## Banff International Research Station Proceedings 2011



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# Five-day Workshop Reports

Five-day Workshop Reports

## Chapter 1

## **Combinatorial Game Theory (11w5073)**

#### Jan 09 - Jan 14, 2011

**Organizer(s):** Elwyn Berlekamp (University of California, Berkeley) Tristan Cazenave (Paris-Dauphine University) Aviezri Fraenkel (Weizmann Institute) Martin Meuller (University of Alberta) Richard Nowakowski (Dalhousie University)

#### **Overview of the Field**

Combinatorial game theory deals principally with two person games of perfect information and without chance elements. It provides techniques for determining who can win from a game position and how. While ad hoc techniques for such analysis are as old as humanity, the modern theory employs more powerful and general tools such as the notion of a game-theoretic value. From a mathematical standpoint, these techniques can be brought to bear to completely solve a wide variety of games. From the algorithmic perspective (that is, when the efficiency of the analysis is considered), there are efficient methods to analyze certain GO endgames and capture races, and various classes of impartial games. In addition, complexity results abound and when a game is provably NP-hard, there are heuristic methods that can be employed. In a hot game, the first player to move can gain a big advantage. Such games, like GO and AMAZONS, frequently decompose into independent sub-games where playing the best local move in a sub-game might be sub-optimal in the global context. The goal is to combine the local considerations into an optimal, or near optimal, global strategy. Indeed, the ancient Asian game of GO is one the last of the classical games of skill in which computer performance has not caught up with humans.

#### **Recent Developments and Open Problems**

Three important topics are: Temperature Theory; misere-play games; and complexity of impartial games. There have been recent strides forward in all three areas of the subject, many directly attributable to collaborations started in previous 'Games of No Chance' workshops at MSRI and BIRS.

1. Temperature theory: how to play when large gains can be made, is a direction of research that has played a central role in combinatorial game theory for many decades. Over the past fifteen years there have been several major advances in temperature theory, and many promising directions for further research have emerged see [2, 6, 8–11, 13–15] for a small selection. Mean and temperature are fundamental invariants of partizan games that quantify the value and urgency of a position. They were studied in the 1950s by Milnor and Hanner, but in the context of modern combinatorial game theory the first rigorous construction was given by Berlekamp, Conway and Guy in the late 1970s [3]. The Berlekamp–Conway–Guy construction applied only to short games, in which repetition is prohibited

and play must end after a finite number of moves. In the ensuing years there has been increasing interest in extending this theory to a wide class of loopy games, those in which repetition is permitted. One such extension was introduced by Elwyn Berlekamp [2] at the first 'Games of No Chance' conference in 1994, and several more recent advances have dramatically increased the scope and sophistication of the theory. These include Fraser's [6] extension of temperature to games with long cycles, and the dogmatic theory of hyperactive positions due to Berlekamp and Spight [15]. These advances suggest numerous possibilities for further research, including a better understanding of cold loopy games; generalizations of heating and cooling to the loopy context; and ultimately, a unified temperature theory that applies to all loopy games. One of the most exciting elements of this theory is its application to the Asian board game GO, which has been a motivating influence in the development of combinatorial game theory. This connection has attracted attention from numerous mathematicians and GO players from Japan and Korea, several of whom have attended previous 'Games of No Chance' conferences (see [12] for example). A further interplay comes from a new heuristic that has been so effective in GO, that of Monte Carlo Tree Search (MCTS) methods (see [5,7] for example). These are sample-based search approaches using Monte-Carlo simulations and selective tree search. They have recently lead to a breakthrough, and considerably closed the gap to the best human players.

- 2. Misere-play Impartial Games: this was a major topic of the 2008 BIRS Games workshop. Recent work (July 2009) by Guo and Miller with Plambeck, Siegel and Weiemerskirsh looking on, suggest a radical change in the mathematical setting and tools. Instead of regarding the games as quotient monoids with a bi-partition they are now encoded as lattice points in rational convex polyhedra. Encodings provided by these lattice games can be made particularly efficient for octal games. The setting of lattice games naturally allows for misere play, where 0 is declared a losing position. Lattice games also allow situations where larger finite sets of positions are declared losing. Generating functions for sets of winning positions provide data structures for strategies of lattice games. The main conjecture is that every lattice game has a rational strategy: a rational generating function for its winning positions. Another conjecture is that every lattice game has an affine stratification: a partition of its set of winning positions into a finite disjoint union of finitely generated modules for affine semigroups. If true, this would give an effective algorithm for solving the games and would represent a great step forward In 2009, Meghan Allen [1] extended to misere partizan games the monoid approach of Plambeck and Seigel that has worked well in impartial games. This involves a tetra-partition of the misere quotient as opposed to a bipartition in the impartial case. Her techniques worked well in characterizing all misere quotients that are isomorphic to that generated by  $* = \{0|0\}$ . Two important questions that are central to furthering the techniques are: if the monoids for S and T are isomorphic when are they isomorphic to that of  $S \cup T$ ? For which class of games is  $* + * = 0 \pmod{q}$  for all g in the class?
- 3. Normal-play Impartial Games: The lattice game approach of Guo and Miller for misere-play games also provides a framework for normal-play impartial games. It provides an algorithm to compute strategies for many heap games in a natural setting. How effective this is for all impartial games is yet to be seen. At the same time Fraenkel & Peled [5] found another computationally effective approach for many impartial games. A pair of integer sequences that split the positive integers I is often—especially in the context of impartial games—defined recursively by A<sub>n</sub> = mex{A<sub>i</sub>, B<sub>i</sub> : 0 ≤ i < n}, B<sub>n</sub> = A<sub>n</sub> + C<sub>n</sub>, n ≥ 0, where mex(S) is the smallest nonnegative integer not in S, and C : I → I. Given x, y ∈ I, a typical problem is to decide whether x = A<sub>n</sub>, y = B<sub>n</sub>. For general functions C<sub>n</sub>, the best algorithm for this decision problem was until now exponential in the input size ω(logx + logy). Very recently it was proved constructively that the problem is actually polynomial for the wide class of approximately linear functions C<sub>n</sub>. This solves constructively and efficiently the complexity question of a number of previously analyzed take-away games of various authors. It is of interest to extend this result in new directions, such as: (i) relax the requirment of C<sub>n</sub> being "approximately linear"; (ii) consider the case where A<sub>n</sub> and C<sub>n</sub> are not necessarily additively related. These extensions may lead to classes of new games not yet imagined.

