise their full potential on seriously large problems and need to be mapped effectively to many-core computing technologies.

The time is ripe for a careful appraisal of these methods and to plan for their future development and adoption. This was the aim for this meeting.

Meeting Particulars

This five day workshop attracted 37 participants which included 10 females and 6 graduate students. The five days included 25 talks of varying length (keynote and contributed talks) as well as an evening whole group brainstorming and planning session.

The meeting saw leading experts in the design and application of r-adaptive methods address the following topics:

- The effectiveness and design of mesh movement strategies to adapt to a function (which may be a solution of a PDE) to minimize interpolation/truncation error or satisfy other considerations. Deriving rigorous results to show that this has been achieved.
- The effectiveness and design of mesh movement associated with changes in the physical domain (free or moving boundary problems) or problems with complex boundary conditions.
- Mesh movement for better mesh quality (mesh smoothing, used in mesh refinement and quality improvement).
- Mesh rezoning in ALE methods (Arbitrarily Lagrangian-Eulerian in computational fluid dynamics).
- Coupling mesh movement to the solution of an evolving PDE. In particular effective strategies for dealing with large scale advection dominated problems.
- Preservation of qualitative solution properties (such as conservation laws, geostrophic balance) under mesh movement strategies.
- Mesh movement on manifolds.
- Computing adaptive meshes with global quality effectively on many–core compute technologies.

The brainstorming session included a discussion on the future of the research area and larger research community in adaptive meshing and r-refinement. This included discussion about

- The development of effective test problems suitable for a wide variety of adaptive meshes, and a comparison of techniques on large scale application problems.
- A permanent website for the research community to share research papers, computer codes, and meeting announcements.

The central goal of this event was to encourage participants to join their expertise for the mutual benefit of developing, testing, appraising and designing, effective moving mesh methods which can be used on challenging problems in the future.

Presentation Highlights

The complete list of talks and abstracts are available on the BIRS website. Here we mention a small sample of a few highlights.

Mikhail Shashkov, a senior researcher in the field, gave a talk entitled Adaptive reconnection-based Arbitrary Lagrangian-Eulerian method. In this talk he presented a new adaptive reconnection-based Arbitrary Lagrangian Eulerian method. This method includes an explicit Lagrangian phase on arbitrary polygonal meshes in which the solution and positions of grid nodes are updated; a rezoning phase in which a new grid is defined - both number of cells and their locations as well as connectivity (based on using Voronoi tessellation) of the mesh are allowed to change; and a remapping phase in which the Lagrangian solution is transferred onto the new grid.

A post-doc Andrew McRae talked about Mesh adaptivity on the sphere using optimal transport, and a moving mesh scheme for the nonlinear shallow water equations. Here the mesh is obtained as the solution of a Monge-Ampere equation, a scalar nonlinear elliptic PDE. This optimal transport approach also generalizes naturally from Euclidean space to manifolds such as the sphere. This method is applied to a finite element shallow water model, as needed in global numerical weather prediction.

In An adaptive moving mesh method for geometric evolution laws and bulk-surface PDEs, John Mackenzie considers the adaptive numerical solution of a geometric evolution law where the normal velocity of a curve in two-dimensions is proportional to its local curvature as well as a general non-geometric driving force. An interface tracking approach is used which requires the generation of a moving mesh. He then considers the generation of bulk meshes for the solution of bulk-surface PDEs in time-dependent domains. The moving mesh approach is then applied to a range of problems in computational biology including image segmentation, cell tracking and the modelling of cell migration and chemotaxis.

Graduate student Avary Kolasinski's talk A surface moving mesh method based on equidistribution and alignment provides an algorithm to improve the quality of the mesh on a surface using a moving mesh method. She constructs a surface moving mesh method based on mesh equidistribution and alignment conditions. She studies various numerical examples using both the Euclidean metric and a Riemannian metric.

In Optimal transformation-based adaptive grids, Paul Zegeling discusses stationary optimal grids for singularly perturbed boundary-value problems. An optimal time-dependent transformation for monotone traveling wave solutions will be proposed. This type of transformation is related to a perturbed method of characteristics. In the final part of the talk, fractional-order differential equations were considered with a discussion of the generation of efficient adaptive grids for these problems.

Jens Lang's talk Adaptive moving meshes in large eddy simulation for turbulent flows discussed adaptive moving mesh methods for the Large Eddy Simulation (LES) for turbulent flows. The characteristic length scale of the turbulent fluctuation varies substantially over the computational domain and has to be resolved by an appropriate numerical grid. The monitor function, which is the main ingredient of a moving mesh method, is determined with respect to a quantity of interest (QoI). These QoIs can be physically motivated, like vorticity, turbulent kinetic energy or enstrophy, as well as mathematically motivated, like solution gradient or some adjoint-based error estimator. Results were presented for real-life engineering and meteorological applications.

A moving mesh finite difference method for non-monotone solutions of non-equilibrium equations in porous media by Hong Zhang presents a moving mesh finite difference method to solve a modified Buckley Leverett equation with a dynamic capillary pressure term from porous media. The effects of the dynamic capillary coefficient, the infiltrating flux rate and the initial and boundary values are systematically studied using a traveling wave ansatz and efficient numerical methods. The governing equation is discretized with an adaptive moving mesh finite difference method in the space direction and an implicit-explicit method in the time direction. In order to obtain high quality meshes, an adaptive time dependent monitor function with directional control is applied to redistribute the mesh grid in every time step, and a diffusive mechanism is used to smooth the monitor function.

Meeting Outcome

Moving mesh methods have passed its early development stage (proof-of-concept and algorithm development) and now the time has come for further mathematical justification, rigorous error analysis, development of more efficient and robust methods and implementations, and broader, more realistic, and large scale applications (for example, for problems in atmospherical sciences, computer science, petroleum engineering, aerospace engineering, and biology).

This was the first meeting in many years which brought together senior and up and coming researchers from diverse areas in the field of adaptive numerical methods for partial differential equations. A fantastic exchange of the latest research in the area resulted, as well as crucial planning for the future of the community.

Participants

Budd, Chris (University of Bath)
Chen, Shaohua (Cape Breton University)
Christara, Christina C. (University of Toronto)
DiPietro, Kelsey (University of Notre Dame)
Haynes, Ronald (Memorial University of Newfoundland)
Hill, Róisín (National University of Ireland Galway)
Huang, Weizhang (University of Kansas)
Hubbard, Matthew (University of Nottingham)
Jahandari, Hormoz (Memorial University of Newfoundland)
Kamenski, Lennard (Weierstrass Institute for Applied Analysis and Stochastics)
Kolasinski, Avary (University of Kansas)
Kopteva, Natalia (University of Limerick)
Lang, Jens (Darmstadt University of Technology)
Lindsay, Alan (University of Notre Dame)
Mackenzie, John (University of Strathclyde)
Madden, Niall (National University of Ireland Galway)
McRae, Andrew (University of Oxford / University of Bath)
Miedlar, Agnieszka (University of Kansas)
Muir, Paul (Saint Mary's University)
Qiu, Jianxian (Xiamen University)
Russell, Robert (Simon Fraser University)

Sarker, Abu Naser (Memorial University of Newfoundland)
Shashkov, Mikhail (Los Alamos National Laboratory)
Sheng, Qin (Baylor University)
Shontz, Suzanne (University of Kansas)
Spiteri, Raymond (University of Saskatchewan)
Stockie, John (Simon Fraser University)
Sun, Weiwei (City University of Hong Kong)
Tang, Huazhong (Peking University)
Van Vleck, Erik (Dept. of Mathematics, University of Kansas)
Walsh, Emily (University of West England)
Wang, Yanqiu (Nanjing Normal University)
Wang, Dawei (Memorial University of Newfoundland)
Williams, JF (Simon Fraser University)
Yang, Xiaobo (China University of Mining and Technology)
Zegeling, Paul (Utrecht University)
Zhang, Hong (Utrecht University)

Chapter 12

Hydraulic Fracturing: Modeling, Simulation, and Experiment (18w5085)

June 3 - 8, 2018

Organizer(s): Anthony Peirce (University of British Columbia), Andrew Bunger (University of Pittsburgh), Emmanuel Detournay (University of Minnesota), Egor Dontsov (University of Houston), Dmitry Garagash (Dalhousie University)

The past decade has seen a significant change in the global energy landscape, largely due to hydraulic fracturing (HF) that has made the extraction of hydrocarbons from gas-rich shale formations economically viable. This process has been enabled by new drilling technology that makes it possible to generate multiple hydraulic fractures from horizontal wells. The rapid expansion of this class of HF is creating concerns about its impact on the environment. Questions are also being raised whether hydraulic fractures could breach impermeable barriers that isolate aquifers from the hydrocarbon bearing formations, thus imperiling the supply of fresh groundwater, or whether they could induce significant seismic events. There are also concerns whether the engineering process has been designed to optimize the recovery of hydrocarbons. The lack of simulation tools that can provide realistic predictions of the geometry and hydraulic conductivity of the HF that have been created and a lack of techniques to characterize these fractures from *in situ* measurements is fueling these concerns. A BIRS workshop was therefore convened to gather input from industry practitioners as well as academic and industry researchers to accelerate the scientific development of the analysis tools required to address these concerns.

Overview of the Field

Despite a long series of investigations on the mechanics of fluid-driven fractures since 1950s, it is only over the last two decades that a coherent understanding of the critical mechanisms at play has emerged. It has been shown that the propagation of a hydraulic fracture is governed by strong nonlinearities associated with fluid flow in the fracture, non-local elastic deformation, fluid leak-off in the surrounding rock, and the fracture propagation criterion [3]. Indeed, even the simplest mathematical model for a single HF propagating in a homogeneous elastic medium involves a coupled system of degenerate nonlinear integro-partial differential equations with a complex multi-scale structure [4, 12, 5, 8, 9, 10, 11]. These equations also involve a singular free boundary problem, in which the front velocity can only be determined by evaluating a distinguished limit. Technical issues brought about by the strong nonlinearity and time-dependence of the governing equations, as well as those associated with the moving boundary problem have hindered the development of efficient computational algorithms to simulate [1, 15] (i) the propagation of multiple hydraulic fractures in complex media and (ii) the transport of proppant (e.g. sand) particles that are added to the injected fluid to create a permeable pathway for hydrocarbon extraction. In order to test these analytic and numerical models, considerable effort has been devoted to performing hydraulic fractures in well controlled laboratory experiments [14].

Recent Developments

Capturing the propagation, interaction, and possible intersection of multiple arbitrary fracture surfaces in a complex solid medium presents the numerical modeler with formidable challenges. Because of the considerable public interest, the development of new numerical models for this purpose has become an area of intense research. These models can be classified into two broad categories: continuum models that treat the solid and the fluid as continuous media [3] and discrete models that treat the solid as a collection of particles in a lattice connected by springs [2], and the fluid as either a continuum or as modeled explicitly as discrete particles. The classical approach to continuum HF modeling has considered boundary integral equation (BIE) formulations of explicit cracks in a homogeneous or piecewise homogeneous elastic medium. This approach has reached some maturity and can capture the multiscale behavior that takes place in the vicinity of the fracture tip [6], but is limited to linear elastic materials and rapidly loses its advantages when dealing with multiple interacting fractures and heterogeneous media. Fully coupled eXtended Finite Element Method (XFEM) models [7, 13] have also been developed that can model heterogeneous solid media and can capture multiscale behavior. However, since the BIE and XFEM formulations rely on explicit representation of fracture surfaces, capturing the propagation and intersection of these in 3D is challenging. Recently, a class of phase field [16] or smeared crack models has also been developed, in which fractures are not modelled explicitly but rather by distributed damage that is represented by a field variable. The primary advantage of both phase field and discrete models is that they are able to capture the evolution and interaction of complex fracture geometries with significantly less effort than the continuum models in which cracks are modelled explicitly. On the other hand, phase-field models are extremely computationally intensive as they involve the solution of a non-convex optimization problem at each time step. Moreover, due to the discrete nature of lattice models and the smeared-out damage representation of cracks by the phase-field approach, it is not clear whether these methodologies will be able, without using prohibitive computing resources, to capture the complex multiscale behaviour characteristic of HF when multiple physical processes compete to determine their evolution. Thus no one computational method is currently able, without further development, to capture all the required physical processes. It is also timely for an update on recent laboratory experiments involving more complex hydraulic fracture situations such as the simultaneous propagation of multiple HF.

Presentation Highlights

Since many of the presentations have been recorded and posted online and all the abstracts are available online we will keep our description of the presentations brief. We have grouped the presentations into seven categories: Industry Perspective, Interaction between HF and natural fractures, Multiple Fracture Interaction, Numerical Techniques (including: DDM/BEM, DEM, XFEM, FEM, Phase Field), The Tip Region, Near-Surface Hydraulic Fractures, Miscellaneous. There were eight industry representatives who gave six talks, there were twenty faculty researchers from universities of whom nineteen gave presentations, and twelve students or postdoctoral fellows of whom eleven gave presentations. All the presentations were thirty minutes in duration including at least five minutes for questions and discussion.

Two presentations were singled out as highlights by the attendees : 1) the analysis by Egor Dontsov of the transition of closely-spaced HF from 'pancake-shaped' fractures propagating in the viscous regime to 'Petal-shaped' HF propagating in the toughness regime, 2) the 3D capture, vizualization by student Will Steinhardt, and mechanism analysis by Shmuel Rubinstein of the formation of fracture steps behind the hydraulic fracture fronts in hydrogels.

1. Industry Perspective:
    - Sau-Wai Wong : HF modeling and design - a perspective on how things have changed from conventional to unconventional reservoirs.
    - Alexei Savitski: Outstanding challenges in modeling HF in unconventionals: What we know and what we cannot do.
2. Interaction between HF and natural fractures
    - Olga Kresse: A stacked height P3D fracture network model and a parallel planar algorithm for the accurate modeling of HF propagating in multiple layered materials.
    - Wei Fu: Crossing criteria at interfaces: HF influenced by spatially varying natural fracture properties.
    - Guanyi Lu: Subcritical crack growth and time dependent HF initiation and propagation.
3. Multiple Fracture Interaction
    - Andy Bunger: A Swarm Theory Framework for evaluating the suitability of models for predicting the simultaneous growth of multiple hydraulic fractures.

- Delal Gunaydin: Laboratory experiments involving the simultaneous propagation of multiple hydraulic fractures.
- Innokentiy Protasov: Simultaneous growth of multiple P3D HF

4. Numerical Techniques

   (a) Displacement Discontinuity (DDM)/Boundary Element Methods (BEM)

   - John Napier: An unstructured triangular mesh model
   - Egor Dontsov: FracOptima models demonstrating the transition for closely spaced HF from ‘pancake-shaped’ fractures propagating in the viscous regime to ‘Petal-shaped’ HF propagating in the toughness regime.
   - Anthony Peirce: The Implicit Level Set Method used in conjunction with the Extended Kalman Filter to monitor HF propagation using tiltmeter measurements.
   - Ali Rezaei: The fast multipole method used for the efficient modeling of HF propagation in a porous medium using the displacement discontinuity method.
   - Sergey Golovin: An efficient implementation of the Implicit Level Set Algorithm for modeling planar HF.
   - Denis Esipov: A direct boundary element simulator for 3D HF propagation.

   (b) Discrete Element Methods (DEM) - Lattice Models

   - Christine Detournay: “Nano-scale” experiments and upscaling - investigation of Kerogen’s effect on hydraulic fracturing using XSite.

   (c) eXtended Finite Element Method (XFEM)

   - Thomas-Peter Fries: Explicit/implicit XFEM crack description for HF with emphasis on transport models on curved crack surfaces.
   - Robert Gracie: How to build a stable and efficient sequential coupling schemes for HF simulation.

   (d) Finite Element Method (FEM)

   - Adrian Lew: Description of a Universal Mesh scheme to perturb FEM meshes to achieve high order accuracy to model thermally and hydraulically driven fractures.
   - Sergey Golovin: Crack propagation in poroelastic medium

   (e) Phase Field

   - Mary Wheeler: Diffusive Fracture Network representations in tight formations.
   - Sanghyun Lee: Phase field modeling for fracture propagation in porous media.
   - Erwan Tanne: A variational phase field model of HF.
   - Keita Yoshioka: A phase field hydromechanical model of reservoir simulation.

5. The Tip Region and Regimes of Propagation

   - Alena Bessmertnykh: Herschel-Bulkley fluid and the representation of proppant packing by a stress jump.
   - Fatima Moukhtari: A semi-infinite HF driven by a shear-thinning fluid.
   - Gennady Mishuris: Analysis of the fluid-induced shear-stress at the tip at the HF tip.
   - Will Steinhardt/Shmuel Rubinstein: Vizualization and instability at the HF front in hydrogels. The detailed investigation of the formation of ‘fracture steps’ behind the fracture front.
   - Dmitry Garagash: Is Linear Elastic Fracture Mechanics (LEFM) justified in hydraulic fracturing?

6. Near-Surface Hydraulic Fractures

   - Thomasina Ball: Magma-driven, gravity/bending and viscosity/toughness
   - Zhiqiao Wang: Universal tip solution - viscosity/toughness

7. Miscellaneous

   - Nancy Chen: Net Present Value Analysis - optimization of well and fracture placement.
   - Robert Viesca: Fluid-induced Faulting: aseismic slip - two asymptotic regimes.
   - Peter Grassl: Multiple cracks from a pressurized spherical cavity.
   - Erfan Sarvaramini: A continuum approach for stimulated rock volume.
   - Emmanuel Detournay: HF in very permeable rocks.

Scientific Progress Made

In addition to a considerable exchange of new ideas this workshop has stimulated a number of planned collaborations among the participants (see comments below). A significant benefit from a workshop like this is the opportunity it provides for students and postdoctoral fellows to meet and learn from researchers whose papers they have only read. This educational opportunity also enables the students to gain perspective on how their research fits into the 'big picture' of research initiatives in the field.

This workshop has fostered the formation of an international team of researchers and practitioners interested in moving the field forward. There was discussion of biennial or triennial meetings in different parts of the world. Indeed, there was an offer by the delegates from Novosibirsk to host such a workshop in 2019 to interact with Russian researchers who have been actively engaged in HF research the past few years.

Below are just a selection of comments solicited from attendees:

Comment from an industry participant:

"It was one of the most effective workshops I had ever attended. The topics discussed range from hydraulic fracture practitioner perspectives to nitty gritty details of various numerical and analytical methods. Diversity in the talks was certainly the key in this successful event. Yet, each day had a clear theme and these presentations on a coherent theme kept the story flow very smoothly. Last not but least, spending consecutive 5 days in somewhat isolated location helped enhance our intimate discussions with other experts and scholars in the field."

Faculty member comments:

1. "The combination of industry and academia was outstanding. It was an academic conference, primarily, but the presence of an active minority from industry kept the discussions honest and ensured we did not stray from the application that provides the reason for working on these problems in the first place.
2. I walked away with tangible benefits that include plans for 2 papers to be co-authored with various cohorts of colleagues from the conference, and my students and I were made aware of and provided with basic training on a powerful package of freely available analysis software that we are starting to use already.
3. The amazing surroundings, healthy lifestyle, and complete freedom from the worries of life provided by the conference center and staff were conducive to my own reflection on research. On the flight home and in the days that followed I outlined proposals on 2 new topics related to hydraulic fracturing.
4. One of my students reflected that this is the first time she really understood where her work fits within the global research community, and knowing the place of the work completely changes her motivation and approach going forward.
5. All of my students were surprised to see how much fun scientists have when they get together to discuss, argue, discover, and encourage together."

Selection of student comments:

1. "Thank you for organizing such an amazing workshop. This workshop brings together people who are conducting cutting edge researches on hydraulic fracturing from all around the world. It also provides a great opportunity to students to learn the most up-to-date knowledge about experiments and modeling in hydraulic fracturing. I am glad to have attended this workshop and have benefited a lot from all the presentations."
2. "I learned from and enjoyed every moment of this excellent workshop. Both the venue and location of the workshop were amazing, but what made this workshop more exciting for me was to meet all the people that I knew by name from their papers and contributions in the hydraulic fracturing field. I think the material presented in the workshop was a thoughtful combination of mathematics, numerical models, and experimental work in the field of hydraulic fracturing. In this sense, the workshop was on top of the edge and being delivered by experts in the field."
3. "Thank you for the invitation to the HF workshop. It was an excellent week of talks. For myself as a PhD student, it was a great opportunity to chat with people in the field that I had read so much of the work of. In particular, talking to Emmanuel about our similar work on near-surface fractures. And also talking to Andy about some related solidification experiments that could be done to investigate magmatic intrusions (which excitingly I should be able to do soon!)."

Outcome of the Meeting

In response to the industry presentations and discussion participants agreed on the formation of a list of open problems/challenges that the newly-formed community can work on. It is anticipated that the various research groups will further develop the algorithms/techniques/experiments they are working on to try to address these problems. One exciting proposal among this list is the establishment of a modeling challenge that has come from practitioners in the field in which existing models fail to predict the outcome of an actual stimulation sequence. This challenge along with as much data as possible would be provided to participants a few months before the next workshop. As an extension of this idea, another participant proposed assembling an easily accessed data base of such modeling challenges.

List of Open Problems

1. The Sinkey Challenge: All future workshops should have a modelling challenge from industry that the modelers/analysts could try their codes/scalings on to see if they can explain the puzzling phenomenon. The proposers would preferably submit the description a while before with as much detail and data as possible.
2. Development of phenomenological models in HF similar to the diffuse damage models described by Mary Wheeler and Erfan Sarvaramini presented. Those models fit the present data which is scarce and the best we can hope for is: geological data, pump rates, mixtures, and finally, production rates. We have to work with this, and the hope for high-quality data in large quantities to verify regimes and influences from rheology, turbulence, etc.
3. Creation of a database of challenging HF stimulation cases from industry in which standard modeling failed to explain the phenomena observed. As much data as possible would be available to modelers in an easily accessible format.
4. The impact of material heterogeneity on hydraulic fracture predictions in physical and numerical settings. Heterogeneities could be at the grain scale (potentially impacting tip behavior), or at a larger, engineering scale.
5. Confirm the multiple crack results presented by a number of speakers in numerical and experimental studies.
6. Near wellbore issues. "Tortuosity" has been recognized for decades but very little is known about horizontal wells, and even for vertical wells there is no systematic theory for predicting, modeling, or deliberately modifying near wellbore tortuosity. Also, all models are static, while it is know that tortuosity is transient. This is a major area where little is known and industry believes is essential, perhaps more than any other single issue, to successful application.
7. Develop criteria to avoid the oscillation instabilities that arise in the modelling of simultaneously propagating, closely spaced, hydraulic fractures.

Participants

Adachi, Jose (Chevron)
Ball, Thomasina (Cambridge University)
Bessmertnykh, Alena (University of Houston)
Bunger, Andrew (University of Pittsburgh)
Chen, Nancy Shengnan (University of Calgary)
Detournay, Emmanuel (University of Minnesota)
Detournay, Christine (Itasca Minnesota)
Dontsov, Egor (University of Houston)
Esipov, Denis (Institute of Computational Technologies SB RAS)
Fries, Thomas-Peter (Graz University of Technology)
Fu, Wei (University of Pittsburgh)
Garagash, Dmitri (Dalhousie University)
Golovin, Sergey (Lavrentyev Institute of Hydrodynamics)
Gracie, Robert (University of Waterloo)
Grassl, Peter (University of Glasgow, School of Engineering)
Gunaydin, Delal (University Of Pittsburgh)
Kresse, Olga (Schlumberger)
Lecampion, Brice (EPFL)
Lee, Sanghyun (Florida State University)
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Chapter 13

Integrative cell models for disease intervention (18w5073)

June 10 - 15, 2018

Organizer(s): Matt Scott (University of Waterloo), Peter Swain (University of Edinburgh), Hans Othmer (University of Minnesota)

Biological processes do not occur in isolation and their appropriate execution requires communication and coordination across the cell. We know that signals are conveyed via interactions between proteins and between proteins and DNA, but such regulatory interactions are not the sole drivers of cellular responses. Changes in the physiological composition of the cell and particularly in the levels of common resources, such as energy and raw materials, also provides a higher level of regulation. The extent of the control provided by this potentially primordial regulation has only recently been appreciated. Yet its effects are felt widely, ranging from the development of antibiotic resistance to the production of chemicals in the biotechnology industry. The broad ambition of this workshop was to foster the development of a new mathematical framework for modelling cellular processes that includes global regulation, either implicitly or explicitly, and so enable quantitative prediction particularly focused on disease intervention.

Overview

Biological cells, whether as single-cell organisms or as part of a tissue, comprise many component subsystems, such as the nucleus and the mitochondria, and execute many processes, such as nutrient uptake, metabolism, biosynthesis, and gene expression, which interact to define the state and function of the cell. These components and processes typically are strongly interacting, but the traditional approach has been to study cellular systems under the implicit assumption that the component or process in question can be understood in isolation from the remaining ones, which merely provide a constant, background environment. This assumption was necessary to make progress in early investigations, but recent research has now shown that the assumption is weak, at best. In systems ranging from microbes to human cancers, the environment and growth rate can affect the level of expression both of single genes, even those with ‘constant’ unregulated gene expression, and of hundreds of genes across the entire genome.

Taken together, these developments question our understanding of cellular regulation and whether the biochemical networks in cells can be usefully decomposed into separate modules, the current paradigm in mathematical and systems biology. This fundamental limitation of existing methods becomes particularly acute in the mathematical modelling of disease states. The interdependence of cellular processes confounds disease modelling in two important ways. First, diseases can induce system-wide changes in gene expression making it difficult to distinguish proximal from distal causes. Second, a lack of modularization in cellular function makes the success of intervention strategies difficult to predict. Often brute-force elimination of what is thought to be the primary molecular cause of disease has no effect: the cell simply compensates through auxiliary and highly redundant channels. What is needed is an understanding of disease that transcends molecular mechanism to provide a system-level view of the phenomenon of how the complex interconnected networks integrate different signals to produce the observed outputs. Gaining this understanding requires mathematical models and new analytical techniques in order to integrate the effects of various levels of regulation and physiology.

Cell physiology imposes strong constraints on how the cell allocates its internal resources. Broadly speaking, to support rapid growth rates, the cell must devote a large fraction of its synthetic machinery to make more of that synthetic machinery. This allocation necessarily comes at the expense of producing other cellular constituents, such as proteins responsible for nutrient assimilation and for repair and maintenance of DNA. As a consequence, in addition to the local, point-to-point concept of regulation, there is a more diffuse and global layer arising from constraints that exist because of the allocation of cellular resources. This primordial regulation has a breadth and impact that could completely dominate local interactions. In other words, the information flow in a cell can be carried by 'signals' as commonly understood – concentrations of specific molecules – but also, perhaps more generally, by macrovariables of the physiological status of the cell. An important example arises in cancer, where the metabolic state both affects and is controlled by up-regulation of transporters and enzymes and by the micro-environment in which a cell finds itself. This can lead to supracellular integration of signals via a process called symbiotic metabolism, in which hypoxic cells produce more lactate that is used by non-hypoxic cells, thereby freeing glucose for cells in hypoxic regions of a tumour. The realization that this global level of control is important in cellular functioning calls for a new class of integrative models for cellular systems.

Quantitatively understanding such physiology-dependent disease modeling poses substantial challenges, both experimentally and particularly mathematically. We do not know what level of description of the 'rest of the cell' is appropriate; we do not know how to correctly connect existing models of different cellular phenomena; we do not know the best type of data to parameterize such modelling or have algorithms in place to carry out this parameterization; we do not even know which cellular processes are core and should be modelled.

Two distinct approaches to this context-dependent modelling are being developed. The first, which we will call coarse-grained modelling, has focused on phenomenological models that aim to capture sufficient information to answer questions of interest with a minimal mathematical description. These approaches have uncovered what appear to be fundamental growth 'laws' demonstrating apparent simplicity – such as linear dependencies on the growth rate – despite the underlying biological complexity [1]. The second methodology, which we will call fine-grained modelling, provides context by including as much of the cell as possible in the model. A recent triumph is the 'whole cell' model of *Mycoplasm genitalium*, a pathogenic bacterium with an unusually small genome, in which, in an engineering feat, models that operate at different spatial scales and over different time scales were linked together and coupled to data to produce a simulation that includes the majority of the biochemical processes we currently know exist in that cell type [2].

The goal of this workshop was to bring together practitioners of both the fine and coarse-grained methodologies along with numerical analysts and those working at the interface of context-dependent modelling with medicine and biotechnology. Our focus was on how physical and biological trade-offs at one level of organization constrain behaviour at other levels. By exploring how both methodologies might be integrated, how models at different scales may be formally combined, and how models might best be simulated and quantitatively compared with data, we aimed to provide the momentum and ideas to develop a framework for physiologically-dependent disease modelling that will drive the field of cellular mathematical biology for the foreseeable future. Different modelling strategies, ranging from Boolean to continuum models, were represented by participants.

The workshop was timely. Experimental advances are generating data on how cellular physiology changes because of both cell growth and human intervention, such as the additions of antimicrobials and of synthetic circuits. New biophysics now allows physiological variables, such as pH, ATP and NADH levels, and membrane potential, to be measured in single cells. Further, automation has led to high-throughput technology that measures physiological variables, such as biomass, pH, dissolved oxygen, fluorescent molecules, levels of NADH and NADPH, and volume, in tens of parallel bioreactors with either continuous or fed-batch growth or at the single-cell level in a so-called 'mother machine' [3]. Mathematical models do not yet exist to allow quantitative comparison with such data: a gap that this workshop aimed to fill.

In addition, context-dependent effects are hindering our understanding of the development of antimicrobial resistance and of tumour development. Models that include cellular physiology can predict growth rate, the standard measure of fitness for microbes. Such information is crucial if we are to reduce antibiotic and anticancer resistance because we have to understand how the molecular mechanisms that confer resistance also determine fitness. A better understanding of how cellular context affects disease and disease intervention at various levels will lead to significant advances in medicine, biology and the biotechnology industry, and our workshop was one step in that direction.

Presentation highlights

Matt Scott (U Waterloo) kicked off the workshop with an overview of physiological constraints on bacterial response to antibiotics [1]. Two cases studies were examined: the first connecting mechanistic parameters to the efficacy of chemical antibiotics [4]; the second connecting pre-infection growth state to susceptibility to phage infection. **Ting Lu** (U Illinois - UC) continued the theme of physiological constraints, but in the context of rational design of synthetic genetic elements in bacteria [5]. The goal is to standardize components to the extent that the design-build-test cycle so familiar in engineering can be efficiently implemented in synthetic biological systems. **David Umulis** (Purdue) showcased a variety of sophisticated mathematical and image-analysis tools he has created for tracking development in zebra fish embryos. These tools were decisive in discriminating a variety of proposed mechanisms for gene expression patterning in the developing embryo [6]. **Tomas Gedeon** (Montana State University) spoke about a generalized theoretical framework for converting large, poorly characterized mathematical models into tractable quasi-Boolean networks [7]. Within this framework, he is able to rapidly identify parameter regimes that are necessary to produce, for example, hysteretic trajectories in the full model [8]. Back-to-back talks in the evening rounded out the first day by returning to operating constraints in bacterial physiology. **Bas Teusink** (VU Amsterdam) presented joint theoretical and experimental work linking elementary-flux-mode analysis of metabolic networks with minimal-constraint criteria in flux balance analysis. Under general hypotheses, he was able to prove that the optimal number of elementary flux modes operating in steady-state are less-than-or-equal-to the number of constraints operating on the system [9]. **Frank Bruggeman** (VU Amsterdam) followed with an extension of the elementary-flux analysis to growth transitions. His object of study was the control structure that steers a bacterial system toward an optimal growth state. He was able, along with Planqué, to prove that the number of metabolites that bind regulator proteins is greater-to-or-equal to the number of environmental parameters to which the system is robust [10].

On the second day, **Edda Klipp** (Humboldt Berlin) spoke about her ambitious research program to create a comprehensive mathematical model of yeast growth, comprised of modular sub-systems characterizing metabolism, gene expression, cell cycle, volume growth, membrane transport and signalling [11, 12]. Moving from microorganisms to multicellular systems, **Hans Othmer** (U Minnesota) presented a mechanistic model for intercellular interactions in the wing disk development of Drosophila. Othmer and coworkers have constructed a detailed kinetic model to inform future experiments. Future work seeks to show that the model recovers both observed scale invariance and uniform growth across the disk. **Erik van Nimwegen** (Biozentrum, Basel) presented a large collection of single-cell data that challenges existing views of regulation in bacteria. First, the novel idea that regulators perform a 'noise-propagation' role in addition to their conditioned response [15]. Second, that the lag-time to respond to a nutrient shift (lactose) exhibits a long-tailed distribution at the single-cell level [14]. According to van Nimwegen, both noise-propagation and long-tailed response distributions serve an evolutionary purpose. **Carla Bosia** (Politecnico di Torino) presented experimental and theoretical work on the growth of human leukemia cells. Bosia uses inoculum size as a means of adjusting proliferation rate, but does not observe the same empirical relations coupling ribosome abundance and proliferation rate that are observed in bacterial systems. Returning to bacterial physiology, **Teuta Pilizota** (U Edinburgh) described a methodology using the flagellar motor of E. coli as an endogenous 'voltmeter' to track intracellular energy levels. This exciting technique was used to quantify the difference between indole and UV radiation damage.

The third day began with **Jia Gou** (U Minnesota) who spoke about theoretical work to both analyze and visualize the variety of possible patterns forming when three ligands compete for a single receptor. **Eldon Emberly** (Simon Fraser) presented examples of spatial organization in bacteria. The first focused on entropy-driven localization of protein aggregates [18, 16]. The second, more recent work using a diffusion-driven ratchet-walker model to analyze intracellular transport via the ParAB system [17]. The final talks of the day were devoted to antibiotic resistance in bacteria. **Mary Dunlop** (Boston U) presented exciting experimental data [20, 21] and mathematical modeling [19] that suggested that transient resistance to antibiotics (via stochastic induction of the MarAB system) predisposes populations to develop permanent resistance. **Rosalind Allen** (U Edinburgh) followed with experimental data and mathematical modeling showing the physiological consequences of cell-wall targeting antibiotics. Though still in the early stages, Allen's phenomenological model was able to recapitulate many of the unusual features of this much-prescribed class of antibiotics.

Kamila Larripa (Humboldt State) started off the fourth day reporting on an industry-driven effort to improve treatment of myeloma (a blood cancer). Larripa and collaborators have developed a mathematical framework to explore effects of specific drugs and their targets. **Luca Ciandrini** (U Montpellier) presented a mechanistic mathematical model of protein translation, based on prior work characterizing ribosome procession as a totally-asymmetric-simple-exclusion process. The work suggests that circularization of mRNA transcripts can lead to increased local concentration of recycling ribosomes and that this effect can be well-quantified by a simple model [22]. **Meriem el Karoui** (U Edinburgh) considered in detail the mechanistic and stochastic elements of DNA damage repair in E. coli. First, the DNA damage response appears to inherit growth-rate dependence from the physiology of the organism. Second, repair proteins repair in low basal abundance, yet the variability is far less than expected [23] – the reason for this is unknown. **Bruno Martins** (Cambridge) used experimental characterization of the circadian rhythms of the cyanobacterium Synechococcus elongatus to illustrate that population heterogeneity can obscure underlying strategies of cell-size homeostasis [25, 24]. Martins has developed a simple mathematical model to quantitatively account for the population heterogeneity. **Ariel Amir** (Harvard) concluded the fourth day with an ambitious survey of past and present mathematical models of bacterial growth and division. In contrast to classical work by Powell, Amir determines conditions under which variance in the division time can increase population growth rate [28, 26, 27].

Jim Greene (Rutgers) began the final day of the workshop with a focus on induced drug-resistance in chemotherapy. A simplified mathematical model was used to explore the control structure that optimizes treatment efficacy. Echoing many of themes of previous speakers, **Stefan Klumpp** (U Goettingen) provided an overview of work coupling bacterial physiology to population heterogenity. The survey included efforts to model the effect of cell growth as an additional pseudo-regulator [29], modulation of the inferred drug efficacy depending on whether the cells are grown in bulk or in a single-cell 'mother machine' '[30], and the physiological characterization of a Bacillus subtilus strain with reduced genome size. **Vahid Shahrezaei** (Imperial College London) presented several efforts to extend coarse-grained physiological models to fission yeast, as well as efforts to provide greater detail in the models [31, 32]. In the final talk, **Peter Swain** (U Edinburgh) outlined a graph-theoretical approach to enumerate and visualize the outcome of competitive evolutionary dynamics. The methodology enables incomplete information to be leveraged to obtain increasingly accurate prediction of the outcome of the competitive evolutionary dynamics [33].

Outcomes and open questions

The two major outcomes of the workshop were the recognition of the surprising similarity between bacterial and cancer models and to identify clear gaps in our knowledge of cell physiology.

As organizers, we deliberately chose participants who likely knew less than 20% of the other speakers. As a result, from side-by-side talks about cancer biology and antimicrobial resistance, it became clear that much of the framework of the mathematical modelling is common between these two very different systems.

Nonetheless, the incorporation of physiological constraints into mechanistic mathematical models is far more advanced in bacterial studies, whereas little in the way of robust empirical relationships linking proliferation rate and the macromolecular state have been established in cancer cell lines. Carla Bosia's work illustrates that one of the major obstacles is determining a reliable method to modulate proliferation rate.

The second major outcome was a broad recognition of how little is known about the coupling between cell growth and DNA replication, even in bacteria. In 2015, several groups used single cell data to establish that in E. coli, the size at birth (s_b) is related to the size at division (s_d) via an adder mechanism, $s_d = s_b + \Delta$, where Δ is a constant (though growth-rate dependent) increment of mass. The mechanism underlying this behaviour remains unresolved. A third of the participants formed an impromptu focus session to clarify the current state of the field. Unpublished data from the van Nimwegen group in particular suggests that the simple 'adder' model is inadequate.

Altogether, the open questions that emerged are:

1. How can we reliably modulate the proliferation rate of human cell lines in a way to sustain exponential growth over many generations?

2. Are the complex adaptations of cancer cell lines (e.g. the Warburg effect) the result of physiological constraints (as appears to be the case in bacteria [34])?

3. How are cell division and DNA replication coordinated in proliferating cells? (This has been an open question for fifty years.)

Participant response

Several of the participants remarked that this workshop was the most productive conference or workshop that they had ever attended. Some of these are reproduced below:

> I wanted to let you know how much I enjoyed the BIRS workshop. Thanks to that meeting I have already initiated two new collaborations (with Erik [van Nimwegen (Basel)] and Ariel [Amir (Harvard)]) and I have learned an enormous amount about both the models currently used for bacterial diseases and also about the potential similarities with models for cancer treatment and drug resistance in cancer (i.e. Kamila [Larripa (Humboldt)] and Jim's [Greene (Rutgers)] talks). I particularly enjoyed the format of the meeting with long talks that allowed for a lot of interactions between the speaker and the audience as well as enough free time to work with specific colleagues and to enjoy the magnificent surroundings. I think that the fact that we were a relatively small group also helped a lot with making the meeting very interactive: I think I had productive discussion with almost all the participants. Last but not least I was very impressed that the gender balance in the meeting was very good which in my experience is rarely the case. The facilities were excellent and the provision of small room with boards for discussion was particularly useful. I also enjoyed the swimming pool! In summary, this was the best meeting I have attended in a number of years. Thanks again for organizing this workshop!
>
> – Meriem el Karoui (U Edinburgh)

This was one of the best conferences I attended, for several reasons:

- The topic was focused enough such that my work has significant overlap with many of the participants. Nevertheless I have not met many of them previously and therefore this was extremely stimulating scientifically, both in terms of feedback and ideas related to my own work as well as learning about recent progress in the field.

- The program was organized in a way that allowed for many off-line discussions, which were often as useful as the formal talks. I hope to keep in touch with new people I met at BIRS, and I think that there is also a good chance that this conference will trigger new collaborations.

– Ariel Amir (Harvard)

The BIRS conference was a wonderful experience. I found it extremely useful to hear about work slightly peripheral to my own area of research, especially from senior and esteemed mathematicians. I work in cancer biology, but a number of mathematical techniques and models being used in bacterials systems are directly applicable to my project– this was wonderful to discover. This has opened up a number of potential directions I plan to pursue, and I have also found some wonderful collaborators. The group was extremely accomplished and I benefitted not just from listening to formal talks, but from the questions I received about my own work. Meals and breaks provided wonderful opportunities for discussion, and the small group size really encouraged this. Big thanks to the organizers and to BIRS for providing such a wonderful scientific program!

– Kamilla Larripa (Humboldt)

Participants

Allen, Rosalind (University of Edinburgh)
Amir, Ariel (Harvard University)
Bosia, Carla (Politecnico di Torino and Italian Institute for Genomic Medicine)
Bruggeman, Frank (VU University)
Ciandrini, Luca (University of Montpellier)
Dunlop, Mary (Boston University)
El Karoui, Meriem (University of Edinburgh)
Emberly, Eldon (Simon Fraser University)
Gedeon, Tomas (Montana State University)
Gou, Jia (University of Minnesota)
Greene, James (Rutgers University)
Iber, Dagamar (ETH Zurich)
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Chapter 14

Advanced Developments for Surface and Interface Dynamics - Analysis and Computation (18w5033)

June 17 - 22, 2018

Organizer(s): Yoshikazu Giga (University of Tokyo), Piotr Rybka (The University of Warsaw), Richard Tsai (The University of Texas at Austin and KTH)

Overview of the workshop themes

This workshop focused on advanced topics involving interfaces, thin domains around them and free boundary problems. These geometric objects are governed by nonlocal, singular or anisotropic motion laws. A particular topic was the partial differential equations (PDEs for short) defined in thin domains around moving interfaces. Effective numerical algorithms for simulating these problems was another leading theme of the workshop.

Some of the top specialists in analysis and numerical methods came to discuss recent advances in above mentioned problems and to present the state of the art both in analysis and numerical computations. The goal was to improve our understanding of the surface and interface dynamics. Below we present the overview of the presentations.

Nonlocal, anisotropic and degenerate diffusions equations The following groups of topics have been discussed during the workshop.

- PDE with singular diffusivity. Among the typical examples are total variation flows for denoising images or anisotropic curvature flows with very strong anisotropy such as crystalline curvatures. These flows describe motion of free surfaces. In these problems motion of surfaces is determined by nonlocal quantities which cannot be written in an explicit way. Even these relatively accessible problems analysis are nontrivial and have been studied for many years. However, if one considers more realistic problems like crystal growth models with general Wulff shape having facets, multi-grain problems or higher order problems involving crystalline mean curvature, mathematical tools are still limited.

  One method to treat these problems is the theory of viscosity solutions, whose scope of applicability is widening. It is based on comparison principle, hence it is restricted to formally 2nd order problems.

  The variational approach presents possibilities of developing another set of methods. But these methods have limitations since they require special structure of the variational models.

  Of course, there is a diffuse interface approach represented by use of reaction diffusion equations. However, the relation to sharp interface approach given above is often not clear, especially for multi-grain problems in materials science.

- Stefan problem with fractional time derivatives. Although the fractional diffusion equations have been studied, the problem of Caputo fractional time derivative is less developed and even simple questions, e.g. concerning existence of solutions, are outstanding. The nonlinear theory that is capable of handling this kind of free boundary problems (e.g. for the position of the head of fluvial sediments) is yet to be developed.

- Modeling and simulating crystal growth. This topic encompasses large networks of grains of different orientations, with grain boundaries moving according to certain notion of curvature.

Numerical algorithms The methodologies discussed in this workshop encompass non-parametric sharp interface models, such as level set methods or the closest point methods, and diffuse interface methods involving phase field approximation. However, the challenges presented in the problems discussed above require non-trivial mathematical formulations before one can apply the standard methodologies and careful numerical approximations in some cases to derive well-conditioned discrete systems.

Topics that have been discussed in this workshop include:

- Generalization of ℓ_1 optimization, augmentation and splitting based approaches for efficient accurate computation of singular diffusion problems.
- Numerical methods for PDEs on manifolds or thin domains around them. There has been significant development in numerical algorithms for PDEs or integral equations on implicitly or non-parametrically defined surfaces. These methods transform equations defined on surfaces into ones defined in thin tubular neighborhoods of the surfaces, and have great potential in dealing with data in the form of point clouds (e.g. surfaces sampled by a finite point set and values of data given on the point set).
- Numerical methods for simulating large network of interfaces and junctions. The leading question is: How to compute junctions under anisotropic motion laws?

Recent Developments and Open Problems

PDEs with singular diffusivity. Progress has been made in several directions within this area. For example, the level-set method is extended to crystalline mean curvature flow in an arbitrary dimensional Euclidean space. Two approaches are presented, one is by A. Chambolle and the other is by N. Požár.

The first method is based on the signed distance function and it applies to a class of evolution problems where the velocity of the interface depends on crystalline mean curvature linearly. In paper [2] the following problem is studied $V = \gamma H_\gamma$, where γ is the surface energy density and H_γ is the anisotropic mean curvature of the surface. The advantage of the approach used by Chambolle is that it applies to a general interfacial energy, see [3].

The second approach is based on the theory of viscosity solutions. It applies when the speed of the interface depends monotonically on the curvature but so far it is restricted to a purely crystalline energy. However, the applicability of both approaches is still limited to the second order problems, because they depend on the comparison principle, see [9], [10].

Several lectures on the recent development of a few versions of the total variation flow were presented during this workshop. One of them was the presentation by P. Mucha, who discussed the anisotropic total variation flow with the ℓ_1 norm anisotropy. Another one was the talk of M. Muszkieta, in which results on the higher order total variation flow with several numerical computations were given.

I. Kim addressed a surprisingly difficult but easy to state problem of preserving the star shape property of sets by the mean curvature flow. This problem remains open.

Stefan problem with fractional time derivative. V. Voller presented an array of problems arising in engineering which fall into the broadly understood anomalous diffusion. This area is rich with problems waiting for rigorous analysis. One of them was studied by T. Namba. He presented an extension of the notion of viscosity solutions to equations with Caputo time fractional derivatives.

Modeling and simulating crystal growth. D.Margetis and J.-G.Liu presented recent development on modeling crystal growth by a high order partial differential equation with exponential nonlinearities. They also offered the analysis of such a high order model, see [13].

S.Esedoglu presented a novel variational formulation for large network of grains with boundaries modeled by different anisotropic interface energies. Based on the new variational formulation, threshold dynamics algorithms with judiciously chosen, averaging kernels are developed. The approach to formulate variational principles and the related algorithms that uses threshold dynamics lead to a wide range of applications involving multiphase problems, see [5], [6].

Numerical algorithms Developments of new algorithms for surface partial differential equations were presented in this workshop. They require extensions of the surface PDEs into a thin tubular neighborhood of evolving smooth surfaces. B. Stinner and K. Decklenick presented algorithms that use a phase field formulation. J. Chu and C. Kublik talked about methods that use an extension approach preserving certain properties of the given equations and integrals. C. Kublik also discussed new work in computing integrals on Lipschitz surfaces, see [4], [12]. A graduate student K. Taguchi gave a new numerical scheme for constrained total variation flow, [18].

Even if we witness progress in several directions, still special variational structure is necessary for advancing studies of these problems.

Other related topics José Mazon presented a development of the theory of harmonic functions and the diffusion equations on graph and metric spaces without any obvious differential or linear structure. This seems to be a new exciting direction. We will present it in more details below.

Juan Manfredi talked about the integral formulas for solutions to the p-Laplace equations. This topic is linked to the stochastic game theory. More details are given below.

Presentation Highlights

We present below ten lectures lectures which are representative of the Workshops main themes.

Mazón: Heat Flow on Metric Random Walk Spaces

The speaker presented results, in the context of "metric random walk spaces", see [16], on

- Ergodicity
- Functional Inequalities and Curvature (such as Poincaré inequality, its relation to isoperimetric inequality, Bakry-Emery curvature)
- Transport inequalities

A random walk m on X is a family of probability measures m_x such that

1. they depend measurably on x;
2. each measure m_x has finite first moment (with respect to the distance).

A metric random walk space is a Polish space equipped with such a random walk. One also has the detailed balance condition,

$$dm_x(y)d\nu(x) = dm_y(x)d\nu(y).$$

Example: in R^N we take a $J \geq 0$ with total mass 1, then we set

$$m_x^J(A) = \int_A J(x-y)dx,$$

where dx is the Lebesgue measure.

Ollivier-Ricci curvature. In Riemannian geometry, positive Ricci curvature is characterized by the fact that "small balls are closer, in the 1-Wasserstein distance, than their centers are". In the framework of metric random walk spaces, inspired by this, Y. Ollivier (JFA 2009) introduces the concept of coarse Ricci curvature changing the ball by the measures m_x.

First, we recall the Monge-Kantorovich problem and the Wasserstein distance.

Definition: Take $x, y \in X$, the Ollivier-Ricci curvature of (X, d, m) along (x, y) is defined as

$$\kappa_m(x,y) := 1 - \frac{W_1^d(m_x, m_y)}{d(x,y)},$$

where W_1^d is the 1-Wasserstein distance with respect to the metric d.

The Heat Flow. Let (X, d, m) be a metric random walk space with invariant measure ν for m. For a function $u : X \to \mathbb{R}$ its nonlocal gradient is

$$\nabla u(x, y) = u(y) - u(x),$$

it is a function in $X \times X$. Likewise we define the m-divergence of a function in $X \times X$

The averaging operator is

$$M_m f(x) := \int_X f(y) dm_x(y)$$

and the m-Laplace operator $M_m - I$. If the invariant measure ν is reversible, the following integration by parts formula is straightforward

$$\int_X f(x)\Delta_m g(x)\, d\nu(x) = -\frac{1}{2}\int_{X\times X} (f(y) - f(x))(g(y) - g(x))\, dm_x(y)\, d\nu(x).$$

This gives rise to a symmetric form, $\mathcal{E}_m$.

Theorem: Let (X, d, m) be a metric random walk space with invariant and reversible measure ν for m. Then $-\Delta_m$ is a non-negative self-adjoint operator in $L^2(X, \nu)$ with associated closed symmetric form $\mathcal{E}_m$, which is Markovian.

The associated continuous semigroup T_t^m solves the associated heat equation.

Infinite speed of propagation and ergodicity The infinite speed of propagation of the heat flow $e^{t\Delta_m}$, i.e.,

$$e^{t\Delta_m} u_0 > 0 \text{ for all } t > 0$$

occurs, whenever $0 \le u_0 \in L^2(X, \nu)$ and $u_0 \neq 0$.

Consider $\Omega = (-\infty, 0] \cup [\frac{1}{2}, +\infty) \times \mathbb{R}^{N-1}$ and the metric random walk space $(\Omega, d, m^{J,\Omega})$, where d is the Euclidean distance and $J(x) = |B_1|^{-1}\chi_{B_1}$. This space has Ollivier-Ricci curvature κ, which is negative.

We now introduce the *m-total variation function*,

$$\frac{1}{2}\int_X\int_X |u(y) - u(x)| dm_x(y) d\nu(x).$$

Therefore, we define the concept of m-perimeter of a ν-measurable subset $E \subset X$ as the m-total variation of the indicator function of E. In the particular case of a graph, this gives the classical definition of a set.

Theorem: If (X, d, m) is a metric random walk space with invariant and reversible measure ν, and $\nu(X) < \infty$, then the following facts are equivalent:

1) Δ_m is ergodic;
2) $\Delta_m \chi_D = 0$ implies χ_D is constant;
3) $P_m(D) > 0$ for every set such that $0 < \nu(D) < \nu(X)$.

Functional inequalities and curvature Let us assume ν is a probability measure. We define the mean and the variance of a function f. Then, we define the spectral gap.

Definition: We say (m, ν) satisfies a Poincaré inequality if there is a $\lambda > 0$ such that

$$\lambda \mathrm{Var}_\nu(f) \le \mathcal{H}_m(f).$$

There is an example of an infinite, weighted linear graph, which does not satisfy the Poincaré inequality.

Remark: Ollivier showed a Poincaré inequality under certain assumptions on the Ricci-Ollivier curvature. The Poincaré inequality at the level of sets implies the following isoperimetric inequality

$$\min\{\nu(D), 1 - \nu(D)\} \le \frac{2}{\lambda} P_m(D).$$

Question: P. Rybka asked about the motivation for studying these problems?

Question: What about Lévy processes? Some cases are covered, but not all: the integrability at infinity becomes an issue – e.g. the process corresponding to the standard fractional Laplacian in $\mathbb{R}^d$ is covered by the theory.

Manfredi – A discrete stochastic interpretation of the dominative p-Laplacian

Dominative p-Laplacian is defined by

$$\mathcal{L}_p u(x) = \frac{1}{p}(\lambda_1 + \ldots + \lambda_{N-1}) + (p-1)/p\lambda_N,$$

where $\lambda_1 \leq \ldots \leq \lambda_N$ are the eigenvalues of $D^2u(x)$. The speaker discussed the relationship between $\mathcal{L}_p$ and the regular p-Laplacian, which the topic of a recent paper, [15].

The ordinary p-Laplacian $\Delta_p^h u$ is given by the formula $\text{div}(|\nabla u|^{p-2}\nabla u) = |\nabla u|^{p-2}\Delta_p^h u$. It is is not difficult to show, (Brustad, 2017), that $\Delta_p^h u \leq p\mathcal{L}_p u$ with equality for radial functions.

Mean values

$$MV_q(v, B_\varepsilon(x)) = \frac{1}{q-1}\frac{1}{|B_\varepsilon|}\int_{B_\varepsilon(x)} v(y)dy + \frac{q-2}{q-1}\sup \sigma \frac{v(x+\varepsilon\sigma(x)) + v(x-\varepsilon\sigma(x))}{2},$$

where σ is what is called a strategy, $q = (p + 4n + 6/2N + 4)$. What is important is to know this for $p = 2$ and for $p \to \infty$

If $\mathcal{L}_p v(x)$, we have the asymptotic mean value property

$$v(x) = MV_q(v, B_\varepsilon(x)) + o(\varepsilon).$$

Fix $x_0 \in \Omega$ and a strategy σ. We will consider a discrete process

$$x_0, x_1, \ldots$$

defined as follows: If $x_0 \in \Gamma_\varepsilon$, we set $x_1 = x_0$ and stop. Otherwise, $B_\varepsilon(x_0) \subset X$. In the latter case, we move one step according to the following rules:

- with probability $1/(q-1)$ select $x_1 \in B_\varepsilon(x_0)$ at random;
- with probability $(q-2)/2(q-1)$ select $x_1 = x_0 + \varepsilon\sigma(x_0)$;
- with probability $(q-2)/2(q-1)$ $x_1 = x_0 - \varepsilon\sigma(x_0)$.

Then, we consider the pay off function associated to the strategy σ,

$$u_\varepsilon^\sigma(x) = E_\sigma^{x_0}[F(x_{\tau_\sigma})],$$

which we call the ε-stochastic solution.

Theorem: Stochastic solution = mean value solution.

"The interesting thing (to me) is that one can actually prove that something satisfies the dynamic programming principle."

One uses the idea of Barles-Souganidis from 1991, exploiting the upper and lower semicontinuous envelopes.

Question by R.Choksi: What was the original motivation of Brustad?
Manfredi: It may have come from the motivation of explaining that result about the sum of p-superharmonic radial functions, the original proofs of which were quite complicated.

Stinner: On a diffuse interface approach to PDEs on surfaces and networks

This is a recent work, performed with the following applications in mind: cluster formation in different situations (cell clusters, foam and bubble clusters, grain boundaries).

These problems led to PDEs on those interfaces. Triple junctions are an important issue. Our approach is a phase field method. We shall describe these interfaces by thin layers. The phase field methodology boils down to the introduction of a bulk phase field $\varphi(t) : \Omega \to \mathbb{R}$, going from 1 to -1 on a strip of size that can be shown to be $\sim \varepsilon$. We look at

$$F^\varepsilon = \int_\Omega \tilde{K}_w(\frac{\varepsilon}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon}W(\varphi)) \text{ as } \varepsilon \to 0.$$

Example: PDE on an evolving surface $\Gamma(t)$, with material velocity $v(t) : \Gamma(t) \to \mathbb{R}^n$

$$\partial_t^\bullet c + c\nabla_\Gamma \cdot v = D^{(\Gamma)}\Delta_\Gamma c + r(c) \text{ on } \Gamma(t),$$

where $\partial_t^\bullet$ is the material derivative.

Idea: smoothing using the phase field with some $\delta_\varepsilon(\varepsilon_\varepsilon) \to \delta_\Gamma$ as $\varepsilon \to 0$. Rigorous convergence analysis as $\varepsilon \to 0$ ($\{\delta_\varepsilon\}_\varepsilon$ given): Elliot - S 2008, Abels - Lam - S 2015, Burger-Elvetun-Schlottbom 2016, Miura 2017.

PDEs on bubble clusters Domains $\Omega^{(i)}(t)$ separated by interfaces $\Gamma^{(i,j)}(t)$ meeting at triple junctions $T^{(,j,k)}(t)$ transported by a continuous solenoidal velocity field v. Species densities: $c^{(i,j)}, \Gamma^{i,j}$. The speaker presented definitions of "Energy", "Chemical potentials" for the system. The potentials drive the evolution of the system.

We approximate the resulting equations in distributional forms with a phase field. Phase variable $\varphi^{(i)}$ for phase i. A constraint: they add up to 1.

A key assumption: along the layer between i and j only φ^i and φ^j are present.

Phase field Ansatz

$$\delta_{\Gamma^{i,j}} \sim \delta_{i,j} = C_\delta \frac{1}{\varepsilon}(\varphi^i, \varphi^j)^2,$$

$$\tau_{T^{i,j,k}} = C_\tau \frac{1}{\varepsilon^2}(\varphi^i \varphi^j \varphi^k)^2.$$

In practice: the phase fields themselves solve PDEs that depend on the surfaces. One must also bear in mind additional conditions in practical applications such as Young's law. This becomes a problem, because we may need this information to calibrate C_τ (the exact form of C_τ may depend on extra modeling assumptions involving higher order terms).

Question: Can you do quadruple junctions?
Answer: No, conceptually probably you could set them up. In the applications I am interested in, they are not stable, so you do not see them.

Question: For the computations, did you do a moving mesh?
Answer: No, we used an adaptive algorithm concentrating in an ε neighborhood of the interface.

Kublik: Applications of distance functions to motions of curves in the plane, and integration over interfaces and unstructured point sets

We are working on a general framework for integrating over interfaces which are implicitly defined. The first part of the talk discussed an MBO (Merriman-Bence-Osher) scheme for two-dimensional area preserving motion by curvature. The normal velocity is

$$v_N = \kappa - \bar{\kappa},$$

where $\bar{\kappa}$ is the average of the curvature on the curve, when if the curve is simply connected. Otherwise, a modified expression is necessary which depends on the number of "holes". A similar thresholding scheme can be used here – the modification arising in the diffusion step.

In the second half of the talk, the speaker discussed a simple, efficient, scheme for computing such boundary integrals. The context is that the boundary is not defined by an specific parametrization (e.g. boundaries evolving in time, with possible changes in the topology). The presented strategy is to derive a volume integral around a tubular neighbor of the interface that is identical to the given integral along the interface. The idea is to approximate the integral over Γ, via an integral over Γ_η, where Γ_η is a properly chosen nearby surface Γ_η is given by a level set of the distance function,

$$\int_\Gamma v(z)dS(z) = \int_{\Gamma_\eta} v(P_\Gamma(y))J_\eta dS_\eta(y),$$

where $P_\Gamma(y)$ is the closest point mapping to Γ. We have that J_η is a polynomial in η $J_\eta = 1 + \eta\kappa$ in 2D (similar formula in 3D). Then, averaging and using the co-area formula, we obtain a volume integral representation of the surface integral, (K-Tanushev-Tsai, 2013). The Jacobian $J(x)$ can be computed from the singular values of the Jacobian matrix of the closest point mapping P_Γ. This offers additional convenience for computation of J and interpreting it, especially for manifolds with boundaries.

The speaker further discussed: (i) how integration along curves with corners and surfaces with creases could be computed accurately by the proposed methodology, but with more elaborate averaging kernels, and (ii) analysis of the algorithm when applied to analyze finite point set that are sampled from manifolds of different Hausdorff dimensions.

Kim: Volume preserving mean curvature flow with start-shaped sets

The speaker considers motion with normal velocity given by,

$$V = -\kappa + \bar{\lambda}_t \text{ on } \Gamma_t = \partial\Omega_t$$

with λ_t such that $\int_{\Gamma_t} V = 0$, so the volume is preserved. Ω_t is assumed to have smooth boundaries and

$$\lambda_t = \frac{1}{\text{Per}(\Omega_t)} \int_{\Gamma_t} \kappa d\sigma.$$

This motion converges exponentially to the sphere (smooth, convex flow). Studies of existence of solutions but uniqueness is open.

Most people care about convex sets and the flow is known to preserve convexity. Also, the curve can undergo topological changes in finite time.

Question: Are there other geometries that are preserved by the flow (other than convexity)? The star-shapedness is expected to be preserved.

The speaker then introduced a strong version of star-shapedness, called ρ-reflection. It turns out that this property is preserved by the motion. To study the flow, we need a notion of weak solution because the flow may develop singularities. The speaker uses two techniques:

1. Notion of a viscosity solution to enable barrier arguments;
2. Variational approach to obtain energy estimates.

The flow considered is the gradient flow for Per(F), the perimeter of the set F, over sets of fixed volume (say 1). The speaker uses minimizing movement to construct the flow. This requires minimizing

$$\text{Per}(F) + \frac{1}{h}\tilde{d}^2(F, E),$$

where E is the set from the previous set and F the current one.

Discrete scheme. Approximate energy:

$$\text{Per}(E) + \frac{1}{\delta}(|F| - 1)^2 + \frac{1}{h}\tilde{d}^2(F, E).$$

When you minimize it, you get a discrete flow $\Omega_t^{\delta,h}$ that converges to the δ-flow with normal velocity,

$$V = -\kappa + \lambda_\delta(|F|), \quad \lambda_\delta(s) = \frac{2}{\delta}(s - 1).$$

This is the δ-flow Ω_t^δ. Now, the speaker uses a modified viscosity-type argument to show that the strong star-shapedness property is preserved. She needs to investigate the convergence of the δ flow.

Result: $\Omega_t^{\delta,h} \to \Omega_t^\delta$ as $h \to 0$ and $\Omega_t^\delta \to \Omega_t$ as $\delta \to 0$. Regularity of δ-flow: the boundary of Ω_t^δ can be locally represented by a Lipschitz graph.

Last result: Assume Ω_t is star-shaped, smooth, preserves volume over time. Then Ω_t is the unique solution of the motion with normal velocity,

$$V = -\kappa + \bar{\lambda}_t,$$

and Ω_t converges exponentially fast to a unit ball. More details can be found in [11].

Chu: Numerical methods for energy minimization problems on surfaces

We look at an energy defined on a surface Γ of the form

$$I_\Gamma(u) = \int_\Gamma F(u, \nabla_\Gamma u) ds.$$

We take an ε-neighborhood of Γ and write $\bar{u}(x) = u(P_\Gamma(x))$, $\frac{\partial \bar{u}}{\partial n} = 0$ (constant extension along the normals). We want to construct an integral formulation $I_{\Gamma_\varepsilon}(\bar{u})$, such that

$$I_{\Gamma_\varepsilon}(\bar{u}) = I_\Gamma(u), \quad \forall u.$$

Questions: Is the minimizer of $I_{T_\varepsilon}(\bar{u})$ equivalent to the minimizer of $I_\Gamma(u)$? The answer is yes.

We derive

$$I_{\Gamma_\varepsilon}(v) = \int_{T_\varepsilon} \tilde{F}(v, \nabla v) dx,$$

where T_ε is a tubular neighborhood around Γ.

Question: Is $\nabla_{\bar{\Gamma}} u(z) = \nabla \bar{u}(z), \forall\, z \in T_\varepsilon$? No, this is only true when $z \in \Gamma$. In fact we have

$$\nabla_{\bar{\Gamma}} u(z) = A(z)\nabla\bar{u}(z),$$

where $A = (1-\eta\kappa_1)\tau_1 \otimes \tau_1 + (1-\eta\kappa_2)\tau_2 \otimes \tau_2 + \delta n \otimes n$. η corresponds to the η level set. There is an extra dimension in the normal direction which gives us a free parameter δ (because the normal derivative is 0).

Question: Choice of δ? δ plays a different role for elliptic than for hyperbolic equations. $\delta > 0$ preserves ellipticity of elliptic equation. $\delta = 0$ is for hyperbolic equation.

Construct an identical volume integral,

$$I_\Gamma(u) = \int_\Gamma F(u, \nabla_\Gamma u) ds = I_{\Gamma_\varepsilon}(v) = \frac{1}{2\varepsilon}\int_{T_\varepsilon} \tilde{F}(x, v, \nabla v) dx.$$

The speaker discussed the boundary (of the tube) treatment: project boundary point ($d = \varepsilon$ or $d = -\varepsilon$) to any point along the normal inside the tube. He also studied the instability (he has a model problem for that). This instability was previously studied by Kreiss, but the speaker studied this for manifolds. He uses the Fourier transform in space and the Laplace transform in time. He studies the existence of unstable modes. For δ large, there is an instability so it is necessary to have small δ.

The speaker discussed a stabilization strategy: add another term to the PDE (already done by Kreiss). He discretizes the integral first (direct method). Looks at obstacle problems and TV-denoising on a torus.

Question asked by a member of the audience: can you solve Maxwell's equation with this method?

Margetis: On the mathematical modeling of crystal facets

The speaker presents a PDE approach with a touch of discreteness in the modeling.

Classical relaxation by surface diffusion Region Ω_t with moving boundary, $\Gamma_t = \partial\Omega_t$, with velocity

$$v_n = -\mathrm{div}_\Gamma J,$$

where J - the surface flux is given by

$$J = -\nabla_\Gamma \mu$$

and μ is the chemical potential.

This model has to be revised in the presence of line defects (steps) and facets (at low temperatures).

Multiple scales Typically, micro- (atomic scale), mesoscale (about 25 nm), macroscale (20 μm). The last two scales are subject of the talk.

How is macroscale facet evolution linked to the step motion? To address this question, one needs to consider 1) PDE away from facets, 2) boundary conditions. Typically for the step flow away from facets, one uses the BCF model. Near a facet, one needs to consider the discrete nature of the problem.

Adatom diffusion On the i-th terrace,

$$J_i = -D_s \nabla \rho_i, \qquad D_s \Delta \rho_i + F = \frac{\partial \rho_i}{\partial t} \approx 0.$$

and Robin-type boundary conditions at bonding step edges. Here, $\rho_i^{eq} = \rho_s e^{\mu_i/T}$ is the Gibbs-Thomson relation, $\mu_i(s,t)$ is the step chemical potential.