#### **Presentation Highlights and Scientific Progress Made**

Monte Carlo methods in combinatorial games (see [4, 7] for example) was a major topic at the workshop. Olivier Teytaud's keynote address, *Monte Carlo Tree Search Method*, was an excellent introduction to the subject by one of the world's experts. He gave a wonderful overview. The easy format afforded by BIRS allowed time for the audience, a mix of computer scientists, mathematicians and assorted graduate and undergraduate students, to ask pertinent questions and to have discussions afterwards. The talk and later discussions gave sufficient details so that several computer scientists where able to produce a Monte Carlo based program for the computer version of the games tournament. Even more impressive was the fact that Jiang Zhujiu, a professional GO player attending the conference, later was able to comment on games played by a GO-playing, Monte Carlo based, program. He also played against the computer and gave comments on the evaluation techniques of the program, providing some very valuable insights.

Formally, Olivier's talk was backed up by presentations by Cazenave and by Mueller both of whom attempting to use Monte Carlo methods to quickly approximate the temperature of a game. Temperature approximation is something that the professional players do very quickly (a top-down approach) but the professional 'scientists' only have a cumbersome, and time consuming, bottom up approach. Again, Jiang Zhujiu's comments were very insightful. There were informal meetings every afternoon to discuss all the Monte-Carlo approaches.

Games form a partial order so it is of no surprise that lattices arise. A major difficulty is that there are few classes of games known which give rise to lattices and in these classes the order grows so large so quickly that little intuitive insight can be gained. (In general, the classes are stratified by 'games born by day n'.) Angela Siegel's talk, *Distributive and other lattices in CGT*, presented two very new and exciting results. A result of Albert & Nowakowski (2011) shows that any closed set of short games generates a distributive lattice. She extended this result to include a subclass of loopy games. She then presented a class of games whose 'born by day n' subclass gives a planar but not distributive lattice, the first non-distributive lattice found in the area. Immediately, a special afternoon session was set up, the outcome of which will be a paper with eight authors. In addition, enough excitement was generated that one of other the graduate students has changed her PhD topic from algebra to lattices in combinatorial game theory.

The researchers favouring impartial games held very active and long informal sessions every afternoon and also during the evenings. A special mention must go to Alan Guo & Mike Weimerskirch's talk, advertised as *Lattice point methods in misere games*. The lattice point method, developed by Ezra Miller& Alan Guo, has more general applications than just misere games. Indeed, during the week it was realized that a problem of Aviezri Fraenkel could be approached with this method. Fraenkel and Weimerskirch led several informal and successful, sessions and a paper is in the works. During the workshop, a class of games was discovered that are, in some sense, minimal in not being covered by Miller and Guo's methods. There is now a PhD student whose topic is to generalize the lattice point method to larger classes of games.

The game of GO is always an important topic. Two linked main themes have always been the implementation of strategies via computers and evaluation of temperature. There was much overlap with the Monte-Carlo methods talks and discussions but there were two non-computer related talks of great interest. Elwyn Berlekamp gave a report of the *coupon GO* tournament held two months earlier in Korea. 'Coupons' are a way of providing a rich environment, an environment that allows a smoother way of evaluating the temperature of a game. Starting from a position in a famous GO game, 6 professional GO players played a round robin tournament playing each other as black and as white. The results were a surprise to the professionals 'players' as well as to the 'scientists'. Each day, the results were also reported in the daily newspapers! The analysis of the games is still on-going. Teigo Nakamura talked about the extensions of his remarkable results first reported in the 2008 BIRS Workshop. His approach to complicated capturing races was to 'cool by 2'. He reported on several (general) situations that have defeated professional GO players even outside of tournament play. Another interesting sidelight was the exposition of the SEKI game by Gurevich but reported by Vladimir Oudalov. This was to take situations that were explicitly not covered by Nakamura's approach and to, essentially, turn the problem into one with linear algebra aspects.

All of the talks resulted in some discussions. We point out just three other highlights.

The first general result in combinatorial game theory is that every impartial game is equivalent to a game of of NIM with exactly one heap and there is a well-defined and algorithmic way of finding the requisite NIM heap. No such game was known for the general partizan theory. That changed with Carlos Santos's talk,

A Non-trivial Surjective Map onto the Short Conways Group showed that every short game is equivalent to position in GENERALIZED KONANE and gave a technique for creating the position.

Neil McKay's talk, *Ordinal Sums with base*, re-started the discussion of how to play HACKENBUSH flowers. This is a long standing question (40 years) of Berlekamp's. This discussion occupied many evenings.

Kyle Burke, a recent graduate and new to academia, had the very pleasant experience of mentioning, in his talk, a complexity problem that interested Erik Demaine. The next day, Erik was able to announce that he and Kyle had solved the problem.

#### **Outcome of the Meeting**

One of the main goals of the Workshop was to create and strength ties between researchers and between fields. In this, the meeting was a huge success. New collaborations happened during the Workshop which will result in several papers. Since the Workshop, this collaboration continued and others have started and now there is active collaboration between groups in North America and Europe where before there was none.

In addition, three graduate students found topics for their PhD theses with the world's experts giving their 'blessing' and advice. The students have already become part of the community and have an international audience for their results. This has given the students a greater sense of pride in and resolve for their work.

Much of the success is due to the BIRS staff who made it easy for us to conduct the business of the Workshop without having to worry about other minor or major details. Given the diverse nature of the researchers in the area of Combinatorial Game Theory, the format, talks in the morning, informal sessions in the afternoon, is ideal. The formal talks allowed the topics for discussion to be laid out then the various well appointed rooms, allowed formation of the informal groups to discuss any of the topics. People could wander between groups and groups could merge when appropriate. The Lounge, itself, deserves to be a co-author on all of the papers that will result from the Workshop.

#### **Participants**

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### Chapter 2

## **Sparse Statistics, Optimization and Machine Learning (11w5012)**

#### Jan 16 - Jan 21, 2011

**Organizer(s):** Alexandre d'Aspremont (Princeton University), Francis Bach (INRIA - Ecole Normale Superieure), Martin Wainwright (UC Berkeley)

The workshop was designed to bring together scientists from three disciplines: statistics, computer science and optimization. Several recent directions of research, among them sparse model selection, matrix completion, robust PCA and graphical model estimation, have successfully exploited the interplay between these three disciplines. However, the standard conferences in these fields do not provide a concentrated opportunity for interaction. Bringing together researchers from various backgrounds for a week at BIRS was an ideal way of making connections.

Overall, the workshop was a great success. Many of the talks provoked lively and engaging discussions, which continued on after the talk through the coffee breaks and meals. Several of the participants actively commented how this workshop was genuinely a working environment, in that the buzz of intellectual activity, discussions and collaboration were continuous.

#### **Overview of the Fields**

Some recent results in model selection and signal processing have recently received a considerable amount of publicity. All of these results all have one point in common: they emerged from a successful collaborations between statisticians, computer scientists, and applied mathematicians, and they relied on mathematical programming in their consistency proofs and implementation performance. Some of the talks in this workshop were part of an effort to push this recipe a bit further and identify broad classes of problems that share common structure. Other talks focused on the problem of deriving sharp model selection conditions, or that of transposing the classical linear regression-model selection results to more exotic settings, including the gene expression networks in discussed in the kick-off talk by Robert Nowak.

#### **Recent Developments and Open Problems**

Several key themes of research following the directions outlines above are listed below.

#### Fast algorithms for structured learning problems

Several talks discussed customized algorithms focused on solving large-scale (or very large scale as in the social networks of I. Dhillon's talk) problems with explicit, polynomial and often accurate complexity bounds

and excellent numerical performance. Classical optimization results are focus on a certain number of standard form problems (linear programs, or more generally conic programs, geometric programming, black-box models with various smoothness assumptions, etc.). Most of the problems discussed during the workshop have a very specific structure which allows significant efficiency gains when properly exploited in the algorithm. Given the popularity and the importance of some of these problems (e.g. NETFLIX challenge,  $\ell_1$ -decoding, etc.) developing specialized algorithms for this class of problems has become a significant direction of work, which was covered by several talks during the workshop.

#### Learning with structured penalties

Beyond the classical  $\ell_1$  or trace norm penalties used for simultaneous variable selection in linear regression or matrix completion, designing structured penalties to account for some prior information on the problem is an active direction of research. These typically arise in imaging for example where relevant variables are often organized in simple connected sets. Structured penalties pose new modeling and computational challenges, and several talks presented efficient results when the structure is modeled as a group.

#### Consistency analysis and convergence rates

A number of authors presented results about the statistical consistency, and associated convergence rates of estimators based on solving optimization problems, both of the convex and non-convex variety. There are various theoretical questions at play here. How fast do the estimates obtained by solving mathematical programs converge to the true but unknown parameters? What conditions on the statistical model are required to ensure convergence? Are the rates obtained optimal, when compared to "oracle" procedures that have no computational limits? What are the differences between methods based on convex formulations, such as  $\ell_1$ -relaxation, and those based on non-convex constraints, such as  $\ell_q$ -constraints? A number of researchers described their recent work in addressing questions of this flavor.

#### **Presentation Highlights**

We summarize some of the workshop presentations in what follows, roughly following the main research directions outlined above.

#### Fast first-order algorithms for structured learning problems

Don Goldfarb discussed alternating direction augmented Lagrangian methods to minimize the sum of several functions subject to convex constraints, in the case where each function is relatively easy to minimize separately subject to the constraints. The algorithm followed both Gauss-Seidel-like and Jacobi-like iterations to compute an epsilon-optimal solution in  $O(1/\epsilon)$  iterations. The talk also discussed accelerated versions that have an  $O(1/\sqrt{\epsilon})$  iteration complexity. For the case where the sum only involves two functions and one of the functions to have a Lipschitz continuous gradient (which is typical in learning applications). These algorithms have a range of applications in matrix completion, robust PCA, covariance selection and linear regression problems with structured penalties. In these large-scale applications, scaling properties of the algorithm are key to practical performance. Numerical experiments were described on problems with tens of millions of variables and constraints.

Inderjit Dhillon presented an algorithm for compressed sensing (or  $\ell_1$ -penalized linear regression) and matrix completion which use hard thresholding to reduce memory usage at each iteration. Convergence results are derived using the same *restricted isometry parameters* that control model selection performance. Numerical performance could be significantly improved by computing only an approximate gradient at each iteration. There is ongoing work to adapt this algorithm to the robust PCA problem (reconstruct a sparse + low rank matrix). Dhillon also discussed specialized matrix factorization techniques that could handle very large scale data sets coming from social networks, where the data tends to be naturally clustered.

Stephen Becker presented recent efficient algorithms solving constrained  $\ell_1$ -minimization, as well as many variants such as the Dantzig Selector, nuclear norm minimization, SVM problems, and composite

problems such as minimizing a combination of the TV norm and a weighted 11 norm. The main argument is the addition of a strongly convex perturbation to the primal objective which allows to efficiently solve the dual problem. An accelerated continuation scheme is used to eliminate the effect of the perturbation. In parallel, Stephen Becker also developed a toolbox for implementing several types of efficient first order algorithms which is specifically designed to handle large-scale learning problems. Efficiently solving learning problems usually meant writing customized code for each specific class, and this toolbox aims to significantly reduce the implementation burden. In the long term- the goal is to integrate into high-level modeling solvers like the package CVX.

#### Linear inverse problems: beyond Lasso and matrix completion

Robert Nowak discussed "active learning" approaches. Most theory and methods for sparse recovery are based on non-adaptive measurements. The talk was focused on sequential measurement schemes that adaptively focus sensing using information gathered throughout the measurement process. It showed in particular that adaptive sensing can be more powerful when the measurements are contaminated with additive noise. While the standard sparse recovery setup involves inferring sparse linear functions, the talk discussed generalizations to the recovery of sparse multilinear functions. Such functions are characterized by multiplicative interactions between the input variables, with sparsity meaning that relatively few of all conceivable interactions are present (a setting akin to multidimensional spin glass models). This problem is motivated by the study of interactions between processes in complex networked systems (e.g., among genes and proteins in living cells). The results presented at the workshop extend the notion of compressed sensing from the linear sparsity model to notions of sparsity encountered in nonlinear systems. In contrast to linear sparsity models, in the multilinear case the pattern of sparsity can significantly affect sensing requirements. Here, the combinatorial dimension is used to characterize the complexity of the multivariate dependence pattern, but making a precise link between the sparsity pattern and the recovery rate remains a challenging problem.