- Step motion and continuum limit (heuristics in 1D): Step velocity leads to $\partial_{\tilde{t}} h = -\partial_x J$, where

$$J = \frac{D_s}{1 + \frac{2D_s}{q\alpha}|\partial_x h|}\partial_x \rho^{eq}$$

  attachment/detachment at bonding steps leads to "Fick's law" for surface diffusion.
- Chemical potential near equilibrium leads to energy $E(h)$.
- Force dipole-dipole interaction model (nearest neighbor).
- Relaxation PDE in 2+1 dimensions, outside facets yields a 4-th order parabolic-like PDE for h. PDE for height profile.

How does the full (nonlinear) Gibbs-Thomson relation affect facet evolution?

$$\partial_t h = \Delta \exp\left[-\beta \mathrm{div}\left(\frac{\nabla h}{|\nabla h|} + g|\nabla h|\nabla h\right)\right],$$

here $\beta = T^{-1}$, $g \geq 0$.

In 1+1 dimensions:

$$\partial_t h = \partial_{xx} \exp[-\partial_x \frac{\partial_x h}{|\partial_x h|}].$$

We neglect $|\partial_x h|\partial_x h$ in the exponent (of facets $\partial_x h = 0$).

The speaker then discussed some further analysis of the newly derived model: the appropriate boundary conditions at facets. The discussion led to free boundary problems. More details can be found in [14].

Liu: Dynamics of a degenerate PDE model of epitaxial crystal growth

This talk complements Dionisios Margetis lecture.

Epitaxial growth is an important physical process for forming solid films or other nano-structures. It occurs as atoms, deposited from above, adsorb and diffuse on a crystal surface. Modeling the rates that atoms hop and break bonds leads in the continuum limit to a degenerate 4th order PDE that involve exponential nonlinearity and the p-Laplacian with $p = 1$, for example. The lecturer discussed a number of analytical results for such models, some of which involving subgradient dynamics for Radon measure solutions.

Particularly noteworthy was how the author dealt with exponentials of singular measures.

Voller: Anomalous infiltration into Heterogeneous Porous media: Simulation and fractional calculus models

Sub-diffusive behavior was demonstrated in some physical systems and with fractional derivative the same behavior can be observed. This motivated that fractional derivatives can be used to model such systems. Problems, where obstacles were considered and the volume of fluid method was used to study how flows go through these obstacles. Two one dimensional measures for the progress of filling was found which gave good agreement with experimental data. The two measures: 1) S: the one dimensional representative front, and 2) F: an effective filling length, the infiltration depth were related to physical parameters such as porosity and the obstacle pattern. The talk was based on [1], [7] and [19].

Questions: fine structures such as fingers? Neglected here but for viscous fluids, no fingering, one still observe sub diffusion.

Does the shape of the obstacles affect the model with the fractional derivative?

Namba: Well-posedness of fully nonlinear PDEs with Caputo time fractional derivatives

Caputo time fractional derivatives were motivated for modeling anomalous diffusion that is observed in heterogeneous media ($\partial_t^\alpha u = \Delta u$). In the talk the notion of viscosity solutions were extended to equations with Caputo time fractional derivatives. Perron's method and comparison principle were used to construct sub and super-solution and to establish the unique existence of viscosity solutions for the initial value problem with Caputo time fractional derivatives. Continuous dependence of the solution on the fraction of the time derivative was also addressed. The talk is based on the following papers, [8], [17].

Questions: Do Caputo time fractional derivatives make sense also for functions that have jumps? Yes!

Scientific Progress Made

There were talks on different models and numerical algorithms for treating junctions and grain boundary motions. Discussions on how to extend surface PDEs into thin domains around interfaces for numerical computation were held. There were lectures on very novel high order PDEs for modeling the dynamics of facets in crystal growth. There were discussion about different nonlocal equations, connection to random walks, and relation between local and non-local diffusions in different domains.

Outcome of the Meeting

Specialists from many disciplines and background took part in the meeting. As a result exchanging ideas from distant area of the Science was facilitated. Indeed, the participants praised the choice of speakers, which conveyed new ideas and viewpoints. This is why one of the outcomes of the meeting was the transfer of knowledge among specialists.

Another outcome, which will turn out to be material, is the meeting of old collaborators, working on joint projects. We expect that the discussions held during the meeting will result in new projects leading to publications.

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Chapter 15

New Trends in Syzygies (18w5133)

June 24 - 29, 2018

Organizer(s): Giulio Caviglia (Purdue University, Jason McCullough (Iowa State University)

Overview of the Field

Since the pioneering work of David Hilbert in the 1890s, syzygies have been a central area of research in commutative algebra. The idea is to approximate arbitrary modules by free modules. Let R be a Noetherian, commutative ring and let M be a finitely generated R-module. A free resolution is an exact sequence of free R-modules $\cdots \to F_{i+1} \to F_i \to \cdots F_0$ such that $H_0(F_\bullet) \cong M$. Elements of F_i are called ith syzygies of M. When R is local or graded, we can choose a minimal free resolution of M, meaning that a basis for F_i is mapped onto a minimal set of generators of $\operatorname{Ker}(F_{i-1} \to F_{i-2})$. In this case, we get uniqueness of minimal free resolutions up to isomorphism of complexes. Therefore, invariants defined by minimal free resolutions yield invariants of the module being resolved. In most cases, minimal resolutions are infinite, but over regular rings, like polynomial and power series rings, all finitely generated modules have finite minimal free resolutions.

Beyond the study of invariants of modules, syzygies have connections to algebraic geometry, algebraic topology, and combinatorics. Statements like the Total Rank Conjecture connect algebraic topology with free resolutions. Bounds on Castelnuovo-Mumford regularity and projective dimension, as with the Eisenbud-Goto Conjecture and Stillman's Conjecture, have implications for the computational complexity of Gröbner bases and computational algebra systems. Green's Conjecture provides a link between graded free resolutions and the geometry of canonical curves. These are just some of the important problems that have seen great recent progress and were discussed at this BIRS meeting. In the following we focus on these four problems in detail. Then we summarize some other meeting highlights and positive feedback from meeting participants.

Recent Developments and Open Problems

The theory of free resolutions and syzygies has seen many spectacular results in the last few years with several long-standing conjectures being resolved. Here we briefly summarize the biggest results and their connections with this workshop.

Buchsbaum-Eisenbud-Horrocks Conjecture

Let k be any field, let R be a regular local ring of dimension n. The Buchsbaum-Eisenbud-Horrocks rank conjecture roughly says that the Koszul complex is the smallest possible minimal free resolution. The conjecture was formulated by David Buchsbaum and David Eisenbud [BE]. The conjecture is also implicit in the work of Horrocks. See [Har]. The precise statement is as follows.

Conjecture 15.0.1 (BEH Conjecture) *Let M be an R module of finite length. Then*

$$\beta_i(M) \geq \binom{n}{i}.$$

Note that if $M = k$, then the minimal free resolution is a Koszul complex and the ith total Betti number is exactly $\binom{n}{i}$. The conjecture has been settled for $n \leq 4$ by Graham Evans and Phillip Griffith [EG2]. A similar statement can be made in the graded case. A special case of this question was proved by Daniel Erman [E].

One can ask the weaker question as to whether the sum of all the Betti numbers is at least 2^n. This is sometimes known as the Weak Horrocks Conjecture or Total Rank Conjecture. In a recent breakthrough, Mark Walker proved the Total Rank Conjecture for all characteristics except 2. Walker gave a talk on his work at the meeting. The proof relies on techniques from K-theory and fits nicely into a one-hour talk. In fact, his result applies more generally to finitely generated modules of finite projective dimension over local complete intersections not of characteristic two or over local rings containing a field of odd, prime characteristic.

Srikanth Iyengar gave a related talk he presented joint work with Walker constructing counterexamples to various generalizations of the Total Rank Conjecture. (See description below.)

Eisenbud-Goto Conjecture

Let $S = K[x_1, \ldots, x_n]$ be a standard graded polynomial ring over a field and let M be a finitely generated graded S-module. We define the (Castelnuovo-Mumford) regularity of M to be

$$\operatorname{reg}(S/I) = \max\{j \mid \beta_{i,i+j}(S/I) \neq 0.$$

Thus the regularity of S/I is the index of the last nonzero row in the Betti table of S/I. David Eisenbud and Shiro Goto showed [EG] that this agrees with the more classical definition of regularity given in terms of vanishing of twists of sheaf cohomology modules. In particular, note that the regularity of an ideal is an upper bound on the degrees of the minimal generators. Thus finding effective bounds on regularity has attracted a lot of attention.

David Bayer and Michael Stillman [BS] gave another characterization of regularity: $\operatorname{reg}(I)$ is equal to the maximal degree of a Gröber basis element of I in the revlex monomial order if we first take a generic change of coordinates. Since Gröbner bases are required for many computational tasks, this means that finding upper bounds on regularity equates to finding bounds on the computational complexity of an ideal. Unfortunately, in the most general setting possible, such upper bounds are quite large. Set $\operatorname{maxdeg}(I)$ to be the maximal degree of a minimal generator of I. A well-known result of David Bayer and David Mumford [BM] and later Giulio Caviglia and Enrico Sbarra [CS] shows that $\operatorname{reg}(I) \leq (2\operatorname{maxdeg}(I))^{2^{n-2}}$, where n is the number of variables.

This doubly exponential bound grows quickly with respect to n. Unfortunately, this bound is nearly optimal. In one construction derived from the so-called Mayr-Meyer [MM3] ideals, Koh [Koh] proved that for any integer $r \geq 1$ there exists an ideal I_r in $S_r = k[x_1, \ldots, x_{22r-1}]$ such that

$$\operatorname{maxdeg}(I_r) = 2$$
$$\operatorname{reg}(S_r/I_r) \geq 2^{2^{r-1}}.$$

Thus doubly exponential behavior cannot be avoided. We note for later reference that I_r is generated by $22r - 3$ quadrics and 1 linear form while the regularity is realized at the first syzygies of I (second syzygies of S/I).

The ideals I_r have many associated primes and embedded primes; in particular, they are far from prime. Better bounds were expected for ideals with some geometric content. This expectation was expressed in the following conjecture:

Conjecture 15.0.2 (Eisenbud-Goto (1984)) *Let $S = k[x_1, \ldots, x_n]$ with $k = \bar{k}$ and suppose $\mathfrak{p} \subset (x_1, \ldots, x_n)^2$ is a homogeneous prime ideal. Then*

$$\operatorname{reg}(S/\mathfrak{p}) \leq e(S/\mathfrak{p}) - \operatorname{ht}(\mathfrak{p}).$$

The condition $\mathfrak{p} \subset (x_1, \ldots, x_n)^2$ is equivalent to saying that the projective variety corresponding to $\mathfrak{p}$ is not contained in a hyperplane and thus is optimally embedded. Such ideals are called nondegenerate. It is worth noting that the right-hand side of the inequality above is always positive for nondegenerate prime ideals.

The Eisenbud-Goto Conjecture can be viewed as an expectation that for ideals with more geometric content, regularity is better behaved. Via the Bayer-Stillman result, this would then ensure that computations involving prime ideals are much better behaved than for arbitrary ideals. Castelnuovo essentially showed in 1893 that smooth curves in $\mathbb{P}^3_{\mathbb{C}}$ satisfy the conjecture. In 1983 Gruson-Lazarsfeld-Peskine [GLP] proved the bound for all curves (smooth and singular) in any projective space. (Remember that $\mathfrak{p}$ defines a projective curve when $\dim(S/\mathfrak{p}) = 2$.) Pinkham [Pi] and Lazarsfeld [La] proved the bound for smooth projective surfaces over $\mathbb{C}$. Ran [Ra] proved the bound for most smooth projective 3-folds over $\mathbb{C}$. Eisenbud and Goto also proved the Cohen-Macaulay case. Numerous other special cases have also been proved.

In 2016, Jason McCullough and Irena Peeva [MP] constructed counterexamples to the Eisenbud-Goto Conjecture. The construction involved two new concepts: Rees-like algebras and Step-by-step homogenization. Given an ideal $I \subset S$, the Rees algebra of I is $S[It]$, where t is a new indeterminate. It defines the blow up of projective space along the subvariety defined by I and thus is important in the resolution of singularities. McCullough and Peeva defined the Rees-like algebra as $S[It, t^2]$. Contrary to the case of the Rees algebra, where defining equations are difficult to find, the defining equations of the Rees-like algebra are easy. Moreover, McCullough and Peeva constructed the entire minimal graded free resolution of the defining prime ideal of any Rees-like algebra. Thus they were able to compute the degree and regularity of these ideals and show that they yield counterexamples to the Eisenbud-Goto Conjecture 15.0.2. Moreover, they showed that there was no polynomial bound on the regularity of nondegenerate prime ideals purely in terms of the degree. A new homogenization was constructed to form standard graded analogs of the non-standard graded prime ideals above.

In more recent work, Giulio Caviglia, Marc Chardin, Jason McCullough, Irena Peeva, and Matteo Varbaro [CCMPV] showed that there is a (necessarily large) bound on the regularity or projective dimension of nondegenerate primes in terms of the degree alone. They also gave new counterexamples to the Eisenbud-Goto Conjecture 15.0.2 that use Rees algebras instead of Rees-like algebras and ones that do not rely on the Mayr-Meyer ideals. Work of Craig Huneke, Paolo Mantero, Jason McCullough, and Alexandra Seceleanu [HMMS4] shows that no similar bound is possible more generally for primary ideals.

While these counterexamples indicate that the Eisenbud-Goto Conjecture 15.0.2 is false in general, it remains open in the smooth case. Suppose $\mathrm{char}(k) = 0$ and $X \subset \mathbb{P}^{p-1}_k$ is a smooth variety. In this case Sijong Kwak and Jinhyung Park [KP] and Atsushi Noma [No] reduced it to the Castelnuovo's Normality Conjecture that X is r-normal for all $r \geq \deg(X) - \mathrm{codim}(X)$. They do so by bounding the regularity of the structure sheaf of X. Sijong Kwak attended the meeting and gave a talk on "$\mathcal{O}_X$ regularity bound for smooth varieties with classification of extremal and next to extremal examples." The proof uses geometric properties of double point divisors from inner projections.

Green's Conjecture

Let $S = K[x_1, \ldots, x_n]$ be a standard graded polynomial ring over a field K. Let I be a homogeneous ideal of S. We denote by $\beta_{ij}(S/I) = \dim_K \mathrm{Tor}_i^K(S/I, K)$ the graded Betti numbers of S/I. Typically one displays the Betti numbers of a module in what is called the Betti table. We place $\beta_{ij}(S/I)$ in column i and row $j - i$. The length of the 2-linear strand of the Betti table is $2\mathrm{LP}(S/I) = \max\{i \mid \beta_{i,i+1}(S/I) \neq 0\}$, and therefore measures the index of the last nonzero entry in the second row in the Betti table.

Green's conjecture concerns the shape of the Betti tables of canonical curves. A projective curve may be embedded into projective space in many ways, but for non-hyperelliptic cruves there is a canonical embedding into projective space. Resolving the associated homogeneous ideal I, one finds that S/I is Gorenstein and has Betti table of the form

	0	1	2	$\cdots$	g-4	g-3	g-2
0:	1	-	-	$\cdots$	-	-	-
1:	-	a_1	a_2	$\cdots$	a_{g-4}	a_{g-3}	-
2:	-	a_{g-3}	a_{g-4}	$\cdots$	a_2	a_1	-
3:	-	-	-	$\cdots$	-	-	1,

where the a_i are the only possibly nonzero Betti numbers and g denotes the genus of the curve. We recall the definition of the clifford index. For a given line bundle $\mathcal{L}$ on C, we set

$$\text{Cliff}(\mathcal{L}) = g + 1 - \left(h^0(\omega \otimes \mathcal{L}^{-1})\right) = \deg \mathcal{L} - 2(h^0(\mathcal{L}) - 1).$$

The Clifford index of C (in the case when the genus of C is at least 3) is the minimum of all Clifford indices of bundles $\mathcal{L}$ with $h^0(\mathcal{L}) \geq 2$ and $h^0(\omega \otimes \mathcal{L}^{-1}) \geq 2$. We can now state Green's Conjecture:

Conjecture 15.0.3 (Green) *The length of the 2-linear strand of the resolution of the canonical ring of a curve of genus g and clifford index c is*

$$2\text{LP}(S/I) = g - c - 2.$$

Equivalently, $a_{g-3} = a_{g-4} = \cdots a_{g-c-1} = 0$ and $a_{g-c-2} \neq 0$ in the Betti table above.

The generic curve of genus g is known to have Clifford index $\lfloor (g-1)/2 \rfloor$. Since the Betti number vanishing condition above defines a Zariski open set, the generic case of Green's Conjecture asserts that there exists a smooth curve whose canonical ring satisfies the conclusion. Special cases of the Conjecture were known, such as for low genus curve, but even the generic case was open until Clair Voisin resolved the generic case in characteristic 0 in 2005 [V1, V2].

At this meeting Claudiu Raicu presented a new proof (joint work with Marian Aprodu, Gavril Farkas, Stefan Papadima, and Jerzy Wayman) of the generic Green's Conjecture that goes further and simplifies Voisin's proof. Their proof uses a vanishing theorem for Koszul modules and connects to other exciting work in [AFPRW]

Stillman's Conjecture

Let $S = K[x_1, \ldots, x_n]$ be a polynomial ring over a field K. View S as a standard graded ring $S = \bigoplus_{i \geq 0} S_i$, where S_i denotes the K-vector space of degree i homogeneous polynomials. Let $I = (f_1, \ldots, f_m)$ denote a homogeneous ideal of S. Around 2000, Michael Stillman posed the following:

Conjecture 15.0.4 ([PS, Problem 3.14]) *Fix a sequence of natural numbers $d_1, \ldots, d_g$. Does there exist a number p such that $\text{pd}_S(S/I) \leq p$, where I is a homogeneous ideal in a polynomial ring S with a minimal system of generators of degrees $d_1, \ldots, d_g$? Note that the number of variables in S is not fixed.*

It follows from Hilbert's Syzygy Theorem that $\text{pd}_S(S/I) \leq n$, but the conjecture does not reference the number of variables. It follows from work of Buch [Bu], Kohn [Ko], and Bruns [Br] that there is no bound on the projective dimension of three-generated ideals. Thus to find any such bound we must at least take into account the degrees of the generators. More recent work of Caviglia (see [MS]) that Conjecture 15.0.4 is equivalent to one where we replace projective dimension by regularity.

Previously, only special cases of the Conjecture had been proved, e.g. [En1, En2, HMMS1, HMMS3, MM2, MM3, AH1]. In 2016, Ananyan and Hocster [AH2] gave a proof of Stillman's Conjecture 15.0.4 in full generality. The bound they prove is generally non-constructive and it remains open as to what an asymptotically tight bound would look like. But they introduced many new ideas that have already had a significant impact on the field. Notably, their result led to the result of Caviglia, Chardin, McCullough, Peeva, and Varbaro [CCMPV] mentioned previously. They also introduced the notion of the strength of a form which we now discuss.

Let $f \in K[x_1, \ldots, x_n]$ with $\deg(f) > 0$. We say that F has a k-collapse for $k \in \mathbb{N}$, if f is in an ideal generated by k elements of strictly smaller positive degree. We say that f has strength k if it has a $(k+1)$-collapse but no k-collapse. For instance, all linear forms have infinite strength. If f is a nonzero form of positive degree then f has strength at least 1 if and only if f is irreducible.

Another new concept was that of a prime (resp. R_i) sequence. A sequence of elements $f_1, \ldots, f_m \in S$ is a prime sequence (respectively R_i -sequence, where $i \in \mathbb{N}$), if $f_j \notin (f_1, \ldots, f_{j-1})$ and $S/(f_1, \ldots, f_j)$ is a domain (respectively, satisfies (R_i)) for $j = 1, \ldots, m$. One of the key observations of Ananyan-Hochster was that F has a small collapse if and only if the singular locus of f is large (i.e. has small codimension). Their proof is a massive yet subtle inductive argument that relies on a technical theorem of Grothendieck. However, their paper also provides other bounds on the number of associated primes, degrees and number of generators of primary components, and more for ideals with a fixed number of generators of fixed degree.

More recently, Daniel Erman, Steven Sam and Andrew Snowden have given two brand new proofs of Stillman's Conjecture. Both rely on a new characterization of infinitely generated polynomial rings via derivations. One of their proofs uses the inverse limit of polynomial rings in an increasing finite number of variables. The other proof uses ultra products. The meeting was fortunate to have Steven Sam give a talk on this paper.

Yet another new proof of Stillman's Conjecture has been given by Jan Draisma, Michael Lason and Anton Leykin [DLL]. Their proof relies on an initial term and Gröbner basis argument. Despite all the progress on Stillman's Conjecture, it remains open as to what the optimal bounds should be in general. Ananyan and Hochster have announced a forthcoming paper giving explicit bounds in the case of ideals generated by quadrics, cubics, and quartics but even these bounds are large and far from optimal.

Presentation Highlights

Including the talks discussed above, there were 22 talks given at the workshop. Here we survey the highlights among those talks.

Hai Long Dao spoke about joint work [DDM] with Allesandro de Stefani and Linquan Ma. Inspired by a question raised by Eisenbud-Mustaţă-Stillman regarding the injectivity of maps from Ext modules to local cohomology modules, they introduce a class of rings which called cohomologically full rings. In positive characteristic, this notion coincides with that of F-full rings, while in characteristic 0, they include Du Bois singularities. They prove many basic properties of cohomologically full rings, including their behavior under flat base change. Ideals defining these rings satisfy many desirable properties, in particular they have small cohomological and projective dimension. Furthermore, they obtain Kodaira-type vanishing and strong bounds on the regularity of cohomologically full graded algebras.

Takayuki Hibi spoke on joint work [HM] with Kazunori Matsuda entitled "Regularity and h-polynomials of monomial ideals." Let $S = K[x_1, \ldots, x_n]$ denote the polynomial ring in n variables over a field K with each $\deg x_i = 1$ and $I \subset S$ a homogeneous ideal of S with $\dim S/I = d$. The Hilbert series of S/I is of the form $h_{S/I}(\lambda)/(1-\lambda)^d$, where $h_{S/I}(\lambda) = h_0 + h_1\lambda + h_2\lambda^2 + \cdots + h_s\lambda^s$ with $h_s \neq 0$ is the h-polynomial of S/I. It is known that, when S/I is Cohen–Macaulay, one has $\mathrm{reg}(S/I) = \deg h_{S/I}(\lambda)$, where $\mathrm{reg}(S/I)$ is the (Castelnuovo–Mumford) regularity of S/I. Hibi showed how, given arbitrary integers r and s with $r \geq 1$ and $s \geq 1$, a monomial ideal I of $S = K[x_1, \ldots, x_n]$ with $n \gg 0$ for which $\mathrm{reg}(S/I) = r$ and $\deg h_{S/I}(\lambda) = s$ could be constructed.

Srikanth Iyengar spoke on joint work with Mark Walker [IW] on "Examples of finite free complexes of small rank and small homology." Given Walker's resolution of the Total Rank Conjecture, one could imagine that there are lower bounds on the total Betti numbers of certain complexes more generally. To the contrary, Iyengar and Walker construct finite free complexes over commutative noetherian rings such that the total rank of their underlying free modules, or the total length of their homology, is less than predicted by various conjectures in the theory of transformation groups and in local algebra.

Satoshi Murai spoke on "h-vectors and the number of generators of fundamental groups," representing joint work [MN] with Isabella Novik. In his talk, he showed how to resolve a conjecture of Kalai asserting that the g_2-number of any (finite) simplicial complex Δ that represents a normal pseudomanifold of dimension $d \geq 3$ is at least as large as $\binom{d+2}{2} m(\Delta)$, where $m(\Delta)$ denotes the minimum number of generators of the fundamental group of Δ. He also showed how to prove that a weaker bound, $h_2(\Delta) \geq \binom{d+1}{2} m(\Delta)$, applies to any d-dimensional pure simplicial poset Δ all of whose faces of co-dimension at least 2 have connected links.

Maria Rossi gave a talk on "A generalization of Macaulay's correspondence for Gorenstein k-algebras and applications." Macaulay's inverse systems give a one-to-one correspondence between Artinian, Gorenstein ideals in $R = k[x_1, \ldots, x_n]$ and finitely-generated R-submodules of the injective envelope of R. Rossi gave a talk on how this picture generalizes to Gorenstein ideals of arbitrary dimension. This is joint work [ER] with Juan Elias.

Hal Schenck spoke on joint work with Matt Mastroeni and Mike Stillman. In his talk entitled "Theta characteristics, Koszul algebras, and the Gorenstein property," Schenck addressed a question of Conca who asked if every quadratic, Gorenstein algebra R of regularity at most 3 is Koszul. They construct a family of counterexamples using the idealization process.

Matteo Varbaro reported on joint work [CV] with Aldo Conca on "Square-free Gröbner Degenerations." They address a conjecture of Jürgen Herzog regarding square-free initial ideals. It is well known that the graded Betti numbers, projective dimension, regularity of the initial ideal of an ideal I are upper bounds for those of I itself. A celebrated result of Bayer and Stillman says that in the degree revlex order and in generic coordinates, these upper bounds become equalities. It had been conjectured by Herzog that this was also the case under any monomial order when the initial ideal was a square-free monomial ideal. Varbaro gave a detailed talk in which he and Conca prove Herzog's conjecture.

Outcome of the Meeting

This meeting brought together 41 researchers in commutative algebra and algebraic geometry. The meeting allowed for participants from far away a chance to talk and collaborate. The participants hailed from Canada, France, Germany, Italy, Japan, South Korea, Spain, and USA.

The meeting was very received very positively with many excellent talks. Several participants reported starting new collaborations as a result of attending the meeting. We include here some of the feedback and testimonials the organizers received regarding the benefits and outcomes of their attendance.

David Eisenbud wrote: "It really was a great workshop. Hightlights for me were the talks reporting on 4 spectacular results:

1. New, simpler proof of Voisin's theorem on Green's conjecture (Raicu)
2. New, very clever and simpler proof of Ananyan-Hochster's result on Stillman's problem (Sam)
3. Wonderful and surprising results on square free initial ideals (Varbaro)
4. Proof of Kalai's conjecture (Murai)

...and lots more.

For my own research, I was particularly happy to interact with Mats Boij, who showed me some things related to inverse systems that I will now publish as part of the next Macaulay2 release."

Takayuki Hibi wrote: "My participation in the BIRS workshop created a motive to write a new paper as well as a new research project. In fact, (a) During the coffee break just after my talk, Marc Chardin kindly made a frank comment about the argument in my talk. His suggestion, in fact, can make our proof much elegant and, as a result, yields a motive to write a new paper. (b) Talking to Adam Van Tuyl over lunch about a conjecture on edge ideals, he agreed with me about making a new joint research project on regularity of edge ideals. Even though each of us have written a lot of papers on edge ideals, I have never had an opportunity to have a conversation with him. This is one of the most productive benefits gotten from participating in the workshop."

Srikanth Iyengar wrote: "Besides giving a chance to catch up and pursue "old" collaborators and collaborations (among whom I count Mark Walker, Claudia Miller and Liana Sega), the conference gave me a chance to talk to Lukas Katthaen. I am not sure this will lead to any theorems right away, but we certainly started a conversation that will be continued. Another benefit of the meeting was that I learnt some new things from Bernd Ulrich's talks that are pertinent to a ongoing project I have with Ryo Takahashi."

Thomas Kahle wrote: "I really enjoyed the workshop and how it helped me to stay up to date with some very recent developments in commutative algebra such as the result by Varbaro and Conca that extremal Betti numbers are preserved under square-free Gröbner degenerations.

Attending the workshop also gave me the chance to renew some long-running collaborations. Together with Lukas Katthän we tested some ideas on random structures in commutative algebra. The wonderful atmosphere at BIRS and Banff makes all this much more enjoyable and effective than collaboration via e-mail."

Paolo Mantero wrote: "This workshop also gave me the opportunity to make progress on two joint projects, one with J. McCullough and one with A. Sammartano; most likely the projects will be done around the end of the Fall semester. I also had the opportunity to discuss research ideas with Matteo Varbaro and Maria Evelina Rossi, which I am very grateful for, since both researchers reside and work in Europe, so without the workshop it is unlikely I could have had this great interactions with them.

Additionally, the workshop helped me strengthen the relation with Greg Smith and Adam Van Tuyl; as a likely outcome I will give talks at their institutions (Queen's University and McMaster University) in the near future. It opens the door to potential future collaborations."

Irena Swanson wrote: "I enjoyed the conference, the talks, and the people very much. Thank you for inviting me. I will be teaching a course on homological algebra on my Fulbright at University of Graz this fall, so connecting with very recent research in the area is very beneficial. I learned much."

Adam Van Tuyl wrote: "I just wanted to write and thank you again for inviting me to conference at BIRS. I really enjoyed the talks, and I came away with a couple of new ideas to play with."

Participants

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De Stefani, Alessandro (University of Nebraska)
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Chapter 16

Spectral Geometry: Theory, Numerical Analysis and Applications (18w5090)

July 1 - 6, 2018

Organizer(s): Nilima Nigam (Simon Fraser University), Iosif Polterovich (Université de Montréal), Justin Solomon (MIT)

Overview of the Field

Spectral geometry is an area of mathematics at the intersection of analysis, partial differential equations and differential geometry. It investigates the properties of eigenvalues and eigenfunctions of the Laplacian and other operators, including their dependence on the geometric, topological and dynamical features of the underlying space (e.g. a Riemannian manifold or a Euclidean domain).

Originally, spectral geometry was motivated by the study of mathematical models of physical processes, such as vibration, heat propagation, oscillations of fluids and quantum-mechanical effects. The quest to better understand these phenomena lead to the development of powerful analytic and numerical methods in geometric spectral theory and also had a profound impact on engineering applications. In recent years, new and somewhat unexpected applications of these techniques to computer science have emerged, notably to shape recognition and machine learning. These applications, in turn, inspire new exciting theoretical and computational challenges.

Spurred by recent fast-paced progress on theoretical and applied aspects of spectral geometry, our workshop brought together experts on theoretical, numerical and applied aspects of this discipline, with the objective to foster interactions and promote new collaborations. To our knowledge, no interdisciplinary meetings of this kind have been held previously, and by all accounts the meeting led to a variety of new research collaborations and open problems.

Recent Developments

There is a long history of fruitful interactions between geometric spectral theory, numerical analysis and computer science. In recent years, the interplay between these fields has reached new heights due to the emergence of increasingly powerful computers, new motivating applications and more efficient numerical algorithms.

Numerical calculations serve as an indispensable source of intuition and are behind many important advances in spectral geometry. In particular, numerical experiments played a stimulating role in recent breakthrough research on nodal portraits of random linear combinations of eigenfunctions (see, for instance, [**?**, **?**, **?**]). Numerical methods are actively used in the rapidly developing theory of spectral minimal partitions (see [**?**, **?**]). For low eigenvalues, numerical experiments are a major source of conjectures in shape optimization problems (see [**?**, **?**, **?**, **?**]). An exciting new trend is to use numerical analysis not only to formulate conjectures, but to actually prove theorems in spectral geometry [**?**, **?**] using rigorous computer-assisted methods.

Some of the most important recent applications of spectral geometry lie in the areas of shape analysis and machine learning (see [**?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**]). These applications are based on the properties of spectral quantities such as heat kernels and eigenfunctions associated with the Laplacian (see, for instance, [**?**, **?**]). As it is now well-understood, the Laplacian on a Riemannian manifold carries a lot of information about intrinsic geometry. To capture the extrinsic geometry of shapes using spectral quantities, however, one needs to use other operators. A natural choice is the Dirichlet-to-Neumann operator, which, incidentally, has been in the focus of intensive research in theoretical spectral geometry in recent years (see [**?**, **?**, **?**, **?**, **?**, **?**, **?**]). The collection of eigenvalues of the Dirichlet-to-Neumann operator is also called the Steklov spectrum, as it is precisely the spectrum of the Steklov boundary value problem. Recent advances in the study of the Steklov spectrum, particularly, of the corresponding geometric invariants, open up a number of promising new applications to shape analysis (see [**?**]).

Accompanying these developments, the design and analysis of high-accuracy discretization methods for spectral problems and optimal design has been the focus of intense research activity in numerical analysis. A plethora of discretization techniques—including methods based on particular solutions [**?**], spectral methods, finite element methods [**?**, **?**] and integral equation methods [**?**]—have been developed. Each of these methods presents both advantages and challenges in the numerical analysis, and this analysis in turn leads us to improved understanding of the properties of the eigenvalues and eigenfunctions of the operators under investigation, and can spark entirely novel areas of development. For example, as described in [**?**], the use of very common Lagrange finite elements for the Maxwell eigenvalue problem was shown to yield the wrong spectrum even on simple geometries, motivating the large-scale adoption of the edge finite elements. The design of numerical methods for inverse problems has lead to the investigation of (nonlinear and non self-adjoint) transmission eigenvalue problems, and this in turn lead to the design of novel methods. The computations were used extensively to enhance our understanding of the situations under which the existence of such eigenvalues could be proven. The design of a boundary integral method for mixed Dirichlet-Neumann eigenvalues of the Laplacian is necessarily intertwined with a careful study of the asymptotic behaviour of the eigenfunctions [**?**].

Upon discretization, the resulting large discrete systems have been coupled to state-of-the-art eigenvalue solvers and optimization methods. Naïve approaches do not suffice, and the design of good algorithms in this area has yielded many interesting and challenging research directions, due to the potentially nonlinear/non-convex nature of the objective function to be optimized. If the eigenvalues are clustered, or if the original spectrum is not discrete, these problems are much harder, see e.g. [**?**].

Another fascinating and important area of investigation seeks to provide computable error bounds and eigenvalue enclosures, e.g. [**?**]. These bounds are crucial if numerical methods are to be used for formulating conjectures.

Finally, practitioners in geometry processing, computer graphics, medical imaging, machine learning, and other computational disciplines have employed spectral geometry to great effect, improving the quality and flexibility of algorithms for a broad range of geometric tasks. The most exciting research in this field requires synthesis of theoretical, numerical, and applied ideas to motivate practical research problems, extract detailed understanding of underlying models, and formulate discrete approximations that provide a stable, faithful link between theory and practice.

Presentation Highlights

In view of the interdisciplinary nature of the workshop, the talks were equally divided into three main themes: theory, numerics and applications. In each theme, one talk was reserved for an overview of the subject. All speakers were advised to give colloquium-style presentations accessible to non-experts.

Theoretical aspects of spectral geometry

A broad historical overview of theoretical advances in spectral geometry from Lord Rayleigh and Hermann Weyl to our time was presented by Michael Levitin. He described some major results on eigenvalue estimates, spectral asymptotics and spectral geometry of the Dirichlet-to-Neumann map. These were recurrent themes during the workshop, and Michael's talk served as an excellent introduction to the subject.

The talks by Dorin Bucur and Mikhail Karpukhin were concerned with shape optimization for Laplace eigenvalues on Riemannian manifolds and Euclidean domains. Dorin Bucur presented his recent work with Antoine Henrot [**?**] on the maximization of the second nonzero Neumann eigenvalue on Euclidean domains. They have shown that among all domains (not necessarily connected) of given volume, the second nonzero Neumann eigenvalue is maximized by a disjoint union of two identical balls. This result extends the 2009 theorem of Girouard, Nadirashvili and Polterovich [**?**] who proved a similar statement for simply connected planar domains. Mikhail Karpukhin reported on his recent joint work with Nadirashvili, Penskoi and Polterovich on a sharp isoperimetric inequality for all Laplace eigenvalues on a sphere [**?**]. It was shown that for any positive integer k, the k-th nonzero eigenvalue on the two-dimensional sphere endowed with a Riemannian metric of fixed area, is maximized in the limit by a sequence of metrics converging to a union of k touching identical round spheres. This proved a conjecture posed by Nadirashvili in 2002.

David Sher and Asma Hassannezhad spoke about recent progress in understanding spectral asymptotics for Steklov-type problems on Euclidean domains. David Sher presented his recent joint work with Levitin, Parnovski and Polterovich on the proof of the two-term asymptotic formula for sloshing (mixed Steklov–Neumann) eigenvalues on planar domains [**?**]. In particular, this result confirmed the 1983 conjecture of Fox–Kuttler [**?**] and could be considered a first step towards obtaining sharp spectral asymptotics for the Steklov eigenvalues (or, equivalently, eigenvalues of the Dirichlet-to-Neumann map) on polygons. Asma Hassannezhad's talk was based on her joint work with Ari Laptev [**?**] on estimates on the Riesz means for the eigenvalues of mixed Steklov problems on Euclidean domains of arbitrary dimension.

Virginie Bonnaillie-Noël presented a collection of analytic and numerical results on spectral minimal partitions. Earlier developments on this topic were mostly concerned with either sums or maxima of the first eigenvalues of a partition. The talk focused on recent advances in the general case of the p-norm of the vector composed by the first eigenvalues of each subdomain of the partition. Some of these results were obtained jointly with Beniamin Bogosel [**?**, **?**].

Yaiza Canzani presented her recent joint works with John Toth and Jeffrey Galkowski [**?**, **?**] on estimates of the averages of Laplace eigenfunctions over Riemannian submanifolds. Particularly strong results were obtained for surfaces with an Anosov geodesic flow, such as surfaces of negative curvature.

Numerical methods

Jeff Ovall presented an overview of discretization strategies and methods for locating the eigenvalues of discrete systems. Naïve implementations of discretizations can lead to problematic results, and this point was highlighted by simple examples. Next, he presented a filtered subspace iteration strategy for (possibly) unbounded self-adjoint operators. The method is analyzed in a fairly general framework. The bulk of the computational effort in the algorithm involves approximating the action of the resolvent at a few points along a contour enclosing the eigenvalues of interest.

David Colton provided a survey of transmission eigenvalue problems. These arise in inverse scattering theory, and are non-self-adjoint in nature. Transmission problems exhibit fascinating spectral properties and many open questions remain: indeed, the existence of the spectrum is only guaranteed under fairly restrictive assumptions on the contrast parameter. Whether these can be relaxed is an interesting open question. A remarkable connection (due to Fioralba Cakoni and Sagun Chanillo) between the location of transmission eigenvalues for automorphic solutions of the wave equation in the hyperbolic plane and the Riemann hypothesis was also briefly discussed.

The spectral indicator method described by Jiguang Sun is an efficient method for determining the location and multiplicity of eigenvalues in the complex plane. The indicators are inexpensive to compute, and the method is memory-efficient even for large spectral problems.

There is an intimate connection between the numerical analysis of wave scattering problems and the calculation of spectra; the family of time-domain spectral methods have typically relied on the availability of eigenfunctions of the Laplacian on a given domain to serve as an efficicent basis. These can, however, be prohibitively expensive to compute on complex geometries. Oscar Bruno described the need for spectrally accurate algorithms for both scattering and spectral problems, and discussed some of the key ideas behind integral-equation based approaches.

Xuefeng Liu presented the recent progress in providing guaranteed eigenvalue bounds in computation. For all but the simplest geometries the eigenvalues of elliptic operators are computed via approximation; it is important to be able to state computable intervals around the approximate eigenvalue within which the true eigenvalue is guaranteed to lie. Such a method is now available using finite element methods, and guaranteed eigenvalue bounding strategies for the Laplace, the Biharmonic, the Stokes, the Steklov operators were presented. A related talk was given by Joscha Gedicke on his joint worith with Carsten Carstensen. He discussed recent results on guaranteed lower bounds for eigenvalues of the Laplace operator on arbitrary coarse meshes using the nonconforming Crouzeix-Raviart finite element method. This approach was shown to yield guaranteed eigenvalue bounds of surprisingly high accuracy.

Francesca Gardini's talk was concerned with the adaptive finite elmeent method for eigenvalue problems. In particular, she explained how this method could be used to approximate multiple eigenvalues and clusters of eigenvalues. Optimal convergence of the method for the Laplace eigenvalue problem in mixed form was also discussed.

Sebastien Dominguez presented his joint work with Nilima Nigam and Jiguang Sun on Jones modes in Lipschitz domains. The Jones eigenvalue problem is an overdetermined problem, where the Neumann eigenvalue problem for linear elasticity is coupled with a constraint on the normal trace of the displacement along the boundary. It is relatively unexplored and has many interesting features, notably its sensitive dependence on boundary geometry. In the talk, existence of eigenpairs for this eigenvalue problem was proved in two and three dimensions, and some numerical results were presented on simple geometries.

The meeting concluded by the talk of Braxton Osting on his joint work with Dong Wang and Ryan Viertel on diffusion generated methods for target valued maps. Diffusion generated methods were discused for minimizing the Dirichlet energy of a function taking values in a wide class of target sets. Applications to finding Dirichlet partitions, generating quadrilateral meshes and solving certain inverse problems were presented.

Applications

Justin Solomon gave a survey of applications of spectral geometry to different disciplines in computer science, including computer graphics, machine learning, and medical imaging. The key theme in his talk was to show how the numerical methods and theoretical results covered in the previous survey talks are incorporated into algorithms that leverage the geometry of scanned shapes and abstract clouds of data points.

Ron Kimmel reported on applications of spectral geometry to surface classification. The classification problem is to find an algebraic representation for each surface that would be similar for objects within the same class and preserve dissimilarities between classes. He discussed how to transform the geometric problem of surface classification into an algebraic form of classifying matrices. The eigenfunctions of the Laplacian with two distinct metrics on a surface are used extensively [**?**]. Another key topic is the connection with deep learning techniques, and a new approach for encoding geometric intuition into modeling, training, and testing. The key idea is to design learning algorithms to use geometric representations and invariants, for applications from shape matching, facial surface reconstruction from a single image, to reading facial expressions [**?**, **?**, **?**].

Etienne Vouga described preliminary results on inverse spectral problems, namely how to embed a piece of geometry given its Laplace–Beltrami spectrum. His talk covered a promising new algorithm leveraging spherical conformal parameterization techniques to pose the problem in terms of optimization over spherical harmonic coefficients. Preliminary experiments show some promise for practical tools that solve the inverse spectral problem numerically.

Mirela Ben-Chen and Amir Vaxman demonstrated the value of spectral geometry algorithms for problems involving vectors and frames on discrete surfaces. Prof. Ben-Chen's talk focused on an operator-based approach to vector field processing, representing fields not as collections of direction vectors but rather as derivative operators discretized as matrices; her work reveals new discretization techniques with structure-preserving properties, as well as applications to field design [**?**, **?**] and simulation [**?**, **?**]. Prof. Vaxman presented efforts to unify directional field processing with subdivision operators for discrete surfaces, providing a representation of vector fields compatible with subdivision-based superresolution.

Hervé Lombaert demonstrated the value of spectral techniques for medical image processing [**?**], in particular correspondence between 3D brain models gathered using MRI. In this domain, spectral algorithms allow for efficient and accurate intrinsic matching of neuroimaging data, enabling tools that transfer labels and other information across multiple scans and subjects [**?**].

Finally, Yu Wang showed that intrinsic surface-based algorithms for geometry processing can be extended to incorporate volumetric information by replacing the Laplacian with the Dirichlet-to-Neumann operator [**?**]. His application of the boundary element method (BEM) enables volumetric shape analysis without tetrahedral remeshing to fill the volume bounded by a surface. Intriguing theoretical questions arise from his work involving the behavior of integral operators involved discretizing the Dirichet-to-Neumann operator in the case of open surfaces.

Outcomes of the Meeting

The intents of this meeting were to (a) capture the state-of-the-art in the theory, numerical analysis and applications of spectral geometry, (b) provide a forum for experts in these typically disparate communities to interact and (c) identify common challenges or problems of mutual interest. As is typical in many mathematical disciplines, several subcommunities of researchers make significant progress with little "cross-pollination", sharing their results with others who may benefit or have ideas for extension.

The current workshop was demonstrably successful in achieving these goals. Longer tutorial and survey-style talks from theory, numerics and applications set a common technical base and vocabulary among the participants. For instance, we saw that the 'stiffness matrix' in finite elements is the 'cotangent Laplacian' in discrete differential geometry. Shorter talks presented the state-of-the-art from the viewpoint of the subcommunities, and the tutorials prepared all the participants to understand some of the recent developments in the field more broadly, as well as to launch meaningful interactions and collaborations. The breaks and open problem sessions generated several interactions and inspired research projects of mutual interest. Here is a sampling of open problems:

Inferring interior structure of Mars from spectral data

The first seismometer is about to land on Mars in November 2018. Amongst other data, it will be able to measure the spectrum of free elastic oscillations of the planet. What can be inferred about the internal structure of Mars from this data? Do discontinuities in the media have a "spectral fingerprint" in terms of heat invariants, Weyl asymptotics, or some other spectral quantity? As a simple first model, one may consider the Neumann spectrum of the Laplace-Beltrami operator on a Riemannian manifold with boundary when the metric has a conormal jump or other singularities across a hypersurface.

This problem was presented by Joonas Illmavirta.

A numerical analysis for the Jones eigenvalue problem in elasticity in curvilinear domains

An unusual eigenvalue problem in elasticity was introduced by D.S. Jones [**?**], in the larger context of fluid-structure and elastodynamic transmission problems. Stated abstractly, the eigenvalue problem is as follows. Let Ω be an open and bounded domain in $\mathbb{R}^d$ with reasonable boundary, and $\lambda, \mu \in \mathbb{R}$ are given constants so that $\mu > 0, \lambda + \frac{2}{d}\mu > 0$. We seek nontrivial $\mathbf{u}$, vector fields in Ω, and $\omega^2 \in \mathbb{C}$ such that

$$\mathcal{L}\mathbf{u} := \mu\Delta\mathbf{u} + (\lambda + \frac{2}{d}\mu)\text{grad}\,\text{div}\mathbf{u} = \omega^2\mathbf{u} \tag{16.0.1}$$

in Ω. On the boundary we enforce the natural boundary condition for the *Lamé* operator $\mathcal{L}$. In addition, we enforce $\mathbf{u} \cdot \mathbf{n} = 0$ on the boundary of Ω, where $\mathbf{n}$ is the unit outer normal to the boundary (defined a.e.). It was only recently established that this constrained eigenvalue problem has a discrete countable spectrum in non-axisymmetric domains with Lipschitz boundaries; it was shown by Hargé in 1990 that the set of C^∞ domains which do not support such a spectrum is dense amongst all possible C^∞ domains. It is clear that any rigid rotation is a Jones mode in a disk, and so zero is an eigenvalue of $\mathcal{L}$ in some instances.

We would like to understand the approximation problem of computing these eigenmodes in curvilinear domains. A standard mesh of triangles will not approximate the boundary exactly, and a consistency error is committed. Certain coercivity constants degenerate in the passage from polygonal domains with many sides to a curvilinear domain, and therefore one question is: In what situations does the Jones spectrum on approximating domains approach the true Jones spectrum, and at what rate? Another question is: Can one develop a stable approximation scheme for the eigenmodes in curvilinear domains?

This problem was presented by Nilima Nigam.

Discrete isoperimetric inequalities

Fine-grained results characterize isoperimetry in terms of the eigenvalues of the Laplacian operator for shapes embedded in the plane; for instance, the shape extremizing the first eigenvalue is a circle. No analogous results, however, are known about discrete Laplacian operators, e.g. the cotangent Laplacian from first-order finite elements on a triangle mesh. Suppose the topology of a triangle mesh with n vertices is fixed. Then, we could consider the first nonzero Laplacian eigenvalue of the mesh to be a function $\lambda(X) : \mathbb{R}^{n\times 2} \to \mathbb{R}_+$, where $X \in \mathbb{R}^{n\times 2}$ gives the positions of the vertices in the plane. Then, we could ask the usual isoperimetric question: What configuration of vertices in X extremizes $\lambda(X)$ subject to a constraint on the area covered by X in the plane?

Similarly, if we fix the boundary of a polygonal region $\Omega \subseteq \mathbb{R}^2$, we have many choices of triangulations in the interior of Ω. A distinguishing feature of the discrete problem is that different triangulations of the same region in the plane may have different spectra. Hence, we can ask: What conditions on a mesh of Ω make for larger or smaller principal eigenvalues?

This problem was presented by Justin Solomon.

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Chapter 17

Around Quantum Chaos (in conjunction with 2018 ICMP in Montreal) (18w5002)

July 15 - 20, 2018

Organizer(s): Dmitry Jakobson (McGill University), Stephane Nonnenmacher (Universite Paris-Sud), Steve Zelditch (Northwestern university)

Introduction

The workshop was focussing on various aspects of "quantum chaos", namely the study of quantum or wave systems, the classical limit of which exhibits some chaotic behaviour. More generally, the talks concerned the high frequency and semiclassical limit of wave propagation in various geometric settings.

Quantum Chaos aims to understand spectra and eigenstates of quantum systems, and relate them to the properties of the corresponding classical dynamical system. The Correspondence Principle in Quantum Mechanics predicts that certain features of the classical system manifest themselves in the semiclassical limit of its quantization. For example, the properties of high energy eigenvalues and eigenfunctions of the Laplacian Δ on a Riemannian manifold should reflect the properties of the corresponding geodesic flow. Other examples include the billiard flow, for spectral problems on manifolds with boundary (Gérard–Leichtnam, Zelditch–Zworski); the frame flow, for the Dirac operator and the Hodge Laplacian (Jakobson–Strohmaier–Zelditch); and branching billiard flows, for systems where the operator coefficients have jump discontinuities (Colin de Verdière, Jakobson–Safarov–Strohmaier).

The workshop gathered specialists studying such problems for various systems, including Riemannian manifolds (with ergodic, completely integrable or mixed geodesic flows), arithmetic manifolds, quantum graphs, as well as random systems. The spectral theory of such systems is studied using a variety of different methods, including microlocal analysis, number theory, the theory of elliptic PDE, probabilistic methods and graph theory. The goal of the workshop was to review the latest progress in the field (including the work related to several fascinating *universality conjectures*), and to facilitate interactions between specialists of different subdomains.

The workshop was organized in conjunction with 2018 ICMP in Montreal that was held the following week. Many workshop participants also took part in the ICMP.

Participants

The workshop attracted altogether 34 participants, among whom 6 graduate students, 3 postdocs and about 5 recently hired academics. A vast majority of the participants stayed the whole week. The origin of the participants was essentially Western Europe and North America.

Detailed report

Monday was devoted to the analysis of high frequency eigenfunctions of Laplace-Beltrami or Schrödinger operators on Riemannian manifolds. The structure of these eigenfunctions can be described in various ways: through their L^p norms (how fast do the norms grow with the frequency?), through their restrictions on submanifolds, through their microlocal concentration properties (that is, their localization properties on the manifold and in Fourier space), through the structure of their nodal set. The interplay between these different aspects has proved very fruitful. Some of the talks focussed on situations of *Quantum chaos*, that is when the geodesic flow on the manifold is chaotic, leading to a certain amount of delocalization for the eigenfunctions.

The first talk was given by Jeff Galkowski. The title was Concentration of eigenfunctions: sup norms and averages. Jeff related the microlocal concentration of Laplace eigenfunctions (that is, their localization in phase space) to their sup-norms and their averages on submanifold. In particular, he presented a unified picture for sup-norms and submanifold averages, which characterizes the concentration of those eigenfunctions with maximal growth. He then exploited this characterization to derive geometric conditions under which maximal growth cannot occur. Moreover, he obtained quantitative gains on possible growth in a variety of geometric settings. The talk was mostly based on joint works with Y.Canzani and J.Toth.

The second talk was given by Semyon Dyatlov, who spoke on Lower bounds on eigenfunctions and fractal uncertainty principle. The talk concerned the following problem. Let (M, g) be a compact Riemannian manifold and $\Omega \subset M$ a nonempty open set. Take an L^2 normalized eigenfunction u_λ of the Laplacian on M with eigenvalue λ^2. What lower bounds can we get on the mass $m_\Omega(u_\lambda) = \int_\Omega |u_\lambda|^2$? There are two well-known bounds for a general manifold M:

(a) $m_\Omega(u_\lambda) \geq c\, e^{-c\lambda}$, following from unique continuation estimates,

(b) $m_\Omega(u_\lambda) \geq c$, assuming that Ω intersects every sufficiently long geodesic (this is known as the *geometric control condition*).

(in both cases $c > 0$ is independent of λ). In general one cannot improve the bound (a) for an arbitrary domain Ω, as illustrated by the example of the "Gaussian beam" eigenstates of the round sphere, which are exponentially concentrated along the equator.

Semyon presented a recent result which establishes the lower bound (b) for *any* choice of Ω if M is a compact surface of constant negative curvature. This bound has numerous applications, such as a control for the Schrödinger equation, the exponential decay of damped waves (no matter how small the support of the damping is), and the full support property for the semiclassical measures associated with the eigenstates. The proof uses the chaotic nature of the geodesic flow on M. The key new ingredient is a recently established *Fractal Uncertainty Principle*, which states that no function can be simultaneously localized close to fractal sets in both position and frequency. This talk was based on joint works with Joshua Zahl, Jean Bourgain and Long Jin.

The first talk of the afternoon was given by John Toth, joint work with X. Wu. It was titled Reverse Agmon estimates for Schrödinger eigenfunctions. Let (M, g) be a compact, Riemannian manifold and $V \in C^\infty(M; \mathbb{R})$. Given a regular energy level $E > \min V$, John considered L^2-normalized eigenfunctions, u_h of the semiclassical Schrödinger operator $P(h) = -h^2\Delta_g + V$ with eigenenergies $E(h) = E + o(1)$ as $h \to 0^+$. The well-known Agmon-Lithner estimates are exponential decay estimates (i.e. upper bounds) for eigenfunctions in the forbidden region $\{V(x) > E\}$. The decay rate is given in terms of the Agmon distance function d_E associated with the degenerate Agmon metric $(V - E)_+\, g$ supported in the forbidden region.

The main result is a partial converse to the Agmon estimates (ie. exponential lower bounds for the eigenfunctions) in terms of Agmon distance in the forbidden region, under a control assumption on the L^2 mass of the eigenfunction in the allowed region $\{V(x) < E\}$ arbitrarily close to the caustic $\{V(x) = E\}$. John explained this reverse Agmon estimate, and then gave some applications to the restrictions of the eigenfunctions on hypersurfaces situated in the forbidden region, along with corresponding nodal intersection estimates.

The next talk was given by Lior Silberman (joint work with S. Eswarathasan), entitled Scarring of quasimodes on hyperbolic manifolds. For M be a compact hyperbolic manifold, the entropy bounds of Anantharaman *et al.* restrict the possible invariant measures on T^1M that can be obtained as semiclassical measures of sequences of Laplace eigenfunctions. On the other hand, if one relaxes the strict eigenfunction condition, but authorizes approximate eigenfunctions ("quasimodes") with a certain precision, the associated semiclassical measures may be less constrained. The precision threshold beyond which the entropy bounds relax corresponds to so-called "logarithmic quasimodes" (the precision depends inverse logarithmically with the approximate eigenvalue). It is thus relevant to construct quasimodes of this precision, which may be associated with more singular semiclassical measures. Generalizing works of Brooks and Eswarathasan–Nonnenmacher (who constructed logarithmic quasimodes concentrated on closed hyperbolic geodesics), Silberman considered hyperbolic manifolds M admitting a totally geodesic submanifold, and then constructed logarithmic quasimodes concentrating on this submanifold.

Etienne Le Masson gave the last talk on Monday, titled Quantum Chaos in the Benjamini-Schramm limit, based on joint works with T. Sahlsten, M. Abert and N. Bergeron. One of the fundamental problems in quantum chaos is to understand how high-frequency waves behave in chaotic environments. A famous but vague conjecture of Michael Berry predicts that they should look on small scales like Gaussian random waves. Etienne showed how a notion of convergence for sequences of manifolds, called the Benjamini-Schramm convergence, can provide a satisfying formulation of this conjecture. The Benjamini-Schramm convergence includes the high-frequency limit as a special case, but provides a more general framework. Based on this formulation, he expanded the scope and considered a case where the frequencies stays bounded but instead the size of the manifold increases. He formulated the corresponding random wave conjecture and presented some results to support it, including a quantum ergodicity theorem.

Tuesday was concerned with the study of nodal sets and critical sets of high frequency eigenfunctions, a topic which has experienced a boom in the last 10-15 years. Examples included the Laplace-Beltrami operator on manifolds or on quantum graphs, as well as the perturbations of the Harmonic oscillator on $\mathbb{R}^n$, where the geometry of the nodal set drastically differs between the allowed vs. forbidden regions of space.

The first talk was by Boris Hanin, titled Nodal Sets and Eigenvalues for Small Radial Pertrubations of the Harmonic Oscillator. In this talk, he presented some recent results (joint with T. Beck) about the behavior near infinity of the nodal sets of eigenfunctions for a small radial perturbation of the harmonic oscillator. For the unperturbed oscillator $P(h) = -h^2\Delta + |x|^2$, the separation of variables allows to write eigenfunctions as products of Laguerre functions and spherical harmonics. For a fixed energy $E_0 > 0$ and small semiclassical parameter $h > 0$, the eigenfunctions with energies $E = h(n + d/2) \approx E_0$ may be composed of spherical harmonics of degrees (= angular momentum) up to h^{-1}. Imposing a radial perturbation, the energy E eigenspace breaks into different energies with different angular momenta. The radial rate of growth for the eigenfunctions is an increasing function of their energy E. The authors' results give precise information about which angular momenta give the largest energies after perturbation, and are able to draw quantitative estimate for the nodal set of these eigenfunctions deep into the forbidden region.

The next talk was by Robert Chang, titled Log-scale equidistribution of nodal sets in Grauert tubes. Let M be a compact real analytic negatively curved manifold. It admits a complexification in which the metric induces a pluri-subharmonic function $\sqrt{\rho}$ whose sublevel sets are strictly pseudo-convex domains M_τ, known as Grauert tubes. The Laplace eigenfunctions on M analytically continue to the Grauert tubes, and their complex nodal sets are complex hypersurfaces in M_τ. S.Zelditch proved that the normalized currents of integration over the complex nodal sets tend to a single weak limit $dd^c\sqrt{\rho}$ along a density one subsequence of eigenvalues. In this talk, Robert discussed a joint work with S.Zelditch, in which they showed that the weak convergence result holds on small scale, namely, on logarithmically shrinking Kaehler balls whose centers lie in $M_\tau \setminus M$. The main technique is a Poisson-FBI transform relating quantum ergodicity on Kaehler balls to quantum ergodicity on the real domain. Similar small-scale quantum ergodicity results were obtained in the Riemannian setting by Hezari-Riviere and Han, and in the ample line bundle setting by Chang-Zelditch.

In the next talk, Graham Cox talked about Nodal deficiency, spectral flow, and the Dirichlet-to-Neumann map. Courant's nodal domain theorem provides a natural generalization of Sturm–Liouville theory to higher dimensions; however, the result is in general not sharp. It was recently shown that the nodal deficiency of an eigenfunction is encoded in the spectrum of the Dirichlet-to-Neumann operators for the eigenfunction's positive and negative nodal domains. While originally derived using symplectic methods, this result can also be understood through the spectral flow for a family of boundary conditions imposed on the nodal set. In the talk Graham described this flow for a Schrödinger operator with separable potential on a rectangular domain, and describe a mechanism by which low energy eigenfunctions do or do not contribute to the nodal deficiency. Operators on non-rectangular domains and quantum graphs were also discussed. The talk represents joint work with G. Berkolaiko and J. Marzuola.

Gregory Berkolaiko gave a talk on Nodal statistics of graph eigenfunctions, based on joint work with L. Alon and R. Band. He started by reviewing the notion of "quantum graph", its eigenfunctions and the problem of counting the number of their zeros. The nodal surplus of the n-th eigenfunction is defined as the number of its zeros minus $(n-1)$, the latter being the "baseline" nodal count of Sturm-Liouville theory. It appears from numerics that the distribution of the nodal surplus of large graphs has a universal form: it approaches a Gaussian as the number of cycles grows. Gregory discussed recent progress towards proving this conjecture. When the graph is composed of two or more blocks separated by bridges, he proposed a way to define a "local nodal surplus" of a given block. Since the eigenfunction index n has no local meaning, the local nodal surplus has to be defined in an indirect way via the nodal-magnetic theorem of Berkolaiko, Colin de Verdière and Weyand. By studying the symmetry properties of the distribution of the local nodal surpluses the authors showed that for graphs with disjoint cycles the distribution of (total) nodal surplus is binomial.

Ram Band gave the next talk titled Neumann domains on manifolds and graphs, based on joint works with L. Alon, M. Bersudsky, S. Egger, D. Fajman and A. Taylor. The nodal set of a Laplace eigenfunction forms a partition of the underlying manifold or graph. Another natural partition is based on the gradient vector field of the eigenfunction (on a manifold) or on the extremal points of the eigenfunction (on a graph). The submanifolds (or subgraphs) of this partition are called Neumann domains. Ram presented the main results concerning these Neumann domains. He compared the situation for manifolds and graphs and related the Neumann domain results in each case to the corresponding nodal domains.

The last talk on Tuesday was given by Junehyuk Jung, titled Boundedness of the number of nodal domains of eigenfunctions. The asymptotic number of nodal domains of eigenfunctions is related with the dynamics of the geodesic flow on the manifold. For instance, if a surface with boundary has an ergodic geodesic flow, then for any given Dirichlet eigenbasis, one can find a density one subsequence of eigenfunctions, for which the number of nodal domains tends to $+\infty$ with the frequency. In this talk, Junehyuk discussed what happens to the unit circle bundle over a manifold. When equipped with a metric which makes the Laplacian commute with the circular action on the fibers, the geodesic flow never is ergodic. Recently he and S. Zelditch proved that among such metrics the following property is generic: for any given orthonormal eigenbasis one can find a subsequence of density one where the number of nodal domains is identically 2. This highlights how the underlying dynamics can impact the nodal counting. Junehyuk sketched the proof in the case of a compact surface of genus $\neq 1$, and presented an explicit orthonormal eigenbasis on the 3-torus where all the eigenfunctions only featured two nodal domains.

On **Wednesday** morning, the talks dealt with the study of resonances, both in the case of hyperbolic dynamical systems (Pollicott-Ruelle resonances) and in quantum disordered systems (Anderson model). The dynamical resonances were investigated using tools from microlocal analysis, thus establishing a direct connection with quantum chaos.

Gabriel Rivière gave a talk titled Witten Laplacians and Pollicott-Ruelle spectrum, based on joint work with N.V. Dang. Given a smooth Morse function and a Riemannian metric on a compact manifold M, Witten defined a twisted Laplacian, which is nowadays referred to as the Witten Laplacian. In light of the recent developpement towards the spectral analysis of hyperbolic dynamical systems, Gabriel discussed some well-known properties and some new ones of these Witten Laplacians. For instance, he explained that the spectrum of this operator converges, in the semiclassical limit, to a certain Pollicott-Ruelle spectrum, describing the decay of correlations for the geodesic flow on M.

The next talk by Frederic Faure was titled Some properties of hyperbolic dynamics from micro-local analysis, joint work with M. Tsujii. In a uniformly hyperbolic system (Anosov system), each trajectory is strongly unstable and its behavior is unpredictable. A smooth probability distribution evolves also in a complicated way since it acquires higher and higher oscillations. Nevertheless, using microlocal analysis, this evolution is predictable in the sense of distributions. It is similar to a quantum scattering problem in the cotangent space, as treated by Helffer and Sjöstrand using escape functions in 1986. In the talk Frederic used wave packet formalism (or FBI transform) and explained how to derive some spectral properties of the dynamics: the existence of the intrinsic discrete spectrum of Ruelle-Pollicott resonances, informations about their distribution (fractal Weyl law, band structure), or estimates on the wave front set of the metastable states associated with the resonances.

The last talk on Wednesday (followed by a free afternoon) was delivered by Martin Vogel, titled Resonances for large random systems. There have been many works studying resonances generated by compactly supported potentials and by potentials which decay sufficiently fast at infinity. However, in the case of random potentials there are only very few results. Martin gave an overview of some recent results in this direction by J. Sjöstrand, A. Drouot and F. Klopp. In particular he discussed his results obtained in collaboration with F. Klopp on the distribution of resonances close to the real axis, and their link to the eigenstates of a full random Schrödinger operator in the localized regime.

The first four talks on **Thursday** concerned various forms of random wave models, which were initially proposed as models describing the statistical properties of quantum chaotic eigenfunctions. These models are now investigated by both probabilists and mathematical physicists, making connections with percolation theory and real algebraic geometry.

Igor Wigman spoke on Russo-Seymour-Welsh estimates for the Kostlan ensemble of random polynomials, based on joint work with D. Beliaev and S. Muirhead. Beginning with the predictions of Bogomolny-Schmit for the random monochromatic plane wave, in recent years deep connections have emerged between the level sets of smooth Gaussian random fields and percolation. In classical percolation theory a key input into the analysis of global connectivity are scale-independent bounds on crossing probabilities in the critical regime, known as Russo-Seymour-Welsh (RSW) estimates. Similarly, establishing RSW-type estimates for the nodal sets of Gaussian random fields is a major step towards a rigorous understanding of these connections. The Kostlan ensemble is an important model of Gaussian homogeneous random polynomials. The nodal set of this ensemble is a natural model for a 'typical' real projective hypersurface, whose understanding can be considered as a statistical version of Hilbert's 16th problem. In the talk, Igor established RSW-type estimates for the nodal sets of the Kostlan ensemble in dimension two, providing a rigorous relation between random algebraic curves and percolation. The estimates are uniform with respect to the degree of the polynomials, and are valid on all relevant scales; this result resolves an open question raised recently by Beffara–Gayet. More generally, the arguments yield RSW estimates for a wide class of Gaussian ensembles of smooth random functions on the sphere or the flat torus.

Yaiza Canzani spoke on Local universality for zeros and critical points of monochromatic random waves, based on joint work with B. Hanin. In the talk she discussed the asymptotic behavior of zeros and critical points for monochromatic random waves on compact smooth Riemannian manifolds, as the energy of the waves grows to infinity.

Damien Gayet gave a talk titled Percolation of random nodal lines. If a real smooth function is given at random on the plane, what is the probability that its vanishing locus has a large connected component? Damien explained some recent answers he obtained with Vincent Beffara to this question, for some natural models coming from algebraic geometry and spectral analysis.

Melissa Tacy gave a talk titled Does it matter what we randomize? The behaviour of quantum chaotic states of billiard systems is believed to be well described by Berry's random plane wave model $u = \sum_j c_j e^{i\lambda x \cdot \xi_j}$, where the c_j are Gaussian random variables. However, in $\mathbb{R}^n$ there are many other candidate waves over which we could randomize. Some are easier to adapt to manifolds than others. In this talk Melissa discussed when (in $\mathbb{R}^n$) we can replace the plane wave $e^{i\lambda x \cdot \xi_j}$ with other waves and how those can be adapted to manifolds.

The last two talks on Thursday as well as the first one on Friday were concerned with wave propagation or wave control in presence of nonsmooth coefficients: control of the Schrödinger operator by an arbitray L^2 control function; propagation of singularities on surfaces with conical singularities, or in presence of a potential with a conormal singularity along a hypersurface.