In a similar vein, Ben Recht's talk focused on further extending the catalog of objects and structures that can be recovered from partial information. It discussed data analysis algorithms designed to decompose signals into sums of atomic signals from a simple set. These algorithms are derived in a convex optimization framework that encompasses previous methods based on  $\ell_1$ -norm minimization and nuclear norm minimization for recovering sparse vectors and low-rank matrices. The talk discussed general recovery guarantees and implementation schemes for this suite of algorithms as well as several example classes of atoms and applications. Beyond simply casting existing recovery result in a new light, and simplifying their generalization, the results also apply to cases which were not covered by the existing literature, such as recovery on the permutation polytope.

#### **Estimation and convergence rates**

Lieven Vandenberghe described a new penalized regression algorithm for autoregressive Gaussian processes. In a Gaussian model, the topology of the dependence graph specifies the sparsity pattern of the inverse covariance matrix. Several topology selection methods based on convex optimization and  $\ell_1$ -norm regularization have been proposed recently. The talk discussed extensions of these methods to graphical models of autoregressive Gaussian time series (AR processes) and focused on the problem of maximum likelihood estimation of autoregressive models with conditional independence constraints and convex techniques for topology selection via nonsmooth regularization. The maximum likelihood estimation problem for AR processes is nonconvex whenever the lag is larger than zero but the talk showed that when the sample estimates have a block-Toepliz (which is the case for the windowed estimate) a convex relaxation of the ML problem is tight, i.e. yields the global optimum. Beyond its statistical implications, this results perfectly illustrate how classical results from linear algebra and mathematical programming can find direct, and unexpected, applications in statistics (guiding the choice of estimator here).

Peter Bühlmann discussed the need for methods for performing causal inference. His talk highlighted the distinction between problems of regression type, versus those of causal or intervention type. He discussed the use of directed acyclic graphs for characterizing causality, and described an algorithm for estimating the DAG equivalence class. This algorithm is computationally efficient and can be shown to be consistent under high-dimensional scaling, including settings when the sample size n is much smaller than the number of

variables *p*. He then discussed an even more challenging problem of inferring causality using a combination of observational and interventional data, and discussed the non-trivial optimization problems that arise from a likelihood-based formulation.

Tong Zhang discussed the use of various types of group-sparse norms for multivariate regression problems. He first demonstrated that the ordinary group Lasso does not achieve information-theoretically optimal  $\ell_2$ -rates for a certain class of group sparse problems. He then discussed a different type of group regularization, which turned out to be related to work discussed earlier by G. Obozinski, for this problem. He proved that it has lower estimation error, in particular matching the information-theoretic limits for a particular type of group structure.

Nati Srebro discussed the use of Rademacher complexity and related quantities for proving bounds on the error of M-estimators, including the Lasso and also closely-related estimators for matrix regression. He showed that various results can be obtained quite directly by reducing certain empirical process quantities to the Rademacher complexity, and then upper bounding it appropriately. He illustrated this line of attack in application to both sparse linear models, as well as versions of matrix completion using both the nuclear norm and a related "max"-norm on matrix space, both designed to encourage low-rank behavior.

#### **Participants**

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## Chapter 3

## Density Functional Theory: Fundamentals and Applications in Condensed Matter Physics (11w5121)

#### Jan 23 - Jan 28, 2011

**Organizer(s):** Eric Cances (ENPC and INRIA) Carlos Garcia-Cervera (University of California, Santa Barbara) Yan Alexander Wang (University of British Columbia)

#### **Overview of the Field**

A complete quantum mechanical description of a solid requires the solution of the many-body Schrödinger equation [8]. The numerical approximation of this equation, however, is impractical: using a straightforward numerical discretization, the number of degrees of freedom grows exponentially with the number of electrons, and therefore only systems with very few atoms can be considered. In [18], Hohenberg and Kohn proved that there exists a universal functional of the electronic density F[u] such that the ground state energy associated to an external potential v can be obtained by minimizing the energy

$$E[u] = F[u] + \int v(\mathbf{x})u(\mathbf{x}) \, d\mathbf{x}.$$
(3.1)

Further refinements of the theory were presented by Levy [21] and Lieb [23].

In (3.1), however, the shape of functional F[u] is unknown, and must be approximated. There are two main approaches for its approximation, which have given origin to what are known as Orbital-Free Density-Functional Theory (OFDFT), and Kohn-Sham Density-Functional Theory (KSDFT).

In OFDFT, the functional F is replaced by an explicit functional of u. The simplest such approximation is the Thomas-Fermi functional [32, 13], and by now several such approximations have been proposed [34, 35, 37, 36, 39]. To achieve good physical accuracy, however, complicated, nonlocal kinetic energy functionals must be used. An example of such functionals is the Wang-Teter functional. Although in principle it captures linear response effects, the kinetic energy is unbounded below, rendering it useless for practical use [2]. Density dependent kernels have been developed, and although they do not seem to suffer from this difficulty, they are not well understood, their numerical implementation becomes cumbersome, and there does not seem to be a systematic way of improving their accuracy.

In a different direction, Kohn and Sham introduced an approximation scheme by decomposing the energy functional F[u] as [20]

$$E[u] = \frac{1}{2} \sum_{i=1}^{N} \int_{\mathbb{R}^{3}} |\nabla \psi_{i}|^{2} \, d\mathbf{x} + \frac{1}{2} \int_{\mathbb{R}^{3}} \int_{\mathbb{R}^{3}} \frac{u(\mathbf{x})\mathbf{u}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} \, d\mathbf{y}, +F_{\mathrm{XC}}[u] + \int_{\mathbb{R}^{3}} v(\mathbf{x})u(\mathbf{x}) \, d\mathbf{x}, \tag{3.2}$$

with  $u = \sum_{j} |\psi_{j}|^2$ , and  $\{\psi_{j}\}$  and orthonormal family of functions in  $L^2(\mathbb{R}^3)$ . The first term is the kinetic energy of N non-interacting electrons, and the other contributions to the energy in (3.2) are Hartree, exchange-correlation, and external potential energies, respectively. The idea of approximating the total energy using non-interacting electrons goes back to the Hartree-Fock method [31]. A fundamental difference is that whereas the Hartree-Fock energy is only an approximation to the true energy, the Kohn-Sham functional is exact. The exchange and correlation energy, however, is not known explicitly, and must be approximated.

There are by now a number of extensions of the Hohenberg-Kohn theorem and the Kohn-Sham approximation scheme to other situations of practical interest, such as Time-Dependent DFT [30], and Current-Dependent DFT [33]. Although all these approaches are in principle exact, it is precisely the quality of the approximation to the exchange-correlation energy that determines the quality of the overall scheme. Among the simplest approximations are the Local Density Approximation (LDA), and the Generalized-Gradient Approximation (GGA), in which the exchange-correlation term is approximated by a functional of the density alone, or the density and its gradient, respectively. Although some of these approximations have proved to be successful in practice, there is currently no real understanding of the actual accuracy of the different models. Furthermore, from a mathematical standpoint, there are not many results even in the simple cases of the LDA and GGA. For the LDA, the existence of solutions is known; however, in the GGA case, the existence is known only for N = 1 [3].

From the numerical point of view, the Kohn-Sham equations also present some challenges. The complexity of the self-consistent iteration introduced by Kohn and Sham scales as  $O(N^3)$ , which is impractical for the study of large systems. In the past twenty years, a number of new methodologies have appeared in the literature, which attempt to exploit the locality of the problem in order to reduce the computational complexity. Locality, in quantum mechanics, refers to the property that a small disturbance in a molecule only has a local effect in the electron density, a phenomenon coined by W. Kohn as *nearsightedness* [19]. Examples of these attempts are the Divide and Conquer methods [38, 1], Orbital Minimization [29], Density Matrix Minimization [22, 17], the Fermi Operator Expansion [16], and, more recently, the Localized Subspace Iteration [15]. There have also been several advances in the design of numerical algorithms for metallic systems [27, 28].

Advances in the numerical computations of DFT have made it possible to study materials with ab-initio simulations, in which the underlying physical model is quantum mechanics.

#### **Objectives of the Workshop**

Since its inception, DFT has been a very popular tool in the physics and chemistry community. In the mathematics community, however, there has not been that much work done, except in a few exceptional cases [2, 1, 3, 6, 7, 24, 25, 26, 12]. One of the main purposes of the workshop was to raise awareness on this important topic by bringing together an interdisciplinary group of experts in the field to discuss the latest developments in the modeling, theory, and simulations of quantum mechanical systems, in the context of density functional theory.

The main topics discussed were:

- Fundamental aspects of DFT: Approximation of the exchange-correlation and kinetic energy functionals.
- 2. Extensions of DFT: Time-dependent, spin-orbit coupling, CDFT.
- 3. Materials modeling: defects.
- 4. Numerical DFT: linear and sublinear scaling methods.

#### **Recent Developments and Open Problems**

From a mathematical viewpoint, much has been learned about the existing models in the past few years. For example, questions of existence of solutions, that had been open for a long time, have been answered [3]; and there has been special interest in the derivation of coarse-grained models from quantum mechanical theories [14, 4, 9, 11, 10, 5].

Numerically, a significant amount of effort has been put to the development of linear scaling techniques and acceleration of the self-consistent iteration. However, a rigorous theory is still lacking.

There have been considerable efforts in an attempt to increase the chemical accuracy of current models, and development of effective theories for complex systems, such as ferromagnetic materials, and topological insulators.

Despite these recent developments, there are still some important open problems. For example, a rigorous derivation of effective models for the treatment of defects in solids in the context of Kohn-Sham DFT or other theories that go beyond DFT, both in the ground state and in dynamics, is still missing. Much has been done in the context of crystalline solids with localized defects, but more needs to be done to understand disordered systems, such as heavily doped and organic semiconductors. Deeper understanding of spin-orbit interactions, as well as relativistic effects, will be necessary for the study of new materials such as ferromagnetic materials, topological insulators. Transport properties are fundamental for the study of electronic systems, however, a rigorous first principles approach is still lacking. This will be of enormous importance for the study of nano-optical devices, and solar cells, for example.

At the more fundamental level, a deeper undersanding of the connection between the many-body Schrödinger equation and reduced theories such as Kohn-Sham or orbital-free DFT is of importance for the systematic development of accurate exchange-correlation functionals with improved chemical accuracy.

#### **Presentation Highlights**

A number of researchers from different scientific areas, some of them not experts in the topics discussed, was invited to the workshop. As a result we had a mixed audience with variable degrees of knowledge on the topics covered in the workshop. We planned four tutorial talks on different topics: Introduction to Quantum Chemistry (Gero Friesecke), Electronic Transport (Roberto Car), Density Functional Theory (Kieron Burke and John Perdew), and Analysis and Algorithms for the Kohn-Sham model (Weinan E and Jianfeng Lu). The tutorials started with an introduction to the topic, and ended with the state-of-the-art and open problems.

The first talk in the workshop was a tutorial on Quantum Chemistry by Prof. Gero Friesecke. The basic many-body Schrödinger equation was introduced, and a number of approximations and reduced models were discussed, with an emphasis on wave-function methods such as Hartree-Fock, the Configuration Interaction method, and the Coupled-Cluster method. Examples were given to describe the accuracy and efficiency of each approach, and for each one its limitations were discussed, which paved the way for a number of open challenges in the field.

The second tutorial was presented by Prof. Kieron Burke (Prof. John Perdew, originally scheduled to deliver the tutorial, was unable to attend the meeting). The main topic was ground-state density functional theory, and a number of topics were discussed. The Kohn-Hohenberg density functional is unknown, and therefore for practical applications it must be approximated. This approximation is not trivial, and some of the currently available functionals, as well as the challenges of developing new improved functionals, were discussed in this tutorial. Some of the difficulties arise from the lack of understanding of the connection between the density-functional and the many-body problem, and part of the tutorial was dedicated to a semiclassical approximation, which could elucidate this connection. Dr. Pina Romaniello discussed this connection from the point of view of many-body perturbation theory in her talk. An alternative approach based on approximating exchange-correlation *potentials* rather than exchange-correlation *energy functionals* was discussed by Dr. Viktor Staroverov.

The following tutorial was presented by Dr. Jianfeng Lu (jointly with Prof. Weinan E, who could not attend the workshop), and focused on some of the mathematical and numerical challenges in the analysis of the Kohn-Sham model. On a more fundamental level, Yan Alexander Wang discussed the differentiability properties of the Kohn-Hohenberg functional in his talk.

The last tutorial was dedicated to the topic of Electronic Transport, and was presented by Prof. Roberto Car. One of the main challenges in the study of electron transport in a quantum system is the issue of collisions. In this tutorial Prof. Car introduced some of the approaches developed for the study of transport, such as the Quantum Boltzmann equation, and after pointing out some of the difficulties, described the development of a Quantum Master Equation. Some of the challenges and open problems were discussed as well. Open systems and the issue of dissipation in a quantum system were also discussed by Prof. Matthias

Ernzerhof in his talk.