Nicolas Burq spoke about Rough controls for the Schrödinger equation on the torus. He presented some results on the exact controllability of the Schrödinger equation on the torus. In a general setting, these questions are well understood for wave equations with continuous localization functions, while for Schrödinger one only has partial results. For rough localization functions, Nicolas first presented some partial results for waves. Then he showed how one can take benefit from the particular simplicity of the geodesic flow on the torus to get (for continuous localization functions) strong results (works by Haraux, Jaffard, Burq-Zworski, Anantharaman-Macia). Finally, for general localization functions (typically characteristic functions of measurable sets) he showed how one can go further, by taking benefit from dispersive properties (on the 2 dimensional torus), to show that in this setting the Schrödinger equation is exactly controllable by any L^2 (non trivial) localization function (and in particular by the characteristic function of any set with positive measure).

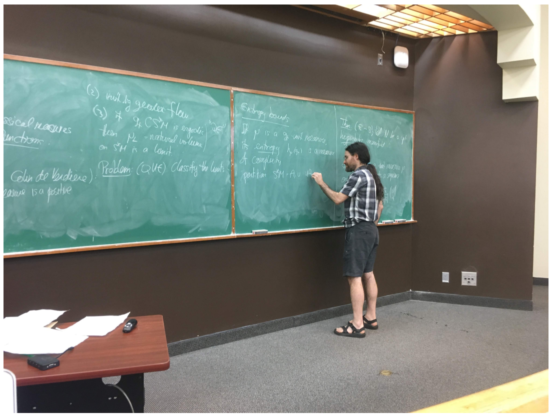
Luc Hillairet spoke on The wave trace on a flat surface with conical singularities. In joint work with A. Ford and A. Hassell, he studies the contribution to the wave trace of diffractive periodic orbits on Euclidean surfaces with conical singularities. Using a new description of the propagator near the so-called geometrically diffractive rays, he is able to compute the leading term of any kind of diffractive periodic orbit.

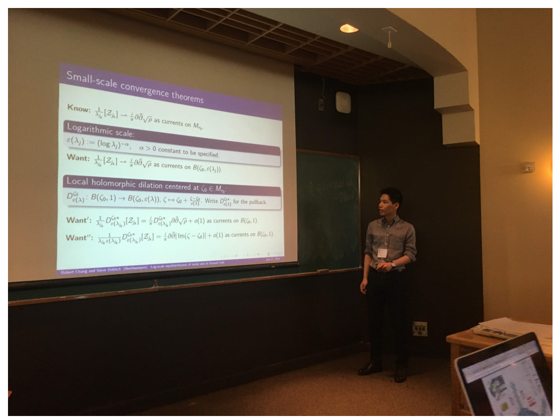
Jared Wunsch spoke on Diffraction of semiclassical singularities by conormal potentials, joint work with O. Gannot. Consider a semiclassical Schrödinger operator $P = -h^2\Delta + V$, where V has a conormal singularity along a hypersurface. The singular structure of V affects the propagation of semiclassical singularities for solutions to $Pu = Eu$, and in particular there is a 'diffraction' of the wavefront set by the interface: singularities are reflected as well as transmitted as they cross the interface transversely. The reflected wave, however, is more regular, with the improvement depending on the regularity of the interface; moreover singularities cannot (for high enough regularity) glide along the interface.

The last conference talk on **Friday** by Semyon Klevtsov described the mathematical theory of the Quantum Hall Effect, more specifically the study of Laughlin states, the fundamental Ansätze of this theory. It was titled Geometry and large N asymptotics in Laughlin states. Laughlin states are N-particle wave functions, successfully describing the fractional quantum Hall effect (QHE) for plateaux with simple fractions. It was understood early on that much can be learned about QHE when Laughlin states are considered on a Riemann surface. Mathematically, it is interesting to know how the Laughlin states depend on the Riemannian metric, the magnetic potential, the complex structure moduli, the singularities – for a large number of particles N. Semyon reviewed the results, conjectures and further questions in this area, and their relation to topics such as Coulomb gases/beta-ensembles, Bergman kernels for holomorphic line bundles, Quillen metric, or zeta regularized determinants.

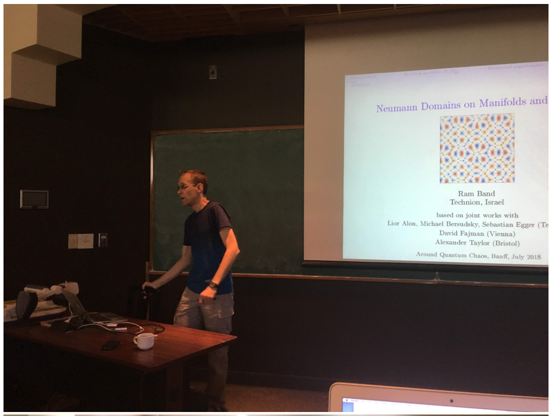
The conference ended around noon on Friday.

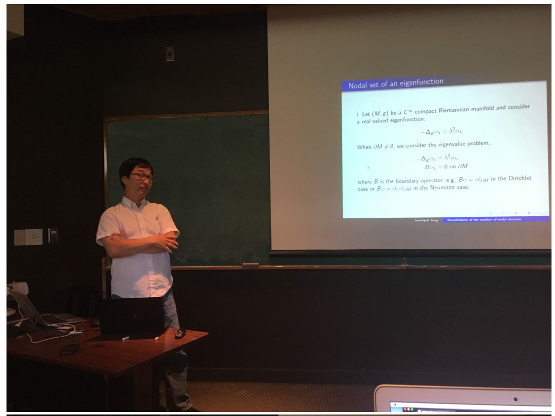
Photos

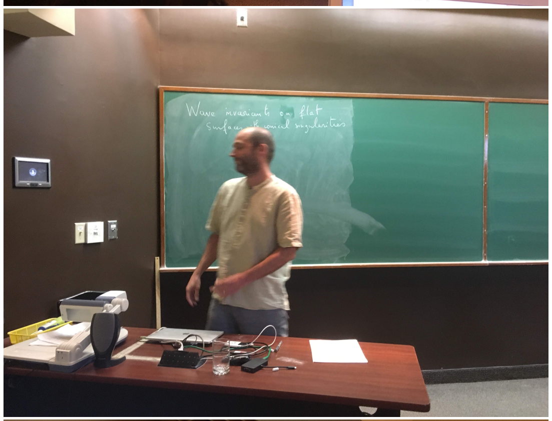


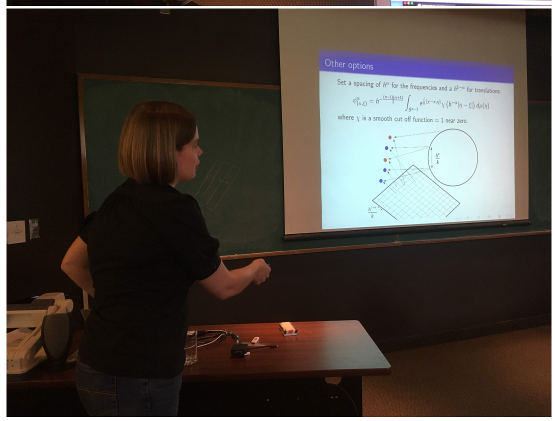

Small-scale convergence theorems
Logarithmic scale

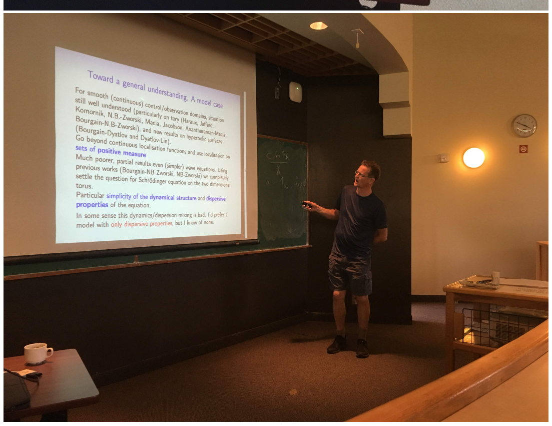

Nodal deficiency, spectral flow, and the Dirichlet-to-Neumann map
Graham Cox
Memorial University of Newfoundland
July 12, 2018











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Chapter 18

Physics and Mathematics of Quantum Field Theory (18w5015)

July 29 - August 3, 2018

Organizer(s): Jan Dereziński (University of Warsaw), Stefan Hollands (Leipzig University), Karl-Henning Rehren (Göttingen University)

Overview of the Field

The origins of quantum field theory (QFT) date back to the early days of quantum physics. Having developed quantum mechanics, describing non-relativistic systems of a finite number of degrees of freedom, physicists tried to apply similar ideas to relativistic classical field theories such as electrodynamics following early attempts already made by the founding fathers of quantum mechanics. Since quantum mechanics is usually "derived" from classical mechanics by a procedure called quantization, the first attempts tried to mimick this procedure for classical field theories. But it was clear almost from the beginning that this endeavor would not work without qualitatively new ideas, owing both to the new difficulties presented by relativistic kinematics, as well as to the fact that field theories, while possessing a Lagrangian/Hamiltonian formulation just as classical mechanics, effectively describe infinitely many degrees of freedom. In particular, QFT completely dissolved the classical distinction between "particles" (like the electron) and "fields" (like the electromagnetic field). Instead, the dichotomy in nomenclature acquired a very different meaning: Fields are the fundamental entities for all sorts of matter, while particles are manifestations when the fields arise in special states. Thus, from the outset, one is dealing with systems with an unlimited number of particles.

Early successes of quantum field theory consolidated by the early 50's, such as precise computations of the Lamb shifts of the Hydrogen and of the anomalous magnetic moment of the electron, were accompanied around the same time by the first attempts to formalize this theory in a more mathematical fashion. Owing to progress and the emergence of new perspectives on quantum field theory, several answers to this question have subsequently been formulated in the 80 years since its birth, illuminating the many facets of this theory. The quest for the ultimate mathematical framework of quantum field theory is still underway.

One of the main motivations for quantum field theory is the description of particle physics. This endeavor culminated in the early 80's in the formulation of the so-called standard model of particle physics, describing quarks, leptons, vector bosons mediating the various forces, as well as the recently discovered Higgs boson. These particles are believed to encompass the visible matter content of the universe, with the exception of dark matter (probably another invisible sector in the standard model) and dark energy. Although the various forces have qualitatively different features – becoming strong effectively at long, respectively short ranges – by the early 70's physicists developed reliable perturbative schemes to calculate quantities of direct physical interest in experiments. These computational techniques typically proceed via Feynman integrals and a systematic control of perturbation theory and renormalization. Open questions, like the convergence of the perturbation theory and infrared problems, motivated axiomatic approaches. It seems that the axiomatic approach that has proven the most vital is the operator algebraic approach. Its scope has widened in the last decades so as to cover more general situations such as thermal equilibrium, non-equilibrium states, or quantum field theory in curved spacetime.

Thermal equilibrium and non-equilibrium states were previously studied mainly in non-relativistic quantum many-body systems and condensed matter physics, where field-theoretical methods and renormalization also play a major role. Modern issues like the thermodynamics of black holes or of the early universe demand the extension of statistical physics to relativistic systems.

The mathematics involved in quantum field theory is very diverse, to the extent that for mathematicians QFT may appear as a collection of many different and completely unrelated formalisms. The underlying principles of quantum mechanics involve spectral theory and the theory of operator algebras, with modular theory playing a major role in modern applications. Perturbation theory naturally uses analysis (for the computation of Feynman integrals) and functional analysis (for questions of convergence, scattering theory, and adiabatic limits). Gauge theories involve tools from differential geometry, and their anomalies are related to cohomological issues. The theory of distributions and microlocal analysis are at the core of the study of states of quantum fields in nontrivial gravitational backgrounds. Modern constructive approaches to path integrals employ stochastic partial differential equations and regularity structures. Numerical high-performance simulations are employed for computations in numerous places. Computer-assisted exact methods, such as the "conformal bootstrap", have gained an increasing importance. (The list is certainly not complete.)

Quantum field theory triggered the development of various mathematical concepts of independent interest, such as non-commutative geometry, vertex operator algebras, tensor categories, random matrices, or topological invariants, to name but a few.

The aim of the workshop was to bring together researchers from different communities interested in various aspects of quantum field theory, so as to explore and vitalize the common roots of their respective approaches and to foster an exchange and comparison of ideas.

Recent Developments and Open Problems

In recent years the research about mathematical structure of quantum field theory made progress in various directions. When organizing this workshop, we decided to focus on the developments that to our minds appeared the most interesting in terms of potential physical applications, as well as from the purely mathematical point of view. Broadly speaking, the areas that we identified as the most interesting by these criteria can be classified as follows:

1. Developments relating **algebraic approaches** to quantum field theory with **perturbative methods**.
2. New ideas in **conformal quantum field theories**, which describe systems in statistical mechanics at the critical point or scale invariant models of particle theory. Among these, we identified the **conformal bootstrap** approach, which is applicable in principle in any dimension, and algebraic methods relating **vertex operator algebras** and non-commutative geometry/operator algebras, which are suitable in two dimensions.
3. **Algorithmic problems** in computing **Feynman integrals**, such as the Laporta algorithm and related ideas.
4. Recent developments in **stochastic quantization/stochastic partial differential equations** (which strictly speaking belong to pure mathematics, however they have strong analogies with quantum field theory).
5. Quantum field theory in **curved spacetime backgrounds**, and microlocal characterization of classes of "states of physical interest".
6. **Mean field approaches** to systems of electrons interacting with electromagnetic fields.
7. Interesting aspects of the **infrared problem** in models with massless particles.
8. **Non-equilibrium** situations in quantum field theory, such as heat waves, non-equilibrium steady states, entropy production, and return to equilibrium.

Our goal was to invite leading researchers representing each circle of ideas as speakers. In our view, this goal has been accomplished. A more detailed overview of the contributions is given in the next section; here we try to explain the context and motivation for our choices.

One major direction of the research over the past decade was an attempt to achieve a synthesis between algebraic and perturbative quantum field theory. This direction has several motivations. One is to put on a firm conceptual foundation the rules for perturbative calculations, especially in the cases where these rules are not clear-cut, or where naive interpretations of the existing rules lead to problems. Examples of this are: Dealing with the infrared problem, which plagues theories with massless particles; finding correct renormalization for quantum field theories on a non-trivial spacetime or e.g. electromagnetic backgrounds without symmetries; renormalization schemes for correlation functions in states other than the vacuum, such as thermal states, non-equilibrium steady states etc. The Epstein-Glaser method turned out to be a convenient tool to carry out such a programme. This method, invented in the 70's, is experiencing in recent years its revival. It works well in quantum field theory on curved spacetime. It is based on the theory of distributions, allowing for renormalization in position space, which is a setting without translation symmetry, where the Fourier transformation is not available. In recent years, complicated analytical questions about the existence and construction of special quantum states in curved spacetimes have been attacked using powerful methods from microlocal analysis instead of the more global technique of Fourier analysis.

One of the most important quantum field theories is quantum electrodynamics (QED). It is often useful to consider its approximate versions, which are easier to study by nonperturbative methods. One such version is the so-called mean-field QED, where charged particles are treated quantum-mechanically and the electromagnetic field is treated classically. The electromagnetic field is divided into a given external part and fluctuations, which are the object of a variational problem. Mean-field QED has been a topic of interesting research involving deep methods from analysis, convex optimization, calculus of variations. In practice, of particular interest are stationary states, but the method is in principle capable of treating non-equilibrium situations as well.

With a similar mix of conceptual and practical motivations, the algebraic viewpoint is exploited to address the notoriously difficult infrared problems in theories with massless particles, thus opening the door to more conceptional treatments of scattering of electrically charged particles and photons. The particularly transparent separation of infra-red and ultra-violet features of perturbative quantum field theories in such a treatment allows for conceptually clear and rigorous proofs of non-renormalization theorems, covering cases of current interest, such as supersymmetric gauge theories and, potentially, supergravity theories.

Algebraic approaches have also received a considerable new impetus from the emergent field of quantum information (QI). Key concepts within this field such a entanglement, capacities, local operations, etc. are naturally formulated in terms of algebraic notions such as entanglement measures, relative entropy functionals, conditional expectations or completely positive maps. While QI historically has been concerned mainly with quantum mechanical systems, it has triggered the interest in the above concepts also in relativistic systems, thus linking QI, for example, with non-equilibrium thermodynamics. Tomita-Takesaki modular theory (a celebrated theory in operator algebras) is used as an important tool when states cannot be described by density matrices.

In practical applications to high-energy physics, once a renormalization scheme is settled upon, calculations of scattering amplitudes typically lead to the problem of evaluating Feynman integrals. Such integrals come with certain parameters, such as masses or the powers of the propagator kernels. Typically, there can exist many relationships between these expressions for different parameters. This naturally leads to the quest for "bases" of independent integrals and algorithms for determining such bases and for computing the corresponding integrals. Such algorithms are thereby not only of practical importance, but also seem to have interesting connections to questions in algebraic geometry and the theory of D-modules.

The idea of stochastic quantization goes back to the early 80's. It is closely related to quantum field theory, especially its Euclidean version. Not surprisingly, stochastic partial differential equations are often affected by divergences of various sorts. A considerable progress how to deal with such divergences has recently been achieved. This progress has triggered renewed interest in various aspects of renormalization.

Conformal quantum field theories form an important subclass of QFT. They are interesting for many reasons: they are relevant for critical phenomena in statistical physics and they have a surprisingly rich structure, which often allows for finding explicit solutions. Besides, they are often good approximations to a realistic description of high-energy physics – note that the Lagrangian of the Standard Model contains only one term that breaks the conformal invariance on the classical level: the Higgs mass term. This approximate conformal invariance is exploited in a recent proposal of Meissner and Nicolai for a quantum field theory that should adequately describe high energy physics over many orders of magnitude beyond the Standard Model.

Conformal invariance is especially rigid in two dimensions. It can be used to describe a large class of models of conformal quantum field theory with rigorous constructive schemes and a complete classification. This classification involves sophisticated mathematical tools such as elements of the theory of categories. Conformal field theory has been developed in various research directions, including the approach based on operator algebras, and a more formal algebraic approach involving the so-called vertex algebras. Heuristically one could expect that the various approaches should be equivalent, however in practice they are not so easy to compare.

In higher dimensions the conformal group is not so large and other tools have to be used in the study of conformally invariant QFT's. One of them is the method of operator product expansions (OPE's). In recent years, there has been a revival of non-perturbative algebraic methods that in essence postulate the OPE of a theory as its defining input. Constraints on the form of this expansion, such as their convergence or associativity, can provide tools to find "exclusion plots" for the conformal data, i.e., the structure constants in the operator product expansion and the conformal dimensions in this expansion. A similar set of ideas, involving constraints on the OPE, seems to be relevant also for QFT's without conformal invariance.

Non-perturbative treatment of quantum field theories (beyond the class of conformal field theories) has a long tradition dating back to works of Glimm and Jaffe, Fröhlich, Nelson, Brydges, Rivasseau, and others. The most traditional subject of this direction of research, usually called Constructive Field Theory, is an attempt to construct interacting models of quantum field theory in various dimensions. It has turned out to be very difficult to construct realistic models in 4 dimensions. In recent years the methods of constructive field theory were applied to construct and investigate some other classes of models, such as hierarchical models and matrix models. They turned out to exhibit many interesting features, which seem to be relevant for realistic theories. Hierarchical models require sophisticated renormalization and lead to interesting phase diagrams. Matrix models are believed to be relevant as approximations of random geometry, and are an important step in our quest for quantum gravity.

Presentation Highlights

There were 14 long talks (55min) and 10 shorter talks (30min).

Long talks:

- Vincent Rivasseau presented the theory of random tensors. It is a theory directly inspired by QFT. It leads to a perturbation theory involving sophisticated versions of Feynman diagrams. Random tensor theory can be viewed as an approach to random geometry, and also as a toy model for quantum gravity in $D \geq 3$ dimensions. Vincent reported on the recent progress in the $1/N$ expansion (in the size of the tensors) and on renormalization group methods for these models. They are believed to be approximate AdS-CFT duals of the Sachdev-Ye-Kitaev model. [1]
- Mathieu Lewin reported on recent progress (achieved with Hainzl, Séré and others) in the so-called mean-field QED. This theory can be thought of as a caricature of the true QED, with charged particles treated quantum-mechanically and classical electromagnetic fields. The electromagnetic field is divided into a fixed external field and a “fluctuation”, which is subject to a variational treatment. It leads to a well-defined nonlinear functional on density matrices of charged particles. Proving the existence of minimizers amounts to establishing the stability of the approximation. The model needs an ultraviolet regularization – for instance, one can employ the Pauli-Villars method. The Landau pole phenomenon appears when one tries to remove the ultraviolet cutoff. The electrostatic case can be treated non-perturbatively, using methods of convex analysis and the calculus of variations. These methods are closely related to the backreaction equation on curved spacetime for quantum fields coupled to the Einstein Equation. [2]
- Detlev Buchholz presented a construction of a certain new C^*-algebra, which can be used to describe observables of interacting non-relativistic Bose particles. The point of departure of this construction is the so-called resolvent algebra, generated by resolvents of field operators. The next step involves taking the gauge-invariant (particle number preserving) part of that algebra. The final C^*-algebra is capable of supporting a large class of interesting many-body dynamics as C^* automorphisms, giving a rigorous meaning to the dynamics generated formally by many-body Schrödinger Hamiltonians with bounded potentials. The state space and ideal structure are particularly rich and the specific dynamics select states and ideals. The algebra has a quasi-local structure, it possesses positive energy representations and asymptotic ground states. Scattering theory can be formulated in this setting. Progress towards the existence of thermal states has been achieved. [3]
- Abdelmalek Abdesselam presented a non-perturbative construction of hierarchical ϕ^4-type models of statistical mechanics on the space of p-adic numbers. The hierarchical structure allows for a rather detailed analysis of the model. In particular, the application of space-dependent renormalization group analysis leads to a definition composite operators, whose anomalous dimensions establish the non-Gaussian nature of theory. By interpreting the infinite hierarchical level as a boundary, an analogy with Witten diagrams in AdS-CFT can be set up. (Talk prepared jointly with A. Chandra) [4]
- Wojciech Dybalski gave a comprehensive overview of infrared features in relativistic and non-relativistic models of many body systems with massless and massive particles. He gave an existence proof for scattering states of electrons, photons and “atoms” in the context of the Nelson model using the Haag-Ruelle ansatz. He emphasized the notable difference between neutral and charged particles, and reported on recent progress made by combining the Dollard formalism with sophisticated methods from scattering theory, which are developed further in his joint work with A. Pizzo. In relativistic quantum field theory, he proposed a general framework for the superselection structure of scattering states, building on ideas of Buchholz et al. He gave an outlook on the “infrared triangle” put forward by Strominger et al. [5]
- Stefan Hollands reported on a longer programme towards a perturbative construction of quantum field theories in generic globally hyperbolic curved spacetimes. The method is based on a combination of essentially algebraic techniques with analytical methods such as scaling/curvature expansions, extensions of distributions to complicated subspaces such as stratifolds, and microlocal analysis. A culmination of this line of research, carried out partly together with Robert M. Wald and based also on work by Radzikowski and by Brunetti and Fredenhagen, is the perturbative construction of non-abelian gauge theories in curved spacetime. Here, one has to combine the algebraic and analytic methods with cohomological methods (the so called BV-complex) in order to control the gauge invariance of the renormalized theory (see also the contribution by Rejzner). [6]

- Mikołaj Misiak gave an overview of the methods and algorithms for computing Feynman integrals of interest in high energy phenomenology, especially in the calculations of various processes beyond the Standard Model. Feynman integrals satisfy a number of identities, which can be obtained via integration by parts. With help of these identities one can reduce Feynman integrals to a finite number of master integrals. These can be solved because they satisfy a coupled system of differential equations. The choice of master integrals is non-unique and seems important from the practical of view, because it often affects the computer time needed to solve a given problem. Mikołaj pointed out several directions for future research, which seem to lead to interesting questions formulated in an abstract algebraic language. [7]
- Krzysztof Meissner analysed the conformal anomaly in theories of fields of various spin and reported on the observation that contributions of different fields in maximally supersymmetric supergravity theories (embedded in conformal supergravity) cancel from $N = 5$ upwards. Based on an argument for the necessity of this cancellation in the cosmological context, he proposed a novel extension of the standard model motivated by maximally supersymmetric gravity theories. In this extension, all masses, being tiny compared to the Planck mass, arise through a soft breaking of conformal symmetry. The model involves an infinite-dimensional hidden $K(E_{10})$ symmetry of $N = 8$ supergravity, whose mathematics and physical implementations remain to be explored. [8]
- Scott Smith presented an overview of stochastic quantization á la Parisi-Wu. He explained how the necessity of renormalization arises in this set-up and outlined different approaches to the problem: regularity structures á la Hairer, paracontrolled distributions á la Perkovski-Gubinelli, or an RG-approach á la Kupiainen. He gave a detailed outline of recent progress for semi-linear stochastic PDEs with stochastic noise of varying regularity (joint with F.Otto, J.Sauer and H.Weber). [9]
- Christopher Fewster reported on ongoing work with R. Verch on the problem of measurement schemes and observables in quantum field theory in curved spacetime. Their basic scenario involved a system coupled to a probe. Both were described in the framework algebraic quantum field theory on curved spacetime. It was assumed that the interaction happened in a compact subset of spacetime and the probe was measured elsewhere. The talk discussed effect-valued measures, their non-selective measurement and joint unsharp measurement of observables. [10]
- Michał Wrochna discussed the importance of Hadamard states in the context of linear quantum field theory in curved spacetime, their applications, microlocal characterization, and methods how to establish them. He gave examples of important Hadamard states in the Schwarzschild black-hole spacetime, recent constructions of Unruh and Hartle-Hawking states, and commented on the non-existence of stationary Hadamard states in the Kerr black-hole spacetime. He presented a microlocal construction of Hadamard states in smooth asymptotically flat spacetimes, and also in analytic spacetimes. The latter construction involves the so-called Calderon projectors, defined after performing a microlocal version of the "Wick rotation". (Talk prepared jointly with C. Gérard) [11]
- Nicola Pinamonti reviewed the construction of thermal equilibrium states of interacting quantum field theories on Minkowski spacetime in the setting of renormalized perturbative algebraic quantum field theory. He compared this modern approach (due to Fredenhagen and Lindner) with other more formal ones á la Landsman and á la Keldysh. He presented results about perturbed dynamics and return to equilibrium. Secular divergences in time are observed in the thermodynamic limit if the initial state is not appropriately chosen. He characterized the asymptotic stationary state as a non-equilibrium steady state (NESS), computed the relative entropy between the NESS and the initial Gibbs state, adapting methods from Araki's perturbation theory. [12]
- David Simmons-Duffin reported on the key ideas and recent progress in the conformal bootstrap approach to conformal field theories. This approach is based on an old idea of Polyakov, Migdal, and others: One tries to exploit the bounds on the so-called conformal data of the theory (the structure constants and dimensions) by writing down the consequences of the associativity law for the operator product expansion ("bootstrap equation"). Recent progress has been achieved thanks to better suited analytical expressions for the so called conformal blocks appearing in those conditions. A concrete algorithm proposed by Rychkov, Rattazzi, Tonni, and others is to test the bootstrap equation via certain well-chosen linear functionals. This algorithm yields exclusion plots in the space of conformal data. Particularly impressive results are available in the 3-dimensional Ising model. [13]
- Sebastiano Carpi reported on the status of the connection between two axiomatic settings: Borcherds' vertex operator algebras (VOA) and the algebraic formulation of chiral conformal QFT á la Haag-Kastler. Both approaches can be used to axiomatize conformal QFT models, even though the original motivation of the first approach was purely mathematical (the "moonshine conjecture" and number theory). Both have complementary advantages that can be transferred to the other, once a suitable "dictionary" has been established. Provided certain energy bounds on their states (the so-called $a_n b$ bounds) are satisfied, unitary VOAs can be turned into Wightman-like fields. One can then introduce nets of local(ized) algebras. Unfortunately, their locality is not automatic. If it holds, then the VOA can be reconstructed from the net via the Fredenhagen-Jörß construction. Many conjectures and questions concerning the representation theory of the two

approaches remain open. [14]

Short talks:

- Daniel Siemssen reviewed some properties of the Klein-Gordon equation on curved spacetimes, which are relevant for applications in Quantum Field Theory. In particular, he described a proof of the existence of a distinguished Feynman propagator on a large class of asymptotically static globally hyperbolic manifold. He also discussed the relationship of the distinguished Feynman propagator with the problem of self-adjointness of the Klein-Gordon operator. [15]
- Krzysztof Gawędzki discussed the time evolution of states called "heat waves" in conformal field theory. These states are defined by a density matrix with non-trivial temperature profiles. Methods using Virasoro symmetry allow us to compute the energy density and currents. Conformal welding techniques (related to the Riemann-Hilbert problem) yield a semi-explicit expression for the exact probability distribution. [16]
- Alessandro Pizzo reported on an unexpected emergence of a non-commutative recurrence problem in the context of non-relativistic scattering theory (as discussed in the talk by Dybalski). He presented various closed form solutions of the recurrence in terms of multi-variate polynomials. This methods leads to results about detailed regularity properties of n-particle wave functions. [17]
- Daniela Cadamuro reviewed the construction of interacting quantum field theories in two spacetime dimensions with a factorizing scattering matrix via an "inverse approach": The S-matrix is taken as an input, and is used to define "deformed" creation and annihilation operators. The associated fields fail to be local, but are localized in wedge-like regions, so that local algebras can be defined as intersections of two algebras of wedge-localized observables. In the case of the Bullough-Dodd model, where the poles of the S-matrix indicate the presence of bound states, one has to add a "bound-state operator" in order to achieve weak commutativity of wedge-localized fields. (Talk continued by Yoh Tanimoto)
- Yoh Tanimoto, in continuation of Daniela's talk, focused on the problem of establishing the Haag-Kastler axioms for the local algebras of the Bullough-Dodd model. This problem involves three steps: the self-adjointness of the wedge-localized generators, their strong commutativity, and finally the "size" of the intersection of two opposite wedge algebras. He reported on the progress in this program. [18]
- Markus Fröb spoke about recent results on the operator product expansion in non-conformally invariant theories. He presented convergence results and estimates on the remainder of the expansion in various theories, originally due to Kopper and Hollands. Furthermore, he explained a flow equation for the coefficients in the operator product expansion, which in principle can be used to self-consistently determine these quantities beyond perturbation theory. When solved in perturbation theory, the flow equation gives a recursive definition of the coefficients which agrees with traditional methods, but is conceptually much clearer. The methods can be generalized to non-abelian gauge theories. [6]
- Kasia Rejzner advertized the application of the Batavin-Vilkovisky formalism in perturbative algebraic quantum field theory with local symmetries (Yang-Mills, effective quantum gravity) on curved spacetime. Using homological algebra, she derived a rigorous quantum Master Equation involving potential anomalies, thereby reinterpreting a formula of Hollands. This approach exhibits the cohomological nature of consistency conditions for anomalies. [20]
- Paweł Duch reviewed the problem of the adiabatic limit (infrared problem) in perturbative QFT with massless particles. He covered the weak adiabatic limit (convergence of correlations and Green functions) and the strong adiabatic limit (construction of fields and their scattering matrix). The existence of the weak adiabatic limit was recently established by him in a large class of models. For the construction of the S-matrix, he reported on his work in progress, which involves a version of ideas of Dollard and Faddeev-Kulish. [21]
- Joseph Várilly reconsidered Wigner's "continuous spin representations" of the Poincaré group, by identifying them with coadjoint orbits of its Lie algebra, in the spirit of the Kirillov approach. Massive and massless orbits have rather different properties. Massive orbits do not have a massless limit. Massless continuous spin orbits allow to define a helicity operator and position operators that are conjugate to the momentum operators. The position operators, however, do not commute among themselves, indicating an intrinsic "noncommutative geometry". The resulting wave-function representation of the one-particle Hilbert space can be cast into a form compatible with the recent "string-localized" second-quantized theory (Mund-Schroer-Yngvason). [22]
- Christian Jäkel discussed QFT on 2-dimensional deSitter spaces. He explained how free quantum fields can be constructed using the theory of representations of the deSitter group $SO(1,2)$. Then he discussed how one can construct interacting fields using the modular theory. He also described a natural generalization of Haag-Kastler axioms to the context of deSitter spacetimes. [23]

Scientific Progress Made / Outcome of the Meeting

The workshop brought together researchers rooted in different communities who address the same subject "Quantum Field Theory", but use widely different concepts and methods, to the extent that they sometimes do not even understand the language of the others. It was our objective to bridge such gaps and thus trigger communication between various communities. The pay-off of such a meeting may not be immediate, but we are convinced that it will develop over time.

For this purpose we gave priority to overview talks. We have the impression that the talks were sincerely appreciated by participants, who engaged in lively discussions during and after the talks. It was visible that many participants were eager to understand the complementary approaches. Most talks were recorded by the BIRS video system, and pdf's of slides are available for all but a few blackboard talks. These documents are valuable resources for who wants to delve deeper into the subjects.

In spite of a large number of talks, there was sufficient time for informal scientific interaction among the participants. Several small groups of participants benefitted from the workshop and its facilities to pursue or initiate joint research projects.

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Chapter 19

New Statistical Methods for Family-Based Sequencing Studies (18w5154)

August 5 - 10, 2018

Organizer(s): Alexandre Bureau (Université Laval), Kelly Burkett (University of Ottawa), Jinko Graham (Simon Fraser University), Ingo Ruczinski (Johns Hopkins University

Overview of the Field

After the era of genome-wide association studies (GWAs) high-throughput DNA sequencing studies became fundamental to isolate the exact causes and contributors of human disease, and to tailor medical treatment to the individual characteristics of each patient ("precision medicine"). While the vast majority of effect sizes for common single nucleotide polymorphisms (SNPs) reported in the GWAS catalogue are small, we now know that much of the heritability for many traits including complex disorders can be explained by rare but highly penetrant variants. These variants have the potential to be used as "genetic biomarkers" in practice, for example to predict disease risk or response to a specific therapy. To detect these rare but highly penetrant variants, family-based study designs are much better suited than population based designs as they provide a way to test co-segregation with disease of variants that are too rare in the population to be tested individually in a conventional case-control study. However, many mathematical and statistical challenges remain in approaches to fully exploit the information in these family based designs. One of the particularly difficult but exciting challenges for bio-mathematicians and statistical geneticists is to account for various types of dependence structures in familial DNA sequencing data, and to develop optimal approaches (in terms of power and scalability) for these time-consuming and expensive studies. Here, dependency can be caused by relatedness among individuals unknown to the investigators, correlation of nearby genetic markers, and/or pleiotropy (i.e. genetic variants affecting multiple traits). This workshop brought together some of the world's leading experts in this field to address these critical and timely issues.

Presentation Highlights

Rare variant sharing

Sequencing DNA in extended multiplex families can help to identify high penetrance disease variants too rare in the population to be detected through tests of association in population based studies, but co-segregating with disease in families. **Alexandre Bureau** and **Ingo Ruczinski** presented a statistical framework based on this paradigm to exploit sequencing data from extended multiplex families [2, 4]. Specifically, when only few affected subjects per family are sequenced, evidence that a rare variant may be causal can be quantified from the probability of sharing alleles by all affected relatives given it was seen in any one family member under the null hypothesis of complete absence of linkage and association. **Ingo Ruczinski** presented the general RVS (rare variant sharing) framework for calculating such sharing probabilities when two or more affected subjects per family are sequenced, showed how information from multiple families can be combined by calculating a p-value as the sum of the probabilities of sharing events as (or more) extreme, and introduced the concept of "potential p-values" to alleviate the burden due to multiple comparisons. He discussed the importance of the rare variant assumption, and the power of the approach. **Alexandre Bureau** later discussed the effect of cryptic relatedness among family founders on the inference, and presented solutions to address the independence violation (see 19). The usefulness of this approach was highlighted in a case study from families with multiple members born with oral clefts, interrogating the sharing patterns of nucleotide and structural variants [3, 6].

Dandi Qiao presented an alternative approach, the gene-based segregation test (GESE) [9]. In contrast to RVS, GESE requires an estimate of variant frequencies to calculate an unconditional probability of segregation patterns (as compared to calculating the probability of sharing conditional on the variant being observed), but otherwise relies on very similar assumptions as RVS. Specifically, GESE (like RVS) assumes only one founder in the family introduced a causal variant in a gene, and limiting the tests to variants with high functional impact is recommended. Further, GESE also calculates the p-value as the sum of the probabilities of all events as or less likely as the observed event. GESE uses the sequence data from affected and unaffected family members, while RVS is based only on sharing among affected subjects, and does not make any assumptions about unaffected subjects.

Exploiting genealogical databases and isolated populations

Genealogical databases have been developed from a variety of data sources. Databases created from systematic civil registers in founder populations contain nearly the complete history of the population and can serve to answer a number of questions about the distribution and history of genetic variants in the population. The largest such database in Canada is the BALSAC database of the Quebec founder population (balsac.uqac.ca). **Simon Girard** gave an overview of this database hosted at Université du Québec à Chicoutimi and containing over 3 million linked records from the Catholic church.

For rare genetic conditions due to a genetic variant likely introduced by a single population founder, **Simon Gravel** presented an approach to estimate the variant genotype posterior distribution over the population founders and, from that founder distribution, estimate the variant frequency in the various regions of Quebec. Assuming the variant entered the population through a unique founder and the genealogy is correct, the variant genotype founder distribution is inferred by "Monte Carlo climbing simulations", where more promising paths are favored by an importance sampling scheme. The resulting bias in likelihood computation is then corrected. The method implemented in ISGen (github.com/DomNelson/ISGen) was applied to Chronic Atrial et Intestinal Dysrhythmia (CAID), an autosomal recessive condition caused by a variant in gene SGOL1 present in Europe with frequency 0.0002. The distribution of the ancestor most likely to have introduced the variant was inferred based on 11 patients tied to the genealogy, and is concentrated on 4 founders. The allele frequencies inferred in the various regions of Quebec matches estimates from population samples. The genealogical approach predicted high frequencies of the causal variant in regions where the available population samples were too small for reliable estimation (e.g. the Charlevoix region), highlighting its potential for orienting mutation screening.

The problem addressed by **Alexandre Bureau** within the rare variant sharing framework for identification of rare disease-susceptibility variants (see 19), was conceptually different but similar in approach. It consisted in estimating the null distribution of rare variant sharing events among present-day affected subjects included in a sequencing study, given a rare variant was seen in any of them, considering the genealogy of these subjects as a single extended pedigree. Solving this problem would have two benefits: controlling for cryptic relatedness (i.e. relatedness that is not captured in typical pedigree structures extending over 3-5 generations) and improving the power of the approach. Like the variant frequency estimation approach of **Gravel**, the present approach has two steps: 1) sampling the distribution of the founder introducing the variant conditional on the genotype of present-day subjects and 2) sampling the transmission of the variant from that founder to the current generation. Step 1) is here much simpler because it conditions on the genotype of a single subject instead of a set of subjects: thus the sampling of the parent transmitting the variant to his offspring is a simple coin toss performed recursively from a present-day variant carrier to a genealogy founder, while step 2) is the same as for frequency estimation, but applies to a more restricted set of subjects. Estimates of the sharing probabilities given any affected subject carries the variant (instead of a specific one) and their associated standard error are obtained by combining results for all present-day affected subjects. This method was attempted on datasets simulated using the 56,800-member genealogy of 217 families from the Saguenay–Lac-St-Jean (SLSJ) region of Quebec comprising 1018 individuals enrolled in an actual study of asthma, extracted from the BALSAC database. The current implementation is however excessively slow when the number of affected subjects exceeds about 10.

A contrasting example of a smaller and older population isolate without genealogical database was provided by **Arthur Gilly** with the Minoean isolates of the Greek island of Crete. With no genealogical database available, standard rare variant aggregation methods to test association with quantitative and dichotomous traits have been applied to genotyping and sequencing data on 1500 individuals from this population, while controlling for relatedness estimated from the genotype data. This analysis in this special population revealed a burden of rare variants in gene FAM189B driven by isolate-specific rare variants.

Gene genealogies

For understanding genetic associations with trait data, it can be useful to model the latent ancestries that give rise to the sample's genetic variability. The gene genealogy is a graph that describes the ancestry or lines of descent of chromosomal segments sampled from the general population. The neutral coalescent provides a mathematical model for the topology and node times of the graph. Several speakers spoke about their work in incorporating the gene genealogy in mapping methodology, including for the discovery of rare variants and extending the modeling to pedigrees.

Jinko Graham presented her work in developing ancestral tree based statistics to find trait-influencing mutations. The ancestry-based approach is motivated by a similar principle as family-based mapping: the similarity in relationships between haplotypes is reflected in similarity between trait values. This suggests examining statistics that capture the degree to which haplotypes from individuals with similar trait values cluster together in the ancestral tree. She discussed an application in which Pearson correlation between tree-defined clusters and disease status was used as a measure of association. This was applied to a dataset consisting of genotype data for diabetes cases and healthy controls. Trees were sampled from their posterior distribution conditional on imputed haplotype data at 55 focal points in a genomic region. The fuzzy pvalue was used to assess the strength of the association. The results highlighted a small number of adjacent focal points where the median of the fuzzy pvalue was low and the spread of the fuzzy pvalue distribution was small, indicating more certainty about the genealogical tree given the data.

Both **Kelly Burkett** and **Renaud Alie** discussed their progress in extending population-based models for the gene genealogy to family data. Kelly Burkett presented her work in extending a Markov chain Monte Carlo approach to sample an approximation of the gene genealogy conditional on genotype data from trios (mother, father, child). Each parents' two unobserved haplotypes correspond to two tips of the ancestral tree and the child's genotypic data restricts the set of parental haplotype configurations. A proposal distribution is then used to update the parental haplotypes while ensuring the child's genotypes remain the same. She applied the sampler to a previously-analysed Crohn's disease dataset and compared results using the trio-based sampler to sampling conditional on imputed parental haplotypes. Results were similar between the two approaches; however, the trio-based sampler showed signs of poor convergence. Renaud Alie spoke about his work developing the pedigree-based coalescent. He proposed using previously developed models for the inheritance of genetic material within the pedigrees at the tips and using the ancestral recombination graph as the model for the relationships between the pedigree founders.

Tree-based association statistics capture the degree to which sequences from disease-affected individuals cluster in the ancestral tree. However, each individual corresponds to two tips of the ancestral tree - one for each of their sequences. Depending on the disease model, it's possible that only one of these sequences actually carries a risk variant. Therefore, a sequence from a case could be misclassified. **Charith Bhagya Karunarathna** described his work comparing the performance of multiple tree and non-tree based association methods in localizing a risk variant. In particular, he compared two versions of the tree-based Mantel test: a naive version where both sequences are classified as a case and an informed version where only the sequence carrying the risk variant was classified as a case. He showed that there was a substantially worse performance for the naive Mantel test relative to all other approaches. The informed Mantel test performed well, but it is an idealized test that cannot be implemented in practice without knowledge of the risk variant. This highlights a challenge to be addressed when developing tree-based association statistics.

Simulation software to test rare variant methods for family data

Simulated genetic data is frequently required for testing new rare variant methods or to compare existing methods. Although many programs for simulating genetic data have been created, they often rely on mathematical models from population genetics that may not be biologically plausible. In addition, programs typically simulate data from unrelated individuals; to generate family data, additional programming or separate software is needed to probabilistically "drop genes" in known family structures. As mentioned in Section 19, public databases contain real genealogical (BALSAC) or genomic data (e.g. 1000 Genomes). These databases are valuable resources for simulating realistic datasets or evaluating algorithms based on probabilistic models. Many of the participants presented simulation software developed by themselves or their colleagues that utilicize these public databases to model the reference population for their simulations.

A number of speakers (e.g. **Briollais, Bull, Choi**) used `Sim1000G` as part of the research that they presented. `Sim1000G`, co-developed by **Laurent Briollais**, can be used to simulate genetic data using a reference population stored in a VCF file that is supplied by the user. In particular, the reference population can be phased data from the 1000 Genomes project. Genetic data for new individuals is generated by sampling from this reference population so that the allele frequencies and linkage disequilibrium patterns are maintained. Unrelated individuals and pedigrees of arbitrary size can be simulated. For pedigree data, two recombination models are available.

Christina Nieuwoudt presented two R packages that she and **Jinko Graham** developed for simulating genetic data on pedigrees ascertained to contain a minimum number of affected individuals. `simRVpedigree` [8] is used to simulate the pedigrees and disease status. The disease model for affected pedigree members includes sporadic cases as well as cases caused by a rare variant segregating in the pedigree. `simRVsequences` can then be used to simulate genetic data for the pedigree members using a model inspired by gene dropping and including recombination events. The sequence data in the founders can be obtained using publicly-available datasets.

Simon Gravel described how a coalescent-based simulation algorithm, `msprime`, failed to capture the genomic structure seen with real data. The distributions of both the length and number of IBD segments between individuals with different familial relationships were quite different between data from "23andme" and the simulated data. Although coalescent-based simulators might reasonably approximate real data over smaller genomic regions, the approximation is poor when simulating large regions since it allows more than two parents per offspring. He is working with collaborators on a simulator, `hybride`, that is based on the forward-in-time Wright-Fisher model rather than the coalescent. By incorporating recent improvements to the representation of gene genealogies used in `msprime` [7], computation time for `hybride` is remarkably fast. Though they are still working on improvements, the software will be available for download in the future.

Variance-components models and identity by descent

Variance-components models are a useful tool for mapping quantitative phenotypes in families. Phenotypes are typically assumed to follow a Gaussian distribution, with a mean that may depend on alleles at a genetic marker of known or hypothesized influence. Overall phenotypic variance within a family is decomposed into *genetic* and *non-genetic* components. In the linear model of the mean phenotype, the genetic component is characterized by a vector of family-specific random effects. The variance-covariance matrix of these family-specific random effects is the genetic component of variance. To assess the evidence for genetic association between the phenotype and alleles at a given genetic marker, the coefficients for fixed allelic effects are tested in the linear model. To assess the evidence for genetic linkage between the phenotype and a particular genomic location, the variance of the random effects is further decomposed into genome-wide and location-specific components. The genome-wide genetic-variance matrix is written as a scalar "polygenic" variance times a kinship matrix summarizing the pairwise relationships in the pedigree. The location-specific variance matrix is expressed as a scalar, location-specific variance times a matrix of pairwise identity-by-descent (IBD) proportions estimated from genetic markers near the location of interest. Linkage corresponds to the scalar location-specific variance being non-zero. Presentations in the workshop extended and/or applied this variance-components model in novel ways. We heard about extensions to accommodate non-Gaussian (e.g., time-to-event or binary) phenotypes, and heterogeneous variance components across families and across ethnic groups. We also heard about methods for estimating kinship matrices and local IBD sharing. The estimates from these methods allow for linkage analysis without the need to know the pedigree relationships between individuals.

Yun-Hee Choi and **JC Loredo-Osti** presented variance-components models for linkage and association analysis of time-to-event and binary phenotypes, respectively. Their generalized linear models for the mean phenotype specify a linear predictor comprised of fixed effects and a vector of family-specific random effects, as well as a link function that relates the linear predictor to the mean. In classic variance-components style, the covariance between family-specific random effects is decomposed into genome-wide and location-specific components. Fixed effects in the mixed model can be viewed as association parameters. By contrast, the location-specific scalar variance in the variance-component model is a linkage parameter. In particular, large scalar variances indicate that the locus-specific contribution to the genetic random effect varies according to the degree of local relationship (i.e. linkage). Choi's model allows for ascertainment of the families through a proband. The likelihood for randomly-sampled (i.e. unascertained) families is corrected by conditioning or adding a penalty term. Issues such as model identifiability and the appropriate null distribution of test statistics for linkage and/or association were discussed by both speakers. Loredo-Osti commented that unrelated individuals may be incorporated as "families" of size one.

Laura Almasy presented methods that allow for genetic variance components that can vary across families. Her motivation for developing these methods was the family-based Collaborative Study on the Genetics of Alcoholism. So far, linkage-mapping studies of alcoholism and its endophenotypes have identified only broad genomic regions of interest. The rationale for her proposed extension is that more detailed modelling of the genetic variance should improve the linkage resolution and provide insight into families segregating different causal loci. Almasy lets the proportion of total variance attributable to the genome-wide and location-specific genetic components vary by family, while holding constant across all families the total variance. In the linear model, fixed effects are also assumed to be the same across families. Examining the resulting family-specific lod scores for linkage leads to insight into which families are contributory to a given linkage peak. Focusing analysis on these contributory families leads to insight into which genes under a linkage peak are contributory, and therefore improved resolution. The results of her linkage analysis highlight the complex nature of alcoholism. Several promising genes and variants were prioritized for further investigation.

Tim Thornton described a variance-components association analysis for two large consortia comprised of multiple ethnic groups. The data for these consortia were collected from different study designs involving families, founder populations and case-control samples. He used variance-components models to account for correlation between related study subjects. The multi-ethnic nature of the subjects leads to a mix of recent relatedness through family structure and distant relatedness through population structure. To account for population structure, he included fixed effects for genetic principal components in the linear model for the mean response. The new approach improves upon competing methods that under-compensate for population stratification at highly-differentiated markers, and over-compensate for population stratification at weakly-differentiated markers. He found that, in multiethnic samples, allowing for the non-genetic variance to be different for different ethnic groups is crucial for unbiased tests of association.

The Workshop included several case studies involving variance-component models and/or IBD. These case studies highlighted the challenges, rewards and insights offered by analysis of sequencing data. For example, **Mariza de Andrade** described whole-genome sequencing of a family with venous thromboembolism and insights gained from linkage and association analysis. **Heather Cordell** described valuable lessons learned from sequencing under a linkage peak in an ongoing study of families with vesico-ureteric reflux. The process of analysis uncovered some pitfalls of working with sequencing data, including variant calls that are highly dependent on the platforms used for sequencing and on the bioinformatics pipeline. **Janet Sinsheimer** discussed a sequencing study of the microbiome of a beetle that lives in family units. The aim of the study was to estimate the heritability of the microbiome. Her results suggested heritability of important bacterial groups. **Simon Girard** used pairwise IBD sharing in the Quebec founder population to identify genetic variants associated with epilepsy.

Elizabeth Thompson discussed methods for estimating kinship matrices and local IBD sharing. The resulting estimates allow for linkage analysis without knowing the pedigree relationships between individuals. Thompson first presented methods for local IBD estimation. She then described how to combine these local estimates to obtain genome-wide measures of kinship. When these estimates are used in linkage analyses of simulated datasets, the likelihood-ratio (lod) curves correctly identify the linkage regions. **Shelley Bull** described an application of inferred local IBD to mapping risk genes for breast cancer using data on affected sisters. The basic premise is that the siblings share disease because of the genomic regions they share IBD, and in particular the susceptibility variants within those regions. If so, more susceptibility variants are expected on haplotypes shared IBD by the sisters than on haplotypes that are not shared IBD. These idea leads to a statistical test of association in terms of inferred IBD and the number of rare variants in a genomic region for the sibship.

Accommodating biased sampling of families

Family studies of genetic diseases typically sample families having one or more affected members. The first affected family member to be included in the study is called the proband, and the set of individuals used to determine family eligibility for the study is called the ascertainment set. As ascertained families do not represent a random sample from the population, statistical methods must account for the biased sampling to avoid biased inference. If we view families as independent, we can understand the ascertainment issues in terms of the likelihood for a single family. Let A be the event that the family is ascertained and Y be the phenotypes (e.g., disease status, or age-at-onset of disease). In heritability studies that do not collect genetic data, the likelihood is $P(Y|A)$. In studies that collect genetic data, G, the likelihood is $P(Y, G|A)$.

In studies that collect genetic data, alternatives to the full likelihood, $P(Y, G|A)$, may be obtained by further conditioning. The prospective likelihood is based on $P(Y|G, A)$ and the retrospective likelihood on $P(G|Y, A)$. As a rule, conditioning ignores information and can lead to a loss of efficiency in statistical inference. However, approaches based on conditional likelihoods may be easier to implement than approaches based on the full likelihood. For example, if ascertainment depends only on Y, then $P(A|Y, G) = P(A|Y)$. We can then argue that the retrospective likelihood is $P(G|Y, A) = P(G|Y)$, so that the ascertainment doesn't matter. Prospective likelihoods can also be easier to implement under certain assumptions. For example, complete ascertainment occurs when every eligible family in the population is ascertained into a study. Under complete ascertainment, $P(A|Y,G) = 1$ for every (Y,G) that meets the ascertainment criteria. Choi et al. (2008) show that the prospective likelihood is $P(Y|G,A) = P(Y|G)/P(A|G)$, which is a penalized prospective likelihood with penalty term $1/P(A|G)$. This simplification allows ascertainment-adjusted methods to be developed as penalized versions of existing prospective methods.

The workshop featured several talks that included the concept of biased sampling of families and ascertainment adjustment. **Lajmi Lakhal Chaieb** presented work investigating the heritability of psoriatic arthritis and its possible dependence on parent of origin. Families were ascertained through a proband only. The phenotype was age-at-onset of arthritis and no genetic data were collected; hence the likelihood is of the form $P(Y|A)$. The ascertainment event A is that the proband develops disease by the time the family is recruited. **Jooyoung Lee** presented methods to estimate risk parameters from time-to-disease phenotypes in studies collecting genetic data. The ascertainment event A is that the proband is alive and affected with the disease and has multiple relatives alive at the time of recruitment into the study. She described how the complexity of the full likelihood, $P(Y,G|A)$, increases rapidly with the family size. To make the problem tractable, she proposed an approximation to $P(Y,G|A)$ that involves the proband and a pair of non-probands from the ascertainment set. Other speakers took retrospective approaches to the analysis of data from their family studies. For example, **Alexandre Bureau** and **Ingo Ruczinski** presented an approach to test for co-segregation of a rare variant with disease. The approach is based on the sharing probabilities, $P(G|Y,A)$, under the null hypothesis of no co-segregation. The ascertainment event A is that there is at least one affected family member and that the rare variant is present in at least one of them. In contrast, **Yun-Hee Choi** took a prospective approach to analysis of her family data. Under complete ascertainment, she adjusts the prospective likelihood by a penalty term to correct for the biased sampling of families. She also assumes that families are recruited through a proband only. The ascertainment event A is that the proband develops disease by the time of recruitment into the study.

Under complex ascertainment, simplifying assumptions for tractable calculations may not be possible. We may then have to resort to Monte-Carlo sampling of ascertained families. Families are randomly sampled from the population and then filtered by the ascertainment criteria. Along these lines, **Christina Nieuwoudt** described her `simRVSequences` R package. This software simulates whole-exome sequence data in families segregating a rare causal variant and allows for different schemes of family ascertainment.

Causal inference using genetic and epigenetic measurements

Inference of causal effects of exposures on health outcomes from observational data gives rise to a large variety of difficult problems. Two contributors to this workshop considered the setting where an exposure A may have a causal effect on a continuous health outcome Y through a mediator variable M, but some of these causal effects may be confounded by a set of factors X [1] (see Figure 19). Both **Karim Oualkacha** and **Xihong Lin** considered studies where DNA methylation at a given genomic site was the mediator variable M, but the problems studied by these two speakers differed. In **Oualkacha**'s talk, the interest lied in establishing the causal effect of M on Y, and A was genotype at a set of genetic markers, to be used as instrumental variables in a Mendelian randomization analysis. Since genotype is fixed at birth, the effect of genotype cannot be confounded by factors acting after birth, so it is assumed that there is no effect of X on A. Mendelian randomization also requires that the genetic markers A selected as instruments have no direct effect on the outcome Y. When these conditions are met, detecting an association between A and Y is evidence of a causal effect of M on Y. With high-dimensional genotype data from genome-wide arrays, selection of the markers to use as instruments A can be performed by penalized least square regression methods such as the Lasso. The difficulty encountered by Oualkacha was that study subjects were grouped in families. A two-step procedure had previously been proposed: 1) use linear mixed models to adjust for relatedness of the subjects and 2) use the residuals from step 1 in variable-selection least-square regression methods. Oualkacha introduced `ggmix`, a two-in-one procedure which controls for relatedness and performs variable selection under linear mixed models. The optimization problem was solved using a block relaxation technique. Initial simulations studies focused on the performance of the approach to select the right set of markers and correctly estimate heritability of M and revealed that `ggmix` is a promising alternative to the two-step approach and the naive Lasso ignoring familial relatedness.

Participants

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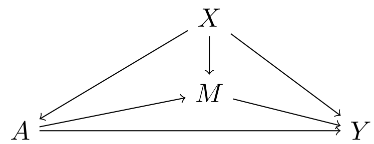
Figure 19.1: Causal diagram between an exposure A, a mediator M, confounding factors X and an outcome Y



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Burkett, Kelly (University of Ottawa)
Choi, Yun-Hee (University of Western Ontario)
Cordell, Heather (Newcastle University)
de Andrade, Mariza (Mayo Clinic)
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Larribe, Fabrice (UQAM)
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Liu, Dongmeng (Simon Fraser University)
Loredo-Osti, J-C (Memorial University)
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Thompson, Elizabeth (University of Washington)
Thornton, Timothy (University of Washington)
Wijsman, Ellen (University of Washington)
Yilmaz, Yildiz (Memorial University)
Zhao, Kaiqiong (McGill University)

Lin was interested in performing classical mediation analysis in unrelated subjects with an exposure A (e.g. smoking) that may affect DNA methylation M at multiple genomic sites, and thus may have a natural indirect effect (NIE) on the outcome Y through M, in addition to a possible direct effect. Earlier work had showed that tests of the NIE were conservative under the null case where there is no association between A and M and no association between M and Y, which is likely to be the case for most methylation sites in a genome-wide analysis[1]. She proposed the divide-aggregate or DAT method to correct conservativeness of NIE tests under standard mediation approaches.

Outcome of the Meeting

The workshop was an opportunity for exchanges leading to new ideas to solve problems faced by participants. For instance, Alexandre Bureau, Ingo Ruczinski and Simon Gravel determined that the software developed by the Gravel group to sample the transmission of variants from founders of a genealogy to present-day individuals could speed-up the same step in the estimation of the null distribution of rare variant sharing statistics in extended families extracted from a genealogical database attempted by Bureau. Also, the suggestion made by Ken Lange at the workshop to subdivide the genealogy into lineages under each founder was later implemented by Bureau in the `RVS` Bioconductor package and enabled exact computations in larger families than had been possible previously.

The workshop gave speakers an opportunity to demonstrate the use of their software in assessing methods for rare variant discovery with family data. As the software described above is freely available, other participants can now use these programs for their own research. For example, `sim1000G` is currently being used by Kelly Burkett's research group for simulating genetic pathway data on trios (mother, father, child). Because it uses real human genetic data, they are able to easily simulate data for human genes in the pathways of interest.

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Chapter 20

Mathematics of the Cell: Biochemical and Mechanical Signaling Across Scales (18w5126)

August 12 - 17, 2018

Organizer(s): Jun Allard (University of California, Irvine), Alexandra Jilkine (University of Notre Dame), Arpita Upadhyaya (University of Maryland)

Overview of the Field

A hallmark of biological systems is their ability to integrate external and internal signals and communicate information at different spatial scales (from molecules, cells and tissues to organs and whole organisms) and temporal scales (microsecond scales of molecular rearrangements to developmental and physiological processes that occur over time scales measured in hours to months). From a mathematical point of view, biological signaling is exceedingly complex, involving a multitude of non-linear interactions.

A seminal application of mathematical ideas to understanding the underlying mechanisms in biological signaling was started by the landmark work of Alan Turing in 1952 [9] on how diffusible chemicals can induce macroscopic biochemical patterns and influence organism development. In the 1960s Lewis Wolpert [10] proposed that biochemical gradients can induce downstream cellular signals and generate different cell types in distinct spatial order.

Following these early studies, a number of mathematically deep ideas have emerged that have had profound impact on biology, physiology and medicine. We now have a better molecular understanding of biochemical signals, and recent work has shown that the mechanical environment plays a critical role in regulating many aspects of cell function such as migration and cell fate determination. Mechanical regulation of cell function appears to be widespread, resulting from a conserved set of physical mechanisms. How cells, tissues, organs and organisms integrate and respond to the interplay of mechanical and chemical signals are frontier problems in biology.

The past few years have witnessed a virtual revolution in the application of quantitative approaches to studying biological systems, stimulated largely by rapidly developing measurement techniques that allow the monitoring of cellular signals with high precision in space and time, as well as the ability to manipulate gene expression and to genetically engineer a variety of cells and model organisms. These new methods now give biologists unprecedented power to test mathematical models, while allowing mathematicians to formulate abstract yet biologically grounded models.

Mathematical cell biology offers an integrative framework allows modern quantitative data to be ordered within predictive models of sufficient abstraction that is amenable to analysis. However, to do so requires bringing together biologists and mathematicians with different areas of expertise. It is essential that mathematicians be aware of the latest biological discoveries, and that biologists be able to actively participate in model development. It is therefore timely to bring together researchers, including young scientists, to reveal the next round of mathematically deep ideas.

Recent Developments and Open Problems

The field of Mathematical Cell Biology has benefited from — and, arguably, emerged into mainstream cell biology with — a series of workshops at BIRS that started in 2005, the first of which was titled "Mathematical Biology of the Cell: Cytoskeleton and Motility" (BIRS 05w5004). This was followed by BIRS workshops in 2011 and 2014. These workshops attracted world-leading biologists and mathematicians, often meeting for the first time, to tackle emerging open questions. The first two meetings focused on the cytoskeleton and cell motility. As the frontiers of knowledge advanced, new questions emerged and the focus of the meeting shifted. The 2014 workshop focused on integrating genes, biochemistry and mechanics. The success of that meeting is evident in the number of collaborations that were initiated at that meeting.

The frontiers of biology have again advanced. Most strikingly, first, new quantitative experimental tools (especially in imaging) are allowing models to be tested and demanding new, integrative models to make sense of a deluge of data. Second, the question of how cells process information — cell signaling — is turning out to be more complex than previously thought, involving not only genes, biochemistry and mechanics, but also collections of cells acting in concert as they interact with their environment, i.e., the tissue, organ or organism in which they reside. In other words, signaling involves biochemistry and mechanics across length scales. This workshop therefore aimed to use the powerful history of the BIRS Mathematical Biology of the Cell workshop series to tackle these emerging questions by enlisting a new generation of researchers.

One of the goals of this diverse group of scientists is to understand the fundamental principles governing cell signaling. This is an ambitious problem because, as noted above (and among many other reasons), it ranges across scales: from single molecules involved in processes such as immune cell recognition and cell division, to integration of environmental signals during cell migration, to cell-to-cell communication involved in wound healing and development. Many of these processes involve the spatiotemporal dynamics of the cytoskeleton which modulates cell mechanics, is critical for cellular force generation, and instrumental in cellular sensing of the chemical and physical environment. This problem is not only of fundamental scientific importance, but also of medical importance, since many new therapies, including cancer immunotherapy, operate by modulating our cell signaling systems.

Participants and meeting highlights

The "inputs" of the participants were diverse along many dimensions. There was representation from United Kingdom, Canada, Australia, and the United States, from research universities, public research institutes (e.g., John Innes Center and Francis Crick Institute) and non-profit institutes (Allen Institute for Cell Science). They came from many types of departments besides Mathematics and Applied Mathematics, with the role of Physics being particularly notable compared to previous years (1.5 of the organizers are appointed in Physics departments), but also including Biology, Medicine, Engineering. Many participants have made fundamental contributions to the understanding of the actin cytoskeleton, the microtubule cytoskeleton, and their role in cell polarization, self-organization of subcellular structures such as the mitotic spindle and cytokinetic ring, and cell size control. In addition to intellectual diversity, the diversity also manifested itself in career stage: 4 graduate students and 7 postdoctoral researchers (the majority of whom presented either talks or posters), 5 pre-tenure principle investigators (the number was due to be higher, but participants were promoted between invitation and participation), and 15 female participants.

Many notable outputs arose from these inputs. As senior researchers in their respective fields, Ken Jacobson and Leah Edelstein-Keshet [4] gave presentations reviewing their decades of contributions (in cell membrane organization and cell motility, respectively) and, especially in the discussions that followed formal presentation, anticipated the next few years: What hypotheses might be confirmed or rejected and what technologies might be enabling or over-hyped. Even more memorable were the presentations by 6 postdoctoral researchers. These were mixed approximately equally between mathematical / computational / theoreticians and experimental biologists — however, in many cases, it was impossible to distinguish this separation from their presentations and discussions because they exuded expertise on both sides of the mathematical-experimental interface. This augurs well for the future of the field of Mathematical Cell Biology. In an anonymous post-meeting survey, one reported that "as a postdoc this was a great opportunity for me to meet researchers who could become collaborators in my future career."

Topics emerging from participants and discussions

The schedule of formal presentations was deliberately not sorted into topics, so that new topics would not be constrained by historically-defined separations, but rather could emerge from the speakers' most current research. As the workshop progressed, we identified five clusters, which we describe in turn below.

The cytoskeleton continues to be a major organizer of researchers (this is fitting, since the cytoskeleton was the theme in the subtitle of previous iterations of this workshop). The cytoskeleton is an integral and ubiquitous part of all eukaryotic cells. Two of the main cytoskeletal components are actin and microtubule filaments, which form networks and higher order structures to determine cell shape and enable the cell to interact with the external environment and mechanical stimuli. Further, these biopolymer filaments undergo dynamic assembly and disassembly in cells. A host of associated proteins regulate these dynamics and crosslink filaments to allow the formation of diverse structures. Additionally, motor proteins are important for transport on these filaments and exertion of forces. These collective dynamics of cytoskeletal filaments, regulatory proteins and molecular motors are important in diverse cellular processes such as cell migration, cell polarization and cell division. Both experimental and mathematical approaches are critical to solving some of the open questions in the field. This workshop brought together scientists from different disciplines and facilitated vibrant discussions on this topic.

Actomyosin Organization

Actin and myosin organization and dynamics is the primary mechanism for force generation in the cell and is hence critical to diverse cellular processes including migration and developmental processes. There were several talks that focused on various aspects related to the organization of actin networks, both in cells and in reconstituted systems from both the experimental and theoretical perspective. The semi-flexible nature of actin filaments and the binding/unbinding kinetics of crosslinkers result in remarkable viscoelastic properties of actin networks, with behaviors such as strain stiffening, nonlinear elasticity and stress-induced reordering. **Moumita Das** spoke about her work on these dynamical mechanical response properties of actin networks. She showed that actin networks can reversibly transition between rigid and non-rigid states (studied experimentally using microfluidic approaches) and that this transition emerges from the assembly and disassembly kinetics of actin filaments as shown from theoretical considerations. Her results highlight how understanding the structural and functional properties of these systems will provide insight into the dynamic response and stability of biopolymer networks. These will be important for predicting behavior across multiple scales — from cells to tissues and may be applicable to tissue repair therapies and soft robotics. **Garegin Papoian** spoke about their work on understanding the emergence of contractility in disordered actomyosin networks as a result of crosslinker binding dynamics. They showed that contractile force dipoles result from the interaction of non-equilibrium dynamics of active motors and passive cross-linkers. Papoian also highlighted an open source software program (Mechanochemical Dynamics of Active Networks – MEDYAN) that his group has developed for simulations of actin and microtubules networks with crosslinking proteins, regulatory proteins and molecular motors. Following this presentation a number of discussions were initiated at this BIRS workshop for further collaborative work. Moving on to cells, **Amy Maddox** [2] gave a cell biologist's perspective on how the actomyosin cytoskeletal network behaves like active living matter, due to the far-from-equilibrium nature of motor contraction and polymerization dynamics. She discussed the contractile behaviors of this network in cells undergoing cell division (cytoskinesis). Her work showed the existence of both positive and time-delayed negative feedback loops that lead to traveling waves of contractility with multiple periodicities of oscillations. Again, they showed that cross-linkers are key elements regulating the frequency of oscillations and that structural reorganizations can give rise to negative feedbacks. These contractility fluctuations may be an emergent property of contractile actomyosin networks. Discussion regarding simulations using MEDYAN as well as mean-field models such as those developed by Das to explain such global behaviors in these networks then ensued. **Orion Weiner** presented his work on higher-level regulation of actin networks, in particular, how the WAVE2 regulatory complex (WRC) self-organizes into ring-like foci. Using super-resolution microscopy they revealed that these act as the fundamental units of organization (templates) of actin sheets which power cell lamellipodia formation during migration, with significant implications for the basic mechanisms underlying motility. He further talked about the use of nanotopographic surfaces to probe curvature sensing by WAVE complex proteins. **Adriana Dawes** talked about the mechanisms underlying the formation of contractile structures called ring channels in the nematode worm, *C. elegans*. Their work used both mathematical modeling (including MEDYAN from the Papoian group) and experimental manipulations to show that two types of myosins motors act in an antagonistic manner to exert orthogonal forces to stabilize these ring channels. **Arpita Upadhyaya** discussed her work on how the actomyosin cytoskeleton self-organizes into characteristic rings during signaling activation in the T cell immune synapse and is responsible for force generation. Finally, **Bill Bement** discussed how the cell cortex behaves as an excitable medium during cytokinesis and the role of both the actin cytoskeleton (which acts as a negative regulator) and membrane organization in this process. He talked about their work on the interplay between chemical and mechanical waves.

Cell Movements: from single-cell to collective cell behavior

A number of talks were devoted to cell motility and the mechanisms underlying directed cell motion from the subcellular single cell level to that of collective motion in multicellular tissues. **Angelika Manhart** addressed the question of how the properties of branched actin networks could be tuned by changing the composition of cofilin (an actin depolymerizing factor). She used mathematical modeling to show that cofilin binding changes the elasticity of actin filaments, which modulated the directionality of actin network growth, thereby directing cell migration. Going to a longer length scale, **Andreas Buttenschoen** showed using a cell based computational model that migrating cells interact with their extra-cellular matrix and can break it down by mechanically adapting to it, with implications for directed cell movements in several biological contexts. Considering even longer length scales, **Rachel Lee** showed that collective motion in epithelial cell clusters can be attributed to a jamming transition and involve an interplay between active cell motility, cell adhesion and cell-cell guidance. **Leah Keshet** gave an overview of her group's work over many years in which they have pioneered the use of mathematical models to couple mechanical interactions between cells to biochemical signaling pathways and thereby predict behavior both at the cellular level (cell migration) to the multicellular level (contractile waves in cell sheets). She highlight some "hot topics" in the field including how the interplay between chemical signaling and mechanical tension which can lead to directed single cell motion as well as collective behavior — in particular how tissue stiffness affects morphogenesis (which was recapitulated by the work from **Otger Campas**).

Several talks focused specifically on **cell movements at the multicellular level** and how cellular interactions led to emergent behaviors at larger length scales. These collective cell behaviors are important during many stages of embryonic development, wound healing and metastases of cancer cells. **Zoltan Neufeld** [8] discussed models for collective migration of cells in different types of geometries — from linear channels to cells in two-dimensional monolayers. Cell motility is regulated by mechanical interactions between cells and their stiffness, resulting in propagating waves. These models are similar to the ones presented by Keshet but extend them by the addition of the external environment as boundary conditions. **Calina Copos** talked about the mechanical coupling between stress fibers and the actin meshworks in cells and how this may facilitate mechanosensing. She continued on the theme of the mechanisms underlying coordinated movements of cells, focusing on the migration of a two-cell system in the ascidian, *Ciona*. She presented her work using computational modeling to study the coupling between actin assembly, actomyosin contractility, cell and extracellular matrix interactions and adhesions to uncover how mechanochemical coordination is achieved in this simple system for collective motion. Insights from this study will be applicable to more complex systems — as were discussed in other talks at the workshop. The theme of cell-cell versus cell-matrix interactions and the interplay between these was discussed again by **James Feng**, who talked about collective migration in neural crest cells, which form clusters that undergo spontaneous persistent migration. He explained this behavior based on models that include biochemical signaling pathways (e.g. modulation of Rho-GTPase) coupled with physical interactions (contact inhibition of locomotion and co-attraction). **Otger Campas** offered an experimental perspective on the mechanical regulation of tissue morphogenesis and how the coordinated motion and deformations of cells direct the elongation of the body axis in developing vertebrates [7]. He presented his work using deformable magnetic microdroplets embedded in tissue to obtain spatiotemporal maps of forces and mechanical properties of the tissue during growth in zebrafish embryos. His work revealed transitions between fluid-like and solid-like tissue states during morphogenesis and suggests that control of tissue mechanical properties could be a fundamental mechanism of morphogenesis. This session highlighted the common themes between mathematical models of collective cellular motion and sparked discussion regarding appropriate coarse-graining approaches that go beyond phenomenological models and can more naturally yield the observed behaviors in cell aggregates. The session could have benefited from additional experimental speakers who could provide a more empirical perspective. Future workshops may wish to emphasize this aspect as advances in imaging and force measurement techniques are beginning to reveal collective behaviors that challenge existing models.

Microtubule organization

Microtubule organization and dynamics is important for many cellular processes including cell division, cell polarization and migration. **Holly Goodson** discussed her work on understanding the fundamental mechanisms underlying dynamic instability of microtubule filaments using computational models to study microtubule behavior at multiple scales from subunits to populations of filaments. Their work helps to establish how system level properties emerge from molecular characteristics in non-equilibrium systems and may be applicable to many biological systems. Returning to the cellular level, a number of talks in the workshop were devoted to studying the role of microtubules and associated proteins in cellular processes — in particular mitosis — in which proper segregation of chromosomes is achieved by the mitotic spindle. **Dan Needleman** spoke about how forces are coordinated to move the mitotic spindle in *C. elegans*. Using laser ablation to perturb the spindle and theoretical models, they have found that pulling forces drive various spindle movements. Their work establishes general principles for a quantitative understanding of spindle positioning and may be applicable to diverse systems. This work also emphasized the deep connections between different active matter systems (e.g. actin and microtubule networks). **Jay Gatlin** talked about experiments using in vitro reconstituted systems in microfluidic devices (to create tunable cell geometries) in order to examine the mechanisms underlying the positioning of the microtubule aster during cell division and dissected the relative roles of cortical pushing, cortical pulling and cytoplasmic pulling. In contrast to spindle positioning, they found that microtubule pushing forces at the cell cortex can generated forces at long length scales and contribute to aster positioning. Turning to theory and three-dimensional modeling, **Meredith Betterton** showed that the mechanical properties of kinetochores and their interactions with microtubules determine the attachment dynamics of mitotic spindles. **Alex Mogilner** talked about how mechanical positioning of nuclei in large multinucleated cells emerge from coordinated actions of microtubules and associated motors [6]. To explain this, he used mathematical ideas from a large body of work on spindle positioning to describe the possible force balance schemes. How the microtubule cytoskeleton interacts with actomyosin networks to create optimal force balance in cells is a topic that has been relatively less explored but would benefit from both experimental and computational approaches.

Intracellular transport and motor proteins

The interiors of cells are not random mixtures of chemicals but are spatially organized, across micrometer length scales and, e.g., in the case of neuronal cells, organized across millimeter scales and above. One of the major drivers of this organization is the action of molecular motors kinesin and dynein, which use microtubules as tracks. While the broad mechanism of these motors is understood, how they combine with microtubule organization and dozens of regulatory molecules to effect control of cell organization is an open mystery. The objects being transported are generically referred to as "cargo". As a first step between understanding how cargo is transported on a single microtubule, **Matt Bovyn** presented an experimental-theoretical collaboration on how motors confront an intersection between two microtubules [1]. The results demonstrate how the angle and separation of the microtubules can tune the "decision" made by the cargo on which route to take. **Alexandria Volkening** presented her work to understand the case where the cargo is a varicosity, pathological subcellular objects present in neurons following brain injuries. In his presentation, **Bill Holmes** discussed the case where the cargo is an insulin granule in pancreatic cells. The motion of these granules relative to the cell periphery not only explain pancreatic function but provide an example of non-Brownian motion, and, specifically, the mathematically curious case of non-Brownian motion near a boundary (in this case the cell boundary). The action of motors is regulated by molecules including microtubule-associated proteins or MAPs. A particularly visually-striking result was presented when **Jonathan Howard** presented striking images of a single MAP interacting with a microtubule using the technique of interference reflection microscopy.

Membrane organization

Another topic that emerged involves the organization of biological membranes, the lipid-bilayer-based elements that form barriers between cells and the outside world, and around many organelles. While the classical view of cell biology holds that these are fluid sheets that contain a few freely-diffusing embedded molecules, recent research is demonstrating much more complexity, and indeed the role of lipids is taking a backstage to the often dense embedded protein. Several talks discussed the spatial organization of these molecules in the quasi-two-dimensional membrane. For **Alan Lindsay**, the embedded molecules were receptors on a spherical cell ready to receive information from freely diffusing ligands. His work demonstrates that different spatial positioning of the receptors on the surface of the sphere leads to different reaction properties between the ligand and receptors. Interestingly, by assuming the diffusing ligand is emitted from a single source and studying (via simulation and analytic methods) how receptor binding varied as the location of the source changes, his work demonstrated the ability of a cell to sense its environment. This work helped emphasize the importance of surface molecule organization, a theme that was highlighted in several other talks. The driver of this spatial organization varied. In the case of **Daniel Fletcher** [3], it was due to the molecule size (normal to the plane of the membrane). In immune cells like macrophages performing phagocytosis ("eating" target pathogens), these molecules are pushed up against the target, and are thus pushed into specific regions depending on their size and how they interact with other molecules. In the case presented by **Ken Jacobson** [5], spatial organization arises from non-diffusion-driven modes of motion. Finally, **Nathan Goehring** presented the example of PAR proteins on the membranes of *C. elegans*, where a dramatic advective motion is driven by the motion of the protein network below the membrane, made of F-actin and termed the cortex.

Outcomes

The activities at the workshop already have notable outcomes. Many of these outcomes emerged from the extended discussions following each presentation. For example, after a presentation in which Nathan Geohring hypothesized about the connection between a (yet-to-be-identified) molecule that flows along the cell membrane by interacting with the cell cortex, Ken Jacobson pointed out a strong, but as-yet-unnoticed, analogy with the behavior of the B Cell Receptor, which moves along the membrane and is associated with the cortex with some similarities.

Many new collaborations emerged from the workshop. We queried the participants two weeks after the conclusion and have identified **9 new collaborations, some of which are already "underway"** (as stated by the participant in the survey). These include the exploration of using the MEDYAN software by Garegin Papoian's research group to accomplish objectives at the Allen Institute for Cell Science. Another example is between Alan Lindsay (Notre Dame) and Jay Gatlin (U Wyoming) on mathematical modeling of nuclear dynamics. Using experimental data from Gatlin lab and mathematical modeling by Lindsay, this collaboration aims to explain how the structure of the nuclear envelope changes in response to protein import. Yet another example is between Alan Lindsay and Angelika Manhart (CIMS, NYU) to build and analyze mathematical models to the explain the size, shape and spatial organization of nuclei in multiple-nucleated fly muscle cells. A description of one collaboration is particularly striking: "One person made a suggestion while at my poster and took it upon themselves to create some code for me. Then they spent 2.5 hours with me one afternoon teaching me how to use it, extending it, and brainstorming about the project."

The future of Mathematical Cell Biology

A discussion on the final evening of the workshop was dedicated to the future of the field of Mathematical Cell Biology. There was unanimous agreement that the idea of **"multiple scales"** (alluded to in the workshop's subtitle "across scales") was becoming more important. It is necessary to connect the tremendous progress in understanding single molecules (e.g., Jonathan Howard's work observing a single microtuble-associated protein with a single microtubule using Interference Reflection Microscopy) to understand how combinations of cells form robust structures in tissues (e.g., the migration of cells during development studied by Otger Campas). This will require new mathematical methods, and applied mathematics is particularly suited to the upcoming challenge of "multi-scale" biology.

Another discussion that emerged was the need to integrate new scientific communities, so that the progress of the Mathematical Cell Biology community continues to have maximal impact, and so that the frontiers of life sciences and other disciplines is integrated into our community:

- There is a particular need for the involvement of **control systems engineering**, where we are seeing hints that the lessons of control theory (in human engineered systems) are emergent in living systems as well.
- There was also a discussion about the appropriate involvement of medicine, here meaning specifically the development of **diagnostics and therapeutics**. This is one of the ultimate goals of biological sciences, and mathematical cell biology being no different. As we approach the integration of our communities, it will become increasingly important to involve diagnostics and therapeutics into meetings like this one.
- Finally, there was discussion about the role of bioinformatics, specifically the tremendous progress being made in **transcriptomics**. Here, the links between things like cell mechanics and transcriptomics is most cloudy: The evidence is unequivocal that the proteins being transcribed (and transcriptionally controlled) have a major impact on cell behavior, including the cell dynamics discussed at this workshop. Yet the nature of the link is unknown.

Participant surveys

Two weeks after the conclusion of the workshop, the organizers sent an anonymous electronic survey to the participants. There were 9 respondents (21%). All ranked it either 9 out of 10 (55.6%) or 10 out of 10 (44.4%) for overall quality. The formal talks were "of excellent quality and variety" and the informal parts of the meeting were "invaluable for sparking new research ideas".

Several comments indicated success in the quest to foster interactions between groups that do not normally interact. We received one comment that "it was super intense for me as a biologist to understand the math talks", a sign that our inclusion of traditionally non-mathematical fields is working (the same respondent scored the overall workshop 10 out of 10). Another said they "met a slice of the field that I don't normally cross paths with at normal meetings."

Suggestions for improvement on the scientific content included "synthesis sessions could be set aside for re-visiting related talks, coming to common ground...", and for posters, that there were "fewer than expected". A valuable suggestion we received in discussion with participants is the scheduling of a session dedicated to funding opportunities for mathematical cell biology.

Future impact

Of the many long-term goals of the field of Mathematical Cell Biology, the one identified by this workshop is to understand cells as signal processing machines, where the machinery is based on the spatial organization of the cytoskeleton, membranes, and the molecules with which they interact. We see evidence for future impact towards achieving this goal. This evidence includes:

- The ($\geq$ 9) new collaborations mentioned above are expected to have an impact beyond the participants themselves, by promoting the idea of successful interdisciplinary collaboration. Many of these are examples of convergence across traditional disciplines, e.g., from Mathematics departments and Biology departments.
- The incorporation of new communities were roughly prioritizes as: Control systems, medical diagnostics and therapeutics, and bioinformatics/transcriptomics.
- The growing emphasis on multi-scale methods that connect single molecules to the behavior of groups of cells in tissues, organs and organisms necessitated the development of mathematics that works "across scales".

Beyond within this field, there are examples on both the mathematical side (e.g., asymptotic approximation methods) and experimental side (internal reflection microscopy) of progress in this field that we expect to have an impact in other areas of mathematics and biology. This workshop continues to provide a potent instance of convergence across scientific and mathematical disciplines.

Participants

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Chapter 21

Regularity and Blow-up of Navier-Stokes Type PDEs using Harmonic and Stochastic Analysis (18w5057)

August 19 - 24, 2018

Organizer(s): Hakima Bessaih (University of Wyoming), Peter Constantin (Princeton University), Jiahong Wu (Oklahoma State University), Kazuo Yamazaki (University of Rochester)

Overview of the Field

Mathematical analysis on the equations of fluid motion have evolved remarkably ever since the pioneering work of Leray [4] in 1930s. While the fundamental question of the existence and uniqueness of a global solution with finite kinetic energy in the three-dimensional case for the Navier-Stokes equations remains unsolved, over these decades mathematicians have contributed to extraordinary advancement in the study of fluid dynamics.

Recent Developments and Open Problems

Very recently, two particular analysis tools have stood out prominently, namely harmonic analysis tools (e.g. [1]) to handle the non-linear terms that involve derivatives, and stochastic analysis tools (e.g. [2, 5]) to study the same equations but forced with noise. Using these tools, we have seen various different results, e.g. global existence of unique solution with dissipative term replaced by a fractional Laplacian or only in selected directions, blow-up of a solution with the structure of the equation slightly modified, and finally the stochastic effects such as whether the noise helps regularize the solution or not.

The objective of this workshop "Regularity and blow-up of Navier-Stokes type PDEs using harmonic and stochastic analysis" at Banff Scientific International Station (BIRS) was to invite various researchers in fluid dynamics working through different approaches to share their work and provide favorable environment for discussion and collaboration among those with complementary background and training who otherwise would not have had this opportunity to interact. The workshop brought together the stochastic and the deterministic communities to share their finding and have a very open discussion on the future research direction of fluid dynamics and in particular Navier-Stokes equations with the goal of helping each other shed some light on how to be more successful in solving the open questions.

Presentation Highlights

The 5-days workshop was scheduled to run everyday. We had deterministic oriented talks by the following experts:

1. Prof. Buckmaster Tristan from Princeton University - Department of Mathematics,

2. Prof. Chae Dongho from Chung-Ang University - Department of Mathematics,
3. Prof. Cheskidov Alexey, University of Illinois at Chicago - Department of Mathematics,
4. Prof. Constantin Peter, Princeton University - Department of Mathematics,
5. Prof. Córdoba Diego, Instituto de Ciencias Matemáticas - Consejo Superior de Investigaciones Cientficas,
6. Prof. Doering Charles, Department of Mathematics, University of Michigan,
7. Prof. Dong Hongjie, Brown University - Department of Mathematics,
8. Prof. Hmidi Taoufik, Université de Rennes1 - Equipe EDP, IRMAR,
9. Prof. Ignatova Mihaela, Princeton University - Department of Mathematics,
10. Prof. Ohkitani Koji, University of Sheffield - Department of Applied Mathematics,
11. Prof. Shvydkoy Roman, University of Illinois at Chicago, Department of Mathematics,
12. Prof. Tarfulea Andrei, University of Chicago - Department of Mathematics,
13. Prof. Titi Edriss, Texas A & M University, Department of Mathematics,
14. Prof. Vasseur Alexis F, University of Texas, Austin - Department of Mathematics,

and the stochastic oriented talks by the following experts:

1. Prof. Ferrario Benedetta, University of Pavia, Department of Mathematics,
2. Prof. Friedlander Susan, University of Southern California - Department of Mathematics,
3. Prof. Glatt-Holtz Nathan, Tulane University - Department of Mathematics,
4. Prof. Iyer Gautam, Carnegie Mellon University - Department of Mathematics,
5. Prof. Maurelli Mario, Technische Universitat Berlin, Institut fur Mathematik,
6. Prof. Romito Marco, Universitá di Pisa, Departimento di Matematica,
7. Prof. Schmalfuss Björn, University of Jena - Institute for stochastic.

It is very rare, if not the first time, to have such an opportunity to intentionally bring experts on the fluid partial differential equations (PDEs) from complementary perspectives and somehow try to bridge our knowledge together. We deliberately tried to order these talks mixed. The talks ranged over not only the Navier-Stokes equations but surface quasi-geostrophic equation from geophysics, flocking models, Korteweg–de Vries equation, Boussinesq equation from oceanography, Muskat equation, Lorenz equation, Kuramoto-Sivashinsky equation, Hele-shaw model, equation of mixing, point vortex model, as well as Burgers equation. There were very good dialogues of what stochastic perspectives may be able to offer when speakers from deterministic perspective gave talks, and similarly how some techniques from deterministic case is difficult but may be extended to the stochastic case. In the direction of research of Navier-Stokes type fluid PDEs there are many results which exist in the stochastic case but not the deterministic case and vice versa. It was very refreshing for many participants how the theory of fluid PDEs, considered from a complementary point of view, lead to so many new techniques and remarkable results.

Between each talk, we typically had breaks of 30 minutes during which participants and speakers were able to engage themselves in deeper discussions through the board outside the lecture rooms. For example, after a talk by a certain speaker, a participant was able to share his progress in a very similar direction and they found out that they had very similar results but proven through different perspectives. Due to their discussion, these two participants will be able to acknowledge each others' works in their papers, which is important in the communication through journal publications.

Scientific Progress Made

We considered that it will be important to have time during which instead of one speaker gives a talk about his/her results, every participant including speakers and non-speakers feel free to share anything, even non-significant computations within their research which have given them concerns or questions. In the direction research of fluid PDEs, there remain so many open problems and unexplored directions of research, which, only if they were shared, will catch much attention and we may quickly see rapid developments. Therefore we reserved Tuesday 16:30 - 17:30, Thursday 16:30 - 17:30, as well as Friday 9:00 - 10:00 and 10:30 - 11:30 for the Discussion periods. During these four rare opportunities, we all sat together, allowed speakers to give additional comments beyond their presentations, sometimes corrections, and also shared open problems as well as general questions.

In particular, an expert in the deterministic PDEs in fluid raised a question of extending the well known result concerning the ergodicity of the two-dimensional Navier-Stokes equations with a hypoelliptic noise on a two-dimensional torus ([3]) to a more general bounded domain. The group of experts on the fluid PDEs forced by noise were able to respond by elaborating on the results which have been obtained, those which have not obtained but are possibly achievable, and finally those which are very difficult and completely open. Again, this was a very good dialogue which was only possible because the groups of researchers on fluid PDEs from complementary perspectives have come together and felt comfortable enough to share their questions honestly and hear feedback directly with one another.

Moreover, on the Thursday 16:30 - 17:30 session, led particularly by the experts with much experience such as Prof. Peter Constantin, Prof. Edriss Titi and Prof. Charles Doering, participants were encouraged to share their open problems, write them on the board and hear thoughts from other participants. In particular, problems concerning exponential decay of a solution to an equation in mixing by Prof. Gautam Iyer, point vortex dynamics by Prof. Marco Romito and numerical analysis by Prof. Adam Larios were written on the board. There were many more problems proposed as very interesting, difficult but perhaps possible candidates for research in the near future, and the board was filled completely and very quickly. Thereafter, many shared their thoughts about relevant results, possible techniques to tackle such problems and difficulty in a very friendly manner. Such a fruitful discussion of sharing problems rather than new results can give us all a better understanding of the directions of research which will be of interest to a wide community of researchers.

Another noteworthy advantage of our workshop was that due to the prestige of the BIRS, its kind accommodation, and the fact that this was not a conference over a few days but an entire week, we were able to attract many renown experts from overseas outside the United States and Canada such as Asia and Europe. Even outside lectures times, during the tours by BIRS, on our way to daily meals at the Vistas Dining Room, walks to the Town of Banff in the evening as well as the trip to Lake Louise on the free Wednesday afternoon, the participants were able to interact with researchers in same field of study with whom they are typically able to communicate only through E-mails or reading papers. In a very relaxed, friendly fashion, every participant was able to share their research results, problems they are facing, and hear feedback from many others, all of which have been extremely helpful and productive for not only research but also motivation and gaining wider perspectives. It is actually very important to spend time together in such non-research activities and have conversations even outside research. It may lead to long term collaboration as well as friendship, helping in particular the young participants build their careers as mathematicians in this international community of fluid dynamics PDEs.

Outcome of the Meeting

This 5-day workshop has opened a new bridge between the deterministic and stochastic community of fluid PDEs. Every participant has enjoyed their time at BIRS fully, as confirmed verbally directly from participants. Due to excellent presentations and deep discussions which took place, many long-term collaborations among the participants who met each others for the first time in this workshop are strongly expected.

Participants

Bessaih, Hakima (University of Wyoming)
Buckmaster, Tristan (Princeton University)
Chae, Dongho (Chung-Ang University)
Cheskidov, Alexey (University of Chicago Illinois)
Constantin, Peter (Princeton University)
Cordoba, Diego (ICMAT Madrid)
Dai, Mimi (University of Illinois at Chicago)
Doering, Charles R. (University of Michigan)
Dong, Hongjie (Brown University)
Drivas, Theodore (Princeton University)
Ferrario, Benedetta (University of Pavia)
Friedlander, Susan (USC)
Glatt-Holtz, Nathan (Tulane University)
Hmidi, Taoufik (Universite de Rennes1)
Ignatova, Mihaela (Princeton University)
Iyer, Gautam (Carnegie Mellon University)
Larios, Adam (University of Nebraska-Lincoln)
Mario, Maurelli (WIAS & Technische Universitaet Berlin)
Martinez, Vincent (CUNY-Hunter College)
Miller, Evan (University of Toronto)

Ohkitani, Koji (The University of Sheffield)
Romito, Marco (Università di Pisa)
Schmalfuss, Bjorn (Friedrich-Schiller-University Jena)
Shvydkoy, Roman (University of Illinois at Chicago)
Tarfulea, Andrei (University of Chicago)
Titi, Edriss (Texas A&M University)
Vasseur, Alexis (University of Texas at Austin)
Wu, Jiahong (Oklahoma State University)
Xu, Xiaoqian (Carnegie Mellon University)
Yamazaki, Kazuo (University of Rochester)
Yao, Yao (Georgia Tech)
Yu, Xinwei (University of Alberta)

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Chapter 22

Tau functions of integrable systems and their applications (18w5025)

September 2 - 7, 2018

Organizer(s): Marco Bertola (SISSA, Italy), Alexander R. Its (IUPUI), Dmitry Korotkin (Concordia University)

Contents

Overview of the Field

The notion of tau-function was coined in the early days of the theory of integrable systems about 40 years ago in works of Jimbo-Miwa-Ueno [JMU81], Segal-Wilson [SeWi1985], Sato[Sa1989] and many others. In the case of celebrated Kadomtcev-Petviashvili (KP) equation the notion of tau-function proposed by Segal-Wilson can be viewed as an extension of the notion of the multi-dimensional theta-function. In works of Jimbo, Miwa and their coworkers the tau-function was introduced as a partition function of so-called holonomic quantum fields on a punctured Riemann sphere; the Jimbo-Miwa tau-function was later proven by Malgrange [Ma1983] to play a primary role in the theory of Riemann-Hilbert problems whose solvability is governed by vanishing properties of the tau-function.

Surprisingly enough, tau-functions of the most celebrated integrable systems like Korteveg de Vries (KdV), KP and Toda equations were proven to appear in fundamental combinatorial models, in particular related to random matrices and geometry of moduli spaces. The most famous example is Witten's conjecture about intersection numbers of ψ-classes on moduli spaces of Riemann surfaces; as it was proved by Kontsevich in 1991, their generating function is a partition function of a random matrix model and, moreover, is a tau-function of the KdV equation. Furthermore, as it was later discovered by Okounkov and Pandharipande [OkPa2005], generating functions of Hurwitz numbers are special tau-functions of Toda's equation. These results were extended to intersection numbers of an arbitrary combination of ψ and κ-classes (Kazarian), to Gromov-Witten invariants (Pandharipande et al) etc.

Tau-functions play a central role in Dubrovin's theory of Frobenius manifolds which formalizes the Witten-Dijgraaf-Verlinde-Verlinde equation of associativity arising in topological field theory. From the point of view of symplectic geometry tau-functions play the role of generating functions of commuting Hamiltonians of a completely integrable system.

Recent Developments and Open Problems

Among recent developments in the theory of tau-functions and their applications are:

– Series of works initiated by conjecture of Gamayun, Iorgov and Lisovyi [GaIoLi2012] who discovered that the coefficient in expansion of Jimbo-Miwa tau-function of Painlevé IV equation coincide with conformal blocks of certain conformal fiels theories.

– The analysis of Jimbo-Miwa tau function allowed to obtain a non-trivial new relation in the Picard group of the space of admissible covers and the moduli space of holomorphic differentials on algebraic curves (Korotkin-Zograf)[KoZo2011] .

– Appearance of tau-functions in the holomorphic factorization formulas for determinant of Laplacian on flat Riemann surfaces with conical singularities (Kokotov, Korotkin), and in the theory of Lyapunov exponents of Teichmüller flow on moduli spaces (Eskin-Kontsevich-Zorich) [EsKoZo2011].

Presentation Highlights

Tau-functions and geometry of moduli spaces.

The moduli spaces of interest to the workshop are associated to algebraic curves: these are moduli spaces of Riemann surfaces, both pointed and non-pointed, Hurwitz spaces, moduli spaces of abelian, quadratic and n-differentials. Generating functions for interesting quantities related to these moduli spaces (Hurwitz numbers, volumes, intersection numbers of various tautological classes etc) coincide, in many instances, with tau-functions of various integrable systems (KdV, Toda, KP). Within this area we found the talks of Chaya Norton who spoke on the symplectic geometry of moduli spaces of projective connections; the symplectic structures that were discovered are related to the geometry of the "double covering" curve, which is associated in a natural way to any quadratic differential (a well known fact in Teichmüller theory). Here tau functions generate the symplectic transformations between different sets of Darboux coordinates, called "homological". Giulio Ruzza discussed the isomonodromic approach to the computation of intersection numbers in the moduli space of open pointed curves; the approach is similar to the original one by Kontsevich [Kon92] starting from an appropriate matrix model with external source [Ale15a]. Tau functions also appeared as generating functions of generalized Hurwitz numbers, counting the branched covers of the Riemann sphere with various weights; in his talk, John Harnad explained a far reaching generalization of the result by Okounkov and Pandharipande [OkPa2005] that identified the generating function for "double Hurwitz numbers" as a particular tau function of the Kadomtsev-Petviashvili (KP) hierarchy. These weighted enumerations can be also represented graphically by a diagram called "constellation". The approach that was explained in the talk relies upon the topological recursion algorithm, pioneered by Chekhov (who was one of the speakers as well), Eynard and Orantin. The algorithm hinges on the notion of "quantum spectral curve"; this is essentially a differential equation whose symbol (the "spectral curve") serves as initial datum for the topological recursion. John explained how, using this approach, they can compute these weighted numbers in terms of the classical objects of the theory of integrable systems.

Within this area we can also list Dimitri Zvonkine's talk; he reported a new result on explicit constructions of classes in the cohomology of $\mathcal{M}_{g,n}$ which are not "tautological", i.e. not a combination of the Ψ-classes. A particularly enticing example is the "simplest" non-tautological class, which appears in the moduli space of genus one surfaces (elliptic curve) with 11 marked points. The main reason is due to a clever interpretation of the classical cusp form (of weight 12) or modular discriminant provided by the twenty-fourth power of the Dedekind η function.

Tau-functions and asymptotics of correlation functions

Correlation functions of various exactly solvable quantum mechanical and statistical models are tau functions associated with isomonodromy deformations of various linear systems. The main analytic issue in these applications of tau functions is their asymptotic behaviour near the relevant critical points. Of a particular importance are the connection formulae between different critical expansions and the evaluation of the constant factors appearing in these asymptotic formulae. These factors, very often, contain the most important information of the models in question. The first rigorous solution of a "constant problem" for Painlevé equations (a special Painlevé III transcendent appearing in the Ising model) has been obtained in the work of Tracy in 1991. Other constant problems have been studied in the works by Basor-Tracy (1992), Krasovsky (2004), Ehrhardt (2006), and in several papers of Its, Deift, Lisovyy and their collaborators starting from 2005. The tau functions that appear in all these works correspond to very special families of Painlevé functions and their extension to the general family of Painlevé transcendents has been a long standing problem in the field . The first rigorous results concerning the general two-parameter families of solutions of Painlevé equations have been obtained only recently in works of Its, Lisovyy, Tikhyy and Prokhorov (2013-2015), and they are based on the combination of the (also recently discovered) conformal block representation of isomonodromic tau functions and on the extension of the original Jimbo-Miwa definition of tau-function given by Malgrange and Bertola. One of the important conceptual outcomes of these results is the realization that the constant factors in the asymptotics of tau functions are the generating functions of certain symplectomorphisms.

Within this scope we found the talks of Gavrylenko, Prokhorov. In his talk Pavlo Gavrylenko explained that the standard principal minor expansion of a Fredholm determinant can be naturally interpreted as multiple sums over partitions (or, equivalently, Maya diagrams). Isomonodromic tau functions of general Schlesinger systems have been expressed as Fredholm determinants and the above expansion provides an explicit combinatorial formula for the general isomonodromic tau function. Interestingly, this approach can be identified with the dual Nekrasov partition function. Gavrylenko also explained how to represent $N \times N$ isomonodromic tau functions as a vacuum expectation value in a vertex-operator-algebra of an N-fermionic CFT; using the combinatorial interpretation alluded above it was explained the terms in the expansion of the combinatorial formula can be identified series over conformal blocks at $c = N - 1$ of a W_N algebra.

The talk by Andrei Prokhorov discussed the relationship between the isomonodromic tau functions of the classical Painlevé equations (in particular Painlevé II and IV) with corresponding classical actions in the Hamiltonian theory (Okamoto) for all Painlevé equations. The main outcome of these relations are certain differential identities which enter in the solution of the "constant" problem in the asymptotic analysis of tau functions. General tau functions display analogous differential identities. He then explained that it is possible to identify the Hamiltonian structure for the isomonodromic deformations corresponding to Painlevé equations and conjecture a generalization thereof to more general cases of isomonodromic deformations.

Tau functions, Fredholm and Töplitz determinants

One of the prime source of tau functions, both in the integrable systems setting and the isomonodromic settings has been determinants of finite or infinite dimensional operators. This was already explained by Segal-Wilson as a general setup to understand the Sato description of the KP hierarchy. In this optics we can frame both Lisovyy and Basor's talks.

Lisovyy reviewed his recent breakthrough results on the general construction of tau functions for Riemann–Hilbert problems. The method relies upon the identification of the "Widom constant" with a tau function (an identification which was originally found by M. Cafasso [Caf2008]). The Widom constant is the expression appearing in the formulation of the Strong Szegö Theorem for either scalar or matrix-valued symbols on the unit circle. This constant is a Fredholm determinant involving the Malgrange-Bertola forms for both the direct and dual Riemann–Hilbert problem. In those cases where either the dual or the direct problem admits an explicit solution, then the Widom constant can be identified with the isomonodromic tau function. This is precisely the setting of Lisovyy's talk, especially in the case of the sixth Painlevé equation. The resulting expansion in the standard Fourier basis yields interesting combinatorics that have been deeply exploited in the context of conformal blocks (see also the talk by Gavrylenko above). The approach extends so far also to Painlevé V and III.

Of similar nature was the contribution by Estelle Basor; she recalled in a very informative way the original result by Widom whereby the large-size asymptotics of determinants of finite–size (block) Toeplitz matrices leads to the strong Szegö theorem (or Szegö-Widom theorem for the block case). As mentioned before, this constant can be described as a determinant of certain operator that is a trace–class perturbation of the identity operator, and therefore admitting a Fredholm determinant expansion. While in the scalar case the computation is explicit in terms of the Fourier coefficients of the logarithm of the symbol, in the non-scalar (matrix) case it is not possible to express concisely the constant. Estelle focused on classes of nontrivial examples of 2×2 matrix symbols where one can still provide an explicit formula; this relies on particular factorization properties of the symbols that are called "root subgroup factorizations". In these cases the Widom constant's computation reduces to finite dimensional linear algebra.

Integrable structures of Quantum Field Theory (CFT)

In a 2012 paper by Iorgov-Gamayun-Lisovyi it was conjectured that the isomonodromic Jimbo-Miwa tau-function is closely related to conformal blocks of certain $c = 1$ conformal field theories. These conjectural formulae have been extended to other classes of theories and other tau-functions (Bershtein-Shchechkin, Marshakov-Gavrylenko and others) and, in the case of PVI, proven by Gavrilenko and Lisovyy. Since the original definition of the Jimbo-Miwa tau-function was inspired by the theory of holonomic quantum fields, this new development is naturally closing the circle of ideas originating from quantum field theory which lie behind the notion of Jimbo-Miwa tau-function.

Shchechkin reviewed his recent result on the proof of a particular power series expansion for the discrete q–Painlevé III tau function. This proof settles a conjecture on a q–deformation of the result by Gamayun-Iorgov-Lisovyy that interpreted the coefficients of the expansion as conformal blocks. The idea of the proof is to exploit its equivalence with bilinear relations on q-Virasoro conformal blocks.

The two talks of Marshakov and Bershtein were naturally linked to each other; Marshakov discussed the interpretation of certain dimer models on bipartite graphs and their partition function in terms of cluster algebras. In this context particularly crafted sequences of mutations of the cluster algebra can be viewed as a discrete integrable dynamical system of Painlevé type; moreover he explained how to find their Lax representation.

Bershtein's talk was the natural continuation of the previous talk, where he constructed special solutions of the discrete equations obtained by deautonomization of certain discrete flows in cluster algebras. These solutions can be written in terms of Riemann Theta functions.

Erik Tonni discussed some analytical results describing the entanglement of disjoint intervals in the context of two dimensional conformal field theories (CFT). In particular, he considered the Renyi entropies and the moments of the partial transpose, which provide respectively the entanglement entropy and the logarithmic negativity through some replica limits. These analytic expressions are obtained as the partition function of the CFT model on some particular singular higher genus Riemann surface constructed through the replica method. He presented explicit expressions in terms of Riemann theta functions for simple models like the compactified free boson and the Ising model and also numerical calculations on different lattice models which give evidence of the correctness of the analytic results.

The talk by Kirill Krasnov was devoted to the discussion of the recently discovered colour/kinematics duality in Yang-Mills theory (Bern, Carrasco and Johansson, 2008). This duality states that the Yang-Mills amplitudes at tree level can be represented as "squares" of the Lie algebraic colour structure. This property is intriguing because it suggests that he Yang-Mills theory has some hidden structure which is invisible in its Lagrangian formulation. The duality is by now well understood in the the self-dual (integrable) sector of the theory. Its role in the full theory is not yet completely known; however it is very encouraging that the famous structure Drinfeld double of the Lie algebra of vector fields plays a central role there.

Tau-functions in the theory of topological recursion and cluster algebras

An alternative method to explore the asymptotic behaviour of matrix integrals (and also more general problems) was developed by physicists and is called the method of topological recursion of Chekhov-Eynard-Orantin which allows to resolve recursively the so-called ”loop” equations. Remarkably, various terms arising in this expansion coincide with tau-functions from the theory of Frobenius manifolds, and also encode important combinatorial quantities like Hurwitz numbers, Gromov-Witten invariants, Hodge integrals etc.

Within this area we can list the talk of John Harnad (already reviewed), David Baraglia, Leonid Chekhov, David Baraglia nicely reviewed the famous construction of Hitchin of an integrable system on the co-tangent space of stable vector bundles on a Riemann surface. This is an algebraically integrable system (meaning that the tori are actually Abelian varieties). He explained how the construction works starting from a spectral curve and how these data are precisely the necessary information to initiate the scheme of topological recursion of Chekhov-Eynard-Orantin. However there is no easy interpretation of the outcome of this procedure in terms of geometric invariant; indeed their meaning is not entirely clear. Nonetheless Baraglia explained that a possible avenue is the theory of special Kahler geometry for the genus zero invariants and Bergman tau functions for the genus one invariants. The interpretation of the higher genera invariants remains a mystery and open problem.

Leonid Chekhov discussed the quantization of the Goldman bracket in the context of SL_k-representations on the moduli spaces $\Sigma_{g,s,n}$ of Riemann surfaces of genus g with s holes and n bordered cusps on the boundaries of the holes. His approach used a certain coordinatization introduced by Fock and Goncharov [FoGa2006] for Teichmüller spaces.

Tau functions in random matrix theory and random processes.

The theory of random matrices and the asymptotical expansion of matrix integrals is an important topic in combinatorics and physics. From a mathematical point of view most matrix integrals can be viewed as tau-functions of various integrable models; this turns out to be true both for finite matrix and as the matrix size tends to infinity.

Rigorous asymptotics analysis of such matrix integrals is based on Deift-Zhou method of steepest descent applied to an appropriate Riemann-Hilbert problem. The approach allows to obtain at the same time the asymptotic of the tau function (or “partition function”) as well as the strong asymptotics of the corresponding orthogonal polynomials, and hence the method is of interest for the two communities of mathematical physicists on one side as well as the community of approximation theory, mostly focused on the asymptotics of the orthogonal polynomials proper. Additionally, the recurrence coefficients of the orthogonal polynomials provide solutions for the Toda equations and also, when viewed in terms of the index, discrete Painlevé equations.

Within this circle of ideas we had the talks of Percy Deift, Tamara Grava, Peter , Anton Dzhamay, Craig Tracy.

Deift tackled a specific problem of the large-n behaviour of the recurrence coefficients for orthogonal polynomials in a $L^2((-1,1), \ln \frac{2k/(1-x)}{d} x)$. These weights (for $k > 1$) are at the center of a conjecture by Alphonse Magnus, which was thus proved. The problem, while specific, has interesting connotations because its solution requires a slightly different technique from the more standard nonlinear steepest descent. The technical reason is that a crucial step (known as the “parametrix”) near the singularity $x = 1$ of the measure cannot be explicitly constructed in terms of known functions. Instead Deift showed how to cleverly use an approximation scheme in terms of Legendre polynomials.

Grava revisited the problem of the asymptotic expansion of the partition function of the one–matrix model when the asymptotic eigenvalue distribution has two connected components (”two-cuts”). While in the one-cut regime it is known that the partition function and all the associated quantities (orthogonal polynomials, recurrence coefficients etc.) admit a regular asymptotic expansion in inverse powers of the size N of the matrix model, when there are two-cuts or more we also find oscillatory terms at every higher order of approximation. The partition function can be approximated using appropriate Theta functions but also an important contribution of Grava and co-authors has been the explicit correct computation of the ”constant problem”, i.e. the overall multiplicative constant (usually dependent on the size N alone) leading the asymptotic behaviour. This is a notoriously difficult problem (see also the talks of Prokhorov and Lisovyy).

More directly related to the classical theory of integrable systems was the contribution of Peter Clarkson, where he explained how the τ function of certain Painlevé equations can be expressed as the Hankel determinant of so–called “semi-classical” weights. His talk provides a concrete and specific realization of an existing framework that relates these Hankel determinants to more general isomonodromic tau functions [BEH2006]. Moreover he showed how the recurrence coefficients of the corresponding orthogonal polynomials can be interpreted as solving specific instances of discrete Painlevé equations.

Anton Dzhamay showed the connection of certain gap-formation probabilities with discrete Painlevé equations (and also with biorthogonal polynomials). In fact these gap probabilities are also tau-functions of the appropriate type (KP or isomonodromic, depending on the model).

It is well-known that gap probabilities of some discrete probabilistic models can be computed using discrete Painlevé equations. However, choosing correct Painlevé coordinates and matching the model with the standard Painlevé dynamics is a highly non-trivial problem. In this talk we show how this can be done using the geometric tools of Sakai’s theory for the model of boxed plane partitions with generalized weights suggested by Borodin, Gorin, and Rains. An important feature of our result is its consistency with the degeneration schemes for the weights matching the degeneration scheme for discrete Painlevé equations.

Random point processes where the correlation are determinants (known therefore as determinantal random point processes) are well known to be related to Fredholm determinants (and tau functions) because the gap-formation probabilities and generating functions of occupation numbers are expressible as such; however there are processes as the Asymmetric Exclusion Process (ASEP) where Fredholm determinants still make a prominent appearance even if the correlations are not determinants; this was the main message of the talk by Craig Tracy. The ASEP is a discrete point process on the line where a particle can jump randomly to the nearest left/right unoccupied site. The probability that the m-th particle from the left is at site x at time t was a breakthrough computation of Tracy and Widom of a few years back. These formulas were expressed in general as sums of multiple integrals and, for the case of step initial condition, as an integral involving a Fredholm determinant. Tracy reported on his more recent work where they obtained a generalization to the case where the m-th particle is the left-most one in a contiguous block of L–particles. These explicit formulæ allow to compute asymptotic behaviour for large time in the Kardar-Parisi-Zhang (KPZ) regime when the initial condition consist of "step-like" data, i.e. there are no particle to the right of the origin and all sites to the left are occupied.

Tau functions, Integrable Systems and vector bundles.

Jacques Hurtubise explored in his talk the deformation theory of bundles. The key to understanding the development of singularities in the solution of isomondromy problems on the Riemann sphere is whether the underlying bundle is trivial or not: for isomonodromy problems over curves of higher genus, the analogous notion is that of stability of the bundle. Hurtubise then showed that isomonodromy deformations provide a natural framework for the study of transverse deformations away from the unstable loci, whether the connection in question is regular, or has regular or irregular singularities.

The talk of Alexander Bobenko focused on his particular brand of integrable discrete systems, which have found wide applications in computer graphics and even, to some extent, architecture. He presented a procedure which allows one to integrate explicitly the class of (checkerboard) incircular nets. This class of privileged congruences of lines in the plane is known to admit a great variety of geometric properties. The parametrisation obtained in this manner is reminiscent of that associated with elliptic billiards. Connections with discrete confocal coordinate systems and the fundamental QRT maps of integrable systems theory were made.

Simonetta Abenda presented recent results (together with P.G. Grinevich) on the association between points of the totally positive Grassmannian and real algebraic-geometric data in the spirit of Krichever that give algebro–geometric solutions to the Kadomtsev-Petviashvili II (KP) equation. These solutions correspond to a certain finite dimensional reduction of Sato's Grassmannian and their asymptotic behavior is known to be classified in terms of the combinatorial structure of the totally non-negative part of real Grassmannians $Gr^{TNN}(k,n)$. Abenda and Grinevich used Postnikov's classification of totally non-negative Grassmannians which associates points of the positive Grassmannian with network graphs. They then made the explicit the correspondence with the datum of a rational degeneration of an M–curve of genus g together with a real, non-special divisor of degree g.

The construction of algebro–geometric solution of integrable hierarchies poses the challenge of effective numerical evaluations of canonical data on Riemann surfaces; in this vein Christian Klein discussed a purely numerical approach to compact Riemann surfaces starting from plane algebraic curves and introduced the necessary notions and approximation algorithms used to carry out numerical computations (mostly using Matlab).

In Atsushi Nakayashiki's talk we heard on a higher genus generalization of the classical Weierstrass σ–function. These multi-variate sigma functions have a series expansion whose coefficients are polynomials of coefficients of the defining equation of the curve which has the very desirable property that it behaves smoothly under degeneration of the curve. In his talk he focused on the degeneration of a hyperelliptic curve of genus g to a curve of genus $g-1$. Using the tau function formalism in the context of Sato's Grassmannian, he represented the limiting sigma function in terms of a sum of lower genus sigma functions.

Another application of isomonodromic deformations to the theory of Frobenius manifolds was presented by Davide Guzzetti. In this context it is necessary to consider particular degenerations of isomonodromic systems where the coefficients of the differential equation become resonant (eigenvalues coincide). The system admits a well–defined limit (relevant then for the application to Frobenius manifold theory) only for certain initial data, which he identified and studied.

Scientific Progress and Outcome of the Meeting

Talks and discussions which took place during the meeting have sewn the seeds of further developments and advances in all the areas presented at the meeting. We only name a few of them.

In the past years it has become clear that there are still unexplored and deep connections between the now-classical theory of isomonodromic deformations and the symplectic geometry of Painlevé equations; the talks of Prokhorov and Lisovyy are a manifestation of this relationship. In fact, one of the outstanding problems in the area is the computation of the "connection constants"; the ratio of the asymptotic expansions of the tau function near its singular points is a function only of the monodromy data (a "constant" relative to the isomonodromic parameters). Its computation poses significant challenges and result are only recently becoming available in papers of Its, Lisovyy and collaborators. This constant appears also to be a generating function of changes of Darboux coordinates. A novel interpretation that emerged during the discussion is that of this constant as transition function of an appropriate line bundle over the monodromy manifold.

As a result of talk of Zvonkine it has become plausible that the Bergman tau function should be a useful tool in construction of new non-tautological classes on moduli spaces of marked Riemann surfaces; until now very few explicit examples of the non-tautological classes are known.

The unexpectedly important role played by the discrete Painlevé equations in conformal field theory was revealed in the talks of Bershtein-Gavrilenko and A.Marshakov; this link allows to expect that rich geometrical structures associated to the discrete Painlev'e equations can be applied to study correlators and conformal blocks of various conformal field theories.

As a result of the talk of Jacques Hurtubise and subsequent discussion involving Baraglia, Bertola, Korotkin, Norton, Harnad, Ruzza, opened the way to generalization of the notion of isomonodromic tau functions to Hitchin integrable systems including their non-autonomous counterpart and higher genus analogues.

Talks by Baraglia and Hurtubise lead also to elucidation of the link between moduli spaces of abelian differentials on Riemann surfaces and spaces of spectral covers of generalized Hitchin systems. In particular, variational formulas on spaces of spectral covers were derived which generalize the celebrated Donagi-Markman cubic to the meromorphic case. A relationship to the topological recursion of Checkhov-Eynard-Orantin was also derived.

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Chapter 23

Affine Algebraic Groups, Motives and Cohomological Invariants (18w5021)

September 16 - 21, 2018

Organizer(s): Nikita Karpenko (University of Alberta), Alexander Merkurjev (University of California at Los Angeles), Anne Quéguiner-Mathieu (Université Paris 13)

Overview of the Field

The theory of affine algebraic groups is a well-established area of modern mathematics. It started as an algebraic version of the massively successful and widely applied theory of Lie groups, pushed forward most notably by Chevalley and Borel. In the hands of Serre and Tits, it developed into a powerful tool for understanding algebra, geometry and number theory (e.g. Galois cohomology). In particular, it provides a way to unify seemingly distinct statements in algebra, geometry and number theory, hence, suggesting new techniques and methods for solving problems in these areas.

For example, the Hasse-Minkowski Theorem and the Albert-Brauer-Hasse-Noether Theorem, which concern respectively quadratic forms and central simple algebras over global fields, can be viewed as special cases of the celebrated Hasse Principle in Galois cohomology of semisimple linear algebraic groups (due to Kneser, Harder, and Chernousov) which unifies these two theorems and provides many new results that would not have been suspected before.

This philosophy has led to a vast number of new techniques that proved useful in many different areas of mathematics such as: quadratic forms (Karpenko, Merkurjev, Vishik), essential and canonical dimensions (Reichstein, Merkurjev), local-global principles (Hartmann, Harbater, Krashen, Parimala, Suresh), motives (Petrov, Semenov, Zainoulline), and torsors (Chernousov, Gille, Panin, Pianzola). For instance, Karpenko proved that some results on isotropy of hermitian forms (related to affine algebraic groups of type A) induce analogous results for symplectic and quadratic forms (groups of types B, C, D), via the theory of algebraic cycles and and the study of Chow motives of projective homogeneous varieties.

Further applications recently emerged in more arithmetic topics, such as the study of arithmetic groups and arithmetic locally symmetric spaces (Prasad, Rapinchuk) and pseudo-reductive groups (Conrad). In the opposite direction, another trend has been using results from finite group theory to prove theorems about algebraic groups (Guralnick).

In this workshop, we brought together specialists and young researchers from these areas, to stimulate new advances and developments, with particular emphasis on recent applications of algebraic groups in algebra, geometry and number theory that establish new links between different areas of mathematics. For example, the following topics have been included: the proof of the Grothendieck-Serre conjecture based on the theory of affine Grassmannians coming from the Langland's program; the breakthrough in the computation of cohomological invariants of degree 3 by Merkurjev based on new results concerning motivic cohomology; Conrad's proof of finiteness of fibers for fppf cohomology over global fields of prime characteristic; and applications of representations with dense orbits inspired by Bhargava's work.

Recent Developments and Open Problems

During the last decade, we observed an explosion of research activity in the area of affine algebraic groups and applications. Below, we describe some topics, where striking results were recently obtained.

The geometric case of the Grothendieck-Serre conjecture (Fedorov-Panin)

Fedorov and Panin have proved this conjecture, stated in the mid-1960's, which says that if a G-torsor (defined over a smooth algebraic variety X) is rationally trivial, then it is locally trivial (in Zariski topology), where G is a smooth reductive group scheme over X. Their proof uses the theory of affine Grassmannians.

This conjecture has a long history: It was first proven for curves and surfaces for quasi-split groups by Nisnevich in the mid-1980's, and for arbitrary tori in the late 1980's by Colliot-Thelene and Sansuc. If G is defined over a field, then the conjecture is known as Serre's conjecture and was proven by Colliot-Thelene, Ojanguren and Raghunathan in the beginning of the 1990's. Ojanguren-Panin-Suslin-Zainoulline proved it for most classical groups in the late 1990's. Finally, Panin-Stavrova-Vavilov gave a proof for isotropic groups. However, no general argument was known up to now. Recently Fedorov and Panin found a new original approach that proves the conjecture in general, using the theory of affine Grassmannians coming from Langlands' program.

Computation of the group of degree 3 cohomological invariants, using motivic cohomology (Merkurjev)

According to J.-P. Serre, by a cohomological invariant, one means a natural transformation from the first Galois cohomology with coefficients in an algebraic group G (the pointed set which describes all G-torsors) to a cohomology functor $h(-)$, where h is, for instance, some Galois cohomology group with torsion coefficients, a Witt group, or a Chow group with coefficients in a Rost cycle module M. The ideal result here would be to construct enough invariants to classify all G-torsors under some affine algebraic group G. The question was put on a firm foundation by Serre and Rost in the 1990's, allowing the proof of statements like "the collection of cohomological invariants of G is a free module over the following cohomology ring" for certain groups G; this theory is expounded in the 2003 book by Garibaldi-Merkurjev-Serre.

Using this theory one obtains a complete description of all invariants landing in degree 1 Galois cohomology for arbitrary G, in degree 2 if G is connected, and in degree 3 if it is simply connected and semisimple (Rost). In a breakthrough recent development, which is the starting point of important research activity, Merkurjev provided a complete description of degree 3 invariants for semisimple groups, solving a long standing question. The full power of his entirely new methods, based on new results in motivic cohomology, still have to be understood. Moreover, even though he describes the finite group of degree three invariants, we often lack a complete description of generators of this group, that is, new invariants have been discovered, that still have to be described.

Length spectra of locally symmetric spaces (Prasad and Rapinchuk)

The answer to the question "Can you hear the shape of a drum?" is famously no. Nevertheless, some variations of the problem where one strengthens the hypothesis or restricts the collection of spaces under consideration has led to situations where the answer is yes. In a remarkable 2009 Pub. Math. IHES paper, Prasad and Rapinchuk introduced the notion of weak commensurability of semisimple elements of algebraic groups and of arithmetic groups and used this new concept to address the question of when arithmetically defined locally symmetric spaces have the same length spectrum. In this paper they also settled many cases of the long-standing question of when algebraic groups with the same maximal tori are necessarily isomorphic. This paper, and the stream of research stemming from it, connects algebraic groups and their Galois cohomology – the central subject of this conference – with arithmetic groups, geometry, and even transcendental number theory.

Applications of algebraic cycles and Grothendieck gamma filtration to invariants of torsors and algebras with involutions (Baek-Garibaldi-Gille-Queguiner-Zainoulline)

Let X be the variety of Borel subgroups of a simple linear algebraic group G over a field k. In a series of papers it was proven that the torsion part of the second quotient of Grothendieck's gamma-filtration on X is closely related to the torsion of the Chow group and hence to the group of cohomological invariants in degree 3 computed recently by Merkurjev. As a byproduct of this new striking connection one obtains an explicit geometric interpretation/description of various cohomological invariants in degree 3 as well as new results concerning algebraic cycles and motives of projective homogeneous spaces.

Genericity theorems for the essential dimension of algebraic stacks and their applications (Brosnan-Reichstein-Vistoli)

Techniques from the theory of algebraic stacks can be used to prove genericity theorems, that bound the essential dimension of those stacks. As an application, new bounds for the more classical essential dimension problems for algebraic groups, forms and hypersurfaces are obtained. These genericity theorems have also been used in particular by Biswas, Dhillon and Lemire to find bounds on the essential dimension of stacks of (parabolic) vector bundles over curves.

Some classification results (simple stably Cayley groups, by Borovoi-Kunyavskii-Lemire-Reichstein, and finite groups of low essential dimension, Beauville and Duncan)

A linear algebraic group is called a Cayley group if it is equivariantly birationally isomorphic to its Lie algebra. It is stably Cayley if the product of the group and some torus is Cayley. Cayley gave the first examples of Cayley groups with his Cayley map back in 1846. Over an algebraically closed field of characteristic 0, Cayley and stably Cayley simple groups were classified by Lemire-Popov-Reichstein in 2006. In 2012, the classification of stably Cayley simple groups was extended to arbitrary fields of characteristic 0 by Borovoi-Kunyavskii-Lemire-Reichstein.

On a different topic, Duncan used the classification of minimal models of rational G-surfaces to provide a classification of finite groups of essential dimension 2 over an algebraically closed field of characteristic 0. Beauville recently used Prokhorov's classification of rationally connected threefolds with an action of a simple group to classify the finite simple groups of essential dimension 3.

Motivic decompositions

Karpenko and Merkurjev gave a description of the motivic decomposition of equivariant compactifications of reduced norm varieties of central simple algebras of prime degree over a field. This result generalizes the classical motivic decompositions of norm quadrics due to Rost, as well as partial results on the case of prime degree 3 obtained by Semenov.

In a different direction, Neshitov, Petrov, Semenov and Zainoulline recently described motivic decompositions of twisted flag varieties in terms of representations of Hecke-type algebras. This creates a link between two different worlds: - the world of motives of generically split twisted flag varieties (i.e, projective homogeneous varieties under an action of a semisimple affine algebraic group such that the group splits over the function field of the variety) on one side and - the world of finitely generated projective modules over certain Hecke-type algebras on the other side.

Presentation Highlights and Scientific Progress Made

Alexander Vishik

In the talk of A.Vishik the idea of *anisotropy* was used to introduce the *isotropic motivic category* $\mathrm{DM}(k/k;\mathbb{F}_p)$, which is obtained from the Voevodsky category by (roughly speaking) "killing" the motives of all anisotropic (mod p) varieties over k. This "local" version of the Voevodsky category is much simpler than the "global" one and has many remarkable properties. As its global counterpart, it has the *pure part* (the analogue of the Chow motivic category) where the classical ("global") Chow groups $\mathrm{Ch} = \mathrm{CH}/p$ are substituted by their quotient $\mathrm{Ch}_{k/k}$ obtained by moding out the anisotropic classes. The notion of *flexible* fields was introduced for which the description is particularly simple, and by passing to which no information is lost. The Conjecture was formulated claiming that, over a flexible field, $\mathrm{Ch}_{k/k}$ coincides with Chow groups modulo *numerical equivalence* (mod p). And so, the "local" Chow motivic category $Chow(k/k)$ coincides with $Chow_{Num(p)}(k)$. This Conjecture was proven for varieties of dimension ≤ 5, for divisors and for cycles of dimension ≤ 2. In particularly, hypothetically (and in the above cases firmly), the "local" Chow groups are finite-dimensional, and any correspondence vanishing over algebraic closure (or even in the topological realization) is zero locally. This provides a natural environment to approach questions like *Rost Nilpotence* and the (mod p) analogues of the *Standard Conjectures*. The "local" motivic cohomology of a point (with $\mathbb{F}_2$-coefficients) over a flexible field were computed. Quite unexpectedly, these encode in themselves the Milnor's operations, which should explain, to some extent, why these operations played such a crucial role in the Voevodsky's proof of Milnor's Conjecture.

Mathieu Florence

In his talk, Mathieu Florence addressed the question of lifting vector bundles to Witt vector bundles. More precisely, let p be a prime number, and let S be a scheme of characteristic p. For any $n \geq 2$, denote by $W_n(S)$ the scheme of Witt vectors of length n, built out of S. The closed immersion $S \hookrightarrow W_n(S)$ can be thought of as a universal thickening of S, of characteristic p^n. Let V be a vector bundle over S.

Question: is V the restriction to S of a vector bundle defined over $W_n(S)$?

He gave a positive answer for line bundles: every line bundle L admits a (canonical and elementary) lift to a W_n-bundle: its n-th Witt lift. Next he considered the case of the tautological vector bundle on the base $S = \mathbb{P}_X(V)$, the projective space of a vector bundle V , defined over an affine base X. The answer is positive again. He also gave an example of a non-liftable vector bundle. Global sections of Witt lifts of line bundles can be naturally described as noteworthy algebraic objects: Pontryagin duals of divided powers of modules over Witt vectors. He ventured to explore connections between Witt vectors and divided powers. In particular, he gave a new functorial description of Witt vectors "by generators and relations", [5].

Skip Garibaldi

Let G be a simple algebraic group over an algebraically closed field k. In case $k = \mathbb{C}$, it has been known for $40+$ years which irreducible representations V of G are generically free, i.e., have the property that the stabilizer in G of a generic $v \in V$ is the trivial group scheme. Recent applications of this to the theory of essential dimension have motivated the desire to extend these results to arbitrary k. We did this in [6], [7], and [8] except for a handful of cases addressed in [9], completing the solution to the problem.

Philippe Gille

This is a report on [10]. Let K be a discretly valued henselian field with valuation ring O and residue field k. We denote by K_{nr} the maximal unramified extension of K and by K_t its maximal tamely ramified extension. If G/K is a semisimple simply connected groups, Bruhat-Tits theory is available in the sense of [13, 14] and the Galois cohomology set $H^1(K_{nr}/K, G)$ can be computed in terms of the Galois cohomology of special fibers of Bruhat-Tits group schemes. This permits to compute $H^1(K, G)$ when the residue field k is perfect. On the other hand, if k is not perfect, "wild cohomology classes" occur, that is $H^1(K_t, G)$ is non-trivial. Such examples appear for example in the study of bad unipotent elements of semisimple algebraic groups. Under some restrictions on G, we would like to show that $H^1(K_t/K_{nr}, G)$ vanishes (see Corollary 3.3). This is related to the following quasi-splitness result.

Theorem. Let G be a semisimple simply connected K-group which is quasi-split over K_t.
(1) If the residue field k is separably closed, then G is quasi-split.
(2) $G \times_K K_{nr}$ is quasi-split.

This theorem answers a question raised by Gopal Prasad who found another proof by reduction to the inner case of type A [14, th. 4.4]. Our first observation is that the result is quite simple to establish under the following additional hypothesis:

(*) If the variety of Borel subgroups of G carries a 0-cycle of degree one, then it has a K-rational point.

Property (*) holds away of E_8. It is an open question if (*) holds for groups of type E_8. For the E_8 case (and actually for a strongly inner K-group G) of Theorem, our proof is a Galois cohomology argument using Bruhat-Tits buildings. We can make at this stage some remarks about the statement. Since K_{nr} is a discretly valued henselian field with residue field k_s, we observe that (1) implies (2). Also a weak approximation argument reduces to the complete case. If the residue field k is separably closed of characteristic zero, we have then $cd(K) = 1$, so that the result follows from Steinberg's theorem. In other words, the main case to address is that of characteristic exponent $p > 1$.

Igor Rapinchuk

Let K be a field. The purpose of this talk was to present new results of [15] in the framework of the following general problem:

(*) (When) can one equip K with a natural set V of discrete valuations such that for a given absolutely almost simple simply connected algebraic K-group G, the set of K-isomorphism classes of (inner) K-forms of G having good reduction at all $v \in V$ (resp., at all $v \in V \setminus S$, where $S \subset V$ is an arbitrary finite subset) is finite?

While the analysis of abelian varieties defined over a global field and having good reduction at a given set of places of the field has been one of the central topics in arithmetic geometry for a long time, particularly since the work of G. Faltings [4], similar questions in various situations involving linear algebraic groups have received less attention so far.

Kirill Zainoulline

This is a report on [18]. Consider a root system Φ together with its geometric realization in $\mathbb{R}^N$, that is we look at Φ as a subset of vectors in $\mathbb{R}^N$ which is closed under reflection operators r_v for each $v \in \Phi$. A basic example of such a realization is given by the vectors

$$\Phi = \{\alpha_{ij} = e_i - e_j \in \mathbb{R}^{2n} \mid i \neq j,\ i,j = 1 \ldots 2n,\ n \geq 1\},$$

where $\{e_1, \ldots, e_{2n}\}$ is the standard basis of $\mathbb{R}^{2n}e$. This corresponds to the root system of Dynkin type A_{2n-1}. Note that $\mathbb{R}^{2n}$ admits an involutive symplectic linear operator $\tau(e_i) = -e_{2n-i+1}$ which preserves Φ. Taking averages over orbits in Φ under τ one obtains a new subset of vectors

$$\Phi_\tau = \{\frac{1}{2}(\alpha_{ij} + \tau(\alpha_{ij})) \mid \alpha_{ij} \in \Phi\}$$

which turns out to be a geometric realization of the root system of Dynkin type C_n. There are other similar examples of root systems (such as D_{n+1} and E_6) and involutive operators τ induced by automorphisms of the respective Dynkin diagrams. The procedure of passing from Φ to Φ_τ by taking averages via τ is called folding of a root system.

In the present paper we are weakening the assumption $\tau^2 = \mathrm{id}$ by considering an arbitrary linear automorphism $\mathcal{T}$ of $\mathbb{R}^N$ that satisfies a separable quadratic equation

$$p(\mathcal{T}) = \mathcal{T}^2 - c_1\mathcal{T} + c_2 = 0, \quad c_1, c_2 \in \mathbb{R}.$$

Hence, introducing the notion of a twisted (quadratic) folding. It would be interesting to extend our construction to affine root systems and higher degree equations.

Our motivating example is the celebrated projection of the root system of type E_8 onto the subset of icosians of the quaternion algebra which realizes a finite non-crystallographic root system of type H_4. This projection has been studied by many authors, among them by Moody-Patera [12] in the context of quasicrystals. More precisely, in this case one considers an operator $\mathcal{T}$ that satisfies the quadratic equation $x^2 - x - 1 = 0$ of the golden section and then takes the projection onto an eigenspace. We formalize such a procedure by looking at a root system $|phi$ as a subset of the Weil restriction $R_{l/k}U$ of a free module U over l where $l = k(x)/(p(x))$ is a quadratic separable algebra over an integral domain k. Then our operator $\mathcal{T}$ is the multiplication by a root τ of p that preserves the root lattice of Φ and partitions the subset of simple roots of Φ. Such data give us a folded representation of Φ. We then introduce a notion of τ-twisted folding as the projection of the root system Φ to the respective τ-eigenspace of $\mathcal{T}$. Observe that for an involution $\mathcal{T}$ this projection coincides with the usual averaging operator.

As an application we use the twisted foldings and moment graph techniques to construct maps from equivariant cohomology of flag varieties to their virtual analogue for finite Coxeter groups. Observe that this follows Sorgel's philosophy to use virtual geometry to investigate combinatorics of Coxeter groups [17].