One important challenge that is still open in the study of quantum systems is the issue of strong correlations, which explains entanglement in quantum systems, and appears in systems with strong magnetic effects and in heavy atoms. Current reduced theories such as DFT are unable to capture this effect. A constrained mean-field approach was presented by Prof. Gustavo Scuseria.

Virginie Ehrlacher discussed the important issue of charge screening for crystals with a defect in the context of Thomas-Fermi-von Weiszäcker (TFW) DFT. A variational model, rigorously derived as the thermodynamic limit of a sequence of finite systems, was presented to model local defects and it was shown that local defects are always neutral. As a result TFW DFT cannot be used to study charged defects.

Prof. Emil Prodan gave a lecture on Topological Insulators, a relatively new class of materials displaying robust physical properties as a result of strong spin-orbit interactions. This is a fairly new area within condensed-matter physics, and where collaboration between mathematics and physics can prove to be fundamental for new discoveries.

Prof. Gang Lu presented a first principles approach for the study of electronic properties in bulk heterojunction solar cells, another area of research that has received much attention recently, and where a multidisciplinary approach could be fundamental.

A study of the properties of large atoms, and its ionization energies, was presented by Kieron Burke. Relativistic corrections for large atoms were discussed by Prof. Jan Phillip Solovej.

A number of talks were dedicated to numerical issues in DFT. The main difficulties in the numerical developments of efficient methodologies for DFT are 1) how to discretize the problem effectively in a way that local effects are captured near the atomic locations while using a reduced number of degrees of freedom, and 2) how to accelerate convergence of the self-consistent iteration. For the former, several ideas were presented, such as the use of enriched basis by John Pask; adaptive mesh refinements by Aihui Zhou, with error estimators discussed by Reinhold Schneider; and the systematic construction of basis functions by solving small local problems in the context of Discontinuous Galerkin FEM by Lin Lin. A detailed analysis of the convergence of spectral approximations was presented by Yvon Maday. With regards to the convergence of the self-consistent iteration, Yakun Chen presented a new idea based on a shooting method that produces a robust and efficient algorithm.

#### **List of Abstracts**

#### **Tutorials**

**Kieron Burke**, Department of Chemistry and Department of Physics, University of California, Irvine. *TDDFT* - *past, present, and future*.

**Roberto Car**, Department of Chemistry and Program in Applied and Computational Mathematics, Princeton University. *Tutorial on Electronic Transport*.

**Gero Friesecke**, TU Munich, Germany. *Some mathematical challenges in quantum chemistry*: I was asked by the organisers not to assume prior expertise in quantum chemistry and density functional theory. So I will start with

- the basic models (many-body Schroedinger equation, with or without nuclear motion), and
- the basic questions (quantities one would like to predict, such as absorption spectra, binding energies, potential energy surfaces for the nuclei and their subsequent use for geometry optimization or MD, and the associated accuracy requirements).

I will then try to give an informal overview over the main approaches that have been developed to reduce the basic equations into computationally feasible electronic structure models: wave function methods including HF, CI, CC, Monte Carlo; reduced density matrix methods; and – very briefly in order not to conflict with the other tutorials – DFT. This will then naturally lead into some of the main challenges.

Jianfeng Lu, Courant Institute of Mathematical Sciences, New York University. *Density Functional The*ory: Analysis and Algorithms: This minicourse will consist of an introduction to density functional theory;

overview of analysis results for DFT; macroscopic limit of Kohn-Sham density functional theory; introduction of algorithmic issues of DFT; overview of some recent results on development of algorithms for metallic (and insulator) system.

#### **Talks**

**Kieron Burke**, Department of Chemistry and Department of Physics, University of California, Irvine. *Non-empirical derivation of density and potential functional approximations*: I will discuss our progress in deriving new approximations for both exchange-correlation and for the non-interacting kinetic energy. A sufficiently accurate kinetic energy functional would make solving the KS equations unnecessary. Semiclassical techniques are applied to yield accurate results as functionals of the potential, rather than of the density. Our most recent calculations reach high accuracy for the ionization energies of atoms.

I will focus on recent work (with Cangi, Lee, Elliott, and Hardy Gross) in which the universal functional of Hohenberg and Kohn is given as a coupling-constant integral over the density as a functional of the potential. Conditions are derived under which potential-functional approximations are variational. Construction via this method and imposition of these conditions are shown to greatly improve the non-interacting kinetic energy needed for orbital-free Kohn-Sham calculations.

Yakun Chen, Department of Chemistry, University of British Columbia, Vancouver, Canada, *Linear-expansion Shooting Technique for Accelerating Self-consistent Field Convergence*:Based on the corrected Hohenberg-Kohn-Sham energy functional (cHKS) [1,2], we present a new method to accelerate self-consistent field (SCF) convergence by utilizing shooting technique. We have developed three different linear-expension shooting techniques (LIST)–LISTd, LISTs and LISTi, by imposing different conditions. Case studies show that overall the LISTi method is a robust and efficient algorithm for accelerating SCF convergence whereas LISTd and LISTs methods are advantageous in the early stage of SCF convergence. More importantly, the LIST method outperforms Pulays DIIS [3,4] and its recent improvements, including EDIIS [5,6] and ADIIS [7].

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- 6. K. N. Kudin, G. E. Scuseria, and E. Cances, J. Chem. Phys. 116, 8255 (2002).
- 7. X. Hu and W. Yang, J. Chem. Phys. 132, 054109 (2010).

**Virginie Ehrlacher**, CERMICS - Ecole des Ponts ParisTech, France, *Local defects are always neutral in the Thomas-Fermi-von Weiszcker theory of crystals*: The aim of this article is to propose a mathematical model describing the electronic structure of crystals with local defects in the framework of the Thomas-Fermi-von Weizsäcker (TFW) theory. The approach follows the same lines as that used in E. Cancès, A. Deleurence and M. Lewin, Commun. Math. Phys., 281 (2008), pp.129177 for the reduced Hartree-Fock model, and is based on thermodynamic limit arguments. We prove in particular that it is not possible to model charged defects within the TFW theory of crystals. We finally derive some additional properties of the TFW ground state electronic density of a crystal with a local defect, in the special case when the host crystal is modelled by a homogeneous medium.