Nicole Lemire

For a central simple algebra A of degree n over a field F, the generalized Severi-Brauer variety $SB(d, A)$ is a twisted form of $Gr(d, n)$, the Grassmannian of d-dimensional planes in n-dimensional affine space. It is well-known that the variety $SB(d, A)$ has a rational point over an extension K/F if and only if $ind(A_K)|d$. We can extend this question to ask about other closed subvarieties of $SB(d, A)$. In particular, we may ask: Under what conditions does $SB(d, A)$ contain a closed subvariety which is a twisted form of a Schubert subvariety of $Gr(d, n)$? We show in [11] that this happens exactly when the index of the algebra divides a certain number arising from the combinatorics of the Schubert cell, using a variation on Fulton's notion of essential set of a partition.

In the classical setting, these Schubert subvarieties are of particular interest as they form the building blocks for the Grothendieck group and Chow group of $Gr(d, n)$. The Chow groups, in the case of homogeneous varieties, and Severi-Brauer varieties in particular, have been much studied, and related to important questions about the arithmetic of central simple algebras. Although the Chow groups of dimension 0, codimension 1 and to some extent codimension 2 cycles on Severi-Brauer varieties have been amenable to study, the other groups are in general not very well understood at all. Algebraic cycles on and Chow groups of generalized Severi-Brauer varieties are even more subtle and less understood. For example, the Chow group of dimension 0 cycles on such varieties are only known in the case of reduced dimension 2 ideals in algebras of period 2. In our work we make some first steps towards developing parallel methods as currently exist for the Severi-Brauer varieties, to compute the codimension 2 Chow groups for the generalized Severi-Brauer varieties of reduced dimension 2 ideals in certain algebras of small index.

Theorem. Let $X = SB(2, A)$ with $ind(A)|12$. Then $CH^2(X)$ is torsion-free.

This computation is done first by using the explicit descriptions of Schubert classes obtained in the first half part of the paper together with other geometric constructions to show that the graded pieces of the K-groups with respect to the topological filtration are torsion free for degree 4 algebras. This quickly gives the result for codimension 2 Chow groups for such varieties. Finally, the theorem follows by an analysis of the motivic decomposition of the Chow motive of $SB(2, A)$ due to Brosnan.

Rostislav Devyatov

For details see [3].

Let G be a simple algebraic group over $\mathbb{C}$ with a simply laced Dynkin diagram. Consider the generalized flag variety G/B, where $B \subset G$ is a Borel subgroup. We are going to study the Chow ring of G/B.

The Chow ring of G/B is generated (as a $\mathbb{Z}$-algebra) by the classes of Schubert divisors in G/B (actually, to define the Schubert divisors canonically, we need to first fix a maximal torus in B, which canonically defines the root system, the Weyl group, and its action on G/B, so we assume that a maximal torus in B is fixed). Denote the classes of Schubert divisors by $D_1, \ldots, D_r$, where $r = rkG$. We will be particularly interested in monomials in classes D_i. Let us say that a monomial $D_1^{n_1} \ldots D_r^{n_r}$ is multiplicity free if there exists a Schubert class X (this is the class of a Schubert variety, not necessarily of a Schubert divisor) such that $D_1^{n_1} \ldots D_r^{n_r} X = [pt]$. Our goal is to answer the following question: What is the maximal degree (in the Chow ring) of a multiplicity-free monomial in $D_1, \ldots, D_r$ (i. e., what is the maximal value of the sum $n_1 + \cdots + n_r$ over all n-tuples $n_1, \ldots, n_r$ of nonnegative integers such that $D_1^{n_1} \ldots D_r^{n_r}$ is a multiplicity-free monomial)? This question is particularly interesting in the case when G is of type E_8, because the answer may be used to compute upper bounds on the canonical dimension of G/B.

The answer to this question for E_8 is 34. More generally, we answer this question for any simple group G with simply-laced Dynkin diagram.

Nikita Semenov

In the present talk we discuss an approach to cohomological invariants of algebraic groups over fields of characteristic zero based on the Morava K-theories, which are generalized oriented cohomology theories in the sense of Levine-Morel. We show that the second Morava K-theory detects the triviality of the Rost invariant and, more generally, relate the triviality of cohomological invariants and the splitting of Morava motives. We describe the Morava K-theory of generalized Rost motives, compute the Morava K-theory of some affine varieties, and characterize the powers of the fundamental ideal of the Witt ring with the help of the Morava K-theory. Besides, we obtain new estimates on torsion in Chow groups of codimensions up to $2n$ of quadrics from the $(n+2)$-nd power of the fundamental ideal of the Witt ring. We compute torsion in Chow groups of $K(n)$-split varieties with respect to a prime p in all codimensions up to $p^{n-1}/(p-1)$ and provide a combinatorial tool to estimate torsion up to codimension p^n. An important role in the proof is played by the gamma filtration on Morava K-theories, which gives a conceptual explanation of the nature of the torsion. Furthermore, we show that under some conditions the $K(n)$-motive of a smooth projective variety splits if and only if its $K(m)$-motive splits for all $m \leq n$.

This is a report on [16].

Maksim Zhykhovich

The classical Hasse–Minkowski theorem says that a non-degenerate quadratic form q over a number field F is isotropic if and only if it is isotropic over all completions of F. This assertion can be reformulated in the language of algebraic cycles and Chow motives. Namely, for the projective quadric Q given by the equation $q = 0$, the Tate motive $\mathbb{Z}(0)$ is a direct summand of the motive of Q if and only if it is a direct summand of the motive of Q_{F_v} for each completion F_v of F.

Moreover, the Hasse–Minkowski theorem readily implies that for every non-negative integer m, the Tate motive $\mathbb{Z}(m)$ is a direct summand of the motive of Q over F if and only if it is a direct summand of the motive of Q over all completions of F. Indeed, this is equivalent to the condition that the Witt index of q is greater than m.

We prove a generalization of the above assertion replacing the Tate motive $\mathbb{Z}(m)$ by a binary motive.

We say that a motive N over an arbitrary field F is a split motive (resp. a binary split motive) if it is a direct sum of a finite number of Tate motives over F (resp. if it is a direct sum of two Tate motives over F). We say that N is a binary motive over F if becomes binary split over an algebraic closure $\bar{F}$ of F.

We work in the category of Chow motives with $\mathbb{F}_2$-coefficients. We consider only non-degenerate quadratic forms. For a non-degenerate quadratic form q over a field F we denote by $M(q)$ the Chow motive of the corresponding projective quadric given by the equation $q = 0$. For a number field F and a place v of F, we denote by q_v the corresponding quadratic form over the completion F_v of F at v. Our main result is the following theorem:

Theorem, [2]. Let q be a quadratic form over a number field F. Let N be a binary split motive over F. Assume that for every place v of F there exists a direct summand ${}^vM$ of $M(q_v)$ that is isomorphic to N over an algebraic closure $\bar{F_v}$ of F_v. Then there exists a direct summand M of $M(q)$ that is isomorphic to N over F.

It follows from our proof of the above theorem that every indecomposable binary direct summand of quadric over a number field is a twist of a Rost motive. Recall that the motive of a Pfister form π over an arbitrary field is isomorphic to a direct sum of twists of one binary motive, which is called the Rost motive of π. Rost motives over an arbitrary field appear in the proof of the Milnor conjecture by Voevodsky.

We remark that over every completion of a number field, all quadratic forms are excellent, and therefore, the structure of their Chow motives is known. Moreover, every motivic decomposition of a quadric with $\mathbb{F}_2$-coefficients can be uniquely lifted to a motivic decomposition with integer coefficients. Therefore, the above theorem holds for motives with integer coefficients as well.

Finally, as an application of the Hasse principle for binary motives we obtain a complete motivic decomposition of the motive of a quadric over any number field with at most one real embedding, for example, over the field of rational numbers $\mathbb{Q}$:

Corollary. In the case when the field F has at most one real embedding, Theorem holds for every split motive N (not necessarily binary).

Nivedita Bhaskhar

Let K be a field and T, a commutative linear algebraic group defined over K. Given L/K, a finite separable field extension, one can define the *norm homomorphism* $N_{L/K} : T(L) \to T(K)$ which sends $t \rightsquigarrow \prod_\gamma \gamma(t)$ where γ runs over cosets of $\mathrm{Gal}(K^{sep}/L)$ in $\mathrm{Gal}(K^{sep}/K)$. The definition of the norm homomorphism can be extended to K-étale algebras in a similar manner. Note that if $T = \mathbb{G}_m$, then $N_{L/K} : T(L) \to T(K)$ is precisely the usual norm $N_{L/K} : L^* \to K^*$.

Now let G be a linear algebraic group defined over K and let $f : G \to T$ be an algebraic group homomorphism defined over K. We say that the *norm principle* holds for $f : G \to T$ over a finite separable field extension (or étale algebra) L/K if $N_{L/K}(\mathrm{Im} f(L)) \subseteq \mathrm{Im} f(K)$. We say that the *norm principle* holds for $f : G \to T$ if for every finite separable field extension (equivalently for every étale algebra) L/K , $N_{L/K}(\mathrm{Im} f(L)) \subseteq \mathrm{Im} f(K)$.

Suppose further that the commutator subgroup G' of G is defined over K. Then every homomorphism $f : G \to T$ factors through the natural homomorphism $\tilde{f} : G \to G/G'$ and it is an easy check that the norm principle for $\tilde{f}$ (over L/K) implies the norm principle for f (over L/K). We say that the *norm principle* holds for G (over L/K) if it holds for $\tilde{f}$ (over L/K).

Let Q be a quadratic form over K. The classical norm principle of Scharlau which asserts that norms of similarity factors of Q_L are themselves similarity factors of Q can be restated in this context to say that the norm principle holds for the multiplier map $M : \mathrm{GO}(Q) \to \mathbb{G}_m$. Similarly Knebusch's norm principle which states that norms of spinor norms of Q_L are spinor norms of Q can be reformulated as the norm principle holding for the spinor norm map $\underline{\mu} : \Gamma^+(Q) \to \mathbb{G}_m$.

Norm principles have been previously studied in especially in conjunction with the rationality or the R-triviality of the algebraic group in question. It was established that the norm principle holds in general for all reductive groups of classical type without D_n components. The D_n case was investigated later and a scalar obstruction defined up to spinor norms, whose vanishing would imply the norm principle, was given. However, the triviality of this scalar obstruction is far from clear and the question whether the norm principle holds for reductive groups with type D_n components still remains open.

If K is a number field, the norm principle was proved in full generality for all reductive groups by P. Gille , so the first widely open and very interesting case is when K is the function field $k(C)$ of a curve C defined over a number field k and the group G in question is of classical type with the semisimple part $G' = \mathrm{Spin}(Q)$. As we show, the validity of the norm principle over K is closely related to the triviality of the kernel of the natural map $H^1(K, G') \to \prod_v H^1(K_v, G')$ where v runs through a set of discrete valuations of K. Therefore the (traditional) local-global approach leads us first to look in detail over completions K_v.

With this motivation in mind, we investigate the D_n case over an arbitrary complete discretely valued field K with residue field k and $\mathrm{char}(k) \neq 2$, restricting ourselves to type D_n groups arising from quadratic forms. In the main result, we show that if the norm principle holds for such groups defined over all finite extensions of the residue field k, then it holds for such groups defined over K (see [1, Theorem 5.1]). This yields examples of complete discretely valued fields with residue fields of virtual cohomological dimension ≤ 2 over which the norm principle holds for the groups under consideration (see [1, Corollary 6.3]). As a further application, we also relate the possible failure of the norm principle to the nontriviality of certain Tate-Shaferevich sets.

Stefan Gille

Let R be a regular semilocal ring containing $\frac{1}{2}$ with fraction field K, and (A, τ) an R-Azumaya algebra with involution of the first or second kind. By second kind we mean that R is a quadratic Galois extension of the fix ring of the involution τ. For $\varepsilon \in \{\pm 1\}$ there is a complex of ε-hermitian Witt groups, the so called ε-hermitian Gersten-Witt complex

$$0 \longrightarrow \mathrm{W}_\varepsilon(A, \tau) \longrightarrow \mathrm{W}_\varepsilon(A_K, \tau_K) \xrightarrow{d^{0,\varepsilon}_{A,\tau}} \bigoplus_{\mathrm{ht} P=1\,, \tau(P)=P} \mathrm{W}_\varepsilon(A_{k(P)}, \tau_{k(P)}) \xrightarrow{d^{1,\varepsilon}_{A,\tau}} \ldots\,,$$

where $k(P)$ is the residue field at the prime P of R, and where we have set $(A_{k(P)}, \tau_{k(P)}) := k(P) \otimes_R (A, \tau)$ and analogous $(A_K, \tau_K) := K \otimes_R (A, \tau)$. We consider this as a cohomological complex with the term $\mathrm{W}_\varepsilon(A_K, \tau_K)$ in degree 0, and denote its cohomology groups by $\mathrm{H}^i(A, \tau, \varepsilon)$.

It is known that this complex is exact if R contains a field. We extended this recently to regular semilocal rings of (very) small dimension.

Theorem A. *If R is a semilocal Dedekind domain then the ε-hermitian Gersten-Witt complex*

$$0 \longrightarrow \mathrm{W}_\varepsilon(A, \tau) \longrightarrow \mathrm{W}_\varepsilon(A_K, \tau_K) \xrightarrow{d^{0,\varepsilon}_{A,\tau}} \bigoplus_{\mathrm{ht} P=1\,, \tau(P)=P} \mathrm{W}_\varepsilon(A_{k(P)}, \tau_{k(P)}) \longrightarrow 0$$

is exact for all $\varepsilon \in \{\pm 1\}$. This sequence is split if R is a complete discrete valuation ring and τ is of the first kind.

This implies by induction that $\mathrm{H}^{\dim R}(A, \tau, \varepsilon) = 0$ for all regular semilocal rings R, from which we then deduce purity for regular semilocal rings of dimension two.

Theorem B. *If the regular semilocal ring R is of dimension two then the complex*

$$0 \longrightarrow \mathrm{W}_\varepsilon(A, \tau) \longrightarrow \mathrm{W}_\varepsilon(A_K, \tau_K) \xrightarrow{d^{0,\varepsilon}_{A,\tau}} \bigoplus_{\mathrm{ht} P=1\,, \tau(P)=P} \mathrm{W}_\varepsilon(A_{k(P)}, \tau_{k(P)})$$

is exact for all $\varepsilon \in \{\pm 1\}$.

There are analogous exact sequences for R-orders in central simple algebras. Let B be a central simple algebra over the fraction field K of the discrete valuation ring R, and Δ a maximal R-order in B. Assume that $\frac{1}{2} \in R$, and that B has an involution of the first kind which maps Δ into itself. Then there is an exact sequence of ε-hermitian Witt groups ($\varepsilon \in \{\pm 1\}$)

$$0 \longrightarrow \mathrm{W}_\varepsilon(\Delta, \tau) \longrightarrow \mathrm{W}_\varepsilon(B, \tau) \xrightarrow{\partial} \mathrm{W}_\varepsilon(\Delta/\mathrm{rad}\Delta, \bar{\tau}) \,,$$

where $\bar{\tau}$ is the by τ induced involution on $\Delta/\mathrm{rad}\Delta$. In case R is complete the 'residue map' ∂ is onto, and this should hold more general for arbitrary discrete valuation rings R.

Outcome of the Meeting

The workshop attracted 40 leading experts and young researchers from Belgium, Canada, France, South Korea, Germany, Israel, Russia, Switzerland, USA. There were 25 speakers in total: 15 talks were given by senior speakers, 9 talks by young researchers and postdocs and 2 talk by a doctoral student.

The lectures given by senior speakers provided an excellent overview on the current state of research in the theory of algebraic groups, their cohomological invariants, and motives. Young speakers were provided a unique opportunity to present their achievements. Numerous discussions between the participants after the talks have already led to several joint projects, e.g. by Auel-Suresh, Chernousov-P.Gille, Karpenko-Merkurjev.

The organizers consider the workshop to be a great success. The quantity and quality of the students, young researchers and the speakers was exceptional. The enthusiasm of the participants was evidenced by the frequent occurrence of a long line of participants waiting to ask questions to the speakers after each lecture. The organizers feel that the material these participants learned during their time in BIRS will prove to be very valuable in their research and will undoubtedly have a positive impact on the research activity in the area.

Below is a feedback of a young participant and speaker from Yale University Asher Auel.

The participants assembled was a great mix of LAG, quadratic forms, motivic, and broader arithmetic geometry people. The lectures (and choice of thematic groupings) were all great. For me, the most inspirational lectures (where I learned something new or surprising) were by Haution, Hoffmann, Bayer-Fluckiger, Garrel, Semenov, and Bhaskhar (in order of the schedule).

For me, the most important part of the workshop is the interactions.

- I had some very useful interactions with Tignol, Saltman, Duncan, Pevtsova, and Karpenko concerning the index of Weil restrictions of Severi–Brauer varieties related to a project I am working on concerning del Pezzo surfaces (one of my questions was fully resolved, and for another, Tignol pointed me to a construction in his book with Wadsworth, which helped provide an example of the phenomenon I was looking for).

- I also had some great conversations with Bayer-Fluckiger and Duncan about the fields of definitions of exceptional curves on del Pezzo surfaces, motivated by her lecture on cubic surfaces (with Duncan, we figured out the easy cases of del Pezzo surfaces of degree 5 and 6, though it's not clear if this will go anywhere until Bayer-Fluckiger and Serre make their work public).

- I had a long discussion (during the Banff airporter ride from the airport) with Lemire about her work on Schubert varieties on twisted flag varieties, where we came up with a host of interesting questions.

- After my talk, there seemed to be a flurry of attempts to prove the nontriviality of unramified cohomology in degree 3 on the product of three elliptic curves over a finite field (a major open question due to Colliot-Thelene). Both Florence and Chernousov had ideas. Actually, Florence had two ideas. His first idea seemed very promising until Parimala and Suresh found a flaw later in the day, but his second idea (using some of the theory he has developed on local systems) is still potentially viable, though I get the feeling that it will be hard to get him sufficiently interested in the questions again to flush the details out. I am sorry that I never circled back to Chernousov to inquire about his idea, so this is reminding me to write to him (which I just did). Then later in the week, Suresh and I came up with yet another strategy based on the some of the work we did together that I reported on during my talk. We are now working out the details together. If this works out, it will be great!

- However, the most sustained interaction was with Krashen. We spent the majority of Wednesday together (both of us fasting because of the Jewish holiday and therefor not hiking) working on several topics. The first was about constructing some kind of algebraic structure that explains when a central simple algebra over a degree 3 extension has trivial corestriction (analogously to an involution of the second kind over a quadratic extension). Asking Tignol, he pointed to some old work of Haile, which turned out to be relevant but not exactly what we needed. The second was about the problem of splitting Brauer classes by genus 1 curves, which I had spoke about at the last LAG meeting in Banff. I had an idea for proving several new cases, and together with Krashen, we managed to get quite a lot! So far only classes of index up to 5 are known, but we were able to prove it for all indices dividing 60. We are writing up the results now. Also, on Wednesday evening, we found ourselves discussing this question also with Hoffmann, with whom we also realized that the question of whether a quadratic form can be made hyperbolic over the function field of a genus 1 curve is also very interesting, and so likely we will write another paper with the three of us.

- I'm sure there were many other interactions of mathematical content.

- Also, after discussing with Andrei Rapinchuk, I decided to apply for a permanent position at UVA.

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Chapter 24

The Traveling Salesman Problem: Algorithms & Optimization (18w5088)

O

Organizer(s): Joseph Cheriyan (University of Waterloo), Sylvia Boyd (University of Ottawa), Amin Saberi (Stanford University)
la Svensson (Ecole Polytechnique Federale de Lausanne) September 23 - 28, 2018

Overview of the Field

The Traveling Salesman Problem (TSP) is one of the central and well-known problems in combinatorial optimization. It has been a source of inspiration and intrigue for decades. In the words of Schrijver [8, Ch. 58], "it belongs to the most seductive problems in combinatorial optimization, thanks to a blend of complexity, applicability, and appeal to imagination". Also see Vazirani [12] and Williamson & Shmoys [13]. TSP has several applications in planning, logistics, and manufacturing. Slightly modified, it appears as a sub-problem in many other areas, such as genome sequencing.

The problem has been studied intensely for over 60 years. Almost all of the emerging new ideas and techniques in the areas of algorithms and optimization have been applied to the TSP. In turn, these efforts have given rise to important new sub-disciplines such as survivable network design.

Despite the attention paid to this problem, its tractability from the point of view of approximation remains poorly understood. For example, the best known approximation algorithm for the symmetric case is a 3/2-approximation algorithm due to Christofides from 1976. On the other hand, existing results on its hardness of approximation seem to be loose (i.e., far from tight), and there is a substantial gap between upper bounds and lower bounds.

Recent Developments and Open Problems

Over the past decade, deep new ideas have been applied to the TSP and closely related problems, and there have been major recent advances. Many of these advances are based on new and beautiful connections with probability theory, coupled with technically difficult exploitation of methods and structures that are studied in combinatorial optimization.

Oveis Gharan, Saberi, and Singh [7] used properties of strongly Rayleigh measures coupled with an elaborate analysis of the structure of near-minimum cuts to obtain the first improvement on the 3/2-approximation guarantee for a key special case called the graphic TSP. Currently, the best result known on this special case is a 7/5-approximation algorithm of Sebő and Vygen [9] that hinges on a probabilistic lemma of Momke and Svensson [5] coupled with an in-depth and novel analysis of structures that are well known in combinatorial optimization.

At the workshop, there was an evening session on open problems, led by Goemans.

Open problem 1: Find a 4/3-approximation algorithm for symmetric TSP. The integrality ratio of the subtour LP relaxation of TSP is at least 4/3.

An, Kleinberg, and Shmoys [1] improved on a 20-year old 5/3-approximation guarantee of Hoogeveen [4] for the s-t path TSP, which is a variant of the TSP; they use a randomized rounding algorithm, and their improvement uses probabilistic methods coupled with an analysis of near-minimum cuts. Very recently, the combination of results by Traub and Vygen [11] and Zenklusen [14] gave a 3/2-approximation algorithm for this problem. Although the approximation factor of 3/2 matches the known lower bound on the integrality ratio (of a well-known LP relaxation), the analysis does not imply an upper bound on the integrality ratio.

Open problem 2: Prove an upper bound of 3/2 on the integrality ratio of the s-t path TSP.

For the Asymmetric TSP (ATSP), Asadpour et al. [3] gave an $O(\log n/\log\log n)$ approximation algorithm by exploiting a connection to thin trees. This connection was further advanced by Oveis Gharan and Saberi [6], and later by Anari and Oveis Gharan [2]. The latter made very interesting connections to the Kadison-Singer problem and proved an $O(poly \log\log n)$ integrality ratio for the problem. It is conjectured that there is a factor 2 approximation algorithm for the ATSP. A key recent breakthrough comes from a fascinating result of Svensson et al. [10] that finally gave a constant factor approximation for the ATSP. The constant factor achieved in that paper is far from the conjectured lower bound of 2.

Open problem 3: Design and analyze a factor 2 approximation algorithm for ATSP. A more modest goal is an approximation algorithm for ATSP with double-digit approximation ratio.

Despite decades of research by some of the best researchers in algorithms and optimization, there are many other tantalizing open questions. We refer the interested reader to Bill Cook's talk in the workshop (see the video posted on the workshop web page) for a comprehensive list and mention only a few here:

Open problem 4: Determine whether there exists a polynomial-time simplex algorithm for optimally solving the subtour-elimination polytope of the TSP. A related question is to determine if there exists a polynomial-time cutting-plane algorithm for this polytope.

Open problem 5: Design and analyze an algorithm for sampling near-optimal node-separators, similar to Karger's method for sampling near-optimal edge-cuts. Such an algorithm would be useful in identifying structures that could be exploited in the cutting-plane method for the TSP.

Open problem 6: Design an algorithm that given an n-city instance of TSP, finds an optimum solution in time $O^*((2-\varepsilon)^n)$.

Presentation Highlights

Bill Cook gave a plenary talk on "Open Problems on TSP." A plenary talk was given by Jakub Tarnawski on his recent breakthrough result (joint with Svensson and Vegh) on a "Constant-factor approximation algorithm for the Asymmetric Traveling Salesman Problem."

Variations of the TSP problem

Stephan Held presented a talk on vehicle routing with subtours, and Zachary Friggstad gave a presentation on linear programs for orienteering and regret-bounded vehicle routing. Viswanath Nagarajan gave a fascinating talk on Stochastic k-TSP. The stochastic version of the k-TSP assumes independent random rewards at vertices and the objective is to minimize the expected length of a tour that collects total reward at least k. Nagarajan discussed both adaptive and non-adaptive solutions. Katarzyna Paluch presented new approximation algorithms for (1,2)-TSP which is a well-studied variant of the TSP where all distances between cities are either 1 or 2. Tobias Moemke presented a talk on the maximum scatter TSP in doubling metrics. This variation has applications in manufacturing and medical imaging.

Thin trees and Asymmetric TSP

Neil Olver, Shayan Oveis Gharan, and Nima Anari presented the thin tree conjecture, its relationship with the ATSP, and different approaches for solving it. The thin tree conjecture is due to Luis Goddyn, and it implies a constant factor approximation for ATSP; see [3] for details. Olver's talk was on pipage rounding, pessimistic estimators and matrix concentration. Anari and

Oveis Gharan presented their approach using "rounding by sampling," as well as geometric methods for solving a weaker version of the conjecture.

Path TSP

Martin Naegele, Vera Traub, and Jens Vygen gave presentations on recent exciting advances on the path TSP. Naegele gave an excellent presentation of Zenklusen's beautiful 3/2-approximation algorithm for path TSP [14], that resolves an intriguing open problem. Traub presented a remarkable recent result (joint with Vygen) on the graphic special case of the s-t path TSP where they achieve an approximation factor of 1.497, thus beating the 3/2 lower bound on the integrality ratio of the general (i.e., non-graphic) problem.

Andras Sebő presented deep connections between the TSP, the postman problem and matroids.

Related problems

There were several presentations on topics related to network design, scheduling, and integer programming. Tom McCormick presented results on strongly polynomial algorithms for problems related to "parametric global minimum cuts," and Thomas Rothvoss presented results on a matroid version of the Santa Claus problem which is a well-known problem in the area of scheduling.

Scientific Progress Made and Outcome of the Meeting

The schedule of the workshop provided ample free time for participants to work on joint research projects. A number of new research projects were initiated during the workshop, while some other researchers used the opportunity to continue to work on projects started earlier. The research talks and the plenary talks were very well received.

Marcin Mucha and Anupam Gupta collaborated on rounding 1/2-integral points of the Held-Karp linear programming relaxation of the TSP. Inspired by Andras Sebő's talk, they focused on the special case where the underlying graph is a 2-cycle and solved that case.

Shayan Oveis Gharan continued his research project with Nima Anari. They had several new insights and resolved some questions they had about approximation algorithms on problems related to counting bases of matroids. Several talks of the workshop also gave them new directions for future research, such as Ravi's talk.

R. Ravi reports that the talks in the workshop gave him a clear overview of the state-of-the-art techniques in designing approximation algorithms for the TSP. This in turn helped him develop and submit (for funding) a new research proposal based on studying some of these techniques in detail and identifying new open problems.

Viswanath Nagarajan reports that the presentations on directed network design problems at the workshop inspired him to focus on the directed Steiner tree problem and the orienteering problem. After the workshop, jointly with a graduate student, he obtained a simple and tight quasi-polynomial-time algorithm for the directed tree orienteering problem.

Hyung-Chan An reports that during the workshop he was able to engage in valuable discussions with his colleagues. He also reports that Naegele's talk on the path TSP [14] was particularly helpful and inspired some new research ideas.

Vera Traub and Jens Vygen made progress on their TSP book project, by learning new techniques during the talks and by discussions with many other participants in the breakout sessions. For example, during one of the discussions, Michel Goemans found a much shorter proof of a result of Henke-Traub-Vygen that says that certain LP relaxations for ATSP are equivalent.

Following Kent Quanrud's talk on fast algorithms for (approximations of) the Christofides heuristic for TSP, Neil Olver and Quanrud investigated whether they can develop even faster algorithms. They are still in the early stages of this research project and they are optimistic.

During the workshop, Hung Viet Le and Vincent Cohen-Addad discussed several research problems on planar graphs and minor-free graphs. They are now working together on designing a PTAS for one of these problems on planar graphs. They report that the workshop provided an invaluable opportunity to learn the state-of-the-art techniques in approximation algorithms for ATSP.

Tobias Moemke started work on a project with Zachary Friggstad to obtain bounds on the integrality ratio for a specific flow problem. The discussions at the workshop led to fresh ideas worth exploring and might lead to substantial improvements.

Vincent Cohen-Addad, Kamyar Khodamoradi, and Zachary Friggstad began joint work on local search algorithms. Inspired by Vygen's talk, Friggstad and Chaitanya Swamy are focusing on an improved approximation algorithm for a well-known problem related to the TSP.

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Chapter 25

Hessenberg Varieties in Combinatorics, Geometry and Representation Theory (18w5130)

October 21 - 26, 2018

Organizer(s): Patrick Brosnan (University of Maryland), Megumi Harada (McMaster University), John Shareshian (Washington University in St. Louis), Michelle Wachs (University of Miami)

Overview of the Field

The topic of this workshop was Hessenberg varieties, which is an exciting area of research lying in the rich intersection of geometry, combinatorics, and representation theory. These varieties were first introduced by De Mari and Shayman in 1988 in the context of computational linear algebra, and more specifically, for applications to the QR algorithm for finding eigenvalues of a complex matrix. Since then, Hessenberg varieties have become important objects in a variety of research areas. The workshop was a great opportunity for mathematicians in disparate fields to share recent results and consider together various interesting open problems and new directions.

In their greatest generality, building on the ideas of De Mari and Shayman, Hessenberg varieties were defined in a 2006 paper by Goresky, Kottwitz and MacPherson [9] for applications to the computation of the orbital integrals that arise in representation theory. Let G be a reductive algebraic group defined over a field $\mathbb{F}$ and let V be an $\mathbb{F}[G]$-module. Fix $s \in V$, a parabolic subgroup P of G, and a P-invariant subspace M of V. The Hessenberg variety $X(s, M, P)$ is defined to be the set of points gP in the partial flag variety G/P such that $g^{-1}(s) \in M$. In most of the discussion below, P will be a Borel subgroup $B \leq G$, V will be the Lie algebra $\mathfrak{g}$ of G with the adjoint action of G, and $M = \mathfrak{m}$ will be a subspace of $\mathfrak{g}$ containing the Lie algebra $\mathfrak{b}$ of B. We write $X(s, \mathfrak{m})$ in this case.

In what follows, we provide a brief overview of past and current work on Hessenberg varieties. We do not claim to be exhaustive.

First, note that $X(s, \mathfrak{b})$ consists of all cosets gB satisfying $sgB \subseteq gB$. The varieties $X(s, \mathfrak{b})$, also called Springer fibers, received much attention from representation theorists during the 1970s and 1980s in the case where s is nilpotent. A highlight of this activity was Springer's description in [Spe79] of irreducible representations of Weyl groups using actions on the cohomology of $X(s, \mathfrak{b})$.

In the original paper on Hessenberg varieties, De Mari and Shayman analyzed $X(s, \mathfrak{m})$ when $G = \mathbf{GL}_n(\mathbb{C})$ and s is a generic (i.e. regular semisimple). The history of and motivation for this enterprise is discussed by De Mari and Shayman in the introduction to [7]. In the same paper, the Betti numbers for such $X(s, \mathfrak{m})$ are determined for a large class of $\mathfrak{m}$. It turns out that in each case the sum of these Betti numbers is $n!$, the order of the Weyl group S_n. The associated Poincaré polynomial is the generating function for a naturally defined statistic on S_n, determined by $\mathfrak{m}$. These permutation statistics interpolate between two well-studied statistics on S_n, the descent number and the length. Here one can see productive interaction between geometry and combinatorics. It is not obvious a priori that the generating functions for the combinatorial statistics in question should be palindromic and unimodal, but this becomes obvious upon applying the Hard Lefschetz Theorem to the Hessenberg varieties. Additional productive interactions followed.

Key results in [7] were generalized by De Mari, Procesi and Shayman in [6]. There, the authors showed that for arbitrary semisimple G, generic $s \in \mathfrak{g}$ and arbitrary $\mathfrak{m}$, the variety $X(s, \mathfrak{m})$ is smooth, the sum of the Betti numbers of $X(s, \mathfrak{m})$ is the order of the Weyl group W, and the Poincaré polynomial is the generating function for a nice statistic on W.

If s is in the subset $\mathfrak{g}^{\mathrm{rs}}$ of regular semisimple elements, then the centralizer $C_G(s)$ is a maximal torus in G and acts on $X := X(s, \mathfrak{m})$. In [21], Tymoczko showed that this torus action satisfies the conditions necessary for the application of the theory developed by Goresky, Kottwitz and MacPherson in [8]. From this, one obtains a combinatorial description of the equivariant and and ordinary cohomology rings of X in terms of the moment graph of X. Using this description, Tymoczko showed that $H^*(X, \mathbb{C})$ admits a representation of W.

Recent work has allowed the determination of the cohomology representations in question when $G = \mathbf{GL}_n(\mathbb{C})$. Shareshian and Wachs conjectured in [14, 15] that the Frobenius characteristic of the graded S_n-representation $\sum_{j \geq 0} H^{2j}(X, \mathbb{C})t^j$ tensored with the sign character, is the chromatic quasisymmetric function $F_{\mathfrak{m}}(t)$ of a graph determined by $\mathfrak{m}$. The chromatic quasisymmetric functions refine Stanley's chromatic symmetric functions, which are generating functions for proper colorings of graphs. (By setting $t = 1$, one gets the chromatic symmetric function originally defined by Stanley in [17].) The conjecture was proved first by Brosnan and Chow in [3] by studying the sheaves on $\mathfrak{g}$ obtained from the cohomology groups $H^*(X(s, \mathfrak{m}))$ by varying s. (This sheaf is a local system on the set $\mathfrak{g}^{\mathrm{rs}}$, and the attached monodromy representation factors through S_n.) Another completely independent proof was given by Guay-Paquet in [10] who used a beautiful theorem of Aguiar, Bergeron and Sottile on Hopf algebras and quasisymmetric functions. When combined with the Brosnan-Chow-Guay-Paquet (BC-G-P) theorem, combinatorial results of Shareshian-Wachs in [15] and Athanasiadis in [2] provide formulas for both the irreducible decomposition and character values of the cohomology representations.

The BC-G-P Theorem gives the possibility of attacking a longstanding combinatorial conjecture using geometry. The Stanley-Stembridge conjecture in [17] asserts that the symmetric function obtained from $F_{\mathfrak{m}}(t)$ by setting $t = 1$ is e-positive, that is, a nonnegative integer combination of elementary symmetric functions. (This conjecture arose from an equivalent conjecture of Stanley and Stembridge in [18] on immanants.) Shareshian and Wachs conjectured in [14, 15] that in fact the coefficient of each t^j in $F_{\mathfrak{m}}(t)$ is e-positive. Given the BC-G-P Theorem, this is equivalent to the conjecture that the representation of S_n on $H^{2j}(X, \mathbb{C})$ arises from a permutation representation in which each point stabilizer is a Young subgroup. Attempts to settle the Stanley-Stembridge and Shareshian-Wachs Conjectures on e-positivity using this equivalence are ongoing. Connections of all of this work with the representation theory of the type A Hecke algebra are described by Haiman in [7] and by Clearman, Hyatt, Shelton and Skandera in [5].

For generic $s \in \mathfrak{g}$, the varieties $X(s, \mathfrak{m})$ are paved by affines. This is easily seen using the theorem of Bialynicki-Birula, and it is the key to the computation of the Betti numbers in [6]. In her 2003 PhD thesis, Tymoczko generalized this result to all s in the case $G = \mathbf{GL}_n$ and used the result to compute the Betti numbers of all the Hessenberg varieties $X(s, \mathfrak{m})$ for $\mathbf{GL}_n$ [20]. This result, which is a crucial input to [3], was generalized recently by Precup to arbitrary reductive groups (for a large class of elements s) [12]. We note that, while the structure of $H^*(X(s, \mathfrak{m}))$ as a graded vector space is essentially known by the above results of Tymoczko and Precup, the ring structure is still somewhat mysterious. Recently, much work has been done in this direction by H. Abe, Harada, Horiguchi and Masuda [1]. Moreover, Horiguchi, Masada, T. Abe, Murai, and Sato have proved that the following three rings are isomorphic: the cohomology of a Hessenberg variety for regular nilpotent s, the Weyl group invariants of the cohomology of a generic s, and the quotient of the polynomial ring by the ideal coming from the logarithmic derivation module of certain hyperplane arrangements. The isomorphism between the first two rings generalizes Theorem A of [1] where it was first proved for $G = \mathbf{GL}_n$. (Theorem 2.1 of [1] was a major influence on the work of Brosnan-Chow who generalized it in a different direction.)

The varieties considered by Goresky, Kottwitz and MacPherson are smooth for generic s, but are not in general paved by affines even when s is generic. Their cohomology is, however, conjectured to be motivated (in the sense used by Arapura) by hyperelliptic curves; this means that for any such Hessenberg variety X, there should exist a surjective morphism $Y \to X$ where Y is a product of hyperelliptic curves. In particular, the Hodge structure on the cohomology of the Hessenberg varieties considered by GKM is supposed to lie in the full tensor subcategory generated by the cohomology of hyperelliptic curves. This has been proved in an interesting special case by Chen, Vilonen and Xue (CVX) [4]. Moreover, CVX compute the sheaves obtained by varying the element s. This is analogous to the work of Brosnan-Chow. However, while the monodromy of the sheaves considered by Brosnan and Chow factor through the symmetric group, the CVX sheaves have infinite monodromy.

Recent Developments and Open Problems

As already noted, the workshop was an excellent opportunity for interaction between mathematicians with disparate interests and expertise. The workshop was successful in facilitating this interaction.

Some of the most exciting recent developments were already summarized in the previous section. Additionally, the following are some specific open problems, in part motivated by these recent developments, that currently drive this research area. Some of these were brought up during a problem session held during the workshop.

1. There are basic geometric questions about Hessenberg varieties which are still open. For example, during our Open Problems Session, Erik Insko asked to describe the singular locus of $X(N, \mathfrak{m})$ in the important case that N is a regular nilpotent.
2. While the theorem of Brosnan-Chow and Guay-Paquet opens the door for a geometric approach to the Stanley-Stembridge and Shareshian-Wachs Conjectures on e-positivity, this has yet to be carried out successfully.
3. Almost all of the combinatorial and geometric work on the varieties $X(s, \mathfrak{m})$ has been in the Lie type A case. The problem of formulating and proving the right conjectures for other simple Lie algebras is currently wide open. For example, there is no known analogue of the chromatic quasisymmetric function $F_{\mathfrak{m}}(t)$ for other Lie types. There is a natural analogue of the Stanley-Stembridge Conjecture that should be investigated. Work of Stembridge in [19] shows that the most obvious analogue of the more general Shareshian-Wachs Conjecture is false, but it is possible that something of this nature is true in many cases. In particular, in the Open Problem Session, Shareshian asked: when is the Weyl group action on the cohomology of a Hessenberg variety a permutation module?

   In connection with this, we mention that, recently, Hiraku Abe and Naoki Fujita have announced results which can be described as a "Weyl character formula for Hessenberg varieties".
4. The representation of W on the cohomology of $X(s, \mathfrak{m})$ described above is determined by an action of W on the moment graph provided by GKM theory. Except in a few specific cases, notably the case of toric Hessenberg varieties, it is not known if this representation arises from an action of W on the variety itself.

   On the other hand, while e-positivity is known in the toric case one would like to have an explicit basis in the equivariant cohomology groups of the Hessenberg variety which is permuted by the Weyl group. This was the subject of a conjecture stated by Chow in the Open Problems Session: he gave a combinatorially defined subset of the equivariant cohomology (in the type A toric case) which is manifestly permuted by the symmetric group and asked whether or not it forms a basis.
5. While the beautiful results of Chen, Vilonen and Xue compute the motive of GKM Hessenberg varieties in one interesting example, the conjecture that all such smooth varieties have cohomology motivated by hyperelliptic curves still seems very hard. Schoen has defined a numerical invariant τX based on the Mumford-Tate groups of a variety X with the following property: if X is dominated by a product of curves then $\tau X \leq 1$ [13]. It may be interesting to compute τX for GKM Hessenberg varieties as a way of gaining evidence for the conjecture. It would also be interesting to try to come up with a conjectural description of the sheaves obtained from the cohomology groups $H^*(s, M, P)$ by varying s. This is done explicitly by CVX in their special case, where the sheaves give rise to representations of the braid group. Perhaps there is a description of these sheaves analogous to the combinatorial description provided by Brosnan-Chow in their proof of the Shareshian-Wachs conjecture.

Presentation Highlights

To start the week, Dr. Hiraku Abe gave a beautiful overview talk on the subject of Hessenberg varieties, setting the stage for the week to come. His main goal was to convey that Hessenberg varieties are a subject lying at an exciting intersection of geometry, algebra, and combinatorics, and that they can be studied from multiple different perspectives. Delving into more detail, he explained how the study of Hessenberg varieties touches upon subjects such as the representations of symmetric groups, hyperplane arrangements, the Stanley-Stembridge conjecture, Schubert polynomials, toric degenerations, integrable systems, (holomorphic) symplectic/Poisson geometry, and the Toda lattice.

Dr. Julianna Tymoczko discussed some of the state-of-the-art techniques for describing and computing the cohomology and K-theory rings of Hessenberg varieties. Two of the techniques which she discussed were the famous Goresky-Kottwitz-MacPherson theory, as well as some known generalizations of the Tanisaki ideal (which describes the cohomology rings of type A Springer varieties as quotient rings). In addition, she discussed her recent work joint with Erik Insko and Alexander Woo, which gives an explicit formula – in terms of Schubert polynomials – for the cohomology and K-theory class of regular Hessenberg varieties in the cohomology of the flag variety.

Dr. Chow presented his recent results joint with Dr. Brosnan which proved the Shareshian-Wachs conjecture. This is a conjecture which links the famous Stanley-Stembridge conjecture in combinatorics, stating that the chromatic symmetric polynomial X_G of an indifference graph G is e-positive. (In fact, Stanley and Stembridge's original conjecture was stated more generally, but Guay-Paquet reduced it to this case.) In the setting of positivity conjectures of this type, it is natural to ask whether X_G is in fact $\mathrm{ch}\rho$ of a naturally occurring representation ρ, where ch is the standard characteristic map. Shareshian and

Wachs had conjectured several years ago that (essentially) the desired representation is the symmetric group representation on the cohomology ring of a regular semisimple Hessenberg variety defined by Tymoczko. The main result of Dr. Chow's recent work, joint with Dr. Brosnan, is a proof of this Shareshian-Wachs conjecture, and Dr. Chow explained the basic ideas of their proof, the most crucial part of which is the identification of the fixed subspaces of ρ by a Young subgroup with the cohomology of a 'smaller' regular Hessenberg variety.

Dr. Guay-Paquet presented his new insights into the role that Hopf algebras play in the theory of the symmetric group representations on the cohomology rings of regular semisimple Hessenberg varieties, and in particular, can explain certain linear relations arising between q-chromatic symmetric functions. Specifically, he explained that there is a (graded connected) Hopf algebra constructed from Dyck paths, and that there exists a natural graded Hopf algebra map from it to the Hopf algebra of quasisymmetric functions. He then explained how this map agrees with the map considered by Shareshian-Wachs and Brosnan-Chow in connection to the Stanley-Stembridge conjecture.

To start the discussions on the second day, Dr. Martha Precup gave an overview of the known results on the Betti numbers of Hessenberg varieties. She explained how combinatorial formulas for the Betti numbers, given in the language of permutations, can be obtained through strategically chosen affine pavings of Hessenberg varieties. As an example application, she presented her theorem that the Betti numbers of regular Hessenberg varieties are palindromic; this is a property of the Betti numbers which is relevant in the study of the Stanley-Stembridge conjecture. Finally, she presented her joint work with Dr. Harada on the cohomology rings of abelian Hessenberg varieties, which gives inductive formulas for the symmetric group representations which appear. In particular, Dr. Precup explained how this result yields a proof of the graded Stanley-Stembridge conjecture in the abelian case.

Dr. Erik Insko followed with a talk whose theme was the study of the singularities of Hessenberg varieties. Much of this study is based on the foundational work of Tymoczko on paving Hessenberg varieties by affines. Building on this, Insko and Yong described the singular locus of Peterson varieties and showed that it is a local complete intersection. Dr. Insko also sketched the follow-up work of Abe-DeDieu-Galetto-Harada showing that regular nilpotent Hessenberg varieties are also local complete intersections. Finally, Dr. Inkso explained his recent joint work with M. Precup which explores the smoothness and the irreducible components of semisimple (not necessarily regular) Hessenberg varieties for the special case when $h(i) = i+1$. In particular, they are able to show that the only singularities that occur are at the intersections of the irreducible components.

In the afternoon, Dr. Mikiya Masuda told us about his joint work with H. Abe and T. Horiguchi on a presentation, by generators and relations, of the cohomology rings of regular semisimple Hessenberg varieties in type A of the form $h = (h(1), n, n, \ldots, n)$. Dr. Masuda began his discussion by reminding the audience of the well-known Borel presentation for the cohomology rings $H^*(Flags)$ of flag varieties, and also stating that, in general, the ring $H^*(Flags)$ does not surject onto the cohomology of the Hessenberg variety. Dr. Masuda then recalled the framework of Goresky-Kottwitz-MacPherson theory, which describes in an explicit combinatorial fashion the equivariant cohomology of flag and Hessenberg varieties. Using this perspective, Dr. Masuda explained how to construct the necessary 'extra classes' which generate the cohomology ring, and proceeded to derive the correct relations among them.

Building on the above work of Abe-Harada-Horiguchi-Masuda (AHHM) on a generators-and-relations presentation of the cohomology ring of regular nilpotent Hessenberg varieties in type A, Dr. Horiguchi presented his results which interpret the generators in the AHHM presentation as a linear combination of Schubert polynomials.

Dr. James Carrell's talk was about the cohomology and equivariant cohomology groups of varieties X equipped with a faithful action of the Borel subgroup B of SL_2. A beautiful theorem of Carrell and Akyildiz says the following: If X is a smooth, projective complex variety and if B acts on X with a unique fixed point, then the fixed point scheme X^B is just the affine scheme $\mathrm{Spec}\,\mathrm{H}^*X$ associated to the cohomology groups of X (with complex coefficients). Later M. Brion and Carrell used this result along with a deep surjectivity result of D. Peterson to compute the cohomology of regular nilpotent Hessenberg varieties. This result played a large role in many of the talks in the workshop. In particular, part of M. Precup's talk consisted of an extensive generalization of the Brion—Carrell theorem.

In talks delivered on Wednesday, October 24, Andy Wilson, Jim Haglund, and Mark Skandera discussed connections between regular semisimple Hessenberg varieites of type A and various combinatorial phenomena. These connections are realized through examination of the chromatic quasisymmetric functions of unit interval orders, which were conjectured by Shareshian and Wachs, and proved by Brosnan and Chow (also independently by Guay-Paquet) to be (essentially) Frobenius characteristics of representations of symmetric groups on the cohomology of the varieties in question.

Drs. Haglund and Wilson discussed LLT polynomials, which were introduced in a 1997 paper of Leclerc, Lascoux and Thibon. These polynomials play a considerable role in the very active study of Macdonald polynomials. Moreover, certain LLT polynomials are closely related to chromatic quasisymmetric functions. Indeed, the chromatic quasisymmetric function of a unit interval graph is a generating function for proper colorings of the graph with the positive integers, while some LLT polynomials are generating functions for all colorings of unit interval graphs. In addition, there are LLT analogues of key questions about chromatic quasisymmetric functions of unit interval graphs (or, equivalently, representations of symmetric groups on the cohomology of regular semisimple Hessenberg varieties). The longstanding Stanley-Stembridge conjecture, already discussed above, also has an LLT analogue, which states that the LLT polynomials under consideration become nonnegative integer combinations of elementary symmetric functions after a simple linear change of variables.

Dr. Skandera discussed his work with Clearman, Hyatt and Shelton on characters of type A Hecke algebras. In this work, the authors address the problem of evaluating such characters on elements of the Kazhdan-Lusztig basis. This basis is indexed by permutations. The main result of Clearman et al. solves this problem for basis elements indexed by permutations avoiding certain patterns. The key result is a combinatorial formula for character values when the permutation avoids the pattern 312. There is a nice bijection between such permutations in S_n and regular semisimple Hessenberg varieties of type A contained in the flag variety $GL_n(\mathbb{C})/B$. It turns out that knowing the values of the irreducible characters of the Hecke algebra on a Kazhdan-Lusztig basis element C'_w, with $w \in S_n$ 312-avoiding, is the same as knowing the irreducible decomposition of the representation of S_n on the cohomology of the corresponding Hessenberg variety. Clearman et al. obtain their results using combinatorial objects called "descending star networks". These descending star networks inspired some informal discussion among the workshop participants, to be detailed in the next section.

In a pair of coordinated talks, Drs. Satoshi Murai and Takuro Abe explained the broader context of the recent work of Abe-Horiguchi-Masuda-Murai-Sato on Hessenberg varieties and hyperplane arrangements. It was shown by Sommers and Tymoczko that the Poincaré polynomials of certain regular nilpotent Hessenberg varieties admit a factorization, the factors of which are parametrized by certain exponents of the Hessenberg ideal. As Drs. Murai and Abe explained, this can be understood in the broader context of free hyperplane arrangements and the Terao factorization of the Poincaré polynomial of the complements of free hyperplane arrangements. They also explained that the cohomology ring of regular nilpotent Hessenberg varieties can be identified with the Solomon-Terao algebra of the hyperplane arrangement corresponding to the Hessenberg ideal. This allows them to derive several interesting consequences, including a computation of the volume polynomial of the Hessenberg variety; moreover, it was pointed out that it seems natural in this context to expect generalizations of these ideas to Schubert varieties and other related varieties.

Dr. Peter Crooks touched upon a different aspect of Hessenberg theory, namely, in its relation with the theory of integrable systems. Completely integrable systems are Hamiltonian systems which exhibit a maximal number of symmetries (in a sense which can be made precise); the symmetries allow us to reduce the number of variables and to build explicit solutions. Dr. Crooks described recent joint work with H. Abe, in which they show how a famous holomorphic integrable system, the Kostant-Toda lattice, can be related to a family of Hessenberg varieties, using Mischenko-Fomenko theory. This work raises the question of whether, and how, this Abe-Crooks construction can be related or altered to a construction of real integrable systems on single Hessenberg varieties (as opposed to families thereof).

Dr. Ting Xue's talk was based on joint work with K. Vilonen and T-H. Chen, which proves an analogue of the Springer correspondence for the symmetric pair $(\mathrm{SL}(N), \mathrm{SO}(N))$. The result can be applied to the family of Hessenberg varieties over the space $\mathfrak{p}$ of trace-free symmetric $N \times N$ matrices: it shows that the monodromy action factors through the Hecke algebra at $q = -1$. This gives an efficient way to compute the cohomology of Hesssenberg varieties associated to the symmetric pair.

Scientific Progress Made and Outcomes of the Meeting

The small size of the workshop meant that all the participants had the opportunity to interact with one another in substantial ways, and many productive informal conversations took place as a result. Below we describe a small sample of some of the mathematical developments that occurred as a result of these interactions. Two are described in some detail in Section 25 and 25, while Section 25 briefly summarizes additional developments.

Hessenberg varieties over finite fields

Brosnan and Shareshian began work on a conjecture relating point counting for regular semisimple Hessenberg varieties, defined over finite fields, and representations of Weyl groups on the cohomology of such varieties defined over $\mathbb{C}$. To explain the conjecture, we need some preparation. Given a field $\mathbb{F}$, a Hessenberg variety defined over $\mathbb{F}$ is determined by the following data: a reductive algebraic group G defined over $\mathbb{F}$ (and therefore over the algebraic closure $\overline{\mathbb{F}}$); a Borel subgroup B of G; a subspace $\mathfrak{h}$ of the Lie algebra $\mathfrak{g}$ of G that contains the Lie algebra $\mathfrak{b}$ of B and is $Ad(B)$-invariant; and an element x of $\mathfrak{g}$ such that $ad(x)$ has entries in $\mathbb{F}$ with respect to some basis for $\mathfrak{g}$. Note that all of these ingredients other than x can be defined uniformly, independent of $\mathbb{F}$. Indeed, one can choose a root datum and from this, one obtains $G = G_{\mathbb{F}}$, $\mathfrak{g}$, B and $\mathfrak{b}$ by then choosing $\mathbb{F}$. Moreover, $\mathfrak{h}$ is determined by an appropriate choice of negative roots in the associated root system, which does not depend on $\mathbb{F}$. Assume that the root datum and negative roots have been fixed. When $\mathbb{F} = \mathbb{C}$ and $x \in \mathfrak{g}$ is assumed to be regular semisimple, the isomorphism type of the associated Hessenberg variety does not depend on the particular choice of x. Thus, given a prime power q, we may assume that x has been chosen to have coordinates (say, with respect to a Chevalley basis for $\mathfrak{g}$ arising from our root datum) in a ring R of algebraic integers with an ideal I satisfying $R/I \cong \mathbb{F}_q$. Now we can reduce x modulo I and use the resulting x_q to define a Hessenberg variety over $\mathbb{F}_q$.

We have now defined (smooth, projective) regular semisimple Hessenberg varieties $X_{\mathbb{C}}$ and X_q, over $\mathbb{C}$ and $\mathbb{F}_q$ respectively. On the one hand, we can consider Tymoczko's "dot action" representation of the Weyl group W of $G_{\mathbb{C}}$ on $H^*(X_{\mathbb{C}})$, as already mentioned above. On the other hand, wne can count, for each finite extension $\mathbb{F}_{q^r}$ of $\mathbb{F}_q$, the number N_r of $\mathbb{F}_{q^r}$ points on X_q and store this information in the zeta function $Z(X_q;t) := \exp(\sum_{r\geq 1} N_r \frac{t^r}{r})$. According to the the celebrated Weil Conjectures (as proved by Dwork, Grothendieck and Deligne), $Z(X_q;t)$ is determined by the eigenvalues in $\overline{\mathbb{Q}_\ell}$ of the Frobenius map σ_q on the ℓ-adic cohomology of the $\overline{\mathbb{F}_q}$-variety X_q. Moreover, the eigenvalues of σ_q on $H^i(X_q;\mathbb{Q}_\ell)$ are algebraic integers of norm $q^{\frac{i}{2}}$. The connected component T of the identity in the centralizer of x_q under the adjoint action of $G_{\overline{\mathbb{F}_q}}$ is a σ_q-invariant maximal torus. There is a standard bijection between the set of conjugacy classes of such tori and the set of conjugacy classes in W. Pick w in the conjugacy class of W corresponding to the class of T in $G_{\overline{\mathbb{F}_q}}$. Assume that w has order n and fix any isomorphism between the group of n^{th} roots of unity in $\overline{\mathbb{Q}_\ell}$ and the group of complex n^{th} roots of unity. We can now state the conjecture.

Conjecture 1 *Under this identification, the multiplicity of a complex n^{th} root α as an eigenvalue of w in the dot action on $H^i(X_{\mathbb{C}})$ is the multiplicity of $q^{\frac{i}{2}}\alpha$ as an eigenvalue of σ_q on $H^i(X_q;\mathbb{Q}_\ell)$.*

Permutation bases for the dot action

As explained in previous sections, we know from the Brosnan-Chow-Guay-Paquet proof of the Shareshian-Wachs conjecture that, in order to prove the Stanley-Stembridge conjecture, it is sufficient to show that the dot-action representation on the cohomology of regular semisimple Hessenberg varieties is a permutation representation in which each point stabilizer is a Young subgroup. This then motivates the natural question: if it is a permutation representation, then can we explicit build a permutation basis for it?

The work of Harada and Precup on abelian Hessenberg varieties shows that, in these cases, the dot action representation is indeed a permutation representation of the appropriate type. Based on these ideas and the question above, Harada, Precup, and Tymoczko began working on the following problem during the BIRS workshop:

Problem 25.0.1 *Let $h : \{1,2,\ldots,n\} \to \{1,2,\ldots,n\}$ be an abelian Hessenberg function. Find an explicit basis of the cohomology $H^*_T(\mathcal{H}ess(S,h))$ that is permuted by the dot action. In addition, for h an arbitrary Hessenberg function, find an explicit basis of the S_n-invariant subspace of $H^*_T(\mathcal{H}ess(S,h))$ (i.e. the trivial subrepresentation).*

One of the reasons this problem is non-trivial is that the dot action does not permute cohomology bases that satisfy upper-triangular vanishing conditions (which are natural in terms of the Goresky-Kottwitz-MacPherson description of the equivariant cohomology). Thus, any basis permuted by the dot action represents an unusual and interesting new basis for the equivariant cohomology of Hessenberg varieties. Moreover, an explicit such basis will also provide new intuition for proving the Stanley-Stembridge conjecture in the non-abelian case.

As is stated in Problem 25.0.1, our goal has two components: namely, the construction of a complete basis for the full representation $H^*_T(\mathcal{H}ess(S,h))$ in the abelian case, and, a construction of a basis for the S_n-invariant subspace (i.e. the "trivial part of the representation") $H^*_T(\mathcal{H}ess(S,h))^{S_n}$ in the general case. We address these separately below.

We know that GKM theory gives an explicit description of the T-equivariant cohomology $H^*_T(\mathcal{H}ess(S,h))$ using the *moment graph* for the T-action. Specifically, in this theory, an equivariant cohomology class in $H^*_T(\mathcal{H}ess(S,h))$ is obtained by assigning a polynomial in $\mathbb{C}[t_1,\ldots,t_n]$ (satisfying certain conditions) to each vertex of the moment graph, which is a permutation. Given $w \in S_n$, the dot action of w maps the polynomial $f_y(t_1,\ldots,t_n)$ assigned to $y \in S_n$ to $f_{wy}(t_{w(1)},\ldots,t_{w(n)})$.

Tymoczko already has a conjectured method for building an explicit basis, as follows. Let X be a matrix with a single nilpotent Jordan block. In [1] it is shown that the cohomology ring of $\mathcal{H}ess(X,h)$ is isomorphic to the S_n-invariants in the cohomology ring of $\mathcal{H}ess(S,h)$. Moreover, work of Mbirika shows that the cardinality of the set of monomials

$$\{t_1^{\alpha_1}t_2^{\alpha_2}\cdots t_n^{\alpha_n} : 0 \leq \alpha_i \leq h(i)-i \text{ for all } i\}$$

gives the Betti numbers of the Hessenberg variety $\mathcal{H}ess(X,h)$ when X consists of a single nilpotent Jordan block. Braden observed that for each $\alpha = (\alpha_1,\ldots,\alpha_n)$ we obtain a GKM cohomology class p^α by setting

$$p^\alpha_e = t_1^{\alpha_1}t_2^{\alpha_2}\cdots t_n^{\alpha_n} \quad \text{and} \quad p^\alpha_w = t_{w(1)}^{\alpha_1}t_{w(2)}^{\alpha_2}\cdots t_{w(n)}^{\alpha_n}$$

for each permutation w. Moreover, the class p^α is S_n-invariant by definition. Thus, we know that these classes are a set of S_n-invariant cohomology classes. If we restrict to those α with $0 \leq \alpha_i \leq h(i)-i$ for each i there are exactly the expected number of them, in each degree. This leads us to the following concrete conjecture.

Conjecture 2 *The set $\{p^\alpha : \alpha = (\alpha_1,\ldots,\alpha_n),\ 0 \leq \alpha_i \leq h(i)-i \text{ for all } i\}$ forms an equivariant permutation basis for the trivial representations appearing in the dot action representation on $H^*_T(\mathcal{H}ess(S,h))$.*

What remains is to prove that the above set of classes is linearly independent; this is one of the main goals of the project undertaken by Harada, Precup, and Tymoczko.

We now describe the second part of the solution to Problem 25.0.1. In the abelian case, the only nontrivial permutation representation which appear in the decomposition of the dot-action representation are the M^λ's where λ has exactly two parts. Combining Conjecture 2 and the inductive description of Harada and Precup yields the necessary tools for defining an explicit permutation basis in the abelian case. The first step is to decompose the moment graph for the T-action on $H_T^*(\mathcal{H}ess(S,h))$ in order to obtain a decomposition analogous to the one given by Harada and Precup. We begin by defining a subset of permutations associated to each maximum independent subset of vertices in Γ_h denoted by W_V for $V \in I_2(\Gamma_h)$. The work of Harada and Precup proves $W_V \simeq S_{n-2}$ and that the induced subgraph of the moment graph corresponding to W_V can be identified with the moment graph for the smaller Hessenberg variety $H_T^*(\mathcal{H}ess(S,h_V))$.

The next important step is to define a permutation basis of equivariant cohomology classes in $H_T^*(\mathcal{H}ess(S,h))$ using this inductive structure. Indeed, as in the case of the trivial part of the representation as discussed above, we already have a candidate basis for the permutation representations corresponding to partitions of at most two parts. What remains to be shown is that this basis is linearly independent, and is also linearly independent when considered together with the permutation basis for the trivial representations given in Conjecture 2 above. Although computations of this form can be non-trivial, the Lie theoretic tools developed by Harada and Precup give us new tools with which to attack this problem.

Harada, Precup, and Tymoczko will work on this problem in June-July 2019 through their participation in the MSRI Summer Research for Women in Mathematics program.

Other interactions

One idea for further study, discussed at the workshop by Skandera and Shareshian, is to try to define analogues of the "descending star networks", discussed by Dr. Skandera in his talk, for Weyl groups other than symmetric groups. Regular semsimple Hessenberg varieties are defined in all Lie types. The main obstacle to developing a combinatorial approach to such varieties is the lack of an analogue to the chromatic quasisymmetric function. One can hope that appropriately defined descending star networks will stand in for chromatic quasisymmetric functions in the development of such an approach. In addition, such networks might shed light on connections between Hessenberg varieties and Hecke algebra representations in arbitrary Lie type.

In another development, Dr. Tymoczko asked during the meeting whether or not every Schubert variety in the flag variety is a Hessenberg variety. Since the meeting, Drs. Shareshian and Precup, together with their collaborator Dr. Laura Escobar, have shown that this question has a positive answer in Lie type A.

Finally, based on Dr. Horiguchi's presentation on his work relating Schubert classes and the elements f_{ij} defining the ideal in the AHHM presentation of the cohomology rings of regular nilpotent Hessenberg varieties, Martha Precup gave an conjecture for an explicit formula – in terms of Schubert classes – for these generators f_{ij}. The advantage of Dr. Precup's conjecture over the known formula is that, firstly, it would generalize to other Lie types, and secondly, it gives an interpretation of the relations f_{ij} in terms of Schubert calculus. If her conjecture can be proven, it would open the door for more investigations into the relationship between Schubert calculus and the cohomology rings of Hessenberg varieties.

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Chapter 26

WOA: Women in Operator Algebras (18w5168)

November 4 - 9, 2018

Organizer(s): Sara Arklint (University of Copenhagen), Astrid an Huef (Victoria University of Wellington), Karen Strung (Radboud Universiteit), Dilian Yang (University of Windsor)

Overview

This report summarizes the organization and scientific progress made at the first workshop for women in operator algebras at the Banff International Research Station in Banff, Canada. The main purposes of the workshop were

1. for women in operator algebras to conduct cutting-edge collaborative research, and
2. to build a network of women working in the field to drive future research collaborations and to alleviate the commonly reported feeling of isolation.

We think that we have achieved both of these aims by using the format from the BIRS workshops "Women in Numbers" where the focus is on research in groups on current problems.

Our workshop had 8 groups, each led by 1 or 2 researchers. Prior to the workshop, the leaders designed a broad outline of a research project, and provided background reading and references for their group. On the first day of the workshop each group briefly outlined the research project they would be working on, and on the last day each group reported on progress made and future directions for the work. See Section 26 below for a report from each group. Several of the groups are planning to meet again this year or are preparing articles for publication.

The workshop had 37 participants from 15 countries (Australia, Brazil, Canada, China, France, Germany, India, Israel, Italy, Korea, Denmark, Netherlands, New Zealand, USA, UK). Unfortunately, 5 woman had to cancel at the very last moment due to visas not being issued, caring responsibilities or illness.

To avoid inviting only researchers we already knew well, we initially invited 28 participants, and then filled the remaining places via an application process. The participants initially invited included the project leaders and researchers whose expertise would enable progress on the projects. The call for applications was very broad via social media; email lists for women in mathematics, women in operator algebras and related fields; e-mail lists for major conferences of interest to operator algebraists. We requested a CV, ranked preferences of 2–3 projects of interest, and a short statement about how their expertise fit with the projects and how they would benefit from participating.

Outcomes of the workshop

The immediate outcomes of the workshop include several new collaborations, a new network of women in operator algebras supported by a website[1] hosted by the Association for Women in Mathematics (AWM) and articles in preparation. Several

[1] https://awmadvance.org/research-networks/woa/

groups reported that they are planning to meet again this year and one group reported that they are preparing a journal article for publication (see the reports from the groups in Section 26 below). The feedback from the participants via an AWM survey and testimonials was overwhelmingly positive (see Section 26).

Scientific progress made: reports from the research groups

The study of operator algebras is a very active branch of functional analysis dealing with problems that are intrinsically infinite-dimensional. Such problems arise in quantum mechanics where, for example, a famous theorem of von Neumann says that the only solutions of Heisenberg's commutation relations are families of operators on an infinite-dimensional Hilbert space. Operator algebras have a rich and remarkably rigid structure, and there is a powerful general theory which makes this precise and applicable. Over the past few decades, operator algebras have influenced diverse areas of mathematics, including number theory, harmonic analysis, knot theory, dynamical systems and ergodic theory.

During the workshop, our groups worked on current research problems in the field. Each group's work is reported below.

Cartan subalgebras of twisted groupoid C^*-algebras

Group members

Anna Duwenig (University of Victoria), Elizabeth Gillaspy (group co-leader, University of Montana), Rachael Norton (Northwestern University), Sarah Reznikoff (group co-leader, Kansas State University), Sarah Wright (Fitchburg State University).

Research synopsis and progress

Let A be a C^*-algebra and let $B \subseteq A$ be a Cartan subalgebra. That is, B is a maximal abelian sub-C^*-algebra of A that contains an approximate unit for A, such that there exists a faithful conditional expectation from A onto B, and the normalizer of B generates A as a C^*-algebra. In 2008, building on earlier work of Kumjian [27], Renault proved [46] that every Cartan pair (A, B) is of the form $(C_r^*(G; \Sigma), C_0(G^{(0)}))$, where $C_r^*(G; \Sigma)$ denotes the reduced C^*-algebra of a twisted, topologically principal, Hausdorff étale groupoid $(G; \Sigma)$, and $G^{(0)}$ denotes the unit space of G. (A groupoid G is a generalization of a group, in which every element has an inverse but multiplication is not globally defined. Thus, each $g \in G$ has two associated units, namely, its source $s(g)$ and its range $r(g)$. Two elements $g, h \in G$ can be multiplied if and only if the source of g equals the range of h. When the only elements in G with $s(g) = r(g)$ are the units themselves, we say G is principal; we say G is topologically principal if G comes equipped with a topology such that the set $\{u \in G^{(0)} : s(g) = r(g) = u \Rightarrow g = u\}$ is dense in $G^{(0)}$.)

However, even if G is not topologically principal, the twisted groupoid C^*-algebra $C_r^*(G; \Sigma)$ may have Cartan subalgebras. This is the case for the rotation algebras A_θ, for example, which can be realized as a twisted group C^*-algebra, $A_\theta \cong C_r^*(\mathbb{Z}^2; c_\theta)$. For any group G, we have $G^{(0)} = \{e\}$, so if G is nontrivial then G cannot be topologically principal. Despite this, other descriptions of the rotation algebras enable one to check that $C_r^*(\mathbb{Z}) \cong C(\mathbb{T})$ is a Cartan subalgebra in A_θ.

The goal of this project is to identify Cartan subalgebras of twisted groupoid C^*-algebras when the groupoid in question is not topologically principal. In the untwisted case, a similar question was investigated by Brown et al. in [13]. Inspired by the Cartan pair $(A_\theta, C(\mathbb{T}))$, we have identified sufficient conditions on a subgroupoid S of a twisted groupoid $(G; \Sigma)$ that ensure $C_r^*(S; \Sigma|_S)$ is a Cartan subalgebra of $C^*(G; \Sigma)$. When restricted to the case of a trivial twist, our theorem recovers [13, Corollary 4.4].

Benefits of the WOA format

The ten-minute presentations given on the first day were extremely beneficial to our group; we recruited a new group member on the strength of that presentation.

Another of our group members was able to join the project thanks to the pre-conference application process. Obtaining her group assignment three months in advance of the workshop gave this team member enough time to familiarize herself with groupoids and Cartan subalgebras, which were new topics for her. This consequently enabled her to contribute to the research during the week at BIRS.

Future plans

Although we proved our main theorem during the week at BIRS, there are still many open questions which we plan to explore, such as the uniqueness of the subgroupoid S and/or the Cartan subalgebra that it generates. Several of these questions are also still open in the untwisted case. We are planning to meet at Northwestern University for a week in May 2019 to continue working on this project, and we will also apply to MSRI's Summer Research Program for Women in the hopes of spending two weeks in July 2019 working on this project at Berkeley.

Index theory and K-theory with applications to arithmetic groups

Group members

Sara Azzali (University of Potsdam), Sarah Browne (The Pennsylvania State University), Maria Paula Gomez Aparicio (group co-leader, Université Paris-Sud 11), Lauren Ruth (Vanderbilt University), Hang Wang (group co-leader, East China Normal University).

Format

Since we had formed a group before the BIRS workshop, on arrival we all introduced ourselves and discussed our connections to the potential research avenues on connections between K-theory, the Baum–Connes conjecture and representation theory. From these discussions we decided on a format which involved us all giving talks connected to the topic (we list the titles and abstracts below). On the first day we presented our plans to the others at the conference. This generated a lot of interest. In particular, Jacqui Ramagge gave us a guest talk on connected joint work by herself, G. Robertson and T. Steger.

Sara Azzali, Discrete groups, counterexamples to the Baum–Connes conjecture, and a localised assembly map

We describe the counterexamples to the Baum–Connes conjecture with coefficients, given by Higson, Lafforgue and Skandalis in [22]. We follow Puschnigg's Bourbaki seminar [42] and focus on the case of discrete groups Γ. The counterexamples are based on the different behaviour of the left and right hand sides of the Baum–Connes map with respect to exact sequences of Γ-algebras: the left hand side is exact in the middle, whereas the right hand side can fail exactness. The discrete group Γ in the counterexample is the so called Gromov "Monster group", in whose Cayley graph one can suitably embed an expander graph.

In the second part of the talk, we report on joint work with P. Antonini and G. Skandalis where we use KK-theory with coefficients in $\mathbb{R}$ to study discrete group actions on C^*-algebras and to give a localised form of the Baum–Connes conjecture [3]. We start with the definition of (equivariant) KK-theory with coefficients in $\mathbb{R}$, which is constructed by means of an inductive limit over II_1-factors [2]. We see how the standard group trace defines a class $[\tau] \in KK^{\Gamma}_{\mathbb{R}}(\mathbb{C},\mathbb{C})$ which is shown to be an idempotent. The image of $[\tau]$ acting on $KK^{\Gamma}_{\mathbb{R}}(A,B)$ by exterior product is called the "τ-part" of $KK^{\Gamma}_{\mathbb{R}}(A,B)$. A Baum–Connes type morphism μ_τ is naturally defined between the τ-parts of the usual left and right hand sides of the Baum–Connes map (where on the right hand side the τ acts via descent). One can show that the τ-form of the Baum–Connes conjecture is weaker[2] than the classical one, but the injectivity of μ_τ still implies the strong Novikov conjecture.

Sarah Browne, E-theory and the Baum-Connes conjecture

We introduced the notion of E-theory and gave properties and understood the relations with both K-theory and KK-theory. After we gave a definition of equivariant E-theory in the papers of Guentner-Higson-Trout [20] and Guentner-Higson [23] and talked about the technicality of composition of elements. There after we described the Baum-Connes conjecture in terms of E-theory and in particular with coefficients to relate to crossed product C^*-algebras. The talk finished with a connection to the speakers' current joint work which may be useful for future avenues.

Maria Paula Gomez Aparicio, Property (T) as an obstruction to prove the Baum-Connes conjecture

The Baum-Connes conjecture gives a way of computing the K-theory of the reduced C*-algebra of a locally compact group. This C*-algebra encodes the topology of the temperate dual of the group and its K-theory is a topological invariant of this topological space. This conjecture, and some generalizations, are still open for some groups having property (T) (e.g $SL_3(\mathbb{Z})$), a rigidity property on groups representations. In this workshop I explained how property (T) appears as an element in the maximal C*-algebra of the group and how it prevents the use of the Dirac-dual Dirac method to succeed. I also explained why a stronger version of property (T) is an obstruction to all the methods that have been used so far to prove the conjecture and that a direction that is still open concerns applying the ideas of Bost, who defined a version of Oka principle in Noncommutative Geometry. Indeed, for higher rank Lie groups, there is a statement that says that proving the Baum-Connnes conjecture is equivalent to prove a Bost's kind of Oka principle for some group algebras. References included [11], [10], [26], [30], [31].

[2](more precisely, it is verified by a Γ-algebra A if the classical Baum–Connes is verified by $A \otimes N$ for every II_1-factor N with trivial Γ-action)

Lauren Ruth, Von Neumann dimension and lattices in algebraic groups

First, we give background on discrete series representations and lattices in algebraic groups. Then we explain the coupling constant, or von Neumann dimension, and how it measures the size of the commutant of a finite factor. Importantly, representations of II_1 factors are classified up to unitary equivalence by their von Neumann dimension, which assumes a continuum of values. In the main part of the talk, we explain a theorem that has its roots in Atiyah's work on L^2-index in [8], which was used by Atiyah and Schmid to realize discrete series representations in [9]; another proof is given in [19]. Let G be a simple algebraic group, with trivial center and no compact factors, having square-integrable irreducible unitary representations; let $(\pi, \mathcal{H})$ be such a representation of G; and let Γ be a lattice in G. The theorem states that the restriction of π to Γ extends to a representation of the II_1 factor $R\Gamma$ on $\mathcal{H}$, and this representation of $R\Gamma$ has von Neumann dimension $\mathrm{d}_p i \cdot \mathrm{vol}(G/\Gamma)$, where d_π is the formal dimension of $(\pi, \mathcal{H})$. We conclude by discussing two results from our dissertation, [47]: calculating the formula in a $\mathfrak{p}$-adic setting by dealing carefully with Haar measure, and obtaining representations of II_1 factors on spaces of automorphic functions.

Hang Wang, Elements in the Baum-Connes assembly map

We introduce for a locally compact second countable group, the universal example of proper actions, the equivariant K-homology and the precise definition the Baum-Connes assembly map. We describe in details the examples of finite groups, free groups, fundamental group of Riemann surfaces, where the Baum-Connes conjecture is true. Using the fact that $SL(2, \mathbb{Z})$ is the $\mathbb{Z}/2$-amalgamated product of $\mathbb{Z}/4$ and $\mathbb{Z}/6$ we are able to label the precise map of the Baum-Connes isomorphism for $SL(2, \mathbb{Z})$, and the generators all come from finite dimensional representations. For $SL(3, \mathbb{Z})$, the difficulty is that we no longer have a nice amalgamated product structure as in $SL(2, \mathbb{Z})$. Therefore, infinite dimensional representations of the group have to be investigated in order to understand the generators of K-homology and K-theory associated to those representations. The references we used here are Valette's "Introduction to Baum-Connes conjecture" Chapters 5, 6 and Natsumi's paper in year 1985 calculating K-theory of the group C^*-algebras of $SL(2, \mathbb{Z})$.

Jacqui Ramagge, Property (RD) for $\tilde{A}_2$-groups, including cocompact lattices in $SL_3(Q_p)$

We proved property (RD) for $\tilde{A}_2$-groups using a geometric argument to prove a Haagerup inequality. That is, we showed that the the operator norm of a group element under the left regular representation on $\ell^2(\Gamma)$ is polynomially bounded by the two-norm of the element, where the polynomial is a function of the length of the element with respect to a length function on the group. We began by giving a geometric reinterpretation of the proof of result of Haagerup on free groups from [21]. By adding one extra idea, we then generalised this to a result on $\tilde{A}_2$-groups as in [45]. By the results of Lafforgue in [29], this proves the Baum-Connes Conjecture for $\tilde{A}_2$-groups.

Outcomes

From all of the discussions and talks for the first half of the week, we then came up with some questions to tackle and ways to attack these together. The project now has a clear structure and we hope to meet again in Shanghai in June 2019.

Semigroup C^*-algebras and simplicity

Group members

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Description of project and outcomes

The project took aim to investigate simplicity of the boundary quotient C^*-algebra $\mathcal{Q}(S)$ associated to a right LCM semigroup with identity (right LCM monoid) S. Simplicity of $\mathcal{Q}(S)$ is proved in [51, Theorem 4.12] under additional assumptions imposed so as to use the characterization of simplicity of étale Hausdorff groupoid C^*-algebras from [12]. We have that $\mathcal{Q}(S)$ is constructed as the tight groupoid C^*-algebra of an inverse semigroup, which should correspond to a "reduction groupoid" of the left inverse hull $I_l(S)$ whose C^*-algebra $C^*(I_l(S))$ models the universal semigroup C^*-algebra of S, see for example, [34, Theorem 5.17].

We started investigating the proof of simplicity from [51, Theorem 4.12], and in particular the construction of the tight groupoid from S. Then we moved on to understand how the conditions on S securing the Hausdorff property can be relaxed if we instead invoke the recent simplicity result for non-Hausdorff groupoids from [15], see in particular their Theorem 4.10.

One reason why it would be interesting to explore this more general, non-Hausdorff universe, is that for arbitrary right LCM monoids without right cancellativity one does not expect their tight groupoids to be Hausdorff. For the class of right LCM semigroups arising from self-similar actions, there is a very interesting simplicity result in [15, Theorem 5.21] which identifies ω-faithful as condition for simplicity of the reduced groupoid C^*-algebra. This should admit useful generalizations.

Our efforts during the workshop concentrated on understanding the various ingredients that go into the construction of $\mathcal{Q}(S)$, and the new subtle points that go into the proof of simplicity from [15]. We have agreed on a plan to move forward with our project. We are grateful to Lisa Orloff Clark who joined our group one morning and gave a short, expert lecture on her recent work in [15].

Quantum majorization in infinite-dimensional Hilbert Space

Group members

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Project description

The research project related to an open problem in quantum information theory (QIT). In QIT, a quantum system is described by a Hilbert space $\mathcal{H}$. The predual of $\mathcal{B}(\mathcal{H})$, the set of all bounded linear operators acting on $\mathcal{H}$, is the ideal of trace class operators $\mathcal{T}(\mathcal{H})$, i.e., $\mathcal{T}(\mathcal{H}) = \mathcal{B}(\mathcal{H})_*$. Note that if $\mathcal{H}$ is finite dimensional, then $\mathcal{T}(\mathcal{H}) = \mathcal{B}(\mathcal{H})$. The study of quantum states and quantum channels is central in QIT. Quantum states, also called density operators, are positive (semi-definite) trace-one operators $\rho \in \mathcal{T}(\mathcal{H})$. We will focus on bipartite states: let $\mathcal{H}_A$ and $\mathcal{H}_B$ be two Hilbert spaces and $\rho^{AB} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ be a state. For two Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$, a quantum channel $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is a completely positive, trace preserving (CPTP) linear map.

Entanglement is one of the key resources that sets QIT apart from its classical counterpart. It is therefore important to quantify this resource, and particular attention is paid to when it is maximal. It should be noted that maximally entangled states do not exist in infinite dimensions as the Schmidt coefficients are an infinite set of nonnegative numbers summing to one, which has no minimal element with respect to majorization, whereas maximally entangled states are minimal elements with respect to majorization in finite dimensions.

Majorization has become an important tool in QIT since Nielsen's theorem (1999) which states that a pure state $|\psi_1\rangle$ shared by two parties can be transformed by LOCC into another state $|\psi_2\rangle$ (that is, $|\psi_1\rangle$ is at least as entangled as $|\psi_2\rangle$) if and only if $\lambda_{\psi_1} \prec \lambda_{\psi_2}$, where λ_{ψ_1} and λ_{ψ_2} are the Schmidt coefficient vectors of $|\psi_1\rangle$ and $|\psi_2\rangle$, respectively, and $\prec$ denotes majorization. This result has become a springboard for various generalizations giving rise to related comparison relations in various contexts.

Many results in QIT are given in the context of bounded operators acting on finite-dimensional Hilbert spaces, and as such these results reduce to results about matrices. The context of infinite-dimensional Hilbert space is of interest to e.g. theoretical physicists, so if a result can be generalized to infinite dimensions it is of interest to do so. Solutions to such open problems are often of independent interest from a pure math standpoint. There are questions of closure and convergence that need to be addressed, issues related to the existence of certain objects in infinite dimensions, and gaps in the literature. In particular, generalizing the various versions of the majorization relation to infinite-dimensional Hilbert space is more than merely incremental in nature. The techniques used during the week relied heavily on operator theory, including comparisons of various norms, and the understanding of small but important details about tensor products of trace-class operators.

Unfortunately, due to a variety of factors (visa issues, family issues, etc.) I. Beltita, P. Ganesan, L. Ismert, and S. Srivastava could not attend. Genesan was able to meet via video chat for a few hours each day, so she was able to be involved remotely. Originally seven group members, the group wound up being three present at BIRS, plus an additional member (Ganesan) via Skype. This setup had its advantages and disadvantages. By the end of the week, we had identified a number of major issues that need to be addressed before attempting to solve the main open problem, and we developed a clear picture of what approach to use.

Twisted Steinberg algebras

Group members

Becky Armstrong (University of Sydney), Lisa Orloff Clark (group leader, Victoria University of Wellington), Kristen Courtney (University of Münster) , Ying-Fen Lin (Queen's University Belfast), Kathryn McCormick (University of Minnesota) and Jacqui Rammage (University of Sydney).

Description of project and outcomes

Jean Renault introduced the notion of a twisted groupoid C^*-algebra in his 1980 thesis and these C^*-algebras have been used in a variety of contexts over the years. Non-twisted groupoid C^*-algebras are themselves a broad class of algebras that includes a number of interesting subclasses, like graph and higher-rank graph C^*-algebras. The class of twisted groupoid C^*-algebras is even broader and there are a few results in particular highlighting this.

Results of an Huef, Kumjian and Sims [24, Theorem 5.2] say that every Fell algebra is isomorphic to a twisted groupoid C^*-algebra. More generally, Renault shows in [46, Theorem 5.9]: If a C^*-algebra contains a Cartan subalgebra, then it is isomorphic to a twisted groupoid C^*-algebra. This result, along with recent progress in the classification program, has placed twisted groupoid C^*-algebras at the forefront of C^*-algebraic research.

In this project, we considered ample groupoids, which are étale groupoids that have a basis of compact open sets. In this case, sitting inside of the groupoid C^*-algebra is a dense subalgebra called the Steinberg algebra [52]. As an analogy, the Steinberg algebra sits inside the groupoid C^*-algebra like the algebra generated by a Cuntz-Krieger family (no closure) sits inside the graph C^*-algebra. Steinberg algebras are gaining popularity as they 1. give rise to a lot of interesting purely algebraic examples and 2. give insight into groupoid C^*-algebras in surprising ways.

Up until now, twisted Steinberg algebras have not been considered. Our first task was to define twisted Steinberg algebras. We took into account the various notions of twisted groupoid C^*-algebras in the literature, and formulated a unified treatment in the purely algebraic setting. From there, we began considering the an Huef-Kumjian-Sims result and Renault's result and are making progressing on proving a purely algebraic version.

Our group will reconvene for 2 weeks in March 2019 at the University of Sydney to continue work on this project.

Quantum principal bundles and their C*-algebras

Group members

Francesca Arici (group leader, Max Planck Institute for Mathematics in the Sciences), Erin Grisenauer (Eckerd College), Chiara Pagani (group leader, Università del Piemonte Orientale).

Noncommutative fiber bundles and spaces

This is project lies at the interface of two important research directions in operator algebra: the theory of C^*-algebras, and Connes' approach to noncommutative geometry (NCG), including the algebraic approach to quantum groups.

The focus of this project is the study of noncommutative spaces and principal bundles over them, starting from the analysis of relevant examples in the literature, with the aim of giving a C*-algebraic description of such objects.

In the purely algebraic setting, a principal bundle over a noncommutative space B consists of an algebra extension $B \subseteq A$ of the algebra B which is H-Galois with respect to a certain Hopf algebra H. The base space B is the subalgebra of (co)invariant elements for the coaction of H on A.

It is less clear how to describe a principal bundle in the C^*- algebraic context. Deepening our knowledge about bundles in the analytic framework is one of the goals of this research project.

Some partial results in this direction were obtained in [7, 6], where the authors described quantum principal circle bundles in terms of Cuntz–Pimsner algebras [41] of self-Morita equivalence bimodules. Prototypical examples of this construction are the inclusions $C(\mathbb{CP}^n_q) \subseteq C(S^{2n+1}_q)$, as well as more general algebra extensions coming from $U(1)$-actions, such as those involving weighted lens and projective spaces [14].

Inspired by these results, we look for a C^*- algebraic characterisation of quantum principal bundles with non-Abelian structure group, inspired by [38]. Current work in progress in a parallel project by the first author suggests that the setting of subproduct systems [49, 57] will help describing Hopf–Galois extensions at the C^*- algebraic level. A relevant class of fundamental examples to be studied are deformations of the $SU(2)$)-Hopf bundle.

A C^*-algebraic version of the symplectic instanton bundle

The q-deformed instanton bundle $\mathcal{O}(S^4_q) \subseteq \mathcal{O}(S^7_q)$ of [32] is an important example of a Hopf–Galois extension which is genuinely noncommutative, in that the structure group is Woronowicz's quantum $SU(2)$ and the total space is a quantum homogeneous spaces of symplectic quantum groups. The total space of this bundle is the symplectic seven-dimensional sphere S^7_q, which is obtained as a quantum homogeneous space for symplectic quantum groups.

During the first days of the WOA week, we have recalled the classical construction of projections that described the modules of sections of the associated vector bundles coming from the representations of $SU(2)$, in order to address the analogous computation for the symplectic sphere S^7 and the corepresentations of the quantum group $SU_q(2)$. These corepresentations are labelled by integers. The projection $\mathfrak{p}_{(1)}$ for the module of sections of the associated bundle coming from the fundamental corepresentation $\mathcal{E}_1$ was constructed in [32].

We have performed lengthy explicit computations and were able to construct the projection $\mathfrak{p}_{(2)}$ for the module $\mathcal{E}_2$, i.e., the module of sections of the associated bundle coming from the weight two corepresentation. In order to do so, we were lead to introduce a suitable ten-dimensional vector subspace of $\mathbb{C}^4 \otimes \mathbb{C}^4$ that can be thought of as a quantum analogue of the second symmetric power of $\mathbb{C}^4$, and that we have denoted by $Sym^2_q(\mathbb{C}^4)$.

Future plans and open questions

1. We plan to construct higher q-symmetric powers of $\mathbb{C}^4$ as maximal standard subproduct systems of Hilbert spaces with prescribed fibres $\mathbb{C}$, $\mathbb{C}^4$, $Sym^2_q(\mathbb{C}^4)$ in the sense of [49, Sec. 6.1]:

$$Sym^n_q(\mathbb{C}^4) = \bigcap_{i+j=n} Sym^i_q(\mathbb{C}^4) \otimes Sym^j_q(\mathbb{C}^4).$$

   To any such product system, one can associate a Cuntz–Pimsner like algebra, as described in [57]. We expect to be able to interpret the resulting algebra as the C*- algebra of the noncommutative symplectic seven-sphere, much as the C*-algebra of the standard symmetric product system over $\mathbb{C}^4$ is the commutative C*- algebra $C(S^7)$.

2. Motivated by the study of $SU(2)$-gauge theories, a parallel goal is that of inductively constructing all projections $\mathfrak{p}_{(n)}$ for $n \geq 2$, possibly giving a unified description, using the higher symmetric tensor powers defined in the previous point. Since the projection $\mathfrak{p}_{(n)}$, is determined by the quantum analogues of the totally symmetric n-th tensors products of ψ_1, ψ_2. We expect powers of q to appear in their expression.

One should observe that, in principle, one could also construct the modules $\mathcal{E}_n$ as maximal standard subproduct systems of Hilbert C*- modules over $C(S^4_q)$ with prescribed fibres $C(S^4_q)$, $\mathcal{E}_1$, $\mathcal{E}_2$. This, however, does not immediately yield the projections, therefore we plan to adopt the more explicit approach described in the two previous points.

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Nuclearity of C^*-algebras of quasi-lattice ordered groups

Group members

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Description of project and outcomes

A C^*-algebra A is <u>nuclear</u> if for every C^*-algebra B there is a unique C^*-norm on the algebraic tensor product $A \odot B$. Nuclearity is an important hypothesis of the classification program for C^*-algebras, and so it is important to be able to decide if a C^*-algebra is nuclear. For example, the C^*-algebra of a group is nuclear if and only if G is amenable.

The question of when the C^*-algebra of a semigroup is nuclear also has deep connections with notions of amenability. In [33, Theorem 6.1] Li studied a subsemigroup P of a discrete group G. He showed, under some hypotheses, that the full C^*-algebra $C^*(P)$ of P is nuclear if and only if, whenever a C^*-algebra A admits an action of G, the reduced and full crossed products of A by the semigroup P are isomorphic. Li's theorem applies, for example, to the quasi-lattice ordered groups (G, P) introduced by Nica in [39]. The project was to find sufficient and checkable conditions for the Toeplitz algebra $C^*(P)$ of a quasi-lattice ordered group to be nuclear.

The existence of generalised length functions, called "controlled maps", from G to an amenable group K is sufficient to ensure that (G, P) is amenable [28, 16, 25]. Given the deep connections between amenability and nuclearity, it seemed reasonable to explore this circle of ideas for nuclearity as well. Indeed, [55] used ideas from [33, Theorem 6.1] to show that a C^*-algebra of a doubly quasi-lattice ordered groups admitting such a controlled map is nuclear.

The Toeplitz algebra is also the C^*-algebra of a Fell bundle extended from P. Properties of controlled maps into $(\mathbb{Z}, \mathbb{N})$ were implicitly used in [48] to prove that Fell bundles extended from free semigroups and from Baumslag–Solitar semigroups are amenable. So it is natural to ask how we might deduce nuclearity of Toeplitz algebras from the amenability of those Fell bundles.

By [50, Example 2.2] every (G, P) gives a category of paths $\Lambda = \Lambda(G, P)$. Spielberg associated a groupoid $\mathcal{G}_\Lambda$ to a category of paths in such a way that C^*-algebra of $\mathcal{G}_\Lambda$ is isomorphic to $C^*(P)$ [50, Theorem 6.3]. So it is possible that nuclearity could be deduced from the results in [50, §9]. To this end, we wanted to know if a "controlled map" of [25, Definition 3.1] satisfies the hypotheses of [50, Theorem 9.8].

During the week at Banff we explored the above strategies and made significant progress. We currently have one paper in preparation and ideas for another.

Generalized Crossed Products

Group members

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Description of project and outcomes

The crossed products C^*-algebras by group actions have long been a source of interesting and elegant examples in the theory of C^*-algebras. One of the most well-studied cases is the case of the crossed product of $C(X)$, for X a compact metric space, by an action of the integers (which is, necessarily, determined by a single automorphism). One reason that these crossed products have been so valuable as examples is that while they are are in some ways complicated, they also have a lot of concrete structure.

There are some interesting generalizations of this construction, one of which is to take a crossed product by a Hilbert A-A-bimodule [1]. This is a generalization in the sense that every crossed product by an action of $\mathbb{Z}$ has a natural $\mathbb{Z}$-grading which allows one to express the crossed product using bimodules instead. In the broadest possible terms, our project is to study structural properties of these generalized crossed products. Of particular interest are those generalized crossed products which are simple, as this allows us to make links to the Elliott classification program. Groupoid C^*-algebras arising from minimal principal étale groupoids provide a different approach to generalizing crossed products of commutative C^*-algebras by the integers. Indeed, the orbit equivalence relation of a minimal dynamical system gives rise to such a C^*-algebra, which is isomorphic to the crossed product.

When studying simple crossed products by group actions, a technique that is frequently used is to find a suitable C^*-subalgebra of the crossed product which is "large enough" to retain most of the structural information of the crossed product while at the same time having a more tractable, recognizable structure. Putnam was the first to use this technique in his work on crossed products arising from Cantor minimal systems, by examining the construction of what we now call orbit-breaking algebras [43]. These have been used successfully in many places to understand the structure of their containing crossed products (see, for example, [37, 54, 56, 35, 36, 53, 18]) and have also been of interest in their own right, as they can also be viewed as C^*-algebras of minimal principal étale groupoids [17, 44].

Definition. Let X be an infinite compact metric space and $\varphi : X \to X$ a minimal homeomorphism. Put $A := C(X) \rtimes_\varphi \mathbb{Z}$. Let $Y \subset X$ be a closed nonempty subset meeting every φ orbit at most once. The orbit-breaking algebra at Y is given by

$$A_Y := \mathrm{C}^*(C(X), uC_0(X \setminus Y)) \subset C(X) \rtimes_\varphi \mathbb{Z},$$

where u is the unitary implementing φ, that is, $u \in C(X) \rtimes_\varphi \mathbb{Z}$ is the unitary satisfying $ufu^* = f \circ \varphi^{-1}$ for every $f \in C(X)$.

In 2011, Phillips introduced a generalization of orbit-breaking algebras which he called large subalgebras [40]. In this more general setting, many properties have been shown to pass between the large subalgebra and its containing C^*-algebra [40, 5, 4]. Although there are cases where this more general setting has proven useful, there is so far a dearth of examples of large subalgebras and their containing algebras that do not come from orbit breaking subalgebra in a crossed product of a commutative C^*-algebra. The goal of this project is to find other examples of large subalgebras, with an aim to exploit the preservation of known structural properties. Our starting point is to look at C^*-algebras which are very similar to crossed products by group actions, namely the two generalizations mentioned above.

Our time at WOA was spent sharing knowledge about Hilbert A-A-bimodules, groupoid C^*-algebras, labeled graph C^*-algebras, and large subalgebras until a candidate for a setting where we might apply the large subalgebra framework emerged. By the end of the week we had identified a (type of) subalgebra of bimodule crossed products which is similar, in spirit, to an orbit breaking algebras of a crossed product $C(X) \rtimes_\varphi \mathbb{Z}$, where the orbit is broken at a single point $x \in X$, the prototypical large subalgebra. We were able to confirm that our candidate is simple if the crossed product is simple, which is known to be a necessary condition for a large subalgebra of a simple algebra.

The next step in our project is to prove that our candidate subalgebras truly are large in the bimodule crossed product. We also hope to find the corresponding large subalgebra in minimal principal étale groupoid C^*-algebras. With these examples in hand, we will then look to prove results on structural properties of generalized crossed products using the properties of the large subalgebras we identified and known results about properties which pass from a large subalgebra to the containing algebra. We are planning to meet again in early spring in Germany or the Netherlands. Exact details are pending confirmation by the host institutions. We have also applied for a two week stay at MSRI during summer of 2019.

Feedback

The Association for Women in Mathematics ADVANCE evaluation team surveyed the WOA participants to provide feedback for the organisers. Of the 37 workshop participants, 31 responded to the survey, yielding an excellent response rate of 84 percent. Of the 31 survey respondents, most (87%) had earned a doctorate degree, and the vast majority (97%) were employed in academia. Graduate students and post-doctorates (39%) were balanced with academics in tenure-track positions (45%), below. This workshop was a new experience for most; almost all (94%) of the participants were newcomers to the Research Conference Collaboration Workshop model. Overall, the survey showed that the workshop was very successful: all participants would attend this conference again. Below are some of the open ended comments from the survey and testimonials supplied to BIRS:

- This was a phenomenal workshop. It was unusually effective in generating meaningful mathematical conversations and results. It also provided a great opportunity to bring together researchers with diverse specialties and to introduce researchers to related fields and questions.
- As far as research goes, I am kind of isolated at my current institution. This workshop was very beneficial for me. It helped me make connections with several people and really make progress on a research project. I am very grateful to the organizers, AWM, and other funding sources for this opportunity.
- It was a great workshop and one of the most friendly conferences/workshops I have been to.
- The workshop was fantastic. The collaborative and supportive atmosphere was totally different than any other workshop I've attended, in the most wonderful way. I think we all felt comfortable, respected and valued as mathematicians. [?] Many of us felt simultaneously that the week was too short, and that a two-week workshop wouldn't be practicable. Maybe a 9-day workshop, including weekends? Or an optional first week that had more of a mini-course structure, followed by the workshop? I also think it's important to support/fund mixed gender collaborations, in addition to the WOA collaboration network.
- The workshop allowed me to have the confidence to ask questions and make the most of a conference unlike any other conference. Being a women only conference it gave me the opportunity to communicate mathematics without having to prove myself. It gave me also a new foresight on job prospects, and actually made me rethink my capabilities as a researcher. I can be a successful researcher! I now have new collaborators with whom I feel comfortable working with.
- This workshop was absolutely remarkable. It provided me with an opportunity to meet and talk maths with outstanding researchers from around the world. During the week, I joined a new collaboration with researchers that I would have never normally had an opportunity to work with. The composition of our group and the structure of the workshop enabled us to prove several preliminary results, which we will develop into a paper in the coming months. Most importantly, this workshop brought together many women in a field with strikingly poor representation of women. The connections formed here, both mathematical and personal, will positively impact the diversity and, consequently, the mathematical developments in our field.
- The meeting was a unique opportunity to meet colleagues that I would not meet at regular workshops and offered me the chance to start a new research collaboration.
- Participating in this BIRS workshop has broadened my knowledge in the research field which I study, as well as new fresh insight of some research questions which I am interested. It was quite an unique experience that in the workshop not only I could have new contacts, but also we started a new collaboration on a research project. It is really good that we could just focus on our research problems during the whole week and achieved some results. On the top of all scientific aspects, I feel very much supported in our discipline through the workshop and the colleagues whom I got to know, which is very valuable for me.

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Chapter 27

Mathematical and statistical challenges in bridging model development, parameter identification and model selection in the biological sciences (18w5144)

November 11 - 16, 2018

Organizer(s): Ruth Baker (University of Oxford), Daniel Coombs (University of British Columbia), Matthew Simpson (Queensland University of Technology)

Overview of the field

Using mathematical models to assist in the design and interpretation of biological experiments is becoming increasingly important in biotechnology and biomedical engineering research; yet fundamental questions remain unresolved about how best to integrate experimental data within mathematical modelling frameworks to provide useful predictions. Traditional approaches incorporating mathematical and computational models in the design and interpretation of biological experiments often rely heavily on heuristic methods that vary from user to user, and from application to application. Not only is the selection of modelling frameworks often subjective, the integration of these modelling frameworks with experimental data is largely driven by individual preferences on a case-by-case basis. **Such variability in scientific practices is at best undesirable, and at worst leads to issues associated with research reproducibility**. Novel mathematical, statistical and computational tools are needed to provide a standardised pipeline that enables experimental data to be used effectively in the development of models, and in model parameterisation and selection.

One key challenge in using mathematical modelling to interpret biological experiments is the question of how to integrate multiplex, multi-scale quantitative data generated in experimental laboratories to improve our understanding of a specific biological question. These data might, for example, include time-series data for the concentrations of key intracellular biological signalling molecules, time-lapse microscopy data visualising the distribution of key cytoskeletal components, or tissue- and organism-scale data describing cell rearrangements or fluid flows. A standard protocol, that includes the design of experiments targeted towards parameterising models, validating specific model hypotheses and inference of underlying mechanisms based on quantitative data, is lacking.

To a large extent these issues are compounded by the fact that attempts to connect quantitative data with mechanistic models are being made in disparate fields of biology that function on a range of spatio-temporal scales: from the study of biochemical signalling networks within individual cells; to tissue-scale models of development, disease and repair; to ecological models of animal populations. At present, a major barrier to progress is a lack of cross fertilisation of ideas, or an awareness of the techniques and methodologies being developed in other fields of specialism. **Our observation is that the lack of cross fertilisation of ideas is because this area of research falls between many established disciplines, such as applied**

mathematics, applied statistics and computational mathematics, and this makes the development of consistent practices and protocols inherently difficult. As such, the broad aim of this workshop was to bring together researchers working in different areas of mathematics and statistics, and on different biological applications, to share and develop their research ideas towards bridging mechanistic model development, parameter identification and model selection using quantitative data.

Recent developments and open problems

Novel mathematical, statistical and computational tools are required to enable models to be developed, parameterised and validated as part of the predict-test-refine-predict cycle essential within biology. The overarching goal of the workshop was to work towards developing the mathematical, statistical and computational tools needed for a standardised pipeline that integrates multiplex, multi-scale quantitative biological data and mathematical and computational modelling. It is extremely timely because the recent explosion in the amount of quantitative biological and ecological data available means that the current disconnect between experimental sciences and mechanistic modelling will widen without interdisciplinary intervention. In addition, international meetings to discuss mathematical and statistical challenges in bridging model development, parameter identification and model selection in the biological sciences have been limited. The workshop focussed on tackling three main problem areas in the field.

Key challenge one: model coarse graining.

In order to resolve the conflict between requirements for including detailed descriptions of multi-scale biological processes into models and being able to efficiently simulate and/or subject models to analytical exploration, coarse graining can be performed. However, with biological data being generated on increasingly fine-grained scales, a significant challenge is to develop coarse graining approaches that retain descriptions of key processes happening across spatio-temporal scales [1, 13]. A relevant example is how to include detailed descriptions of tissue perfusion, that include descriptions of flow within blood vessels, into models that aim to understand tumour growth and, ultimately, determine optimal cancer treatment protocols.

Key challenge two: efficient methods for computational inference.

Computational inference methodologies target the posterior distribution (probability of the parameters given the observed data for a specific model), and are required when estimating models of biological systems as the likelihood function is generally analytically intractable (see *e.g.* [20]). There are significant challenges associated with computational inference that were discussed within the workshop. A key challenge, that was the focus of many discussions, is the development of understanding of when and where it is appropriate to use different types of inference methodologies, and how to quantify the errors associated with them.

Key challenge three: experimental design, model selection and uncertainty quantification.

Experimental design and data collection need to be optimised with respect to the specific biological or ecological question of interest and the model used to interrogate it [12]. The field currently lacks standardised approaches to model-driven experimental design. In addition, existing methods for model selection (encoding different biological hypotheses) can return different outcomes [18], and become difficult to interpret in the context of complicated models and noisy data, which is fast becoming the norm in the field. Methods for quantifying uncertainty include those that aim to understand how system outputs are affects by uncertainties in inputs such as parameter values (forward uncertainty propagation), and those that aim to measure discrepancies between data collected from a given experiment and the predictions of a mathematical model of that experiment (inverse uncertainty quantification). Uncertainty quantification is not routinely performed, however, the development and standardisation of methods to report and discuss uncertainty is key to the integration of modelling within the biological toolbox.

Presentation Highlights

The participants of the workshop included representation from Australia, Canada, New Zealand, Norway, United Kingdom, and the United States, with a range of career stages represented, from early-stage doctoral students, through postdoctoral research assistants, research fellows, tenure-track faculty and principle investigators. The participants were united by the use of common methodologies and ideas, that bring with them the same key challenges, on very different biological applications. As such, none of the participants, knew more than a handful of others in advance of the meeting. This common bond, and the small-scale nature of the workshop ensured that many new links and collaborations were formed; the meeting has really stimulated the development of a new research community.

Darren Wilkinson kicked off the meeting with an excellent talk outlining methods for Markov process parameter inference [21]. Darren compared some of the different “likelihood free” algorithms that have been proposed, including sequential ABC and particle marginal Metropolis Hastings, paying particular attention to how well they scale with model complexity.

Mattias Chung continued this theme, discussing the challenges in parameter inference for biological systems with noisy data, model uncertainties, and unknown mechanisms. Here, parameter and uncertainty estimation problems are typically ill-posed, meaning solutions do not exist, are not unique, or do not depend continuously on the data. Furthermore, experimentalists face a dilemma between accuracy and costs of an experiment. Mattias discussed new developments for parameter and uncertainty estimation for dynamical systems [8], as well as novel techniques for optimal experimental design [7], using three example applications.

Adelle Coster gave a very focused presentation about building models of glucose tolerance [6], with an emphasis on constructing useful mathematical models that capture biological processes at the level of a cell. In particular Adelle wishes to create models and compare predictions to experimental data so that she can rank the importance of various features and processes encoded in the data, and to make informed decisions about which model provides the “best” description of observations, by combining mean-field experimental data as well as observations of experimental noise.

Gary Mirams presented recent work regarding mathematical models of ion channel modelling with application to cardiac modelling [10]. Gary explained that to make progress in the field he needs to propose models, undertake an identifiability assessment to be sure that the models are identifiable given the types of data available and this leads to questions of optimal experimental design and questions of parameter inference, all of which feedback into the original question of model proposition. Gary’s talk was used as the basis for a longer group discussion on the following day (see below).

Adam MacLean spoke about models of kidney development and inference, with a focus on branching processes during morphogenesis [11]. A key tool to connect models and experiments is approximate Bayesian computation, with a focus on identifying the key parameters in relatively complicated experimental data. Adam’s model takes the form of an individual based model simulating stochastic cell migration and cell proliferation, with a continuous field of growth factor, which influences cell proliferation into neighbouring lattice sites giving rise to branching structures. Experimental data are movies from explants, giving rise to questions about comparing images from movies with images from simulations. Summary statistics are the area of the epithelia and the number of branches and ABC rejection is used to sample the posterior distribution. The main novelty is to use ABC rejection to generate an intermediate result and then refine the result using AABC, finding that branching is most sensitive to branching parameters.

Alex Browning spoke about identifying parameters in a continuum model of malignant invasion where malignant melanoma cells migrate, proliferate and degrade surrounding skin tissues [4]. Alex presented a typical continuum PDE model and a set of experimental data showing the invasion of the malignant population into the surrounding skin. Measurements of experimental noise allow the construction of an exact likelihood and Alex showed that invasion depth versus time is insufficient to distinguish between the three parameters in the model. Alternatively, Alex showed another two sets of experiments without skin tissues that allowed him to simplify the model and use Bayesian learning to learn parameters from one experiment and apply them to the next experiment. Overall, the new approach leads to well-formed posterior distributions that agree with some previous parameter estimations.

Michael Plank presented a stochastic birth-death model developed to describe populations of plants with no movement, and the key effect is to incorporate spatially-driven competition so that individuals undergo a constant birth rate, but a density dependent death rate to reflect the impact of competition for nutrients and space. Stochastic simulations reveal how the spatial competition affects the model outcomes and standard mean-field arguments do not account for such spatial effects. The construction of a spatial moment model, whereby interactions between pairs of individuals are accounted for, was presented and the numerical solution of the governing equations provides a good match to the stochastic simulations [2]. A key aspect of the presentation was to explain how the ecology-based model with no movement might be extended to apply to a model of cells in which cells are able to undergo proliferation, death and movement events.

Rob Deardon spoke about building discrete time S-I-R models of disease spreading with the key aim of working in real time. Working in a Bayesian framework with an explicit likelihood, the main aim is that key features are not observed since real cases give no idea of the infectious period. Instead there are measurements of reporting time or notification time. This means the simulation times are an issue since the MCMC algorithm needs to cover the joint posterior of the model parameters, incubation periods, delay periods and parameters describing the delay periods. The main idea is to speed-up using a simpler simulation framework called an emulator, which Rob explained and showed promising results leading to significantly faster computation times [14].

Dennis Prangle gave a presentation about inference on stochastic differential equations using methods from machine learning, called variational inference, with the aim of obtaining results faster than MCMC [17]. The key features of the approach is to take a Bayesian approach with partial observations with the main goal of inferring the parameters in the model, making use of the fact that the likelihood is tractable. Example calculations confirm the computational efficiency of these methods.

David Campbell gave a presentation starting with a case study in parameter estimation from the Dow Chemical company in 1981 with serious identifiability problems. With a poorly defined relationship between data and potential model structures Dave proposed several methods to learn about the problem by relaxing the proposed model structure, using the data to learn about how best to model the data and provide quantitative information about when parameters are identifiable or not [16].

Alexandre Bouchard-Cote spoke about difficulties with high-dimensional problems by focusing on well-known ODE models and MCMC Bayesian inference, discussing case studies of benchmarking MCMC methods, most of which fail except for a technique called parallel tempering, which is a novel method with the input of a Markov Chain where the output is a higher performance Markov Chain [3]. Examples, observations and implementation rules of thumb follow.

Thomas Prescott presented recent work that takes a multi-fidelity approach to approximate Bayesian computation for stochastic models of biochemical processes [15]. The key advance in the presented method is the use of a low-fidelity model to try and make an early accept or reject decision for a given parameter sample from the posterior. In the context that simulation of the high-fidelity model is instead required for this decision, the use of a common noise input to correlate output from the low- and high-fidelity models (using ideas from the multi-level Monte Carlo literature) allows for computational savings.

Ramon Grima gave a presentation motivating the kinds of data of interest reflecting single cell level signals of underlying gene networks, focusing on temporal snapshots so that measurements of temporal moments is the key quantity of interest. Grima shows that the posterior mode using moment-based inference methods is fast and accurate, and some analysis comparing the approximate results and exact results suggests a form of the systematic error in the likelihood approximation [9].

Simon Cotter gave a presentation about accelerated importance sampling to deal with MCMC sampling that are curved and thin ("banana shaped") and that often arise when variables cannot be easily observed. Without good ideas of the manifold, issues arise in standard methods, such as Metropolis Hastings or Importance Sampling. The idea is to work with Parallel Adaptive Importance Sampling (PAIS) and Transport Maps to Importance sampling, these ideas borrowed from applying Transport Maps to MCMC algorithms [5]. In general the transport maps are multidimensional Gaussians that can be sampled very simply. Implementations are discussed.

Barbel Finkenstädt Motivated her work by considering observations of a circadian oscillator with a delay and explores challenges associated with experimental measurements of such oscillators and demonstrates how to use an adaptive MCMC algorithms to estimate model parameters and then outlines methodologies that might be relevant to exploring spatial structure and spatial patterns [19].

Scientific Progress Made

Daily discussion sessions were used to isolate key problems / challenges faced by a range of the attendees, and to attempt to make progress towards tackling them. We focussed on a different problem, and used a different format each day, to stimulate discussion, new ideas and collaborations.

Day 1 discussion – "Burning questions"?

The meeting was perhaps fairly unique in the sense that it brought together researchers from a range of different application fields, and so no attendee was familiar with all others in advance of the meeting. As such, the meeting began with an introductory session, where participants introduced themselves, their research interests, and a "Burning question for the workshop". These questions provided the basis for the group discussions during the rest of the week. A sample of the points raised during this session are listed below.

- What can the process of model inference in biology learn from other disciplines? What makes biology unique, and where can biology borrow?
- We have two versions of the same model: a deterministic parametric model, data and inference; or a stochastic parametric model, internal noise, data, inference. What are sensible criteria for model choice?
- When selecting between models encoding different hypotheses, how do we cope with all our models being 'wrong'?
- How can / should we learn from imperfect models?
- Is there a role for benchmark data(/model) analysis tasks in this field?
- How can we leverage machine learning tools for inference?
- How can mathematical models be applied clinically to directly inform treatments for individual patients?
- How can we construct fast and accurate inference methods for single-cell data?
- How do we combine modern machine-learning approaches with mechanistic models?
- When, and how much, should we care about identifiability for biological models?
- How can we develop appropriate inference schemes for models that cross multiple scales?
- Which classes of model assumption can be assessed? Can assumption impact be measured / quantified?
- What are the best ways to balance objectives in optimization problems with mixed types of data?

The questions outlined above were the subject of many talks, and of subsequent discussions (both formal and informal). **Importantly, we are aware that such discussions between participants are continuing well after the workshop, and these discussions have the potential to lead to new scientific discoveries and the establishment of new scientific partnerships that would not have been created without the workshop**.

Day 2 discussion – "What should Gary do"?

Within his talk on Day 1, Gary Mirams posed lots of questions relevant to the workshop participants, centered around model development, parameter identifiability and optimal experimental design in the context of ion channel modelling. As a basis for concrete discussions, the Day 2 discussion involved participants working in small groups to suggest avenues for Gary to explore. Themes and ideas relevant to a range of projects that came out of the discussion were

- Would using a correlated error structure be appropriate? To what extent is heteroskedasticity an issue? Can cross validation help in exploring the noise structure?
- Can input signals be designed and / or modified to discriminate between different models (i.e. is model-guided experimental design possible)? Can the number of possible models be reduced iteratively by variation of the input signal? When should we use the simplest adequate model in place of the "best" model?
- Can we learn anything by attempting to fit a mixture of all postulated models? Can machine learning help with model design?
- What metrics are useful in comparing models and data?

Day 3 discussion – "Best practices for reporting"

The discussion on day 3 entered around best practices for reporting. The discussion involved participants working in small groups to identify the current practices, and how those could be improved in the future. The discussions were divided into five areas:

Benchmark experimental data sets. In field such as image analysis and machine learning, the availability of experimental data sets that can be used to test new algorithms has been vital to progress in the field. However, no such data sets exist for problems in parameter inference and model selection. Issues that were discussed in this respect included the lack of a repository where authors could submit data, access to high quality data (with a clear description of any pre-processing steps taken), whether different models and implementations would provide similar results. A recommendation going forward is that authors should post full data sets (wherever possible) within a publicly accessible repository, and provide a link to it within any published research article.

Bench-marking problems. Discussions were centered around the different types of problems for which algorithm bench-marking is necessary, including those associated with parameter estimation, model selection, approximations and models. The creation of synthetic data sets was recommended, along with the use of modular approach for different aspects of modelling and inference.

Software best practices. With increasingly sophisticated models, data sets and inference approaches now routinely in use, the use of software best practices is vital, yet not generally adopted. The group recommends that all software should be modular, well-documented and developed using version control.

Repositories / software packages / Journals. One issue raised is the current lack of an obvious "home" for papers in this newly emerging field, and the potential for a Special Issue was discussed as a means to raise the profile of the field. Github was widely viewed as a good platform for hosting software / code arising from research projects, but the group suggested that code / software should also be included within publications (and deposited in a journal repository, as is currently the case for Supplementary Material).

Publication best practices. The group recommended publishing at least pseudo-code to accompany (where relevant) all research papers, and that any code submitted with a manuscript should also be peer-reviewed. They recognised that there needs to be a greater awareness of the contributions of researchers in developing code / software, and that all code should be published with papers, as should data (experimental and synthetic).

The overwhelming point that came out of the Day 3 discussion, was the importance of building a new research community for the field, to promote collaboration and the sharing of ideas and best practices.

Day 5 discussion – "All models are priors" debate

The discussion on Day 4 took the form of a lively debate over whether "All models are priors". This raised some interesting points over how to approach modelling and inference!

Outcome of the Meeting

The meeting has seeded a new community in the broad field of quantitative approaches to biology and ecology, that is focussed on connecting models and quantitative data using statistical techniques. Going forward, it will be important to maintain this momentum, by having a similar meeting perhaps every 2-3 years that brings together the community to share and recent results and developments, and establish new collaborations, by having small focussed meetings to work on key problems, and by putting together a special issue for publication in an interdisciplinary journal (such as *Journal of the Royal Society Interface Focus* or *Bulletin of Mathematical Biology*).

Participant response

Alex Browning. I am a fairly new PhD student, who has only undertaken a few research projects in the past. The BIRS workshop gave me a fantastic opportunity to present and discuss my work and ideas with a large number of new connections that I made. I believe it aided me enormously in terms of future prospects, as well as future research ideas.

Simon Cotter. It was one of the most productive and gratifying workshops that I have ever been on. The scientific programme was superb, and the organisation by everyone at BIRS was top-notch. It was also a stunning location and I thoroughly enjoyed my trip. In short, it was well worth the long journey, and I hope that I will get a chance to visit again in the future.

John Fricks. The BIRS workshop was especially helpful in providing insights on which computational frameworks and tools to use in order to move my research forward. I made a lot of great contacts and met potential collaborators with whom I expect to keep in contact. One of the important takeaways from the meeting was a plan for this to be a first step in building a broader community.

Priscilla Greenwood. This was an outstanding workshop for me in terms of making important new contacts: Adelle Coster from Sydney, whom I was able to help with a problem she presented in her talk, also had time to get acquainted and plan to meet again. In addition, after my talk, we found many points of common interest with Ramon Grima from Edinburgh, and discussed for several hours. We have already exchanged several of our papers and also other references. This contact may well lead to joint work. Will keep you posted. The workshop, in general, was excellent. It brought together people who had several different approaches (a number centered around approximate Bayesian computation, a rather new version of MCMC which reduces computing time in complex models with much or little data) to inference for ODE, SDE and SPDE-type models arising in all sorts of math-bio settings, cell biology (very important current topic) and epidemiology, various medical applications, and so on. Most of the participants, mostly from UK, North America and Australia-New Zealand, had not met. So the group tended to assemble as a whole, rather than breaking into small circles of old buddies as sometimes happens. I felt that I left with lots of new friends! An outstanding contributor was one of the organizers, our own Dan Coombs, who set a number of discussion topics which drew lively, inclusive, sometimes heated discussion, one of these sessions each day. I was lucky and very much pleased to be part of this workshop!

Participants

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Chapter 28

Unifying Themes in Ramsey Theory (18w5180)

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Overview of the Field

Ramsey Theory has its official origins in the work of Frank Ramsey almost 100 years ago, showing that order can be found in large enough structures. But the idea was also present at about the same time in the work of Issai Schur and Bartel Leendert van der Waerden for example. This was followed by a long and intensive period of research in this direction, notably by Béla Bollobás, Paul Erdös, Ronald Graham, Alfred Hales, Robert Jewett, Jarik Nešetřil, Vojtěch Rödl, Bruce Rothschild, Joel Spencer among many others.

Then Timothy Gower's positive solution to the homogeneous space problem of Banach in the early 90's triggered renewed interest in Ramsey Theory of structures. This was followed by the work of Alexander Kechris, Vladimir Pestov and Stevo Todorcevic uncovering close connections between the Fraissé theory of amalgamation classes and homogeneous structures, Ramsey theory, and topological dynamics of automorphism groups of countable structures, leading to surprising results by connecting the study of continuous actions of topological groups on compact spaces, usually referred to as compact G-flows.

More recently, Ramsey Theory has further expanded throughout Mathematics and there is an intense level of broad activity based on Ramsey Theory connecting various areas and techniques throughout Mathematics. This includes new and continued research to universal structures and graphs, geometric and Euclidean spaces, Banach spaces, topological dynamics, metric and Polish spaces, logic and set theory, using varied techniques from probability to group theory and model theory.

This activity is exemplified by the following recent conferences and workshops:

- Homogeneous Structures, BIRS, 2015
- Sesquicentennial Ramsey Theory Conference, Devnver University, 2014
- Hausdorff Trimester Program on Universality and Homogeneity, Hausdorff Institute, Bonn 2013
- Workshop on the Concentration Phenomenon, Transformation Groups and Ramsey Theory, Fields institute, Toronto 2010
- Workshops on Homogeneous Structures, Leeds 2011 and Prague 2012

And the following current workshop specifically for highly qualified personnel:

- Modern Methods in Ramsey Theory, Ramsey DocCourse, Prague 2016

Recent Developments and Objectives

Mathematicians typically work with fundamental objects containing very rich structures. These include for example the rational numbers, the Rado graph, and the Urysohn space just to name a few, each exhibiting deep symmetry and universality. Indeed all countable linear orders will be found inside the rational numbers, all countable graphs will be found in the Rado graph, and similarly all countable metric spaces will appear as subspaces of the Urysohn space. The process of finding nice substructures within such large structures is a central theme of Ramsey Theory, and it is thus natural and the purpose of this workshop to study these methods and impact to other mathematical areas.

The principal objectives were to first promote continued interactions between different fields of mathematics affected by these recent developments, including researchers in the areas of analysis, combinatorics, dynamical systems, geometry, group theory, measure theory, metric and Polish spaces, model theory and logic in general. However we aimed at an important development and formally pursue the ongoing efforts at unifying Ramsey Theory themes into the mature subject area and theory that it has become.

This was a major undertaking and thus we also proposed to focus on specific unifying goals, including:

- Understand when a Ramsey-theoretic pigeon-hole principle allows a density version.
- Explore the relationship between axiomatizations of different parts of Ramsey theory such as the finite and infinite.
- Investigate a categorical approach that could explain the relationship between dualities in Ramsey theory; in particular we are still missing a finite dual Ramsey theory when we add forbidden configurations.

Some of the mainstream recent themes and methods that have emerged include:

- Universal objects
  Examples include the Fraïssé theory in logic and generalizations in model theory, universal graphs in combinatorics, the universal Urysohn space in topology, universality in algebraic geometry.
- Homogeneous structures
  Automorphism groups of homogeneous structures, Polish groups and topological dynamics, structural Ramsey theory, constraint satisfaction, omega-categoricity and amalgamation constructions, metric homogeneous structures, and classification results.
- Ramsey spaces and the underlying abstract theory of Ramsey Theory
  This work constitutes major efforts in formalizing and unifying in infinite-dimensional Ramsey theory, bringing together deep combinatorial methods which have had tremendous impact over the last 80 years in areas as diverse as functional analysis, dynamical systems, set theory, topology and much more.

Presentation Highlights

In November 2018, 41 of the top researchers in Ramsey theory met at the BIRS in Banff for the Unifying Themes in Ramsey Theory conference. The workshop was another formidable opportunity to regroup these specialists, learn about the latest developments, work together and exchange ideas. Moreover we had an unusually large cohort of young people including graduate students and postdoctoral fellows, a major success in itself.

What makes Ramsey theory so special is that it has wide ranging impacts in diverse fields in mathematics. The participants gave talks showing how Ramsey theory has impacted fields like graph theory, topological dynamics, set theory, model theory, operator algebras, logic and statistics. To facilitate open discussion in the spirit of a workshop, every “speaker” was given 45 minutes, with instructions to talk only for 30 of these and reserve at least 15 minutes for interactions with the audience; this worked quite well as it stressed the message of audience participation.

Here are four talks we selected as particularly important representatives of the workshop and worth watching for any mathematicians:

- Aleksandra (Ola) Kwiatkowska: “Universal minimal flows of the homeomorphism groups of Wazewski dendrites“.
  Watch it because: Ola presents a nice structure that answers two big problems in the field.
- Jordi Lopez-Abad: “Approximate Ramsey properties of Banach spaces”.
  Watch it because: Jordi is doing cutting edge research on important open problems, and explains his thinking with clear examples and computations.
- Jaroslav Nešetřil: “Unifying Themes in Ramsey Theory”.
  Watch it because: This gives an important unifying perspective on the place of Ramsey theory in mathematics.

- Stevo Todorcevic: "Concluding Remarks – Unifying Themes in Ramsey Theory".
  Watch it because: Stevo gives very deep and insightful perspectives on the connections of Ramsey theory to other fields.

Monday – Day 1A – Combinatorics and Ramsey classes

To kick off the conference, Jaroslav Nesetril gave a nice overview of the types of Ramsey theorems, problems and perspectives we are likely to see this week. He told us about how Mendel (the biologist) was the first to use the $\binom{n}{k}$ notation. Of the many important questions related to Ramsey theory, Nešetřil mentioned two:

- Are there other good tools for showing that a graph has high chromatic number?
- Does the class of graphs that forbid C_4 have a Ramsey expansion?

The second talk was supposed to be given by Michael Kompatscher, but he was unable to travel to Canada because of illness. So Mike Pawliuk gave the second talk in his place, about connections to data science, big data, statistics and machine learning. Coincidentally Pawliuk could have presented Kompatscher's talk since it was about joint work.
Ramsey theory is a natural perspective to use when studying the structure of large data sets. Big data, machine learning, and neural nets can all be profitably seen through this lens. Pawliuk followed on recent work of Calude and Longo ("The Deluge of Spurious Correlations in Big Data") by providing meaningful interpretations of basic Ramsey results in the setting of statistics. His first example was to interpret Goodman's Theorem in this context. He further layed out some of the current research in the area, presenting open problems relevant to researchers in Ramsey theory, and advertising some soon to be published work in these fields. Hopefully this will spur even more sophisticated connections of Ramsey theory with big data. This contained joint work with Michael Waddell, Columbia University.

Matej Konecny gave the final talk of the morning, showcasing new results that capture the completion algorithms of many different classes of metric spaces. Completing large cycles to a complete metric graph is an important step in showing that a class has a Ramsey expansion. This technique has become more and more explicit in recent years.
A large portion of the known Ramsey classes are essentially classes of ordered binary symmetric structures, for example the Kn-free graphs, Sauer's S-metric spaces, Cherlin's metrically homogeneous graphs, Braunfeld's Lambda-ultrametric spaces or Conant's generalized metric spaces. All of these can be shown to be Ramsey using the Hubicka–Nesetril Theorem and some variant of the shortest path completion. Konecny studied the limits of the shortest path completion and introduced the semigroup-valued metric spaces — a general framework which includes all the aforementioned classes. He found their Ramsey expansions and proved EPPA. Konecny conjectured that every primitive strong amalgamation class in a finite binary symmetric language can be understood as a semigroup-valued metric space. This is joint work with Hubicka and Nešetřil.

Monday – Day 1B – EPPA/Hrushovski property

Natasha Dobrinen started the afternoon with a chalkboard talk showcasing new results about big Ramsey degrees. She showed how she overcame the difficulties with the random graph to find the big Ramsey degrees for graphs that forbid small complete graphs. At its core she was able to sidestep a difficulty that the Sauer construction presented by starting where the Sauer construction ends.
In this talk, Dobrinen used techniques of logic, particularly set theory, to determine upper bounds on the big Ramsey degrees of the universal homogeneous k-clique-free graphs, for each k greater than two.

Jan Hubicka highlighted exciting work that he's been doing about general methods of proving the EPPA (Hrushovski property) for various classes of metric spaces. He was able to breathe life into the idea of valuations first presented elsewhere.

Finally, Marcin Sabok presented work showing that the class of hypertournaments does not have EPPA. It uses natural generalizations of the ideas present in Herwig-Lascar. It does not say anything about the (very hard) prized problem "Does the class of tournaments have EPPA?"
It is an open problem whether the Hrushovski extension property holds for tournaments. Sabok showed that it is equivalent to a problem concerning a profinite topology and a characterization of closed f.g. subgroups in this topology. During the talk he discussed a generalization of the latter problem to a family of profinite topologies.

The day ended with a small group of us going on a fast hike of Tunnel mountain.

Tuesday – Day 2A – Dynamics

The morning session focused on the fruitful connections that topological dynamics has had with Ramsey theory through the KPT correspondence.

Friedrich Martin Schneider gave the first talk which presented the "Gromov-Milman" perspective on the KPT correspondence. We saw a Gromov result that is a concentration of measure result, which corresponds to a Ramsey result through the KPT correspondence. Martin then showed us a stronger version of Gromov's result, answering a question of Pestov.
The work of Kechris, Pestov and Todorcevic has revealed a close connection between Ramsey theory of model-theoretic structures and topological dynamics of their automorphism groups, providing a rich source of examples of extremely amenable topological groups. Next to Ramsey theory, there is a second pathway to extreme amenability of topological groups: the phenomenon of measure concentration, which was exhibited in the 1970s by Milman (extending an idea going back to the work of Levy) and linked with extreme amenability in Milman's groundbreaking joint work with Gromov. In the late 1990s, Gromov offered a far-reaching generalization of the measure concentration phenomenon: the concentration topology on the space of metric measure spaces. Inspired by the striking applications of measure concentration in topological dynamics, Pestov suggested to study manifestations of Gromov's concentration to non-trivial spaces in the context of transformation groups. In the talk, Schneider reported on his recent progress in that direction, focusing on automorphism groups of metric model-theoretic structures and connections with Ramsey theory. Whereas for discrete structures dissipation and reasons related to ergodic theory prevent any kind of concentration, the situation is quite different in the continuous case.

Colin Jahel, a graduate student, gave an impressive talk about the semigeneric directed graph, answering an open problem from Pawliuk's thesis. Colin presented results that unified techniques for proving unique ergodicity, and sidestepped using probabilistic arguments.
A Polish group G is said to be uniquely ergodic when every minimal G-flow admits a unique invariant probability measure. For various examples of amenable automorphism groups of Fraïssé structures, it has been shown that this property holds. Jahel proved that this is also true in the only remaining case in Cherlin's classification for directed graphs: the semigeneric directed graph. This work follows from the papers of Angel-Kechris-Lyons and Pawliuk-Sokic, however it uses a new method not relying on the probabilistic method. Jahel also discussed the fact that the class of uniquely ergodic groups is closed under extension.

Andy Zucker rounded out the morning by giving an alternate perspective on the work of Colin (who is a coauthor). He discussed the dynamical perspective of the amenability and metrizable flows. This work is another step in Andy giving a very clear picture of what is happening with the universal minimal flows. This is one of the clearest, most straightforward talks about this topic I've ever seen.
From the audience, Stevo Todorcevic mentioned a nice (classical) result that if the product of two spaces contains a copy of $\beta\mathbb{N}$, then one of the factors must contain a copy of it. In this way, $\beta\mathbb{N}$ is an "irreducible" space.
Zucker showed that for Polish groups, the property of having metrizable universal minimal flow is preserved under group extensions; if G is Polish, H is a closed normal subgroup of G, and both M(H) and M(G/H) are metrizable, then M(G) is metrizable. In the case that G is non-Archimedean, this theorem has consequences in structural Ramsey theory for which we do not know a combinatorial proof. This is joint work with Colin Jahel.

Tuesday – Day 2B – Applications of Ramsey theory

The afternoon session featured subtle uses of Ramsey theory underlying key theorems. This made many of the results possible, even if they didn't directly invoke Ramsey results.

Wieslaw Kubis started the afternoon by presenting results about uniform homogeneity, Katetov functors and mixed sums of Fraïssé classes. The mixed sum construction is a type of "bipartite" construction where each part is a Fraïssé structure. While he used this construction to provide a counterexample, it is also a broadly useful construction.
A model M of a fixed first-order language is called homogeneous if every isomorphism between its finitely generated submodels extends to an automorphism of M. Theory of homogeneous models was developed by Fraïssé (1954) and now belongs to the folklore of model theory. Kubis discussed a stronger version of homogeneity, where extending partial isomorphisms is functorial, in the sense that it preserves compositions. He calls it "uniform homogeneity". This property implies that the automorphism group of M contains isomorphic copies of all automorphism groups of its finitely generated submodels. It turns out that most of the well known countable homogeneous models are uniformly homogeneous, which is implied by the existence of so-called Katetov functor, studied recently by Masulovic and the author. Nevertheless, there exist finite homogeneous models that are not uniformly homogeneous. Kubis presented an example of such a model which has 6 elements. It is not clear whether there exists a smaller model with this property. We shall also present countable infinite homogeneous models that are far from

being uniformly homogeneous. One of the examples has the property that its automorphism group is torsion-free, while among the automorphism groups of its finite submodels one can find arbitrarily large finite products of finite cyclic groups. The talk is based on two works, one joint with S. Shelah, another one joint with B. Kuzeljevic.

Milos Kurilis followed up with a proof of Vaught's conjecture in the case of monomorphic functions. This result quietly uses the fact that chainable uses Ramsey type-results. It was a remarkably understandable talk (to me a non-expert in model theory), despite the technical nature of the material. In his talk Milos produced one of the most beautiful diagrams ever seen in a math talk.
A complete first order theory of a relational signature is called monomorphic iff all its models are monomorphic (i.e. have all the n-element substructures isomorphic, for each positive integer n). Kurilis showed that a complete theory T having infinite models is monomorphic iff it has a countable monomorphic model, and confirmed the Vaught conjecture for monomorphic theories.

The final talk of the afternoon was David Hartman, who ended the day with a high-energy punch. David separated two closely related embedding properties with lots of examples and constructions. The final payoff for the day was a nice construction of the Rado graph partitioned into finitely many pieces.
This talk provided a story of equality of homomorphism-homogeneous classes. Cameron and Nesetril [1] suggested a novel notion of homomorphism-homogeneity for relational structure that requires every local homomorphism between finite induced substructures extends to homomorphism to the whole structure extending thus a classical notion of ultrahomogeneity in sense of Fraïssé. Depending on types of local homomorphism as well as the extending one it is possible to define various types of homomorphism-homogeneity, e.g. monomorphism-homogeneity extending local monomorphism to homomorphism. Mentioned work was an onset of wide classification program attempting to describe corresponding homogeneity classes. Already in this work there was a question about equality of classes HH and MH which was answered by Rusinov and Schweitzer 4 years later for countable undirected graphs. Later, with Hubicka and Masulovic [3], Hartman studied L-colored graphs, graphs having their edges as well as vertices colored by partial ordered set L, and showed conditions under which classes HH and MH are equal for finite L-colored graphs. Hartman extended this result by considering countably infinite P,Q-colored graphs, graphs coloring vertices and edges by two different partially ordered sets P and Q, and showed that necessary as well as sufficient condition for equality of classes MH and HH is that Q is a linear order [4]. This was joint work with Andres Aranda.

1. P. J. Cameron, J. Nesetril (2006), Homomorphism-homogeneous relational structures, Combinatorics, probability and computing 15(1-2): 91-103.
2. M. Rusinov, P. Schweitzer (2010), Homomorphismhomogeneous graphs, Journal of Graph Theory 65(3):253-262.
3. D. Hartman, J. Hubicka, D. Masulovic (2014) Homomorphism-homogeneous L-colored graphs, European Journal of Combinatorics 35: 313-32.
4. A. Aranda, D. Hartman (2018), Morphism extension classes of countable L-colored graphs. Preprint at arXiv:1805.01781.