**Matthias Ernzerhof**, Department of Chemistry, University of Montreal. *Density functional theory for open systems: Theory and applications*: We describe a generalization [1] of ground-state DFT that preserves its formal structure, i.e., the basic equations remain unchanged, while the external potential and the electron density become complex valued functions instead of real valued ones. As a consequence, the ground-state energy is also replaced by a complex energy, which is interpreted as a resonance-state energy. Resonance states are metastable and their lifetime is proportional to the inverse of the imaginary part of their energy. A suitable choice of the external complex potential enables one to model systems such as metastable molecules

on surfaces and electron transport [2] through molecular electronic devices. We discuss [3] several applications of our theory as well as limitations of existing exchange-correlation energy functionals to represent the complex exchange-correlation energy.

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- F. Goyer, M. Ernzerhof, and M. Zhuang, J. Chem. Phys. 126, 144104 (2007); M. Ernzerhof, J. Chem. Phys. 127, 204709 (2007).
- 3. Y. Zhou and M. Ernzerhof, in preparation.

Lin Lin, Program in Applied and Computational Mathematics, Princeton University. Adaptive local basis for Kohn-Sham density functional theory in Discontinuous Galerkin framework: Kohn-Sham density functional theory is the most popular electronic structure theory in chemistry and material science. Numerically Kohn-Sham density functional theory gives rise to a matrix eigenvalue problem. The eigenfunctions (also called orbitals) are non-smooth with localized features in real space around atom sites. A proper discretization on a uniform mesh generally requires a large number of plane waves to capture the localized feature, therefore resulting an eigenvalue problem with large matrix dimension. The matrix dimension can be reduced by incorporating parameterized empirical basis functions suggested by chemical intuition such as using atomic orbitals, but the basis functions have to be tuned finely and manually in order to obtain comparable accuracy as that in uniform mesh. We present a new scheme that constructs the basis functions adaptively by using the eigenfunctions from Kohn-Sham theory defined on a local region. The resulting basis functions capture the localized feature of the global eigenfunctions by definition. The basis functions are local and are discontinuous in a global level, and the global eigenfunctions are reconstructed from these discontinuous basis functions in Discontinuous Galerkin framework. Numerical examples indicate that the new scheme achieves dimension reduction effectively and automatically. The local nature of the basis functions leads to a sparse matrix eigenvalue problem, which allows to be combined with the recently proposed sparse matrix technique (selected inversion technique) to further reduce the computational cost for both insulating and metallic systems. (Joint work with Weinan E, Jianfeng Lu and Lexing Ying)

**Kenneth A. Lopata**, Pacific Northwest National Laboratory. *Modeling fast electron dynamics with realtime time-dependent density-functional theory*: The response of matter to external fields forms the basis for a vast wealth of fundamental physical processes ranging from light harvesting to nanoscale electron transport. Accurately modeling ultrafast electron dynamics in excited systems thus offers unparalleled insight, but requires an inherently non-linear time-resolved approach. To this end, an efficient and massively parallel real-time real-space time-dependent density functional theory (RT-TDDFT) implementation in NWChem is presented. The implementation is first validated against linear-response TDDFT and experimental results for a series of molecules subjected to small electric field perturbations. Next, non-linear excitation of green fluorescent protein is studied, which shows a blue-shift in the spectrum with increasing perturbation, as well as a saturation in absorption. Finally, the charge dynamics of optically excited zinc porphyrin is presented in real-time and real-space, with relevance to charge injection in photovoltaic devices.

**Gang Lu**, Department of Physics, California State University Northridge. *Exciton Diffusion in Organic Solar Cells: First–Principles Investigations*: Exciton diffusion length and time are among the most important factors that govern the performance of organic solar cells and light-emitting diodes. Understanding exciton diffusion process in organic semiconductors such as conjugated polymers from firstprinciples represents a crucial aspect of designing high-efficiency solar cells. We have developed a first-principles approach based on time-dependent density functional linear response theory with the Casida's formalism to describe the energy and many-body wave-functions of excitons. The non-adiabatic ab initio molecular dynamics is used to calculate phonon-assisted transition rates between localized exciton states with the spontaneous emission determined by the dipole approximation. With Monte Carlo simulations, we are able to calculate the exciton diffusion length, time, and diffusivity for a prototype polymer system P3HT, and have obtained excellent results comparing to experiments as well as physical insight into the microscopic nature of exciton diffusion.

The work was partially supported by NSF-Solar grant DMR-1035480.

**Yvon Maday**, Laboratoire Jacques Louis Lions, Université Pierre et Marie Curie, Paris, France and Division of Applied Mathematics, Brown University, USA, *Two-grid method for the approximation of nonlinear* 

*eigenvalue problems*: Approximation of non linear eigenvalue problems represent the key ingredient in quantum chemistry. These approximation are much computer demanding and these approximations saturate the ressources of many HPC centers. Being nonlinear, the approximation methods are iterative and a way to reduce the cost is to use different grids as has been proposed in fluid mechanics for various non linear problems as the Navier Stokes problem. We explain the basics of the approximation, present the numerical analysis and numerical results that illustrate the good behavior of the two grids scheme. This work has been done in collaboration with Eric Cancès and Rachida Chakir.