After the presentations we had a problem session, where participants in the conference shared problems of interest. Here are the mostly-complete notes I took.

Ending the day, Wieslaw Kubis lead us in a problem session about the weak amalgamation property. About half the participants showed up and many people contributed to the discussion. Finally, at 8:30 (almost 12 hours after starting) we called it a day.

Wednesday – Day 3A

Wednesday contained only talks in the morning.

Martin Balko explained the project of ordered Ramsey numbers. He started by surveying the classical results about (usual) Ramsey numbers and contrasting them with the ordered versions. In many cases the bounds on the ordered/unordered Ramsey numbers are very different, even in the case of paths.
An edge-ordered graph is a graph with linearly ordered set of edges. Balko introduced and study Ramsey numbers of edge-ordered graphs, called edge-ordered Ramsey numbers. We prove some basic properties of these numbers for general edge-ordered graphs and we provide some stronger estimates for special classes of edge-ordered graphs. Balko also posed some new open problems and compare edge-ordered Ramsey numbers with the standard Ramsey numbers of graphs and with ordered Ramsey numbers, which are Ramsey numbers for graphs with linearly ordered vertex sets. This was joint work with Mate Vizer.

Lionel Nguyen Van Thé followed up by reminding us about Erdos-Rado type results about canonical colourings and equivalence relations. Big Ramsey results would become a recurring theme in this workshop. This talk stirred the most discussion about how it relates to canonical functions in other areas (like algebra).
One of the numerous strengthening of Ramsey's theorem is due to Erdös and Rado, who analyzed what partition properties can be obtained on m-subsets of the naturals when colourings are not necessarily finite. Large monochromatic sets may not appear in that case, but there is a finite list of behaviors, called "canonical", to which every coloring reduces. The purpose of this talk was to remind certain not so well-known analogous theorems of the same flavor that were obtained by Prömel in the eighties for various classes of structures (like graphs, hypergraphs, or Boolean algebras), and to show that such theorems can in fact be deduced in the more general setting of Fraïssé classes.

The final talk of the morning was Sam Braunfeld, who gave an overview of the classification of homogeneous finite-dimensional permutation structures. Sam compared and contrasted his results with Cameron's 2002 classification. This type of work is of particular interest to people in structural Ramsey theory, who use these catalogues as a source of interesting examples.
Braunfeld discussed the classification of homogeneous finite-dimensional permutation structures, i.e. structures in a language of finitely many linear orders, recently completed in joint work with Pierre Simon. After constructing the catalog of such structures, Braunfeld presented some of the key concepts in the classification, primarily coming from Simon's work on linear orders in omega-categorical structures. Braunfeld also touched on the Ramsey property for these structures, which may be viewed as Ramsey expansions of certain metric-type structures. This was joint work with Pierre Simon.

In the afternoon, some of us hiked up to Sundance Canyon, others went up Tunnel mountain, and others up Sulfur mountain.

Thursday – Day 4A – Set Theory and Logic

Thursday's schedule was anticipated to be rather heavy, but the speakers were very gentle to the audience and it ended up being one of the best days of the conference.

Martino Lupini started us off by explaining his intuition for his recent results about the generalized Tetris operations relating to Gower's theorem. In particular he showed us how he used a perspective from non-standard analysis and the idempotent ultrafilter proof of Hindman's theorem.
Lupini presented an ultrafilter proof of the infinitary version of the Gowers theorem for multiple tetris operations. Bartosova and Kwiatkowska previously gave a constructive proof of the corresponding finitary version, which has applications to the dynamics of the Lelek fan.

Francisco Guevara Parra gave a talk about Tukey orders and local Ramsey theory. This was one of the few talks to show the application of Ramsey theory to topological groups, and infinite combinatorics.
In [4] the authors used the Local Ramsey theory to prove that a countable Frechet group is metrizable if, and only if, its topology is analytic. Guevara Parra used this result together with the connections between the Tukey ordering and topology found in [2] to give a characterization of separable metrizable groups. Guevara Parra also proved that a separable group is metrizable if, and only if, it is Frechet and the the ideal of converging sequences to the identity is Tukey below some basic order that is analytic. Results in this direction have been obtained before in [1].

1. S. Gabriyelyan, J. Kakol and A. Leiderman. On topological groups with a small base and metrizability. Fundamenta Mathematicae, 229 (2015) 129-157.
2. S. Solecki and S. Todorcevic. Cofinal types of topological directed orders. Ann. Inst. Fourier, Grenoble, 54, 6 (2004), 1877-1911.
3. S. Todorcevic. Introduction to Ramsey spaces. Annals of Mathematics Studies, No 174, Princeton, 2010.
4. S. Todorcevic and C. Uzcategui. Analytic k-spaces. Topology and its applications, 146-147 (2005) 511-526.

David Chodounsky ended the morning with a problem motivated by set theoretic forcing, but of independent interest to those studying Ramsey theory. David stirred up interest in his question about Halpern-Lauchi ideals. He also gave us a survey of the landscape of HL ideals including a very nice map of the known implications.
A special case of the Halpern–Lauchli theorem implies that for a given 2-coloring of a perfect binary tree there exist a perfect subtree and an infinite set A of levels such that the coloring is monochromatic on nodes of the subtree coming from levels in A. We say that a collection of infinite sets R is (HL) if the statement can be strengthened by requiring that the set of levels A is in R instead of just infinite. This HL-property of R is equivalent with R being a reaping family (of subsets of omega)

indestructible with Sacks forcing, or equivalently some forcing adding a real. We are primarily interested in indestructible ultrafilters, Chodounsky proved the HL-property for various classical co-ideals. Thsi was joint work with O. Guzman and M. Hrusak

Thursday – Day 4B

Jordi Lopez-Abad gave us a very nice presentation of various approximate Ramsey properties. He put special effort in to give examples and pictures and it was very appreciated. We saw that some of the studied objects were "shapes" where the boundary is kind of blurry, but you can still tell the difference between a square and a hexagon. This context is "almost Euclidean". There was a lot of motivating intuition here.
Lopez-Abad discussed the Ramsey and other related properties in the context of Banach spaces and similar categories.

Michael Pinsker described canonical functions but, funny enough, not the "canonical functions" he originally wanted to talk about! The motivation for his talk is a nearly complete paper he wrote in 2002 that contained a critical false lemma. This lemma is an (infinite) Ramsey theory problem, and Michael was hoping to spark some renewed interest in it.
A function from one first-order structure into another first-order structure is called canonical if it sends tuples of the same type in the first structure to tuples of the same type in the second structure. This regularity notion for functions has found numerous applications in model theory, universal algebra, and theoretical computer science since its invention 7 years ago. In particular, it facilitates the understanding of self-embeddings, endomorphisms, and polymorphisms of structures, and has been applied, for example, in the classification of reducts of structures and in the study of certain computational problems related to them.

Any function between two countable structures gives rise to canonical functions in a natural way, provided its domain structure has the Ramsey property, and its goal structure is ω-categorical. Pinsker outlined a new proof of this fact using the framework of topological dynamics, and presented the recent discovery that under certain conditions also the converse holds, i.e., the possibility of obtaining canonical functions in that way implies the Ramsey property for the domain. He moreover outlined the main applications mentioned above, and the most important open problems connected to canonical functions.

Aleksandra (Ola) Kwiatkowska gave the final talk for the day, and it was one of the best of the conference. Ola showed that an obscure (but natural!) Fraïssé class (the Weiewski dendrites) negatively answers two fundamental (and related) questions in the field (Does every omega-categorical structure have a precompact Ramsey expansion?). David Evans had given an answer to this in 2016, but Ola's example is more natural, and provides a counterexample to some other conjectures as well.
For each $P \subseteq \{3, 4, ..., \omega\}$, Kwiatkowska considered Wazewski dendrite WP, which is a compact connected metric space that can be constructed in the framework of the Fraïssé theory. If P is finite, Kwiatkowska proved that the universal minimal flow of the homeomorphism group H(WP) is metrizable, and she computed it explicitly. This answers a question of Duchesne. If P is infinite, Kwiatkowska showed that the universal minimal flow of H(WP) is not metrizable. This provides examples of topological groups which are Roelcke precompact and have a non-metrizable universal minimal flow with a comeager orbit.

After dinner, Michael Hrusak led a working session about Ramsey-type problems on Borel Ideals, including several open questions. You can watch the video of it.

Friday – Day 5A – New Frameworks

The final day, like Wednesday, only had talks in the morning. The theme of the morning was new frameworks and directions for Ramsey theory.

Noé de Rancourt opened the talks with a discussion about Ramsey spaces, and specifically, what kind of results can you get if you don't have a pigeonhole principle in that space. Ramsey spaces are very nice combinatorial objects that capture the essential Ramsey behaviour of many geometric objects; it is related to combinatorial forcing. Noé showed us how to relate these to games and local Ramsey theory.
Strategical Ramsey theory was developed in the nineties by Gowers in the setting of Banach spaces; it is an alternative to standard infinite-dimensional Ramsey theory in this setting where the natural pigeonhole principle does not always hold. In this talk, de Rancourt presented an abstract formalism for strategical Ramsey theory, which also allows to recover more standard results relying on a pigeonhole principle, like Galvin-Prikry's theorem. As an application, de Rancourt explained how we can deduce, from this formalism, new Banach-space dichotomies. These dichotomies are part of a common work in progress with Wilson Cuellar-Carrera and Valentin Ferenczi.

Dragan Masulovic showed us how the tools of category theory can be used to view and prove dual results in Ramsey theory. He showed us the value and type of isomorphism of categories in the Ramsey context. There was a special attention to making the results usable and practical for the non-category theorist.

Generalizing the classical results of F. P. Ramsey from the late 1920's, the structural Ramsey theory originated at the beginning of 1970's. We say that a class K of finite structures has the Ramsey property if the following holds: for any number $k \geq 2$ of colors and all $A, B \in K$ such that A embeds into B there is a $C \in K$ such that no matter how we color the copies of A in C with k colors, there is a monochromatic copy B' of B in C (that is, all the copies of A that fall within B' are colored by the same color).
Showing that the Ramsey property holds for a class of finite structures K can be an extremely challenging task and a slew of sophisticated methods have been proposed in literature. These methods are usually constructive: given $A, B \in K$ and $k \geq 2$ they prove the Ramsey property directly by constructing a structure $C \in K$ which is Ramsey for B, A and k.
In this talk, Masulovic explicitly put the Ramsey property and the dual Ramsey property in the context of categories of finite structures. He uses elementary category theory to generalize some combinatorial results and using the machinery of very basic category theory provide new combinatorial statements (whose formulations do not refer to category-theoretic notions) concerning both the Ramsey property and the dual Ramsey property. Masulovic stressed that it was Leeb who pointed out already in early 1970's that the use of category theory can be quite helpful both in the formulation and in the proofs of results pertaining to structural Ramsey theory.

Stevo Todorcevic gave concluding remarks for the conference, in particular stressing Dual Ramsey results. Stevo also put in perspective the development of Ramsey expansion, with its roots in the work of Ramsey himself, followed by that of Baumgartner, Galvin and Laver, and all the way to the general Fubini problems on Polish spaces with Baire measurable colourings.

And with that, we wrapped up this iteration of the Ramsey theory meeting.

Open Problems

A list of open problems was collected, including the following.

Andy Zucker

Note. This question was solved at the conference after the problem solving session, please contact Andy for more details.

Definition: Let $\mathcal{F}$ be a Fraïssé class, $\mathbb{F} = \text{Flim}(\mathbb{F})$, $A \in \mathcal{F}$. We say that A has **Big Ramsey Degree (BRD)** $k < \omega$ iff

1. $\forall r > k$, we have $\mathbb{F} \to (\mathbb{F})^A_{k,r}$, and
2. There is an $f : \text{Emb}(A, \mathbb{F}) \to k$ which is "unavoidable'.'

Let $\mathcal{F}$ be the class of finite sets with an equivalence relation and a convex linear order. So $\mathbb{F}$ is a convex ordered 2-distance ultrametric space, which has infinitely many infinite classes, each class densely linearly ordered, and teh set pf classes also densely linearly ordered.

Question. Does $\mathcal{F}$ have finite BRD?

It was suggetsed by the audience to look at Laver's construction and infinite dimensional Halpern-Lauchli.

Matěj Konečný

Say that we want to prove Ramsey for a class $\mathcal{C}$ (with binary relation E, which is a complete graph). We study which incomplete structures have completion in $\mathcal{C}$. (This is motivated by Herwig–Lascar and Hubička–Nešetřil.) There is often a *finite* class $\mathcal{F}$ (possibly after eliminating imaginaries) such that as long as no elements of $\mathcal{F}$ have a homomorphism into your structure, then you can complete your structure into $\mathcal{C}$.

This usually comes along with automorphism preservation, stationary independence relation (SIR), coherent EPPA, APA. Note that coherent EPPA and APA imply ample generics. The class of "two-graphs" is interesting.

Definition: The class of "two-graphs" is triple systems where each collection of 4 vertices contains an even number of triples.

Note two-graphs do not have APA (easy example) and SIR. Their Ramsey expansion is adding back the graph and a linear order. However we still can prove the following theorem (not using Herwig–Lascar).

Theorem: They all have EPPA.

(But we cannot prove coherent EPPA.)

Question 1. Do two-graphs have ample generics?

Question 2. What about other reducts (of the random graph)? E.g. do "complementing graphs" have EPPA?

Mike Pawliuk

Definition: The statement "Permutation Hales-Jewett for a template abc" is the statement:

Fix a size t. For any number of colours r, there is a large enough N such that for every colouring of the words in $\{a,b,c\}^N$ there is a variable word $w(x,y,z)$ with disjoint variable parts $I_1, I_2, I_3 \subset [0,N]$ such that

1. $|I_1| = |I_2| = |I_3| = t$, and
2. The words $w(a,b,c), w(a,c,b), w(b,a,c), w(b,c,a), w(c,a,b), w(c,b,a)$ all have the same colour. (Note that each letter can only be used once!)

Note that a, b, c could contain repetitions, and there's nothing special about three elements and variable sets. This question makes sense for more general templates. This is special because the size t is given in advance of the N. In regular Hales-Jewett, this is an impossible demand; For example, take the colouring of words given by:

$$\chi(f) = \left\lfloor \frac{\sum_{i<N} f(i)}{t} \right\rfloor \text{mod} 2$$

Some known facts:

- Template $11\ldots122\ldots2$. This is a straightforward application of Ramsey's Theorem (for cliques of size t times the number of letters in the alphabet).
- Template $11\ldots122\ldots23$. This is the major Ramsey result in the Leader-Russell-Walters 2012 paper [1]. This uses VdW's theorem in a sophisticated manner.

These are the two simplest problems that are open (and were asked in LRW 2012).

Question 1. Permutation Hales-Jewett for the template 1234.

Question 2. Permutation Hales-Jewett for the template 112233.

The proof of either of these would immediately imply that a certain structure in Euclidean space is "Euclidean Ramsey".

Theorem: [Leader-Russell-Walters, 2012] Permutation Hales-Jewett for all templates $123\ldots n$ implies "all transitive (Euclidean) sets are (Euclidean) Ramsey".

[1] Leader, I., Russell, P. A., & Walters, M. (2012). Transitive sets in Euclidean Ramsey theory. Journal of Combinatorial Theory, Series A, 119(2), 382-396.

Noé de Rancourt

Let X be countable. Consider a set $S(X) \subseteq P(X) \setminus \{\emptyset\}$ Borel. Here P, Q, R denote elements of $S(X)$.

This is meant to model concrete situations, where X is a structure and $S(X)$ is the set of subspaces of X. To avoid pathological counterexamples[1], we suppose that the following condition is satisfied: for every $P \in S(X)$, there exist $Q, R \subseteq P$ such that $Q \cap R = \emptyset$.

Examples:

1. $X = \mathbb{N}, S(X) = [\mathbb{N}]^\infty$.
2. $X = E \setminus \{0\}$, where E is a countably infinite dimensional vector space over a countable field $\mathbb{F}$, and $S(X)$ is the set of infinite dimensional subspaces of X.

Definition: The space $(X, S(X))$ satisfies the **pigeonhole principle (PHP)** if for all $A \subseteq X, \forall P, \exists Q \subseteq P$ such that either $Q \subseteq A$ or $Q \subseteq A^c$

Example 1. above satisfies PHP (this is the usual pigeonhole principle) and example 2. satisfies PHP if and only if $\mathbb{F} = \mathbb{F}_2$ (the "if" part is Hindman's theorem).

With a little bit more structure, you can prove an infinite dimensional Ramsey-type result in such a space, even without PHP (with PHP, you will get the results you are used to, e.g. Galvin-Prikry for example 1.). But with PHP these results are valid for Suslin sets, whereas whitout it, you cannot go beyond analytic. The counterexamples in the case without PHP are built by a coding method. More generally, there seems to be a link between PHP and questions of complexity. (See Noé's talk for more context.) Noé's question is about a possible new example of this phenomenon.

Definition: A set $A \subseteq X$ is **dense** if for all P, there is a $Q \subseteq P$ such that $Q \subseteq A$.

Note that this is a $\mathbf{\Pi}^1_2$ property.

Theorem: Suppose PHP holds. Then A is dense iff for all P, $P \cap A \neq \emptyset$.

[1] After the problem session, such a counterexample was found by Marcin Sabok: take $X = \mathbb{N}$ and $S(X) = \{\mathbb{N}\}$ (this is not his original counterexample, but his idea was similar).

Proof: If A is dense, then in particular $\forall P \ P \cap A \neq \emptyset$. To prove the converse, remark that "A is not dense" means $\exists P \ \forall Q \subseteq P \ Q \nsubseteq A$; but using PHP, $\forall Q \subseteq P \ Q \nsubseteq A$ implies $\exists Q \subseteq P \ Q \subseteq A^c$. The result follows.

This result shows that under PHP, the property "being dense" is $\mathbf{\Pi}^1_1$.

Question 1. Do we have the equivalence between

1. $(X, S(X))$ satisfies PHP.
2. The property "being dense" is $\mathbf{\Pi}^1_1$.

Question 2. Furthermore, in case PHP does not hold, what can be the complexity of "dense"?

Question 3. Can it be $\mathbf{\Pi}^1_2$-complete?

Martino Lupini

Assume all metric spaces are complete with unique geodesic. Hardeman spaces ar such structures equiped with a function symbol assigning the midpoint between two given points.

Fact. Hardeman spaces have amalgamation (along convex sets).

So you should have a Fraisse limit if it is separable, and if so it would be a "non-positive curvature" Urysohn space.

Question. Is there a universal object for this class?

This appears to be a question in geometry. You can't always write these (finite) spaces as the convex hull of finitely many points, and we know Hilbert spaces don't work.

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Chapter 29

Model Theory and Operator Algebras 18w5155)

ovember 25 - 30, 2018

rganizer(s): Ilijas Farah (York), Isaac Goldbring (UC Irvine), Dimitri Shlyakhtenko (UCLA), ilhelm Winter (Münster)

verview of the Field

erator algebra has developed into a field of its own since the time of von Neumann. C^*-algebras and von Neumann algebras be represented as algebras of bounded operators on a Hilbert space and although the relevant topology is different in the dy of these algebras (the operator norm for C^*-algebras and the weak-$*$ topology for von Neumann algebras), both classes ve interesting ultraproduct constructions. The class of C^*-algebras is closed under the usual norm ultraproduct while the class II_1 factors is closed under the tracial ultraproduct. Although it took 40 years to notice, the existence of these ultraproduct nstructions highlights that model theory has a role to play in the subject. There are many interesting current directions to sue but we concentrated on three general themes:

- Interaction with the Elliott classification programme
- Relationship with free probability
- Model theoretic considerations

There are several things that model theory brings to the table in this endeavour. First of all, the theory of an algebra is invariant which is complementary to many of the operator algebraic invariants on offer. The utility and consequences of ognizing when two algebras do not have the same theory will be highlighted below. Second, model theory provides methods constructing examples which are different from those in operator algebra. The primary example is model theoretic forcing ich plays a prominent role in [8]. Although to date the examples constructed have been modest, refocusing attention on the nstruction of specific examples with this technique in mind could pay dividends. Third, the notion of an elementary class in ntinuous logic is a common generalization of both the class of C^*-algebras and II_1 factors. Model theory can be used for h clarifying concepts and identifying good questions to ask. The key is to identify at an abstract level what role the language playing and what model theoretic properties are present. Two examples of this appear in [9] where model theoretic properties strongly self-absorbing algebras are discussed and [10] where isomorphism classes of ultrapowers are considered.

e Elliott classification programme

iott had conjectured that the category of separable, simple, nuclear C^*-algebras is equivalent to the category of certain K-oretic invariants. The original conjecture had generated an impressive body of work, some of which (notably [25] and [28]), essitated its reformulation. After a succession of spectacular technical breakthroughs, (notably [20], [19], [26], [27], [4], l [6]), a restricted version of Elliott's conjecture has been confirmed. The regularity properties that distinguish 'classifiable' and 'non-classifiable' C^*-algebras are only to a limited extent detectable by K-theoretic invariants or by any well-behaved functorial invariants. Interestingly all known counter-examples to classification by K-theoretic invariants are distinguished by their continuous first order theories. $\mathcal{Z}$-stablity (perhaps the most prominent regularity property of nuclear C^*-algebras) is an elementary property ([8]), and the existence of a nuclear C^*-algebra without the UCT (perhaps the most mysterious regularity property of nuclear C^*-algebras) is equivalent to the existence of a particular first-order theory of C^*-algebras omitting certain types. One of the highlights of [8] is the insight that many regularity properties related to the classification programme are equivalent to a particularly nice form of omitting types in continuous logic. The properties include nuclearity, nuclear dimension n, decomposition rank n and many more; conspicuous by its absence is exactness. This raised the intriguing possibility that model theory could play a role in the resolution of the Toms-Winter conjecture and a complete resolution of the quasidiagonality conjecture (although substantial progress on this has already been made; see [27]). More specifically, the technique of model theoretic forcing could be used to construct examples with given regularity properties and provide counter-examples to certain conjectures. In the positive direction, in [17] it was proved that weaker versions of the UCT problem and the quasidiagonality problem imply that all nuclear, stably finite, C^*-algebras are quasidiagonal; this purely C^*-algebraic result was proved using model theoretic forcing.

Free probability and model theory

Free probability theory provides a probabilistic framework for understanding free groups factors. Some of its most powerful tools come from the connection to random matrix theory, which can be naturally placed into the context of ultraproducts of matrix algebras and the quantitative study of matricial approximations. Among interesting free probability approaches is one called linearization, where a matrix trick replaces non-commutative rational functions of n-tuples of variables by corners of matrices whose entries are linear in the variables. It would be instructive to explore this in connection with model-theoretic ideas.

For a free group F_n on n generators, $L(F_n)$ is the corresponding group von Neumann algebra. The celebrated free group factor problem asks if all non-abelian free group factors on finitely many generators are isomorphic. It is known that they are all either isomorphic or all not isomorphic. A model theoretic variant of this problem is to ask if all of the $L(F_n)$'s for $n > 1$ have the same theory as II_1 factors. Of course, if they don't then one has a very strong answer to the free group factor problem. On the other hand, if they do have the same theory then this provides a partial explanation for why the free group factor problem is difficult. There are no known examples of explicitly given, elementarily equivalent, C^*-algebras or II_1 factors which are not isomorphic.

A related problem asks whether $L(F_n)$ is pseudo-finite for $n > 1$. That is, is $L(F_n)$ elementarily equivalent to an ultraproduct of matrix algebras viewed as von Neumann algebras. All of the free group factors and ultraproducts of matrix algebras have the same universal theory (they are R^ω-embeddable). Property Γ is an elementary property ([11]) and all of these examples fail to have Γ so they agree on at least one highly interesting sentence with two quantifiers. Little else is known. It is also not known if the theories of ultraproducts of matrix algebras are all the same. It is known that there is either 1 such theory of ultraproducts or continuum many. Understanding the answer to this question requires an understanding of the asymptotic behaviour of formulas in large matrix algebras. A potential strategy for resolving the model theoretic version of the free group factor problem would be to show that every free group factor is pseudo-finite and that all ultraproducts of matrix algebras have the same theory.

Model theoretic considerations

In [10], the model theory of operator algebras resolved the McDuff problem regarding the isomorphism types of ultrapowers of separable II_1 factors and their relative commutants. The question was (slightly rephrased): given a separable II_1 factor M, are all ultrapowers of M by non-principal ultrafilters on $\mathbb{N}$ necessarily isomorphic and also are the relative commutants isomorphic. The answer is no but the reason is very interesting. One shows that the relevant concept is the model theoretic notion of stability and when one transports this notion to the class of C^*-algebras and asks the corresponding question, one gets exactly the same answer although of course for different local reasons. Since [10], the model theory of operator algebras has matured and it became a subject in its own right.

Much work in classification has gone into analyzing Connes' work [5] on injective factors and transferring the techniques into the study of C^*-algebras. With the long term goal of feeding into this programme, a model theoretic study of the hyperfinite II_1 factor and strongly self-absorbing algebras was initiated.

On the II_1 factor side of the equation, much is known about the model theory of the hyperfinite II_1 factor R. R is a prime model of its theory (it embeds elementarily into any other model of its theory; interestingly it embeds into any II_1 factor and if that factor is a model of the theory of R, then the embedding is automatically elementary; [3]). The theory of R is not model complete ([15], [11]). Although it is possible that the theory of R is $\forall\exists$-axiomatizable there is speculation that this theory could be undecidable [13].

On the C*-algebra side, the corresponding algebras are the strongly self-absorbing algebras. We say that a separable and tal A is strongly self-absorbing if $A \cong A \otimes A$ and any two unital *-homomorphisms from A to $A \otimes A$ are approximately tarily conjugate. There are only a handful of known strongly self-absorbing algebras: $\mathcal{Z}$, UHF$^\infty$ (any UHF algebra of nite type), $\mathcal{O}_\infty$, $\mathcal{O}_\infty \otimes$ UHF$^\infty$ and $\mathcal{O}_2$. It is an open question if this list is exhaustive; potentially, if there is a missing ongly self-absorbing algebra, model theoretic forcing could help to find one. In any case, the model theory of strongly self-orbing algebras is well understood ([9]). As with the hyperfinite II$_1$ factor, they are the prime models of their theory in the guage of C*-algebras. They again have the automatic elementarity mentioned above. Little is known about the theories of ongly self-absorbing algebras except that two non-isomorphic strongly self-absorbing algebras have distinct theories.

One intriguing issue that arises in the study of strongly self-absorbing algebras in either context is the role played by relative commutant inside an ultrapower or the central sequence algebra. That is, for a separable algebra A, one considers $\cap A^U$ for a non-principal ultrafilter U on $\mathbb{N}$. Model theoretically, the role of the ultrapower is clear: it is a countably saturated del. This saturation implies that the central sequence algebra is always quantifier-free saturated and in important instances actually an elementary submodel (as it is in the case that A is strongly self-absorbing). There is no general model theoretic nstruct similar to the relative commutant and it would be extremely interesting to investigate the exact formal properties ich makes this such an important tool in the study of operator algebras.

The role of the notion of saturation in the general model theoretic study of operator algebras cannot be overstated. As ntioned above, full saturation and quantifier-free saturation play their usual roles as in any model theoretic study. In [7], ery weak form of saturation (countably degree-1 saturated) is discussed. This level of saturation is shared by all coronas separable C*-algebras like the Calkin algebra which is known not to be quantifier-free saturated. This provides simplified ofs of Kasparov's technical lemma among other things. This theme was also picked up in [29] where it is shown that certain -algebras, rough analogues of the Calkin algebra, are also countably degree-1 saturated. This restricted form of saturation uld play a key role in the construction of a K-theory reversing automorphism of the Calkin algebra.

There is value in continuing the study both of general elementary properties of C*-algebras and II$_1$ factors. It was widely ieved amongst those working in the area that there should be continuum many distinct theories of II$_1$ factors. This sus-ion was confirmed in [2] where it was shown that McDuff's original family of continuum many pairwise non-isomorphic arable II$_1$ factors were indeed not elementarily equivalent. The proof proceeded by showing that any two ultrapowers of tinct members of the family were nonisomorphic. It would be interesting to isolate particular sentences that distinguish these tors. In [14], Ehrenfeucht-Fraïssé games were used to at least give upper bounds for the quantifier complexity of sentences tinguishing these factors. A related problem would be the study of the model-theoretic fundamental group of a II$_1$ factor. particular, finding an example of a II$_1$ factor with proper first-order fundamental group would give another proof of the stence of continuum many non-elementarily equivalent II$_1$ factors.

ecent Developments and Open Problems

e following list of problems highlights some of the aspects of the interaction between model theory and operator algebras.

jas Farah

$\mathcal{Q}$ be the universal UHF algebra and let $\mathcal{R}$ be the hyperfinite II$_1$ factor. Are $\mathcal{Q}$ and $\mathcal{R}$ elementarily equivalent *in the language C*-algebras*? In other words, do $\mathcal{Q}$ and $\mathcal{R}$ have isomorphic ultrapowers (again, as C*-algebras)? Note that a positive answer plies that $\mathcal{R}$ is an MF-algebra.

Related questions are: Is there a unital map from the Jiang-Su algebra $\mathcal{Z}$ to the (norm)central sequence algebra of $\mathcal{R}$? Does theory of $\mathcal{R}$ in the language of C*-algebras have a nuclear model?

A positive answer to this question would imply that $\mathcal{R}$ is quasidiagonal, answering a prominent open problem. More cisely, the quasidiagonality of $\mathcal{R}$ is equivalent to $\mathcal{R}$ and $\mathcal{Q}$ having the same universal theory.

Another related question, asked by Chris Schafhauser, is whether R has a theory of a $\mathcal{Z}$-stable C*-algebra? Although R elf cannot absorb $\mathcal{Z}$ tensorially, a positive answer is equivalent to every separable elementary submodel of R absorbing $\mathcal{Z}$ sorially.

n Hayes

l a tracial C*-algebra (A, τ) Hayesian if there is a trace-preserving embedding $A \hookrightarrow \prod_{\mathcal{U}} M_n(\mathbb{C})$, where the latter ultra-duct is the C*-algebra ultraproduct equipped with the trace obtained by taking the $\mathcal{U}$-ultralimit of the normalized traces on $M_n(\mathbb{C})$. Call a discrete group Γ Hayesian if the tracial C*-algebra $(C_r^*(\Gamma), \tau_\Gamma)$ is Hayesian, where τ_Γ is the canonical ce. Which groups are Hayesian? By standard arguments, this is equivalent to an assertion about the universal theory of $(\Gamma), \tau_\Gamma)$ ([**?**]). Here are some facts about Hayesian groups:

- Amenable groups are Hayesian. ([27]).
- $\mathbb{F}_2$ is Hayesian. ([18]).
- Free products of Hayesian groups are Hayesian (Reference?)
- Direct products of exact Hayesian groups.

Are there any non-Hayesian groups? Is the amalgamated free product of Hayesian groups over an amenable amalgam once again Hayesian?

N. Christopher Phillips

Fix $p \in (1, \infty)$. A *unital L^p-operator algebra* is a Banach algebra $\mathcal{A}$ such that there is an L^p-space $L^p(X, \mu)$ and an isometric unital Banach algebra homomorphism $\mathcal{A} \hookrightarrow \mathcal{B}(L^p(X, \mu))$. They appear to be closed under ultraproducts and are clearly closed under ultraroots (in fact substructures), so form an axiomatizable class in the language of unital Banach algebras. What are natural axioms?

Alessandro Vignati

A result of K.P. Hart implies that if X and Y are two nontrivial continua, then $C(X)$ embeds into an ultrapower of $C(Y)$. It is also known that there is no metrizable continuum X such that $C(Y)$ embeds into $C(X)$ for all other metrizable continua Y. In particular, this implies that for every metrizable continuum X, there is a metrizable continuum Y such that $C(X) \equiv C(Y)$ but $X \not\cong Y$. For specific X, find examples of such Y. For example, find Y such that $C([0,1]) \equiv C(Y)$ but $[0,1] \not\cong Y$.

In another direction, suppose that X and Y are locally compact spaces such that $C(\beta X \setminus X) \equiv C(\beta Y \setminus Y)$. What can we say about $C_0(X)$ vs. $C_0(Y)$. Also, under the same assumption, if one assumes CH, do we know that in fact $C(\beta X \setminus X) \cong C(\beta Y \setminus Y)$?

Isaac Goldbring

Call a McDuff II_1 factor *strongly McDuff* if it is isomorphic to one of the form $M \otimes \mathcal{R}$ for M a non-Gamma II_1 factor. Can an existentially closed (e.c.) II_1 factor ever be strongly McDuff? As partial progress, if the non-Gamma factor M is *bc-good* (to be defined shortly), then $M \otimes \mathcal{R}$ is not e.c. Here, M is bc-good if it has a w-spectral gap subfactor N (meaning that $N' \cap M^{\mathcal{U}} = (N' \cap M)^{\mathcal{U}}$ for which $(N' \cap M)' \cap M \neq N$. This leads to the question: is every non-Gamma factor bc-good?

Wilhelm Winter

By [**?**], a separable, nuclear, C*-algebra satisfies the UCT if and only if it has a Cartan masa. A major open question is whether or not all strongly self-absorbing (ssa) algebras satisfy the universal coefficient theorem (UCT). Towards that goal, here are some intermediate questions. View the set of ssa algebras as a category whose morphisms are unital $*$-homomorphisms up to approximate unitarily equivalence. This category has an initial object, namely the Jiang-Su $\mathcal{Z}$, which has a Cartan masa. Can you prove that the initial object has a Cartan masa without actually knowing that it is $\mathcal{Z}$? Also, one can ask the same question for the category of ssa algebras of the form $A \otimes M_{2^\infty}$ where A is ssa. This also has an initial object, M_{2^∞}, which also has a Cartan masa.

Questions on opposite algebras

It is a major open problem whether every simple, separable, nuclear C*-algebra A is isomorphic to its opposite algebra, A^{op}. (The answer is positive if simplicity is dropped, if nuclearity is relaxed to exactness, and nonseparable examples exist.) Every C*-algebra that is classifiable by its Elliott invariant is isomorphic to its opposite algebra. The following two questions are about C*-algebras not isomorphic to their opposites.

Ilan Hirshberg

Is there a C*-algebra A such that $A \not\equiv A^{\mathrm{op}}$? (If yes, how 'nice' can A be? Can it be unital, simple, ...?) Nonseparable examples given in [**?**] are elementarily equivalent to Elliott-classifiable C*-algebras, and therefore elementarily equivalent to their opposites.

Christopher Phillips

ppose that A is a unital, simple, purely infinite C*-algebra. Is there a state φ on A which can be distinguished up to unitary ivalence in the sense that for every automorphism α of A there is a unitary u in A such that $\varphi \circ \alpha = \varphi \circ \mathrm{ad}_u$? (If A is a tal C*-algebra with a unique tracial state τ, then one has $\tau \circ \alpha = \tau$ for every automorphism α of A.)

The motivation for this question comes from the argument in [23], where it was proved that if M is a II_1 factor not morphic to its opposite and A is a separable, weakly dense, elementary submodel of M (considered as a C*-algebra), then A ot isomorphic to A^{op}. A positive answer would provide a purely infinite, simple, C*-algebra not isomorphic to its opposite.

n Hirshberg

here any natural model-theoretic meaning to looking at structures that resemble ultrapowers except one uses βX for X an itrary locally compact space (e.g. $\mathbb{R}_+$, which shows up in practice) rather than just βI for I a discrete set? Is there a corre-onding logic for which this is well-behaved? Are there parallels to usual model-theoretic facts about ordinary ultrapowers? at uses does this construction have?

ther problems

e of the most prominent open problems in the theory of operator algebras is whether all II_1 factors associated with nonabelian e groups (the so-called 'free group factors') are isomorphic. A variant of this question is whether all free group factors are mentarily equivalent. (Or equivalently, whether they have isomorphic ultrapowers.) The answer to this question is positive if l only if the free group factors $L(F_2)$ and $L(F_3)$ (or any other $L(F_m)$ and $L(F_n)$, for $m \neq n$) are elementarily equivalent.

The C*-variant of this question has a negative answer. The reduced group C*-algebra $\mathrm{C}^*_r(F_m)$ has the K_1-group equal to ^{r}, and therefore these algebras are pairwise nonisomorphic. But the following is open.

mitri Shlyakhtenko

e all reduced group C*-algebras associated with finitely generated free nonabelian groups elementarily equivalent?

One approach to giving a negative answer to this question would be to show that the K_1-groups of the ultrapowers of free up C*-algebras are nonisomorphic. Since each $\mathrm{C}^*_r(F_m)$ has stable rank 1, its K_1-group is equal to $\mathcal{U}(\mathrm{C}^*_r(F_m)/U_0(\mathrm{C}^*_r(F_m))$. us the question reduces to the followig:

Is the homotopy relation on the unitary group of $\mathrm{C}^*_r(F_m)$ definable?

Or even more specific: Is there $n \in \mathbf{N}$ such that every unitary in $\mathrm{C}^*_r(F_m)$ homotopic to 1 can be approximated in norm up < 2 by a product of n exponentials of self-adjoints, each of norm at most π? A positive answer to this question would imply t the K_1 group of $\mathrm{C}^*_r(F_m)$ belongs to the eq of this algebra ([**?**]), and in turn give a negative answer to the above question.

resentation Highlights

s workshop brought together experts in operator algebras and model theory. The first two days of the meeting were domi-ed by three tutorials that provided a fresh look at the background material.

abor Szabo, Introduction to C*-algebras

ill give an introduction to the theory of C*-algebras. Starting from the basics, we will treat spectral theory in some detail, minating in the Gelfand-Naimark theorem. We will cover the GNS construction, with highlight being that every abstract -algebras can be realized as a C*-algebra of bounded operators on a Hilbert space. We will then discuss other construc-ns/examples such as certain universal C*-algebras or inductive limits. If there is time, I will give a rough outline of the iott classification program.

lrian Ioana, Tutorial on von Neumann algebras

the first lecture, I will review basic notions and constructions of von Neumann algebras. The second lecture will be devoted property Gamma and McDuff's property for II_1 factors. In the third lecture, I will discuss the isomorphism problem for rapowers of II_1 factors.

Lecture 1: Define vN algebras and state the bicommutant theorem. Introduce tracial vN algebras and the hyperfinite II_1 tor. Group and group measure space vN algebras.

Lecture 2: Define property Gamma and discuss the connection with inner amenability of groups. Define McDuff's property. Examples of II_1 factors that are Gamma but not McDuff.

Lecture 3: The ultrapower construction for tracial vN algebras. Discuss dependence on the choice of the ultrafilter and examples of II_1 factors with non-isomorphic ultrapowers.

Martino Lupini, Tutorial on model theory

Lecture 1: Structures, ultraproducts, and formulas

I will introduce the fundamental notions of logic for metric structures, such as formulas and ultraproducts. I will then explain how C^*-algebras and von Neumann algebras fit into this framework.

Lecture 2: Axiomatizability and definability

I will present the crucial model-theoretic concepts of axiomatizability and definability, and then provide many examples from the theory of operator algebras.

Lecture 3: Nuclearity and omitting types

I will discuss how nuclearity can be captured model-theoretically, and how this opens up the possibility to use constructions from model theory to produce interesting new examples of nuclear C^*-algebras.

Leonel Robert, C^*-algebras of stable rank one and their Cuntz semigroups

I will talk about recent joint work with Antoine, Perera, and Thiel. We have shown that the Cuntz semigroup of a separable C^*-algebra of stable rank one is inf-semilattice ordered, i.e., has finite infima and addition is distributive over infima. We use this to gain new insights into the structure of these Cuntz semigroups and to answer a number of questions on C^*-algebras of stable rank one. We are able to remove the assumption of separability in some of these applications using model theoretic tools.

Christopher Schafhauser, On the classification of simple, nuclear C^*-algebras

I will discuss some recent joint work with José Carrión, Jamie Gabe, Aaron Tikuisis, and Stuart White, which provides a new abstract approach to the classification of simple, nuclear C^*-algebras.

Aaron Tikuisis, The Toms-Winter conjecture and complemented partitions of unity

The Toms-Winter conjecture postulates that three very different-looking regularity-type conditions coincide for separable simple infinite-dimensional amenable unital C^*-algebras. The different conditions are (i) finite nuclear dimension, (ii) Z-stability, and (iii) strict comparison of positive elements. In the first half of my talk, I will say some things about this conjecture and its important connections to the classification of C^*-algebras.

In the second half of the talk, I will discuss a key concept used in the proof that (ii) implies (i), called complemented partitions of unity (CPoU). As I will explain, this concept provides a method for gluing local witnesses of open types in tracial GNS representations to global witnesses (satisfying the type uniformly over all traces). I will explain complemented partitions of unity in the context of this local-to-global type satisfaction device.

This is joint work with Jorge Castillejos, Sam Evington, Stuart White, and Wilhelm Winter.

Stefaan Vaes, Classification of regular subalgebras of the hyperfinite II_1 factor

I present a joint work with Sorin Popa and Dimitri Shlyakhtenko. We prove that under a natural condition, the regular von Neumann subalgebras B of the hyperfinite II_1 factor R are completely classified (up to conjugacy by an automorphism of R) by the associated discrete measured groupoid. The key step in proving this result is the vanishing of the 2-cohomology for cocycle actions of amenable discrete measured groupoids and the approximate vanishing of the 1-cohomology. This leads us to a new notion of treeability for equivalence relations. I also discuss (non-)classification results for amenable discrete measured groupoids.

Bradd Hart, Correspondences and model theory

In joint work with Goldbring and Sinclair, for tracial von Neumann algebras M and N, we show how to capture the notion of an M-N correspondence model theoretically. We use this correspondence framework to study σ-finite von Neumann algebras and the uniform 2-norm on a C^*-algebra with respect to a collection of states. The role of the ultraproduct will be highlighted for its guidance in determining the correct languages in these cases.

sebio Gardella, Equivariant model theory and applications to C^*-dynamics

e use of (central) sequence algebras in the theory of operator algebras has a long history, dating back to McDuff's characteri-ion of those factors which absorb the hyperfinite II_1-factor. Applications in the context of C^*-algebras are both abundant and -reaching, and they often appear in connection with classification of C^*-algebras. Central sequence algebras are fundamental ls in the study of strongly self-absorbing C^*-algebras, which themselves have tight connections with the Elliott classification gramme. This has prompted a deeper study of ultrapowers and (central) sequence algebras, where model-theoretic methods ve become predominant. Ultrapowers and relative commutants have also been a crucial tool in the study of group actions operator algebras, dating back to the classification of amenable group actions on the hyperfinite II_1-factor. A more recent tance of their use in the equivariant setting is the study of strongly self-absorbing actions. As such, equivariant (central) uence algebras are interesting objects whose systematic study is justified by their wide application in the literature. In this k, we report on joint work with Lupini, where we consider actions of a compact group on a C^*-algebra as a structure in the mework of continuous model theory. The realization that the continuous part of the ultrapower of a G-C^*-algebra is just its rapower as a structure in the new equivariant language, allows us to establish interesting properties, including saturation and ś's theorem. We give various applications to C^*-dynamics, including to strongly self-absorbing actions as well as to Rokhlin mension.

kael Rørdam, Non-closure of quantum correlation matrices and certain factorizable maps, traces on free oduct C^*-algebras, and Connes Embedding Problem

show that the convex set of factorizable quantum channels on a fixed matrix algebra of size at least 11 which factor through te dimensional C^*-algebras is non-closed, and that there exist factorizable quantum channels on matrix algebras that require ancilla of type II_1. We also give a new and simplified proof of the result by Dykema, Paulsen and Prakash that the set of chronous quantum correlations $C_q^s(5,2)$ is non-closed. One can describe factorizable quantum channels on a given matrix ebra in terms of traces on the unital free product of that matrix algebra with itself. We give a description of which of these ces correspond to factorizable maps that can be approximated by ones with finite dimensional ancilla, and we relate this to Connes Embedding Problem.

This is a joint work with Magdalena Musat.

n Hirshberg, On C^*-algebras not isomorphic to their opposites.

each C^*-algebra A, one can construct its opposite A^{op}, which is the same as a Banach space, only with the order of ltiplication is reversed. It is a long-standing and difficult open problem whether there exists a simple separable nuclear -algebra which is not isomorphic to its opposite. I will survey some of the known results and techniques, focusing on the clear case, and discuss a joint paper with Ilijas Farah ([**?**]) in which we construct a simple nuclear non-separable example.

C. Phillips, The Continuum Hypothesis implies existence of outer isometric automorphisms of the l^p Calkin gebra

$p \in (1, \infty)$. We show that the Continuum Hypothesis implies that the l^p Calkin algebra $Q(\ell^p) = L(\ell^p(\mathbb{Z}))/K(\ell^p(\mathbb{Z}))$ isometric automorphisms which are not given by conjugation by invertible isometries in $Q(\ell^p)$. Depending on what is done ween now and the time of the talk, we will describe progress towards proving that it is consistent with ZFC that there are no h isometric automorphisms.

This is joint with with Andrey Blinov.

cientific Progress Made

ring the breaks and evenings, the participants worked in smaller groups. Only time will tell what progress resulted from this eting, and we will list only the progress that we are aware of.

Inspired by Robert's talk and recent Thiel's construction of ultraproducts of Cuntz semigroups, several participants gave a gh outline of a formal model-theoretic framework for Cuntz semigroups. Giving a model-theoretic framework for the study Cuntz semigroup is a major challenge.

A group of participants worked on the early 1970's problem of Brown, Douglas, and Fillmore, asking whether the Calkin ebra can have a K-theory reversing automorphism. By a 2011 work of Farah, it is known that forcing axioms imply a negative wer. A new alley of attack on this prominent open problem, combining KK-theory with some set-theoretic considerations, been outlined.

The recent major progress in Elliott's classification programme, reported in talks by Schafhauser and Tikuisis, inspired many conversations. In particular, the principle CPoU (Central Partitions of Unity) can be restated as a transfer principle from the theory of type II_1 von Neumann algebras to the theory of the so-called strict closures of C^*-algebras. (The latter comes from a generalization of the seminal work of Ozawa on W^*-bundles, [22].) The independently developed model theory of correspondences, reported in Hart's talk ([16]), appears to be tailor-made for studying strict closures of C^*-algebras.

Vaes reported a major breakthrough in our understanding of regular subalgebras of the hyperfinite II_1 factor $\mathcal{R}$ ([24]). The Connes Embedding Problem, one of the most famous problems in the theory of operator algebras, was the subject of Rørdam's talk (see [21]).

Connections to set theory were addressed on the last day of the meeting, in the talks by Hirshberg and Phillips.

Outcome of the Meeting

The talks at this meeting were of an exceptionally high quality. All speakers were given a full hour, and the majority of the talks were given in the old-fashioned way, using chalk and blackboard. This encouraged lively discussions that always continued well past the end of the talk and throughout the meeting.

Participants

Ben Yaacov, Itaï (Université Lyon 1)
Browne, Sarah (Pennsylvania State University)
Chifan, Ionut (University of Iowa)
Courtney, Kristin (WWU Münster)
Dabrowski, Yoann (Université Claude Bernard Lyon 1)
Elliott, George (University of Toronto)
Farah, Ilijas (York University)
Fox, Alec (University of California, Irvine)
Gabe, James (University of Glasgow)
Gardella, Eusebio (University of Muenster)
Goldbring, Isaac (University of California at Irvine)
Hart, Bradd (McMaster University)
Hayes, Ben (University of Virginia)
Henson, C. Ward (University of Illinois at Urbana-Champaign)
Hirshberg, Ilan (Ben Gurion University of the Negev)
Houdayer, Cyril (Université Paris-Sud)
Ioana, Adrian (University of California San Diego)
Ivanescu, Cristian (MacEwan University)
Jekel, David (UCLA)
Kerr, David (Texas A&M University)
Lazzaro, Steven (McMaster University)
Lupini, Martino (Victoria University of Wellington)
Musat, Magdalena (University of Copenhagen)
Peterson, Jesse (Vanderbilt University)
Phillips, Chris (University of Oregon)
Pisier, Gilles (Texas A & M University)
Robert, Leonel (University of Louisiana at Lafayette)
Rordam, Mikael (University of Copenhagen)
Schafhauser, Christopher (University of Waterloo)
Sherman, David (University of Virginia)
Sinclair, Thomas (Purdue)
Skoufranis, Paul (York University)
Spaas, Pieter (University of California San Diego)
Szabo, Gabor (University of Copenhagen)
Thiel, Hannes (University of Münster)
Tikuisis, Aaron (University of Ottawa)
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gnati, Alessandro (KU Leuven)
hite, Stuart (University of Glasgow)
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Chapter 30

Shape Analysis, Stochastic Mechanics and Optimal Transport (18w5151)

ecember 9 - 14, 2018

rganizer(s): François-Xavier Vialard (University Paris-Dauphine), Martin Bauer (Florida ate University), Martins Bruveris (Brunel University London), Tanya Schmah (University Ottawa), Stefan Sommer (University of Copenhagen)

verview of the Field

e mathematical and computational analysis of shape and shape changes has, over the last few years, been at the center focused research efforts, driven by a wide range of applications, from biological imaging to fluid dynamics. Problems in as as diverse as shape optimisation, functional data analysis and computer graphics can all be formulated in terms of shape lysis.

Mathematically, shape analysis combines ideas from infinite-dimensional Riemannian geometry, geometric mechanics, d dynamics and, recently, also sub-Riemannian geometry and stochastic analysis. This interplay of different areas continues historically very fruitful exchange of ideas between geometry, mechanics and applications.

In many instances, shape spaces can be endowed with the structure of an infinite-dimensional Riemannian manifold. Ex- ples include the shape space of curves or surfaces in Euclidean space, the space of densities as well as more general spaces mappings. The diffeomorphism group in particular plays a central role in the field of shape analysis and medical imaging.

The main objective of the workshop was to bridge the gap between shape analysis, stochastic geometric mechanics and plied optimal transport communities and to advance research that crosses the boundaries of the three fields in addition to mmunicating important challenges in shape analysis to researchers in stochastic geometric mechanics and optimal transport.

ape analysis and medical imaging

e space of images is acted upon by the diffeomorphism group and, in the spirit of Grenander's pattern theory [1], differ- es between images can be encoded by diffeomorphisms. In this way medical images can be investigated with the help of emannian metrics on the diffeomorphism group. One of the major applications of Grenander's pattern theory is in com- ational anatomy [2], a field that uses modern imaging techniques, such as magnetic resonance, computed tomography and sitron emission tomography, to perform a precise computational study of functional and anatomical morphology. Currently, extension of statistical tools such as kernel PCA and regression, that are well understood in the linear setting, to finite and nite-dimensional Riemannian shape manifolds is of great interest to the medical imaging and computer vision communities. s in addition provide links with geometric statistics [3], statistical analysis of data taking values in geometric spaces.

Stochastic geometric mechanics

Shapes observed in nature exhibit variations that are often best described stochastically. Thus there is a need, arising from applications, for stochastic shape models, that would enable statistical analysis of shape populations and describe stochastic nonlinear shape variations in a geometrically intrinsic way. The diffeomorphism group, which describes shape variations through its action on shape space [4], allows us to transfer developments happening in the new and growing field of stochastic geometric mechanics to problems in stochastic shape analysis.

Recent work has shown that the Euler-Poincaré equation on the diffeomorphism group has a stochastic analog [5], derived from a stochastic variational principle, that yields natural stochastic models of shape evolution. The diffeomorphism group can be equipped with a Lie group structure giving rise to Brownian type flows that are mapped from the Lie algebra to the group. Lagrangian Navier-Stokes flows [6] also constitute an alternative approach to stochastic flows. In very recent work, it has been shown how such flows can induce stochastic shape evolutions [7] but very little is known about their properties, such as existence, invariant distributions or ergodicity. Stochastic geometric mechanics is still a new field, and the similarity between stochastic flows on finite-dimensional Lie groups and stochastic flows on shape spaces induced by the diffeomorphism group enables developments in both fields to be transferred between them. For example, Riemannian stochastic models in shape analysis are used to construct stochastic models in geometric mechanics, whose definition relies on the affine connection. The workshop had as an objective to introduce in the shape community models from stochastic geometric mechanics, and to link ideas from shape analysis back to geometric mechanics.

Optimal transport

Independently, optimal transport has seen significant development as an area of pure mathematics. One can consider optimal transport as a special case of Riemannian shape analysis, with shapes being probability densities. Improved numerical methods, such as Monge-Ampère type solvers and entropic regularization schemes, have recently expanded the applications of optimal transport to include computer vision, biomedical imaging, machine learning and statistics. Compared to optimisation problems encountered in shape analysis, those in optimal transport often stand out by being convex, thus simplifying and speeding up computations. Nevertheless, embedding optimal transport into the more general framework of shape analysis allows one to consider possible extensions of optimal transport; for example the recently developed unbalanced optimal transport was partly inspired by ideas in shape analysis.

In turn, stochastic variants of optimal transport such as the Schrödinger problem of minimizing the relative entropy with respect to a Wiener process does not, at the moment, have a counterpart in stochastic shape analysis or stochastic geometric mechanics. An important outcome of entropic regularization of optimal transport is the development of algorithms that allow for fast computations of entropically regularized transport maps. For many problems in shape analysis, for example the computation of geodesics on the diffeomorphism group, computational time is still prohibitive for large scale applications. Ideas from optimal transport could prove useful in developing new numerical methods for these problems.

Presentation Highlights

We here discuss the topics presented in the range of excellent talks at the workshop. These highlights start with optimal transport and related topics followed by geometry of diffeomorphisms and hydrodynamics, stochastic geometric mechanics and stochastic shape analysis, and finally mathematical foundations of shape and image analysis.

Applied optimal transport and related topics

Talks concerned with optimal transport started with Ana-Bela Cruzeiro who presented an extension of the Schrödinger problem to Lie group valued processes. The infinite dimensional case and its connection with fluid dynamics ([8]), currently an open research area, was also touched upon. In particular it is not known how to obtain more regularity for the weak generalized flows associated to the Navier-Stokes equations through optimal transport methods and how to approach compressible Navier-Stokes equations.

On the space of probability densities, Christian Léonard presented a reformulation and a generalization of the so-called entropic interpolation of Wasserstein geodesics in terms of Newton equations on the space of densities ([9]). He was able to present a general contraction inequality for the Schrödinger problem on a Riemannian manifold with Ricci lower bound.

Other talks in optimal transport were centered on extensions of optimal transport and applications. Based on [10], semi-discrete numerical solutions of unbalanced optimal transport were presented by Bernhard Schmitzer and interesting connections and applications in fluid dynamic for the generalized Camassa-Holm equations were presented by Andrea Natale as in [11]. Unbalanced optimal transport appears to have applications not only in quantization but more surprisingly in crystallization.

Tryphon Georgiou presented a numerical approximation to optimal transport using Gaussian approximations, and also sented extensions of optimal transport to vector valued and matrix valued optimal mass transport. Based on a matrix ntinuity equation, the Linblad equation known in quantum theory was obtained as a gradient flow of the Von Neuman entropy ich is a non-commutative counterpart of the pioneering result of Jordan-Kinderlehrer-Otto. An open question of interest in s field consists in providing a unified framework to all these generalizations of optimal transport to cone valued measures.

Tom Needham introduced the Gromov-Monge quasimetric, which is a notion of distance between arbitrary compact metric asure spaces that blends the Monge formulation of optimal transport with the Gromov-Hausdorff construction. He dis-sed applications to metric trees, which appear in shape analysis and data visualization. Alice Le Brigant spoke on optimal antization on Riemannian manifolds, which is the problem of finding the best (with respect to Wasserstein distance) finite crete approximation to a given probability distribution. She presented a new online algorithm as well as an application to nmarizing air traffic complexity in which she compared summaries using discrete optimal transport.

Carola Schönlieb has shown the use of the Wasserstein distance in unsupervised learning of regularizers in inverse imaging blems such as tomography, the Wasserstein distance being here approximated via the dual formulation on the space of Lipschitz functions. Another use of optimal transport was proposed by Jean Feydy in shape matching where a similarity ergence [12] was built upon entropic regularization. Importantly, numerical advances on the computation of these metrics a large number of data were shown.

On the numerical side of optimal transport, Jean-David Benamou presented the extension of the Sinkhorn algorithm to a lti-marginal setting as in [13] for the simulation of the generalized incompressible Euler equation which was introduced by enier in the 90's. The Sinkhorn algorithm is known to converge linearly with respect to a Hilbert norm in the case of standard imal transport with two marginals. Although the multimarginal scheme proposed by Jean-David Benamou is variational and vably convergent, it is an open question to prove the linear convergence with respect to a modified Hilbert norm.

Related to these generalized incompressible Euler equations, Andrea Natale presented, as in [11], a generalized Camassa-lm equation based on the unbalanced optimal transport problem, which is related to Bernhard Schmitzer's talk. He has roduced a convex relaxation of the Camassa-Holm equation à la Brenier. The main open question is the tightness of this axation in dimension greater or equal to 2. Andrea Natale showed that in a particular case this relaxation was tight and his nstruction was similar to the one proposed by Cy Maor in his vanishing distance result on the diffeomorphism group.

These optimal transport talks have shown that generalizations of optimal transport are a very active topic of research in nnections with fluid dynamic, quantum theory and practical applications. In all these talks, the entropic interpolation stands and was a central tool for practical use and extensions, and also motivated theoretical developments.

eometry of the diffeomorphism group and mathematical hydrodynamics

e first series of talks on infinite dimensional Riemannian geometry concerned the geometry of the diffeomorphism group he particular context of mathematical hydrodynamics. Boris Khesin focused in his talk on the geometry of the Madelung nsform, which is known to relate Schrödinger-type equations in quantum mechanics and the Euler equations for barotropic-e fluids. He presented a recent result by himself, K. Modin and G. Misiolek [14] in which they showed that the Madelung nsform is a Kähler map (i.e. a symplectomorphism and an isometry) between the space of wave functions and the cotangent ndle to the density space equipped with the Fubini-Study metric and the Fisher-Rao information metric, respectively.

Gerard Misiolek's lecture centered around Arnold's geometric picture [15] for the incompressible Euler equations as odesic equation on the group of diffeomorphisms of the fluid domain equipped with a L^2-metric given by fluid's kinetic ergy. Misiolek gave a detailed overview of the study of the exponential map of this metric and described several recent ults concerning its properties. These investigations of the geometric properties of the L^2-metric on the group of volume pre-ving diffeomorphisms date back to the seminal paper by Ebin and Marsden [16], in which they proved local well-posedness l uniqueness of the solutions to the corresponding geodesic initial value problem. These techniques have been later extended he class of right invariant Sobolev metrics on the full diffeomorphism group. This observation lead to geometric interpre-ons of many prominent equations of mathematical hydrodynamics, including for example the Camassa-Holm [17, 18] or V-equation [19]. In his talk Stephen Preston discussed how many of these one-dimensional Euler-Arnold equations can be ast in the form of a central-force problem

$$\Gamma_{tt}(t,x) = -F(t,x)\Gamma(t,x),$$

ere Γ is a vector in $\mathbb{R}^2$ and F is a nonlocal function possibly depending on Γ and Γ_t. Angular momentum of this system is cisely the conserved momentum for the Euler-Arnold equation. In the solar model, breakdown comes from a particle hitting origin in finite time, which is only possible with zero angular momentum. In his talk Preston discussed some conjectures l numerical evidence for the generalization of this picture to other equations such as the μ-Camassa-Holm equation or the Gregorio equation. Klas Modin presented a recent result with Martin Bauer [20] in which they prove extensions of the n and Marsden result to higher order Sobolev metrics on diffeomorphism groups that are only invariant with respect to volumorphisms. This study reveals many pitfalls in going from fully right invariant to semi-invariant Sobolev metrics; the regularity requirements, for example, are higher. Nevertheless the key results, such as no loss or gain in regularity along geodesics, can be adopted.

While these previous talks focused mainly on properties of the geodesic spray (geodesic initial value problem resp.), the lecture of Cy Maor studied a different geometric question that arises in this context: properties of the geodesic distance induced by right invariant metrics on diffeomorphism groups and in particular the question whether it is positive between distinct diffeomorphisms or not. In this talk he presented a recent preprint by him with Robert Jerrard [21] which shows that the geodesic distance on the diffeomorphism group of an n-dimensional manifold, induced by the $W^{s,p}$ norm, does not vanish if and only if $s \geq 1$ or $sp > n$. The first condition detects changes of volume, while the second one detects transport of arbitrary small sets. In particular he discussed how the failure of these two conditions enables the construction of arbitrarily short paths between distinct diffeomorphisms. This work extends previous results on vanishing geodesic distance by Michor, Mumford and others [22, 23, 24, 25].

Stochastics in geometric mechanics and shape analysis

The talks on stochastics in geometric mechanics and shape analysis concerned symmetry reduction for two different stochastic models, the stochastic variational principle in Lie groups by Arnaudon, Chen, and Cruzeiro [6] and the variational model by Holm [5], together with particle samplers for Feynman-Kac measures on path spaces.

Ana-Bela Cruzeiro's presented the variational principle and Euler-Poincaré reduction of [6]. The setting is a left- or right-invariant metric on a general Lie group. Noise is introduced in Stratonovich form through a set of vector fields on the Lie algebra, and the resulting stochastic perturbations are transported by the push-forward of left-translation to the group. From this, a stochastic action functional is derived. Critical points of this functional are then shown to be amenable to Euler-Poincaré reduction in a setting resembling the deterministic case (see e.g. [26]). In particular, the motion can be described by

$$\frac{d}{dt}u(t) = \mathrm{ad}^*_{\tilde{u}(t)}u(t) + K(u(t))$$

with

$$\tilde{u}(t) = u(t) - \frac{1}{2}\sum_i \Delta_{H_i} H_i$$

and subsequently reconstructed to the group. In the reconstruction equation, a coupling term appears that comes from the Itô to Stratonovich conversion terms.

Alexis Arnaudon discussed the stochastic model of [5] in the context of shape analysis. Stochastic perturbations are here introduced by perturbing the Hamiltonian that before perturbation comes from a right-invariant metric on e.g. the diffeomorphism group. This leads to a different variational principle, again with Euler-Poincaré reduction for critical paths, however in a different form than considered by Cruzeiro et al.. In coadjoint form, the reduced dynamics are governed by

$$d\mu(t) + \mathrm{ad}^*_{dX}\mu(t) = 0$$

with

$$dX = udt - \sum_i \partial_\mu \Phi_i(\mu) \circ dW_t^i \quad \mu = \frac{\partial l(u)}{u}$$

where Φ_i constitute a basis for the noise and l is a reduced lagrangian. Arnaudon showed how the stochastic dynamics through the action of the diffeomorphism group descend to shape spaces, e.g. the landmark shape space. Here, Arnaudon related the model to Langevin dynamics in different forms, particularly the stochastic model of [27], and he introduced a dissipation term on the Hamilton equations as a general link between the two stochastic landmark equations.

Marc Arnaudon discussed continuous time Feynman-Kac measures on path spaces. There equations are central in applied probability, PDE theory, and quantum physics. Arnaudon presented a new duality formula between normalized Feynman-Kac distributions and their mean field particle interactions. This allows rerversible particle Gibbs-Glauber samplers for continuous time Feynman-Kac integration on path spaces. Arnaudon in addition discussed new estimates for propagation of chaos for continuous time genealogical tree based particle models, allowing sharp quantitative estimates of the convergence rate of particle Gibbs-Glauber samples.

Mathematical Foundations of Shape and Image Analysis

Several of the talks on Shape and Image analysis concerned new developments for the LDDMM-framework [28]. The first in this direction was by L. Younes, who presented recent work on equivolumic layers estimation in the cortex. B. Gris described a constrained version of LDDMM and showed how this approach can help to understand the variability within a population of pes. A crucial ingredient for deformation based approaches such as LDDMM is the construction of efficient data attachnt terms. Towards this aim, N. Charon presented several deformation models on spaces of oriented varifolds, which embeds ny previously considered geometric structures like curves, surfaces but also orientation distribution fields. In particular he cussed compressing/quantizing oriented varifold representations in order to numerically accelerate diffeomorphic registra- procedures. D. Kuang presented a completely different method for nonlinear image registration using unsupervised neural works. This led to some discussion about the relative merits of, on one hand, data driven methods such as Kuang's, and on other hand, variational and geometric methods such as LDDMM.

A central concept in LDDMM is the momentum vector field; in a related theoretical talk, T. Ratiu introduced a new neralization of the momentum map concept: a group-valued momentum map, inspired by the Poisson Lie setting.

A second theme in this part of the workshop consisted in the study of intrinsically defined metrics on spaces of geometric ects, such as curves or surfaces. E. Klassen presented a new Riemannian metric on the space of vector valued one-forms, that potential applications for the shape analysis of surfaces. The proposed metric is a direct generalization of the elastic metric ociated to the SRV framework [29], that has been proven successful for the analysis of unparametrized curves. Related to s talk was the presentation of P. Harms, who showed that (fractional) Laplacians depend real analytically on the underlying emannian metric in suitable Sobolev topologies. As an application he presented local well-posedness of geodesic equations (fractional) Sobolev metrics on the space of mappings. While these two talks focused mainly on the existence and form geodesic curves, M. Rumpf studied the existence and construction of spline curves in the context of Riemannian shape ces. In his talk he introduced a variational time discretization for the spline energy, that leads to a constrained optimization blem over discrete paths on the manifold. Existence of continuous and discrete spline curves is established using the direct thod in the calculus of variations and the convergence of discrete spline paths to a continuous spline curve follows from the convergence of the discrete to the continuous spline energy.

utcomes of the Meeting

s meeting provided an excellent occasion to open discussions and develop connections between several related fields: Aped optimal transport, methods involving diffeomorphic matching, the so-called large deformation by diffeomorphisms, and chastic geometric mechanics. Different applications context have shown fundamental differences as well as similarities. In dition, the link between these fields and fluid flows was discussed several times in the talks.

A central discussion topic at conference was the question of finite explosion time of Brownian motion on landmark spaces. consider the LDDMM landmark manifold [30] with metric inherited from a right-invariant metric on the diffeomorphism up. This Riemannian manifold has a global representation as an open subset of Euclidean space. It is thus not compact, ich raises the question of finite time blowup of Riemannian Brownian motion. Several recent works use the landmark Brown motion in applied settings [31, 32] which underlines the interest in the existence question. Furthermore, understanding the cture in the Brownian case may shed light on similar questions for stochastic shape models such as discussed in the talks his workshop. We made significant progress on this question by finding sharper conditions for finite time collision of the dmarks. Current ongoing work evolves around evaluating these conditions to either prove or disprove finite time explosion.

In informal discussion about applications to medical image registration, tips and tricks were shared, and a divergence of nion appeared about the likelihood of large practical improvements over the current state of the art, given that the practical istration problem isn't entirely well-posed.

In addition several new projects and discussions have been initiated during the workshop, including: Cy Maor and Philipp rms on the physics of stress and strain in shape analysis; Martin Bauer, Nicolas Charon, Philipp Harms and Martin Rumpf cussed a new collaboration to obtain a numerical framework for shape analysis of surfaces with respect to higher order bolev metrics; Tryphon Georgiou and Tanya Schmah discussed the restriction of the Wasserstein metric to the space of ussian mixtures. Martin Bauer, Klas Modin and Cristina Stoica discussed and started a new project related to the existence 'peakon' singular-suported solutions for non-Newtonian fluids.

articipants

naudon, Marc (Université de Bordeaux)
naudon, Alexis (Imperial College London)
uer, Martin (Florida State University)
namou, Jean-David (INRIA)
aron, Nicolas (Johns Hopkins University)
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vdy, Jean (Ecole Normale Supérieure)

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Harms, Philipp (University of Freiburg)
Joshi, Sarang (University of Utah)
Khesin, Boris (University of Toronto)
Klassen, Eric (Florida State University)
Kuang, Dongyang (University of Ottawa)
Le Brigant, Alice (ENAC - Ecole Nationale de l'Aviation Civile)
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Miolane, Nina (Stanford)
Misiolek, Gerard (University of Notre Dame)
Modin, Klas (Chalmers University of Technology / University of Gothenburg)
Natale, Andrea (Inria)
Needham, Tom (Ohio State University)
Pennec, Xavier (Université Côte d'Azur and INRIA)
Preston, Stephen (Brooklyn College)
Ratiu, Tudor (Shanghai Jiao Tong University)
Rumpf, Martin (University Bonn)
Schmah, Tanya (University of Ottawa)
Schmitzer, Bernhard (TU Munich)
Schönlieb, Carola-Bibiane (University of Cambridge)
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Younes, Laurent (John Hopkins University)

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Two-day Workshop Reports

Chapter 31

Impact of Women Mathematicians on Research and Education in Mathematics (18w2043)

March 16 - 18, 2018

Organizer(s): Lillian Beltaos (Nikola Tesla Historical Society of Alberta), Amenda Chow (York University)

Overview of the Field

It is well known that women in mathematics have historically been unrecognized and under represented in their significance to the field. The extent of this social and historical oversight came to light at this workshop. The eminent women mathematicians are not well known even among those who teach the material that is directly related to their work and are unaware of this failing to credit them appropriately. The purpose of this workshop was to bring forward the lives and research of some – a small number – of these women and to encourage the participants to engage in initiatives that would correct the history by giving these women a prominence in curriculum and associated courses on the topic of women in mathematics.

Recent Developments and Open Problems

The workshops three working groups provided an opportunity for exploring recent developments and open problems. One working group addressed the need to introduce courses that focus on women in mathematics, either through already existing history of mathematics courses or developing specific courses on women in mathematics. Finally, reaching out to history and science departments and collaborating with those departments to highlight and include the women in mathematics in appropriate courses.

Another working group focused on mentorship and collaboration in research. To this end, a new collaborative research model in mathematics, mostly geared to younger women mathematicians who are taking a leave of a year or two to raise children, to enable them to carry out ongoing research without interruption, has emerged. This new model is now being considered for implementation. It also recognized that a formal support from organizations that have access to funding beyond local levels, should be explored to further access to women in mathematics and introduce associated programs and infrastructure.

The third working group focused on promoting women in mathematics through art based activities such as role playing, music composing and creative writing including poetry and comics. Discussions on how to incorporate such an approach to traditional mathematics courses such as calculus, statistics and algebra were explored.

resentation Highlights

e program included broad topics in mathematics, covering algebra, number theory, calculus, topography, statistics, math logy, physics, cryptology, graph theory and education. It highlighted, repeatedly, the challenges and opportunities that these men had to achieve to gain productive and distinguished status, at times many years later as the social fabric of the past did open the educational opportunities for women in general. The sample of these scientists, each having their own story, clearly ngs out strong and determined individuals who refused to be stopped by the blockages to their education and employment. me used men's names to break through with their research. Some opposed their family stigmas of "girls not needing to be ucated". Some experienced rejection for employment based on their gender, and were not granted degrees that they earned, many years after completion of the program.

cientific Progress Made

s workshop acknowledges the need to recognize the contributions of women in mathematics and other science-related ciplines. Some ways to do this are: developing mentorships and collaboration networks and/or designing a history of women mathematics courses. The networking opportunities with new professional links created has been invaluable to participants furthering research and developments.

utcome of the Meeting

e workshop highlighted a need to examine, not just the past circumstances of the challenges that women have had pursuing thematics, but also, recognizing that even today, women are underrepresented in higher education institutions as researchers l professors of mathematics. To this end, the workshop delivered a powerful message of engagement into carrying on with at has been started at the workshop by considering organizing a similar workshop in two years and assessing the impact of workshop with identification of projects and research initiatives that will take place over this period.

articipants

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ltaos, Lillian (Nikola Tesla Historical Society of Alberta)
ltaos, Andrew (University of Waterloo)
ltaos, Angela (University of Alberta/NRC Nanotechnology Research Centre)
own, Hannah (University of Alberta)
rak, Katie (University of Calgary)
ro, Karen (Grant MacEwan University)
rrero, Gustavo (Athabasca University)
tral, Minnie (Xavier University)
ow, Amenda (York University)
nnolly, Dennis (University of Lethbridge)
Vries, Gerda (University of Alberta)
Dieu, Lauren (University of Calgary)
ropolski, Anastassia (Rice University)
rcia, Amanda (University of Waterloo)
rofsky, Susan (University of British Columbia)
as, Ruth (University of Hawaii at Manoa)
pler, Charles (Mount Royal University)
nson-Leiva, Rose (San Francisco State University)
mley, Allysa (York University)
inali, Sreyasa (Nikola Tesla Historical Society of Alberta)
ayes-Tang, Sarah (University of Toronto)
ynhardt, Kieka (University of Victoria)
sili-Chatzi, Dionysia (University of Ottawa)
odal Persad, Veda (Thompson Rivers University)
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Chapter 32

Ted Lewis SNAP Math Fair Workshop 2018 (18w2221)

April 27 - 29, 2018

Organizer(s): Sean Graves (University of Alberta) Tiina Hohn (MacEwan University) Ted Lewis (SNAP Mathematics Foundation & U of Alberta)

Introduction

The SNAP Foundation is a non-profit organization whose mandate is to encourage the development of mathematics learning resources at the classroom level with very little retraining of the teaching staff, with very flexible budgets, and by utilizing the energy and natural curiosity of the students themselves. The main theme of the BIRS workshop was, "What is a SNAP math fair and how to organize a math fair in your classroom". The presenters mostly consisted of teachers/educators who shared their math fair experiences and success stories.

The first SNAP type math fair was designed in Edmonton by Mike Dumanski and Andy Liu in 1997-1998. Since then, a large number of schools in Alberta and beyond have adapted the SNAP math fair to their needs. The SNAP program has been spread through similar workshops and conferences, and mainly by teachers themselves.

SNAP received its initial funding from the Canadian Mathematical Society and from private donations. PIMS, the Pacific Institute for the Mathematical Sciences, has been a long time financial supporter of our math fairs. BIRS, the Banff International Research Station, has provided funding for the BIRS math fair workshops that have been held in Banff on a regular basis. Currently, our major supporter is Thinkfun - a company that develops a variety of excellent puzzles.

Puzzle Resources

- www.mathfair.com
- www.galileo.org
- www.puzzles.com
- www.thinkfun.com
- www.classic.csunplugged.org

018 Workshop Highlights

major theme of this year's Ted Lewis SNAP Math Fair Workshop was to point out connection of puzzles with the Alberta ucation K-9 Mathematics Program of Studies. *Puzzles and Math Connections*, a new resource developed by Ted Lewis and esa Sutherland, has recently been made available to teachers. The booklet connects various math fair puzzles to specific comes in the Alberta curriculum as well as the American standards.

A second document resulted from the workshop pointing out how math fair addresses the front matter of the Alberta K-9 riculum. Some of the ways that math fair fosters a child's mathematics education are as follows.

Student will...

- gain understanding and appreciation of the contributions of mathematics as a science, philosophy and art,
- exhibit a positive attitude toward mathematics,
- engage and persevere in mathematical tasks and projects,
- contribute to mathematical discussions,
- take risks in performing mathematical tasks,
- exhibit curiosity.

A subsidary result of this year's workshop was the realization that the idea of math fair is not as well known amongst berta teachers as we originally thought. An area of improvement that we agreed to focus on is working to spread this idea to ger audiences. Presenting at teachers conventions and targeting math consultants accross the Alberta districtics should help.

018 Workshop Feedback

s workshop is so helpful for giving people the confidence to try something new. I found it helpful this year to hear how ferent people do their Math Fairs. It's validating to hear that there is no one way that is necessarily better than others, as long kids have choices and are engaged in the process. The other piece that I really enjoy is connecting with other teachers and ving opportunities to hold conversations, share ideas, etc. I always leave feeling motivated!

articipants

drea, Caitlin (preservice teacher)
hworth, Michelle (University of Alberta)
own, April (Peace Wapiti Schools)
rrows, Andrew (Edmonton Public Schools)
nnor, Janessa (Grasslands School District)
Astous, Hélène (Edmonton Catholic Schools)
saulniers, Shawn (University of Alberta)
aves, Sean (University of Alberta)
nderson, Kari (UofA Grande Prairie Campus)
debrandt, Maxine (Mother Earth's Children's Charter School)
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wis, Ted (SNAP Mathematics Foundation & U of Alberta)
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yer, Alyssa (Edmonton Public Schools)
cLeod, Vanessa (Edmonton Public Schools)
ller, Leann (Peace Wapiti Schools)
chols, Ryan (Edmonton Schools)
sanen, Trevor (University of Alberta)
rsaud, Barbara (University of Alberta)
tipas, Erin (Edmonton Public Schools)
lushin, Beth (Grasslands School District)

Press, Lorraine (Edmonton Catholic Schools)
Radloff, Erin (Edmonton Public Schools)
Radtke, Jennifer (Edmonton Public Schools)
Raju, Bindya (Calgary Board of Education)
Sarango-Loayza, dalton (Edmonton Catholic Schools)
Shaw, Dolph (Edmonton Public Schools)
Strungaru, Nicolae (MacEwan University)

Chapter 33

Restructuring IEEE VIS for the Future 18w2230)

une 15 - 17, 2018

rganizer(s): Hans Hagen (University of Kaiserslautern), Daniel Keim (University of onstanz), Tamara Munzner (University of British Columbia), Stephen North (Infovisible), anspeter Pfister (Harvard University)

ntroduction

EE VIS, the premier conference in the field of visualization, is at a crossroad: for many years it has been subdivided into the Vis, InfoVis, and Visual Analytics conferences. There is now considerable appetite to consider alternative structures, such a more unified conference, that may better enhance vibrancy and growth. Our goals are to preserve intellectual diversity ile promoting organizational consistency. A subcommittee (Hagen, Keim, Munzner, North, and Pfister) has been charged by VIS Executive Committee (VEC) to guide this decision-making process, which started in 2016.

Two similar workshops were held in the summer of 2018, at Dagstuhl in Wadern, Germany, and BIRS in Banff, Canada, he cornerstones that provided a broad cross-section of the community a voice into the set of options under consideration. itees included the VEC, VIS Steering Committees, selected members of recent and upcoming VIS Organizing Committees, many earlier-career researchers. The recommendations that arose from these workshops will shape the future of our flagship ue and thus the field of visualization for the coming decades.

rocess

e organizers invited 144 visualization researchers and practitioners who held current and recent organizing and steering mmittee positions and people who participated in the early career meet-up at VIS 2017, which was mainly tenure-track ulty who are ultimately going to lead the future of the VIS conference. The notably high acceptance rate of about 70% icated that the topic of the workshops resonates with the community. Ultimately we had 43 attendees at Dagstuhl and 47 endees at BIRS, including some last minute cancellations.

The participants wrote one-page statements that were shared before the meeting. The organizers gave an initial briefing frame the discussion regarding goals, scenarios, and lenses through which to evaluate them, and concerns and challenges. ticipants made short oral statements highlighting key points from their one-pagers. After a brainstorming session to propose ics for breakout meetings, the organizers grouped the topics into themes. There was a series of breakout meetings, with nary sessions to discuss the results and iteratively re-organize the themes based on progress made. Participants submitted e-page follow-up reflections a few weeks after each workshop.

Unification

A vast majority of attendees were in favor of unifying the three conferences. Although the separation of V-I-S (VAST–InfoVis–SciVis) has a historical basis, it raises many issues. Newer attendees of the VIS conference do not understand the separation and find it confusing. Another problem is that the separation may not align well with paper submissions, in which multiple aspects of visualization are involved that cross-cut the three historical areas. The discussion covered both internal and external unification.

A first step towards external unification, primarily affecting authors, was to allow authors to submit to either V-I-S conference or VIS in general and in the latter case let the PC chairs decide by which of V-I-S conference sub-committees the paper is reviewed. Another proposal was to immediately move to a uniform set of publication mechanisms across all three V-I-S tracks so that they all have conference-only and short papers in addition to TVCG papers. A proposal for external unification, primarily affecting attendees, was to have paper sessions integrated across all three V-I-S tracks. All three steps towards external unification could be implemented immediately, and are independent from an internal unification of the reviewing process.

Proposals for internal unification focused on how the current three-part chairship for organizers from each of V-I-S could be improved. A PC structure based on an area chair model was discussed, where the key questions are the number of areas, exactly what the categories are, the right balance between continuity of existing categories and vibrancy from changing them, and the governance process of how these decisions are made. There was debate over whether starting with the existing three conference areas as the categories, possibly with the addition of a fourth multicategory track, would be a useful first step or a counterproductive diversion from real change.

Publication Model

The publication model was extensively discussed. One major issue is that submission to V-I-S is possible only once a year. Some attendees expressed a desire for a rolling submission model, with several deadlines throughout the year, to increase the number of potential reviewing rounds with the goals of decreasing the burstiness of work for both authors and reviewers and potentially increasing review quality due to less time pressure. However, concerns were raised that increasing the number of submissions to the VIS conference in this way would very likely hurt the submissions to other conferences such as EuroVis and PacificVis and the TVCG journal, to the detriment of the health of the field as a whole.

Another extensive debate revolved around a journal-only option, where journal papers would only be possible through the TVCG umbrella (rather than the current dual-track policy that VIS runs its reviewing and publishes proceedings as a special issue and in addition all TVCG papers have talks at VIS). Although there is substantial overlap between the pool of people who review for both venues and are VIS papers chairs or TVCG associate editors, TVCG policies could be changed abruptly by IEEE Computer Society dictate or by decisions made by its constituencies. Concerns were raised that relinquishing our flagship publication track to an entity that is not under the direct control of the VIS community might be unwise.

There were also suggestions on improving the review process while reducing the burden on individual reviewers and the appropriate target for acceptance rates. There was a desire to accommodate multiple levels of effort and quality under the VIS umbrella because some attendees have goals that do not align with publishing TVCG journal papers. Some suggested adding partnerships with other journals. A substantial majority of attendees were in favor of short papers with a later deadline than the full papers (in the same spirit as EuroVis).

Attendees of the workshop also made several suggestions for new publication formats including explainer sites, online demos, and open source contributions. There was also discussion about improving the quality of some of the presentations into more TED-like talks that would be approachable by a general audience. In general, these new contribution formats need more consideration.

Practitioners

There was strong agreement of the need to attract more practitioners, even as there was a great deal of controversy over who these people are and how we might connect with them more effectively. There was discussion of the many different kinds of practitioners that we might attract and what terms these non-academics might find appropriate for themselves. There was also debate about what kinds of content and mechanisms would align with their incentives, and many noted that papers are not rewarded outside of academia. The suggestion of an option to offer a lower-cost one-day ticket was made, in conjunction with the idea that the technical program could be structured to make one-day attendance more attractive to various types of participants.

rowth in Size, Breadth, and Depth

r the ideal growth in size, there was no consensus. Suggestions ranged from keeping the current size (about 1,000 attendees) aiming for gradual increases up to double in current size, to massive expansion to the size of the CHI conference.

There was a clear wish to increase the range of VIS, both concerning increasing the breadth of targeted topics and the depth our impact on the world including adjacent fields. The suggestions included having more parallel sessions and including new ics such as education.

Also, there was extensive discussion of how to increase the diversity of the community to keep it healthy, covering both nographic diversity (increasing the participation of underrepresented groups including gender, race) and intellectual diversity creasing the participation of people from other fields and of non-academics). In this context, several significant issues were sed: How to start something new in the ecosystem of the VIS conference? How does the entire VIS system relate to adjacent ds such as scientific computing and data science? How can the field do more to recognize the practical successes we have eady had, and highlight them to attract practitioners?

pplication Papers

ere was a clear consensus that we need more application papers. Although the suggestions on this topic were varied, an ion that had strong support was to immediately establish a separate application track for papers, with appropriate reviewing eria that differ from the current call for research papers. This unified track would accept papers from all areas of V-I-S, ependently of any other unification efforts that might take more time to work out for the research papers. A suggestion about ving mini-symposia on designated topics also received positive feedback.

overnance

ere was concern that the upper levels of the organization (VGTC ExCom) are not flexible enough to respond to changing uations and needs by acting on them, due to insufficient turnover and a very top-down structure with a great deal of control m the VGTC chair. For comparison, the SIGGRAPH ExCom has nine elected positions (not just one) and one seat for a past ir (not seven). There was agreement that the VEC would need to change composition in a unified VIS, but no discussion of ncrete alternatives to the current structure. The participants generally agreed there should be a well-defined Code of Conduct the conference itself, not just for the preparation of submitted papers.

ivergence

e two workshops were designed to have many commonalities but also to allow divergent themes to arise from the different s of participants. The most obvious points of divergence were a much more detailed discussion of the journal-only option at gstuhl and the area chair publication model at BIRS.

ext Steps

e committee will report these findings to the Visualization Executive Committee (VEC). This report constitutes an executive nmary; a more detailed version, including a set of committee recommendations, will be distributed to the VEC and the nmunity and discussed at an open meeting at the VIS 2018 Conference in Berlin. The committee would like to thank gstuhl and BIRS for their hospitality and generous support of our endeavors.

articipants

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hapter 34

etreat for Young Researchers in tochastics (18w2239)

ctober 12 - 14, 2018

rganizer(s): Chris Hoffman (University of Washington), Yaozhong Hu (University of Alrta), Ed Perkins (UBC)

verview

s was the fourth annual meeting of the PIMS Postdoctoral Training Centre in Stochastics (PTCS). The Retreat offers an portunity for young researchers in pure or applied probability from Western Canada and Washington state to interact, comnicate their recent results and ongoing research programs and initiate new collaborations. Eight of the nine postdoctoral ows affiliated with PTCS spoke at the meeting. The 25 participants included postdoctoral fellows from U. Washington, U. Alberta and UBC, Ph.D. students from U. Saskatchewan, U. Calgary, U. Alberta and UBC, and faculty from U. Calgary, U. berta, U. Victoria, U. Regina, and UBC.

The response from the participants after the retreat was hugely positive.

resentation Highlights

umanti Podder (UW) spoke about her joint work [1] with Ander Holroyd, Avi levy and Joel Spencer on second order ic and random trees. A sample problem is given by the logical complexity of the statement that a tree is finite, or infinite. initeness can be expressed by an 'existential monadic second order (EMSO) sentence', but finiteness cannot. This logical ult does not preclude the possibility that for a class of random trees, there exists an EMSO sentence that with probability does detect finiteness. Podder shows this is not possible for Galton-Watson trees with a Poisson offspring law. The proof ceeds by an elegant mapping of the problem into a set of games. The result holds for more general offspring mechanisms the proofs require the offspring law to have full support, although it is expected to be true much more generally. After a estion of Yinon Spinka, a discussion ensued on whether or not there is an EMSO sentence that detects finiteness with positive bability.

Sarai Hernandez (UBC) spoke about her ongoing joint work with Omer Angel, David Croyden and Daisuke Shiraishi on ling limits of Uniform Spanning Trees (UST) in 3 dimensions. In dimension 2 the scaling limit is SLE(8) and in high nensions it is believed to be super-Brownian motion, but in intermediate dimensions (like 3) the non-Gaussian limits that are icipated are notoriously difficult to find, let alone study. For Loop Erased Walk, Kozma [2] had shown that along dyadics re is a scaling limit in 3 dimension as random sets with the Hausdorff metric but little is know about this non-Gaussian it. Given Wilson's algorithm, there is a close connection here with limits of UST's. The striking result of Sarai and her authors is that rescaled UST's in 3 dimensions converge in the space of paths (and so also in the space of random sets) to a iting object. This ancestral structure gives us some additional insight into this limiting object. They are currently working on extending this groundbreaking result to convergence in the space of metric spaces equipped with the Hausdorff-Gromov topology.

Liping Xu (UW) presented some very recent work with Zhenqing Chen on pathwise uniqueness for finite-dimensional stochastic differential equations (SDE's) with multiplicative noise and non-Lipschitz drifts driven by a Lévy process. The classical results here for Brownian motion with additive noise were resolved some forty years ago by Zvonkin [4] and Veretennikov [3]. The analogue of Zvonkin's original transformation is still the tool being used but obtaining the required regularity of this map for integral operators when dealing with multiplicative noise is a much more difficult problem. Xu first presented recent work of Chen, Zhang and Zhao which establishes pathwise uniqueness for "α-stable-like" Lévy processes and β-Hölder continuous drift for $\beta > 1 - \alpha$. The latter is sharp as classical results of Tanaka, Tsuchiya and Watanabe showed. However, the rather specific nature of the noise should not be needed here. Dr. Xu's recent result extends this work by allowing one to add much more general Lévy processes which have an α-stable-like component. The result is intuitive but establishing the analogue of Zvonkin's transformation in this non local setting when $\alpha < 1$ is quite interesting.

Yinon Spinka (UBC) spoke on the problem of determining whether or not a given translation-invariant random field on $\mathbb{Z}^d$ is a finitary factor of an i.i.d. process (ffiid). Spinka presented various sufficient conditions for a translation invariant process on $\mathbb{Z}^d$ to be ffiid. The conditions include a spatial mixing properties for Markov random fields, monotonicity and uniqueness of the Gibbs measure. Quantitative results on the tails of the coding radius were also presented (exponential or polynomial decay of tails). Here stronger mixing properties of the Markov random fields lead to faster decay of tails. Finally, he presented applications to various well-known models from statistical physics such as the Potts model, proper colorings and the random cluster model.

The lively Open Problems Session featured 5 problems from math finance and insurance, population genetics, and coding theory. Noah Freeman asked for the distribution of the ordered excursion length of the sticky Brownian bridge–note that the conditioning here is not singular as . Yinon Spinka asked Noah about considering the Brownian path up to the time when the local time hits 1 (instead). Noah pointed out this law in the non-sticky case is different. Ed Perkins discussed it with Noah hiking up Tunnel Mountain and felt Yinon's model may be more relevant to the sticky case than the bridge case and they agreed that conditional on the local time at 0, one should get a scaled Poisson-Dirichlet law and so it reduces to the law of this local time which looks quite accessible. Spinka asked a follow up question from his lecture on finitary coding. Tony Ware asked about 'Hawaiian options': this is an option which is traded in energy markets, where on exercise of the option (call or put) the holder receives an option of the other type, put or call. The infinite time horizon causes some difficulty in valuation, and there was a lively discussion on approaches to the problem.

Outcome of the Meeting

The level of talks at this Retreat was extremely high in terms of content and presentation. Five of the ten lectures were given by outstanding young female probabilists from U. Alberta, U. Calgary, U. British Columbia and U. Washington. The Open Problems Session was also particularly successful. For example, the day after his presentation Tony Ware announced that as a result of the discussion he had made significant progress on the Hawaiian options problem.

A number of the participants wrote after the meeting, all expressing thanks for a stimulating meeting. Yaozhong Hu (CRCI at U. Alberta) pointed to new connections made with faculty and young researchers at U. Calgary.

During the meeting it was agreed that after the funding for the Postdoctoral Training Centre for Stochastics stops, we should continue these annual meetings featuring young researchers in Probability from PIMS sites. It was felt that a 3-day meeting might be better to offer more time for informal discussion. With recent hires in Probability at U. Alberta and U. Victoria, both those sites were discussed. Tony Ware suggested we meet for a day or two at U. Calgary and then move on to BIRS for another two days.

Participants

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Chapter 35

CS-Can/Info-Can State-of-the-Discipline nd Planning Retreat (18w2240)

ovember 16 - 18, 2018

rganizer(s): Kellogg S. Booth (UBC), Yvonne Coady (University of Victoria), Doina Precup IcGill University), Carey Williamson (University of Calgary)

A representative group drawn from the Canadian Computer Science (CS) community gathered in Banff in November 2018 discuss the future of our discipline. The attendees included a diverse selection of about 30 Canadian CS academics, students, l industry representatives, all of whom were extremely passionate about CS research, education, and innovation. The retreat s organized by CS-Can/Info-Can [10], which is the new national organization for Computer Science in Canada. The retreat ped foster a shared vision for the organization, and identified how it can better support the evolving needs of CS in Canada.

verview of the Field

mputer Science as a discipline is about 50 years old, having emerged from its mathematical and engineering roots in the e 1960's and early 1970's at most academic institutions in Canada, and subsequently coming to the forefront as a significant entific discipline within the past three decades.

Modern CS is typically characterized into three branches: Theory (e.g., algorithms, graph theory, complexity theory, numer- l analysis, optimization), Systems (e.g., operating systems, networks, distributed systems, computer architecture, databases, gramming languages), and Applications (e.g., artificial intelligence, computer graphics, human-computer interaction (HCI), tware engineering, gaming). Canada is a recognized world leader in several areas of CS, such as Artificial Intelligence (AI), eory, and HCI.

The CS discipline continues to grow and evolve, with Machine Learning (ML), Data Science, and Cyber-Security as three mples of areas of significant growth at many Canadian universities [9]. There are also many emerging multi-disciplinary as based on important applications of CS that are increasingly receiving attention (e.g., augmented reality, digital humanities, lth informatics, and social computing).

ecent Developments and Open Problems

e most vexing problem for CS in Canada has been the lack of a visible and effective national organization. Although the mer CACS/AIC (Canadian Association of Computer Science/Association d'Informatique Canadienne [1]) had existed for out 25 years, it was viewed as a "heads only" administrative organization based on a departmental membership model that l minimal engagement with research funding organizations such as NSERC, and low visibility among faculty members hin its constituent departments. The recent transition from CACS/AIC to the new CS-Can/Info-Can organization (launched September 2016) is intended to help the organization have much more impact on the discipline and on the role of CS within nada. CS-Can/Info-Can is modeled in part on the 40-year-old Computing Research Association (CRA [6]) in the United

States, as well as on other national academic organizations in Canada (e.g., Canadian Association of Physicists [2], Canadian Mathematical Society [4]). Its mandate is CS research and education.

One general trend in CS globally right now is growing enrollments, especially at undergraduate levels, with a 20-50% increase in students in recent years [7, 8, 11]. The same trend has occurred in CS departments across Canada, as students see new opportunities in areas such as ML, data science, social networking, mobile computing, and entrepreneurship. While this is great for our discipline, it is difficult to accommodate these students without additional budgetary resources, and many CS departments in Canada are facing this challenge right now.

Another pernicious problem in CS and Engineering disciplines is achieving diversity, especially for female enrollment, which is typically only 10-15% of the undergraduate student population at most institutions. Curiously, CS enrollment was much closer to being gender-balanced in the 1980's, but has seen a steep decline in female enrollment since then. While recent efforts at remediating this problem are starting to have an impact, with female enrollments nearing 25-30% at some institutions, there is still a long way to go to reach gender parity. Furthermore, the CS pipeline needs to consider all aspects of diversity, not just gender (which itself is undergoing a significant transition from its historical binary dichotomy to a broader and more nuanced understanding), since there are many other under-represented groups (e.g., First Nations). Addressing these diversity issues is important for the long-term health of the discipline.

Another perennial issue for CS researchers is finding the right balance between fundamental (theoretical) research and applied (practical or industry-oriented) research. The trend in our national funding agencies is toward partnership programs featuring university-industry interaction. However, an over-emphasis on this type of applied research has the potential to polarize our community into "haves" and "have-nots". Furthermore, Canada's Information and Communication Technology (ICT) industry is uniquely characterized by a preponderance of Small and Medium Enterprises (SMEs), not all of whom have the resources to undertake partnership programs like larger companies do. This is especially true of start-up companies that do not have well established research groups that can partner with academic researchers. As a result, CS as a discipline feels disadvantaged by some of these granting programs. While multi-disciplinary collaborative research programs are definitely a viable opportunity for CS, oftentimes the focus is on using CS as a tool to advance research in other disciplines, rather than focusing on CS research itself. As a result, CS researchers sometimes see themselves marginalized in these programs, which is why CS is often under-represented in major grant applications. These issues have been well-documented [13] by the former (2011-2016) NSERC CS Liaison Committee [12], which in turn helped spur the creation of CS-Can/Info-Can.

Presentation Highlights

The retreat was structured into a combination of plenary sessions for all attendees, and working breakout sessions for subgroups of the attendees.

The opening plenary session helped set the general context and goals for the retreat. Specific highlights included the perspectives shared by the representative from the US-based CRA (Andy Bernat), as well as the strategic views on governance and policy articulated by Arvind Gupta (University of Toronto) from his senior leadership experiences at MITACS and UBC. Other plenary sessions were used for brainstorming vision and mission statements for CS-Can/Info-Can, and to share results from the breakout sessions.

The breakout sessions were designed to address particular issues identified prior to the retreat and refined on site. There were six breakout sessions, with themes on Membership, Education, Research, Industry, Outreach, and Communication. Each attendee participated in three of the six breakout sessions, which were run concurrently (two at a time). The breakouts allowed deeper small-group discussions on the chosen topics, with results brought back for sharing with the group as a whole in subsequent plenary sessions.

The notes and blackboard photos from all of the sessions have been collected and archived into the Google Documents maintained by the leadership of CS-Can/Info-Can as resources for the working groups that will continue activities initiated at the retreat. A summary of the discussions and recommendations will be shared with the Canadian CS research community at the next CS-Can/Info-Can Annual General Meeting, which will take place at McGill University on June 3-4, 2019.

Progress Made

Substantial progress was made on new vision and mission statements for CS-Can/Info-Can. We need a vision statement that is pithy, meaningful, and easy to articulate both within and outside of the CS community. The mission statement will make this vision more concrete, by outlining the specific thrusts to address the needs of our CS stakeholder communities. A working group was identified at the retreat and tasked with completing our vision and mission statements, which will then be shared with the larger group.

The retreat helped build a stronger sense of community for those in leadership positions within CS in Canada, who share a nilar vision for our discipline, and much passion for it as well. One tangible result was raising the collective awareness about initiatives taking place across the country (e.g., outreach, K-12 CS education, industry collaborations, research funding op-tunities, Can-CWiC [3], CUCSC [5], UCOSP [14]), several of which we believe can be brought together under the umbrella CS-Can/Info-Can. Another tangible result was the formation of a set of working groups to follow up on selected retreat ics (e.g., Diversity Committee, Vision/Mission statement working group, Industry Advisory Board, mentoring network for ge research grant applications).

utcome of the Meeting

e retreat was viewed as a success by the organizers, as well as the attendees. One major outcome was the set of initial steps defining a vision for CS in Canada, which will help CS-Can/Info-Can in its ongoing strategic planning. Another important come was clearly identifying the many different stakeholder groups for CS in Canada (e.g., government, industry, K-12, ding agencies, under-represented groups), and identifying strategies to address their specific needs. Last but not least, the reat helped build the "people network" of key CS leaders (past, present, and future) across the country, and identify resources help move our discipline forward.

As with any strategic planning exercise, the hard part still remains, namely identifying and carrying out an actionable plan t makes a difference. As a group, however, we are extremely optimistic about the future of CS in Canada as a research-ed academic discipline and as an important contributor to the Canadian economy and society at large. Our retreat at BIRS helped galvanize a shared vision for CS that will allow CS-Can/Info-Can to become a much more effective and impactful ional organization.

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Focused Research Group Reports

Chapter 36

The crystal structure of the plethysm of Schur functions (18frg224)

April 1 - 8, 2018

Organizer(s): Mike Zabrocki (York University), Franco Saliola (Université du Québec à Montréal)

Our focused research group consisted of Laura Colmenarejo, Rosa Orellana, Franco Saliola, Anne Schilling and Mike Zabrocki. We worked at the BIRS station from April 1 until April 8 (except Rosa Orellana who left on April 6).

The problem

The irreducible polynomial representations of GL_n are indexed by partitions with at most n parts. Given such a representation indexed by the partition λ, its character is the Schur polynomial

$$s_\lambda = \sum_{T \in \mathrm{SSYT}(\lambda)} x^{\mathrm{weight}(T)}. \tag{36.0.1}$$

Composition of these representations becomes composition of their characters, denoted $s_\lambda[s_\mu]$ and this operation is known as the operation of plethysm. Composition of characters is a symmetric polynomial which Littlewood [Lit44] called the (outer) plethysm. The objective of our focused research group project is the resolution of the following well known open problem.

Problem 36.0.1 *Find a combinatorial interpretation of the coefficients $a^\nu_{\lambda,\mu}$ in the expansion*

$$s_\lambda[s_\mu] = \sum_\nu a^\nu_{\lambda,\mu} s_\nu. \tag{36.0.2}$$

In the last more than a century of research in representation theory, the basic problem of understanding the coefficients $a^\nu_{\lambda,\mu}$ has stood as a measure of progress in the field. A related question that we felt was an important first step in the resolution of Problem 36.0.1 is the following second approach to understanding the underlying representation theory.

Problem 36.0.2 *Find a combinatorial interpretation for the multiplicity of an irreducible S_n module indexed by a partition λ in an irreducible polynomial GL_n module indexed by a partition μ.*

We will discuss briefly below why the resolution of Problem 36.0.1 will also solve Problem 36.0.2, but we generally believe that the second question we are considering can be used as a guide for the resolution of the first.

We arrived at Banff with two different approaches to this research. Some preparation for this meeting was carried out by email in the weeks before in a discussion about how the different ways of looking at the underlying combinatorics and representation theory are related.

Overview of the direction of research

With five people working intensely on this problem we mainly focused on two different (but ultimately equivalent) approaches. Working as two groups, we followed the main ideas of each others progress with the intention that ideas about what would be successful from one approach could be translated to the other .

The first approach was to use the restriction coefficients from GL_n to S_n as a guide to computing the coefficients $a_{\lambda,(r)}$ (a subset of the full plethysm problem, but we expect that this base case could serve as a guide to the more general plethysm problem). The Schur function s_μ is the character of an irreducible polynomial GL_n module and, since the symmetric group S_n is embedded in GL_n, it can also be considered as the character of an S_n module. We are then looking for the multiplicity of an irreducible S_n module indexed by a partition λ in the irreducible GL_n module indexed by the partition μ. There is a theorem due to Littlewood [Lit50] that this multiplicity is equal to the coefficient of s_μ in the plethysm expression $s_\lambda[1+s_1+s_2+s_3+\ldots]$. Due to other combinatorial considerations, it suffices to understand the plethysm $s_\lambda[s_r]$ to resolve this question.
An idea from a talk by Arun Ram [Ram2017] that we had discussed before arriving at BIRS encouraged us to look closely at an insertion algorithm that combinatorially described the decomposition of $V_n^{\otimes k}$ into S_n irreducibles. The decomposition of $V_n^{\otimes}$ into GL_n irreducible modules is well understood combinatorially through crystals and the Robinson-Schensted-Knuth insertion algorithm. We began with a new insertion algorithm (similar to, but not the same as, the insertion algorithm Ram described in his talk) and then found that the dynamic reading word of Loehr and Warrington [LW12] could be used as a guide to make it compatible with the usual crystal structure of $V^{\otimes k}$. This approach looks extremely promising and it has been the subject of two follow-up research meetings in April.

The second approach that we considered in parallel with the first was to put a crystal structure on combinatorial objects representing the monomial expansion of plethysms. The papers of Marc van Leuwen [vL99] extending the work of Carré and Leclerc [CarLec95] describe the crystal structure of combinatorial objects representing the monomial expansion of $s_2[s_\lambda]$ and $s_{11}[s_\lambda]$ known as domino tableaux. Our main focus here was to extend the known crystal structure on these domino tableaux to ribbon tableaux to compute $s_\mu[s_\lambda]$ for partitions of μ larger or equal to 3. A note at the end of [vL99] indicated that this idea was tried and was known to be difficult, but we had hoped that almost two decades of research and understanding of crystals might make this approach amenable. In particular, the technique of tableaux switching, which recently also has played an crucial role in Schubert calculus, seems to be an important ingredient in this approach.

Participants

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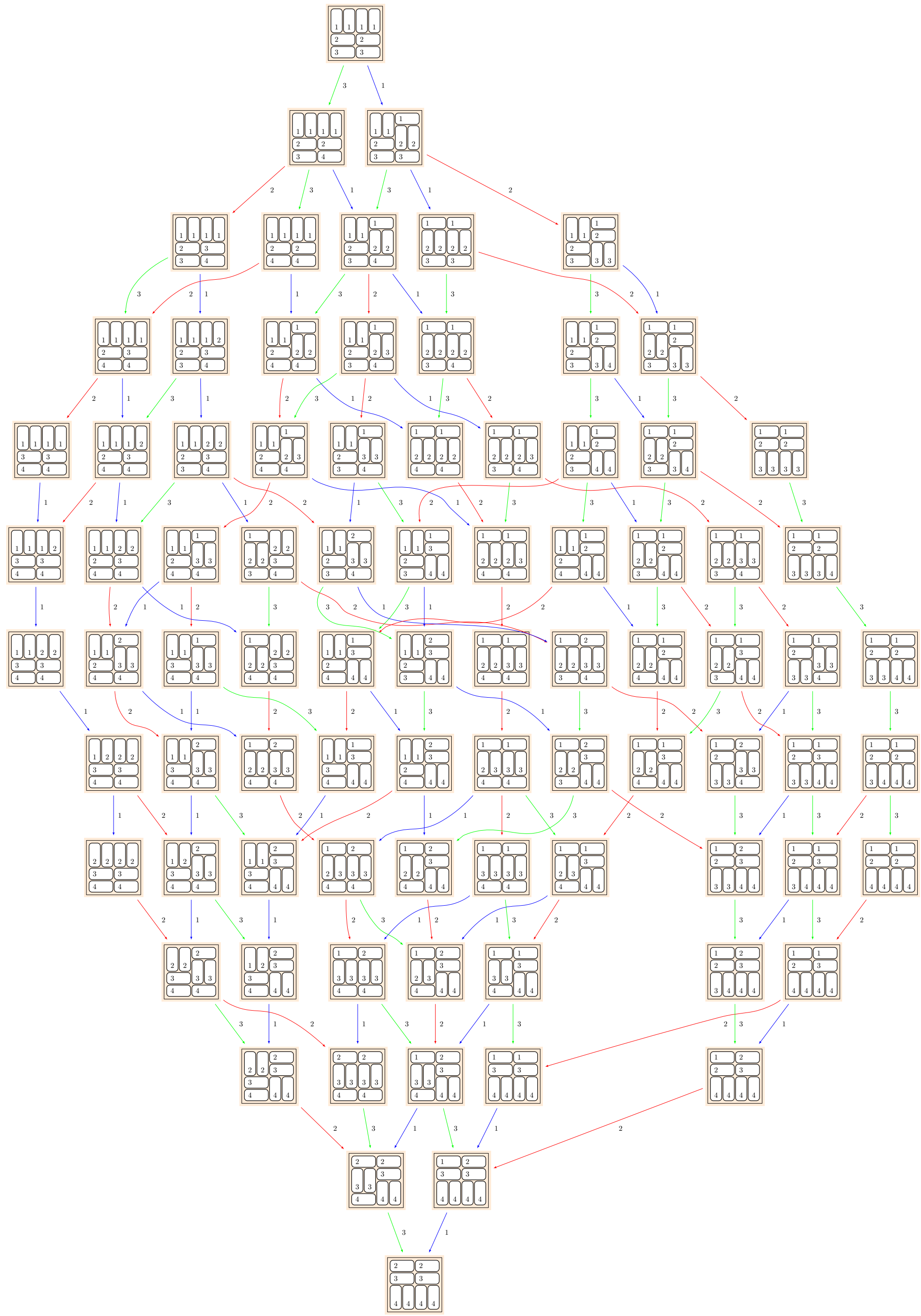

Figure 36.1: A connected component of the crystal structure on the set of domino tableaux of shape 4444. This component corresponds to the Schur function s_{422} appearing in the plethysm $s_2[s_{22}] = s_{2222} + s_{3311} + s_{422} + s_{44}$.

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Chapter 37

Stability Indices for Nonlinear Waves and Patterns in Many Space Dimensions (18frg225)

June 17 - 24, 2018

Organizer(s): Margaret Beck (Boston University), Graham Cox (Memorial University), Christopher Jones (UNC Chapel Hill), Yuri Latushkin (Missouri)

Overview of the Field

Assessing the stability of distinguished states of a nonlinear partial differential equation is a key step in understanding the behavior of the physical system modeled by the equation. Stability here means the robustness of the dynamics to perturbations in initial conditions from a particular state. The distinguished state may be a nonlinear wave, pattern or coherent structure arising in applications such as optics, fluids, chemical reactions, neuroscience, and ecology. Its stability indicates its physical realizability, while any instability suggests more complex dynamics, and understanding the nature of such instabilities can be used as a jumping off point for understanding the organization of the nonlinear dynamics away from the unstable state.
For instance, consider a system of reaction-diffusion equations

$$u_t = \Delta u + F(u)$$

on a bounded domain $\Omega \subset \mathbb{R}^n$, where $u(x,t) \in \mathbb{R}^N$ and $F\colon \mathbb{R}^N \to \mathbb{R}^N$. It is well known that the stability of a stationary solution $\hat{u}$ is determined by the spectrum of the linearization

$$Lv = \Delta v + \nabla F(\hat{u})v.$$

The case of a scalar ODE, where $n = N = 1$, is well understood. In this case Sturm–Liouville theory relates the stability of $\hat{u}$ to its geometric properties (e.g. number of critical points). The Maslov index generalizes this theory to systems of ODEs in the special case that the operator L is selfadjoint; see [3] for a recent application.
The Maslov index has also been used to obtain stability criteria for multi-dimensional problems, but in general is very difficult to compute. Other methods that exist in multiple dimensions, such as the Evans function on channel domains, and variational methods for Hamiltonian systems, apply only in special cases. For the above reasons, our workshop emphasized the following generalizations of Sturm's oscillation theory:

1. non-symmetric systems of ODEs—we focused on extending the definition of the Maslov index to non-Hamiltonian systems, which allows us to study non-selfadjoint eigenvalue problems $Lv = \lambda v$.
2. PDEs (selfadjoint or otherwise)—here we focused on developing new tools for multi-dimensional stability, as well as finding new tools for efficiently computing the already developed Maslov index.

Recent Developments and Open Problems

The following sections summarize the major topics discussed during our program, including recent developments, progress made during the course of the workshop, and topics of future research.

The fat Lagrangian Grassmannian and the generalized Maslov index

Let (V,ω) be a symplectic vector space of dimension $2n$. The Lagrangian Grassmannian is the submanifold of the Grassmannian of n-planes $\Lambda \subseteq Gr_n(V)$ consisting of n-planes that are isotropic with respect to ω. It is a homogeneous space diffeomorphic to $U(n)/O(n)$ and has fundamental group $\pi_1(\Lambda) \cong \mathbb{Z}$. Therefore continuous loops $f\colon S^1 \to \Lambda$ are classified up to homotopy by an integer invariant, called the Maslov class.

Fix a $P \in \Lambda$ and define $Z := \{W \in \Lambda \mid W \cap P \neq \{0\}\}$ to be the set of Lagrangian n-planes which intersect P non-trivially. We call Z the "train" or the "Maslov cycle." It represents a homology class which is Poincaré dual to a generator of $H^1(\Lambda,\mathbb{Z}) \cong \mathbb{Z}$. Consequently, if a loop $f\colon S^1 \to \Lambda$ intersects Z in a sufficiently generic way, the Maslov index of f is equal to the geometric intersection number of f with Z (see [1, 12]).

An open problem is to construct a "Fat Lagrangian Grassmannian"; that is, a subspace $F \subseteq Gr_n(V)$ strictly larger than Λ which satisfies

i) $H^1(F;\mathbb{Z}) \cong \mathbb{Z}$ so that one can assign a Maslov index to loops in F, which

ii) equals with the geometric intersection number with the train $Z_F := \{W \in F | W \cap P \neq \{0\}\}$.

In the case $n = 2$, such an F has recently been constructed; this was presented by Tom Baird at the workshop. Graham Cox presented some work he had done relating the generalized Maslov index to the Turing instability phenomenon.

During discussions, it was observed that F in $Gr_2(V)$ is contains the complement of the Lagrangian Grassmanian of a different symplectic structure. This works as follows: Identify $V = \mathbb{H}$ with a one dimension quaternionic vector space. In particular, $\mathbb{H}$ admits three orthogonal complex structures I, J, K satisfying the quaternionic relations. Each of these determines a symplectic form $\omega_I, \omega_J, \omega_K$ in the standard way. Suppose that $P \subset V$ is Lagrangian with respect to both ω_I and ω_J. Then the fat Lagrangian Grassmannian F_I corresponding to I contains the complement of the Lagrangian Grassmannian Λ_J determined by J. This observation implies that Hamiltonian flow with respect to ω_J will preserve a dense open subset of F_I. Furthermore, given appropriate initial conditions, it should be possible to violate the Hamiltonian property to some degree while still remaining inside of F_I. This hopefully will allow Maslov index methods to be applied in non-Hamiltonian situations.

Sturm oscillation theory for non-local operators

Non-local operators naturally appear in fluid mechanics, mathematical physics, mathematical finance, and in probability theory (see, for example, [2, 4, 5, 9]). The spectral properties of such operators play an important role in the study of stability of solitary waves for several nonlinear dispersive models, e.g., generalized Benjamin–Ono equation, Benjamin–Bona–Mahony equation, and the fractional non-linear Schrödinger equation. One of the main open problems in the spectral theory of the associated linearized operators is finding sharp estimates on the number of nodal domains of the eigenfunctions.

Several recent results (cf., e.g., [2, 5, 9]) rely on an elegant reformulation of the problem in terms of the Dirichlet-to-Neumann maps for higher-dimensional local operators, the Courant nodal domain Theorem, and the combinatorics of noncrossing partitions. The obtained bounds do not match their counterparts from the standard (i.e., local) Sturm oscillation theory and have not been shown to be sharp.

Since most of the classical tools (such as Sturm comparison results, shooting argument) do not seem to be applicable in the study of nodal domains for non-local operators, it is natural to approach this topic using the recently discovered symplectic properties of the operators in question. We therefore propose to investigate the "Maslov-index" program for the fractional Laplacian.

Problem 1. Reformulate the eigenvalue problem for the non-local operators in terms of the intersection of certain Lagrangian planes (i.e., generalize [10, Theorem 3.2] to the case of fractional Laplacian).

Problem 2. Establish a relation between the eigenvalue counting function and the Maslov index of the Lagrangian planes (i.e., extend [10, Theorem 3.3] to the case of fractional Laplacian).

Problem 3. Investigate monotonicity of the crossings/conjugate points for a fixed spectral parameter.

Problem 4. Estimate the Maslov index to obtain a bound on the eigenvalue counting function in terms the number of zeros of the eigenfunctions.

The Souriau map and the Evans function

One of the main achievements of the workshop was realization of the fact that Maslov index computations are closely related to a construction of the infinite dimensional Evans function. The Evans function is a Wronskian-type determinant which is an analytic function of the spectral parameter λ. It is equal to zero at the points of the spectrum of the differential operator under consideration. The Evans function is usually constructed by means of certain subspaces parametrized by the spectral parameter. The intersection of these subspaces is nontrivial if and only if the respective value of the spectral parameter λ is a zero of the Evans function. To detect if these subspaces indeed have a nonzero intersection we propose to employ the widely used in the Maslov index theory Souriau map $W(\lambda)$ (cf. [7, 8]). This is a unitary operator whose spectral flow through -1 is a count, including both multiplicity and direction, of the number of times these subspaces intersect. We obtained some preliminary results indicating that -1 belongs to the spectrum of $W(\lambda)$ if and only if certain perturbation determinant, $E(\lambda)$, constructed by means of $W(\lambda)$, is equal to zero. Thus, $E(\lambda)$ may serve as an infinite dimensional Evans function. We stress that one of many possible definitions of the Maslov index is given in terms of the spectral flow of eigenvalues of the Souriau map through -1.

Geometric phase

An alternative approach to counting the eigenvalues inside a simple closed curve is given by a geometric phase defined in the Hopf Bundle and its generalizations. The idea is that a stability index can then be determined by taking a curve that would be known a priori to contain any potential unstable eigenvalues. The theory was developed in a paper by Grudzien, Bridges and Jones [6] in the context of traveling waves. There is an alternative formulation of phase in terms of Stiefel bundles and one topic discussed was whether this phase contains any extra information. The structure group of the bundle will be $U(n)$ in this case and not simply $\mathbb{S}^1$. There is therefore the potential for extra information. The geometric phase also offers the possibility of an alternative index for stability in problems on multi-dimensional domains. This is the main focus of our effort for generalizing the geometric phase. It is analogous to defining the Evans Function for a multi-dimensional domain, but offers the possibility of circumventing some of the technical issues in defining the full Evans Function. The formulation of a geometric phase will then be based on infinite-dimensional bundles. We considered the work of Quillen [11] and others as a basis for this formulation. While we did not resolve the problem and, indeed it looks challenging, we were able to lay out a clear plan for moving forward.

The Spatial Evolutionary System (SES)

Another major topic of discussion was the spatial evolutionary system—a reformulation of a semilinear elliptic PDE as a first-order infinite-dimensional dynamical system. In its simplest form it says that the PDE $\Delta u = F(u)$ on $\mathbb{R}^n$ is equivalent to the system

$$\frac{df}{dt} = g, \quad \frac{dg}{dt} = F(f) - \frac{1}{t^2}\Delta_{\mathbb{S}^{n-1}} f - \frac{n-1}{t} g,$$

where f and g are functions on $\mathbb{S}^{n-1}$, parameterized by t. More generally, it describes the evolution of the Cauchy data

$$f(t) = u\big|_{\partial\Omega_t}, \quad g(t) = \frac{\partial u}{\partial n}\bigg|_{\partial\Omega_t}$$

on a one-parameter family of hypersurfaces, where $\{\Omega_t\}$ is a family of domains that shrinks to a point as $t \to 0$.

So far we have been able to prove the equivalence of the SES to the original PDE in a wide variety of settings. Moreover, we have shown that the linearized equation admits an exponential dichotomy. This means at each time t_0, the space of data $(f(t_0), g(t_0))$ can be split into two complementary subspaces: one consisting of solutions that grow exponentially as $t \to -\infty$, and one of solutions that decay exponentially in the same limit. The latter of these two spaces, the so called unstable subspace, arises in the construction of the multi-dimensional Maslov index and Evans function. Thus the SES gives a new dynamical interpretation of this object, which we believe will be useful in linear stability computations.

Outcome of the Meeting

At the meeting we made significant progress on ongoing projects (the SES and the generalized Maslov index) and new projects (the multi-dimensional Evans function), and started discussing new stability tools as well as new applications of our existing machinery (the geometric phase, oscillation theory for non-local operators). Overall the meeting was very productive, and led to many new ideas with the potential for significant impact on the study of dynamical stability in multiple spatial dimensions.

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Chapter 38

Investigating Linear Codes Via Commutative Algebra (18frg220)

July 22 - 29, 2018

Organizer(s): Susan Cooper (University of Manitoba), Alexandra Seceleanu (University of Nebraska–Lincoln), Stefan Tohăneanu (University of Idaho), Adam Van Tuyl (McMaster University)

Overview of the Field

The importance of coding theory to the digital era that we live in cannot be overstated. Our research meeting aimed to explore the relationship between the theory of error-correcting codes and the more classically studied fields commutative algebra and algebraic geometry, with the goal of establishing a toolset of joint relevance.

A linear code of length s is a linear subspace $\mathcal{C}$ of a finite dimensional vector space K^s over a finite or infinite field K. A linear code of length s and dimension $\dim_K(\mathcal{C}) = n$ is often viewed as the row space of a $n \times s$ matrix G. The Hamming distance d of $\mathcal{C}$ is the minimum number of nonzero entries in a nonzero element (codeword) in $\mathcal{C}$. The numbers s, n and d are called the parameters of $\mathcal{C}$, and the code with these parameters is termed an $[s, n, d]$-code. A central theme to the study of codes is the determination of their minimum Hamming distance, which is a measure of the code's error correction capability.

Hamming distance has a nice geometric interpretation: if the columns of the generating matrix G are viewed as coordinates for a set of points $X = \{P_1, \dots, P_s\}$ in projective space $\mathbb{P}^{n-1}$ and if these points are distinct, then, setting $\mathrm{hyp(X)} =$ the maximum number of points among $P_1, \dots, P_s$ that are contained in a hyperplane, gives $d = n - \mathrm{hyp(X)}$. This description of Hamming distance gives a first glimpse at the crucial role that the geometry of zero-dimensional projective schemes plays in coding theory.

It may be the case, however, that some of the columns of the generating matrix G are proportional vectors. Note that adding proportional columns does not change the set of points X, however it does change the row space of G and hence the code $\mathcal{C}$. In this situation, one must keep track both of the set of distinct points arising from the columns of the generating matrix and their respective multiplicities. This data is represented algebraically by means of a fat (non-reduced) point scheme $Y = m_1P_1 + \cdots + m_sP_s$, where m_i is the multiplicity of the point P_i, i.e., the number of columns of G proportional to the coordinate vector of P_i.

Evaluation codes are a class of codes of great practical importance which can be defined in the language of polynomials. Let $S = K[t_1, \dots, t_n] = \oplus_{d=0}^{\infty} S_d$ be a polynomial ring over K with the standard grading and let X be a finite subset of $\mathbb{P}^{n-1}$ as above. The vanishing ideal of X is the ideal generated by the homogeneous polynomials vanishing on X. For each $d \geq 0$ there is a linear map of K vector spaces

$$\mathrm{ev}_d : K[t_1, \dots, t_n]_d \to K^s \quad f \mapsto \left(\frac{f(P_1)}{f_0(P_1)}, \dots, \frac{f(P_s)}{f_0(P_s)} \right), \quad \text{where } f_0(t_1 \dots, t_n) = t_1^d.$$

The kernel of ev_d is precisely the set of degree d polynomials in $I(X)$, denoted $I(X)_d$, and the image of ev_d is a linear code denoted by $\mathcal{C}_d(X)$ and termed an evaluation code. The case $d = 1$ gives the linear code associated to the matrix G whose columns are the points in X; this represents the K-linear map ev_1.

Recent Developments and Open Problems

The correspondence between reduced point schemes in projective spaces and codes has been established and studied from a commutative algebra point of view in [7] and [5]. In [11], numerical invariants of point schemes are used to bound invariants of the corresponding linear codes and vice-versa. Specifically Tohăneamu and Van Tuyl prove the following bounds hold true in the case $Y = m_1P_1 + \cdots + m_sP_s$: $d \geq \alpha(Y) - m(Y)$. Here $\alpha(Y)$ is the smallest degree of a hypersurface passing through $P_1, \ldots, P_s$ with multiplicities $m_1, \ldots, m_s$ respectively and $m(Z) = \max\{m_1, \ldots, m_s\}$. A natural generalization is the following

Problem 1 *Investigate whether the stronger inequality $d \geq \mathrm{reg(X)} - \mathrm{m(X)} + 1 \geq \alpha(\mathrm{X}) - \mathrm{m(X)}$ holds, where $\mathrm{reg(X)}$ (the Castelnuovo-Mumford regularity) is the least degree in which the Hilbert function of X agrees with the number of points of X (counted with multiplicity).*

The classical notion of Hamming distance, which is central to coding theory, has been generalized to a family of generalized Hamming weights in [12]. One can ask

Problem 2 *Is there a characterization for generalized Hamming distances for evaluation ideals in terms of the geometry of the set of reduced points X or the fat point scheme Y analogous to the complement to the maximum number of points contained in a hyperplane characterization given in section 1?*

We have seen in section 1 how generator matrices and evaluation maps produce codes, but in turn these matrices and maps respectively can be produced from graphs or, more generally, from simplicial complexes. Let $G = (V, E)$ be a simple graph on vertex set $V = \{1, \ldots, n\}$, and with $s = |E|$ edges. We assume that G is connected. A cutset of G is a set of edges in E such that when it is removed it disconnects the graph. Consider the linear code with generating matrix of size $n \times s$, where each column corresponds to an edge $[i, j] \in E(G)$ and the entries of that column are zeros, except for the i-th and j-th entries which are 1 and -1 respectively. By [11], the minimum distance d of the linear code generated in this manner is equal to the size of the smallest cutset of G. If G is a planar graph, then this is equal to the smallest size of a simple cycle in the dual graph of G. We ask

Problem 3
1. *When is the linear code constructed from the a graph as described above a minimum distance separable (MDS) code? That is, when is $\mathrm{d} = s - n + 2$, where n is the number of vertices, s the number of edges and d is the size of the smallest cutset?*
2. *Is the code associated to the dual graph $G^{\perp}$ the dual to the code constructed from the graph G?*

When K is a finite field, the basic parameters (length, dimension, and minimum distance) of the evaluation codes $\mathcal{C}_d$ associated to the set $\mathbb{T}^{s-1} = \{[(x_1, \ldots, x_s)] \in \mathbb{P}^{s-1} : x_i \in K^* \text{ for all } i\}$ are known for each $d \geq 0$ (see [6] and [9]). The finite set $\mathbb{T}^{s-1}$ is called the projective torus of dimension $s - 1$ over K and $I(\mathbb{T}^{s-1}) = (t_2^{q-1} - t_1^{q-1}, \ldots, t_s^{q-1} - t_1^{q-1})$. In general, when considering evaluation codes for proper subsets $X \subset \mathbb{T}^{s-1}$, the basic parameters of $\mathcal{C}_d$, especially the minimum distance, can be hard to determine even when $d = 1$. Let G be a simple graph with p vertices $V = \{1, \ldots, p\}$ and q edges, and let $\mathbb{X}$ be the algebraic toric set parameterized by all monomials y_iy_j such that $[i, j]$ is an edge of G, that is the coordinates of every point in $\mathbb{X}$ are given by evaluating all the monomials y_iy_j corresponding to edges of the graph at a point in $\mathbb{T}^{s-1}$. In this case, we say that $\mathcal{C}_d(\mathbb{X})$ is the parameterized linear code of order d associated to $\mathbb{X}$.

Problem 4 *For certain families of graphs, determine the generators of $I(\mathbb{X})$, the regularity of $S/I(\mathbb{X})$, and the minimum distance of the linear codes $C_d(\mathbb{X})$ associated to the given graphs (the length of the codes, $|\mathbb{X}|$, is already known by [8]).*

Presentation Highlights

Susan Cooper introduced the paradigm that relates linear codes and the geometry of zero-dimensional schemes in projective space, as described in the first section. The focus of her talk was on obtaining bounds of the Hamming distance for linear codes using algebraic parameters of homogeneous ideals in polynomial rings. In particular, she highlighted two results from

[11] which give bounds for a linear code with generating matrix G whose columns correspond to a fat point scheme $Y = m_1P_1 + \cdots + m_sP_s$ on a set of points $X = \{P_1, \ldots, P_s\}$. On one hand, if $m_1 \geq m_2 \geq \cdots \geq m_s$ then the following inequalities hold for the Hamming distance d

$$m_1 + \cdots + m_{d(X)} \geq d \geq m_{\mathrm{hyp(X)}} + \cdots + m_s.$$

On the other hand, if $m_1 = \cdots = m_s = m$ (the case of a uniform fat point scheme), then d can be bounded in terms of $\alpha(X)$, the minimum degree of a hypersurface passing through all the points in X and in terms of a homological invariant of $I(X)$ termed the minimum socle degree. The speaker proposed several strategies, such as trimming, a procedure originating in the paper [1], which gives a good handle on the Hilbert function of a fat point scheme and asked how minimum distance behaves under this operation.

Ştefan Tohăneanu talked about interpreting the Hamming distance of a code in terms of ideals generated by products of linear forms. Let $\ell_1, \ldots, \ell_s \in R := \mathbb{K}[x_1, \ldots, x_n]$ be linear forms such that $\langle \ell_1, \ldots, \ell_s\rangle = \langle x_1, \ldots, x_n\rangle$ and let $\mathcal{C}$ be the code whose generating matrix has as columns the coefficients of the linear forms. For $1 \leq a \leq s$, we define the ideal generated by $a-$fold products of these forms to be the ideal of R

$$I(a) := \langle \{\ell_{i_1} \cdots \ell_{i_a} | 1 \leq i_1 < \cdots < i_a \leq s\}\rangle.$$

De Boer-Pellikaan [4, Exercise 3.25] noticed that $d(\mathcal{C}) = \max\{a | \mathrm{ht}(I(a)) = k\}$ (here ht denotes the height of an ideal), a fact which can be extended to recover the generalized Hamming weights as well. The speaker presented a conjecture from [10] which states that the ideals $I(a)$ have linear graded minimal free resolutions, as well as partial results which support this conjecture.

Maria Vaz Pinto talked about evaluation codes on toric sets. When K is a finite field and

$$\mathbb{X} = \{\, [(x_1^{v_{11}} \ldots x_p^{v_{1p}}, \ldots, x_1^{v_{s1}} \ldots x_p^{v_{sp}})] : x_i \in K^* \text{ for all } i \,\} \subseteq \mathbb{P}^{s-1},$$

one says that $\mathbb{X}$ is the algebraic toric set parameterized by $y^{v_1}, \ldots, y^{v_s}$ (s monomials in n variables, $y^{v_i} = y_1^{v_{i1}} \ldots y_n^{v_{in}},\ v_{ij} \in \mathbb{N}$). The speaker considered the parameterized linear code of order d associated to $\mathbb{X}$, $\mathcal{C}_d(\mathbb{X})$. She highlighted some remarkable properties of these parametrized linear codes, such as the dictionary establishing equivalences between the length of the code and the degree (multiplicity) of the vanishing ideal $I(\mathbb{X})$ or the dimension of the code and the value of the Hilbert function for $S/I(\mathbb{X})$ in degree d. She pointed out that a good description for the Hamming distance is still elusive in many important cases.

Rafael Villarreal proposed in his talk a broad generalization for the notion of Hamming distance. Instead of studying the distance of a linear code by converting the generating matrix into a set of points X in projective space and using the linear aspects of the geometry of these points, as encoded by the $\mathrm{hyp(X)}$, one can start with any homogeneous ideal I in a polynomial ring and define a generalized $\mathrm{hyp_I(d, r)}$ function that encodes the maximum degree of a subscheme $X \subset V(I)$ that is also supported on the intersection of r hypersurfaces of degree d which are linearly independent modulo the ideal I. The talk was dedicated to exploring properties of this new function and the way they generalize previously known results. The speaker also presented a computer program designed to efficiently approximate the generalized Hamming distances for a code based on the use of initial ideals (Gröbner bases).

Scientific Progress Made

A substantial amount of algebraic and homological techniques are available to commutative algebraists in order to analyze properties of varieties embedded in affine or projective space. Familiarity with these techniques has allowed the participants of this focused research group to bring their expertise to bear on several issues of current interest in coding theory introduced in section 2. By recasting some central notions of coding theory into algebraic language we were able to strengthen and generalize them to many new settings. Our main contributions consist of: (1) developing a notion of generalized minimum distance functions motivated by the generalized Hamming weights of [12] and (2) analyzing several families of codes built from graphs, which include linear codes whose generator matrix is a signed incidence matrix of a simple graph and toric codes parametrized by monomials encoding edges of a graph.

Generalized minimum distance functions

This new notion generalizes the notions of distance existent in coding theory using the algebraic-geometric invariant of a scheme called degree (or multiplicity). Let $S = K[t_1, \ldots, t_n] = \oplus_{d=0}^{\infty} S_d$ be a polynomial ring over a field K with the standard grading and let $I \neq (0)$ be a graded ideal of S. We denote the degree of S/I by $\deg(S/I)$. The function $\delta_I : \mathbb{N}_+ \times \mathbb{N}_+ \to \mathbb{Z}$ given by

$$\delta_I(d, r) := \begin{cases} \deg(S/I) - \max\{\deg(S/(I, F)) |\, F \in \mathcal{F}_{d,r}\} & \text{if } \mathcal{F}_{d,r} \neq \emptyset, \\ \deg(S/I) & \text{if } \mathcal{F}_{d,r} = \emptyset, \end{cases}$$

is called the *generalized minimum distance* function of I, where $\mathcal{F}_{d,r}$ is the set

$$\mathcal{F}_{d,r} := \{\, \{f_1, \ldots, f_r\} \subset S_d \mid f_1, \ldots, f_r \text{ are linearly independent modulo } I, (I\colon (f_1, \ldots, f_r)) \neq I\}.$$

To compute $\delta_I(d, r)$ is a difficult problem, hence one of our aims is to introduce lower bounds for $\delta_I(d, r)$ which are easier to compute. One of our main results shows that there exists a function $\mathrm{fp}_I(d, r)$ termed the footprint function which is a lower bound for $\delta_I(d, r)$ and is easier to compute. We also explore other notions of generalized minimum distance such as the generalized minimum Loewy distance, which is better behaved with respect to non-reduced scheme structures and could provide a satisfactory answer to problems 1 and 2 of section 2. Moreover, since we make use of computational algebra programs in our research, we have programmed routines compatible with the computational algebra system Macaulay 2 for computing and analyzing these new invariants.

Codes from graphs

In our second project, we analyze codes arising from graphs $G = (V(G), E(G))$ with n vertices and s edges. Let A_G be the matrix whose columns correspond to the oriented edges of G: if $\{k, l\}$ is the j-th edge then the jth column of A_G has zeros in all of its positions, except in the entries (k, j) and (l, j) of A_G, wich are equal to 1 and -1, respectively. If G is connected, $\mathrm{rank}(\mathrm{A_G}) = \mathrm{n} - 1$ and the rows of A_G span a $[\,q,\, n-1,\, d_1(C)\,]$-linear code $\mathcal{C}$. We prove that, if G is a connected graph that is not a tree and X is the set of points whose coordinates are given by the columns of A_G, then the Castelnuovo-Mumford regularity of $I(X)$ is 2. We also classify the graphs that give rise to MDS codes, partially answering problems 3 and 4 of section 2.

Outcome of the Meeting

Although there are many meetings devoted to general advances in coding theory, there have been no opportunities to date for mathematicians specifically interested in commutative algebraic methods applied to coding theory to get together and exchange ideas for collaboration purposes. We feel that our meeting has marked an important first step in this regard and we thank BIRS for its support.

We expect that our collaboration will give rise to two research articles [2, 3], one for each of the projects described in sections 4.1 and 4.2 of this report.

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