John E. Pask, Lawrence Livermore National Laboratory, USA. Partition-of-unity finite elements for large, accurate quantum mechanical materials calculations: Over the past few decades, the planewave (PW) pseudopotential method has established itself as the dominant method for large, accurate, density-functional calculations in condensed matter. However, due to its global Fourier basis, the PW method suffers from substantial inefficiencies in parallelization and applications involving highly localized states, such as those involving 1strow or transition-metal atoms, or other atoms at extreme conditions. Modern "real space" approaches, such as finite-difference (FD) and finite-element (FE) methods, can address these deficiencies without sacrificing rigorous, systematic improvability but have until now required much larger bases to attain the required accuracy. Here, we present a new real-space FE based method [1,2] which employs modern partition-of-unity FE (PUFE) techniques to substantially increase the efficiency of the real-space representation, thus decreasing the number of basis functions required correspondingly, by building known atomic physics into the FE basis: without sacrificing locality or systematic improvability. We discuss the weak formulation of the required Poisson and Schroedinger problems in the Kohn-Sham solution and the imposition of Bloch-periodic boundary conditions. We present both pseudopotential and all-electron applications, with attention in the latter case to the approximation of the singular solution outside Sobolev space H1 using a basis in H1. Finally, we highlight recent progress and open questions relating to generalized eigensolvers and parallelization. Initial results show order-of-magnitude improvements relative to current state-of-the-art PW and adaptive-mesh FE methods for systems involving localized states such as d- and f-electron metals and/or other atoms at extreme conditions.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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**Kieron Burke**, Department of Chemistry and Department of Physics, University of California, Irvine. *Density Functional Theory, and the Persistence of Chemistry in the Limit of Large Atomic Number*: This talk applies the orbital-based Kohn-Sham density functional theory to compute the first ionization energies of hypothetical non-relativistic neutral atoms with up to Z=3000 electrons, within the sp or main block of the periodic table [1]. The ionization energies and density changes upon ionization are extrapolated to the limit of infinite atomic number Z. We find well-defined limits that depend upon the chosen column of the periodic table. Thus the periodic table becomes perfectly periodic in this limit. The limiting ionization energies are smaller than those from the real periodic table, but still increase across a row or period. The finiteness of the limiting ionization energy is remarkable, because the total energy of the neutral atom varies as . An sp chemistry of unusually long, weak bonds likely persists in the limit The simple local density approximation for the exchange energy appears to give an exact or nearly-exact exchange contribution to the ionization energies and energy averaged over a shell. Proving or disproving these conclusions rigorously is a challenge to mathematical physics.

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**Emil Prodan**, Department of Physics, Yeshiva University. *Predictive ab-initio simulations of Topological Insulators: Fundamental Challenges*: Topological Insulators represent a new class of materials displaying robust physical properties triggered by a strong spin-orbit interaction. Based on qualitative and sometime empirical models, several topological insulating materials have been predicted and then discovered experimentally. Ab-initio simulations of such materials have start appearing in the literature and some of these

simulations were even used to predict new classes of topological insulators. However, the ab-initio simulations of these systems with strong spin-orbit interaction are facing daunting challenges, especially when predictive power is needed.

In this talk I will first briefly summarize the status of the field, touching on the following points: what is a topological insulator, what are the robust properties and how are they triggered by the spin-orbit interaction, what materials are known to display the effect? Then I will discuss the status of the existing ab-initio simulations and start listing the emerging challenges. I will present the status of the Density Functional Theory for systems with strong spin-orbit interaction and touch on several key points that need practical solutions in order to efficiently apply the theory to the complex topological materials.

**Pina Romaniello**, Universitae Paul Sabatier, Toulouse, France and European Theoretical Spectroscopy Facilities (ETSF), F-91128 Palaiseau, France. *DFT: insight from MBPT*: Density functional theory (DFT) has become over the years one of the few well-established theoretical approaches for calculations on realistic systems. The basic idea of DFT is to replace the many-body problem with an effective one-particle description in which the many-body effects of the system enter through an exchange-correlation potential that is a functional of the density of the system. This functional is not known and needs to be approximated. Designing new functionals that are generally applicable is an hard task. A way to follow is to pass through Many-Body Perturbation Theory (MBPT) [1]. In this framework, the many-body effects of the system are contained in the self-energy, which thus plays a similar role as the exchange-correlation potential in a density-functional context. Also the self-energy needs to be approximated. However in MBPT approximations can be found in a systematic way, although MBPT in itself is too costly for realistic systems. Therefore, passing through MBPT has the advantage that approximations with a clear physical meaning can be designed more easily than in the context of density functionals and introduced in a second-step into the computationally more efficient DFT. In this work I will focus on MBPT and I will show how one can improve the currently used approximations [2,3]; I will also discuss how to translate the physical insight acquired in MBPT into DFT.

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- 3. G. Lani, P. Romaniello, and Lucia Reining, in preparation.

**Reinhold Schneider**, TU Berlin. A posteriori error estimators in Density Functional Theory and Hartree-Fock: We present an a posteriori error analysis of the discretization of error in the Kohn Sham energies, resp. the Hartree Fock energy. The analysis is based on duality techniques as developed for goal oriented error estimators. Basic assumptions are similar to those imposed for a priory estimates, e.g. Cances et al.. We consider the error estimators for the orbital functions, taking the unitary invariance into account, as well as for the density matrix directly. This is joint work with S. Schwinger (MPI Leipzig), and most material is from his recent PhD thesis.

Gustavo E. Scuseria, Department of Chemistry, Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA, guscus@rice.edu. Strong Correlations from Constrained Mean-Field Approaches: This presentation will discuss mean-field approaches for describing strong correlations. The methods that we have developed allow for symmetry breaking followed by a restoration step. We work both with wavefunctions and density matrix functionals. In both cases, symmetry breaking is constrained to an active space. Constrained-pairing mean-field theory (CPMFT) [1-4] yields a two-particle density matrix ansatz that exclusively describes strong correlations. The model wavefunction breaks electron number conservation and is correct only on average but expectation values calculated from the effective two-particle density matrix contain no particle number fluctuations. On the other hand, Constrained Unrestricted Hartree-Fock (CUHF) theory [5, 6] limits spin and space symmetry breaking to an active space. Based on it, we have recently proposed a novel approach for obtaining high-spin ROHF wave functions by imposing constraints to UHF. The constraints can be selectively released in an active space but imposed elsewhere. If the active space is properly chosen, our CUHF method greatly benefits from a controlled broken-symmetry effect while avoiding the massive spin contamination of traditional UHF. We have also applied Lowdins projection operator method to CUHF and obtain multireference wave functions with moderate computational cost. Singlet-triplet energy splittings show that our constrained scheme outperforms fully unrestricted methods. This constrained approach can be used in spin density functional theory with similar favorable effects.

- 1. Strong correlations via constrained-pairing mean-field theory, T. Tsuchimochi and G. E. Scuseria, J. Chem. Phys. 131, 121102 (2009).
- Constrained-Pairing Mean-Field Theory. II. Exact treatment of dissociations to non-degenerate orbitals, G. E. Scuseria and T. Tsuchimochi, J. Chem. Phys. 131, 164119 (2009).
- Constrained-Pairing Mean-Field Theory. III. Inclusion of Density Functional Exchange and Correlation Effects via Alternative Densities, T. Tsuchimochi, G. E. Scuseria, and A. Savin, J. Chem. Phys. 132, 024111 (2010).
- Constrained-Pairing Mean-Field Theory. IV. Inclusion of corresponding pair constraints and connection to unrestricted Hartree-Fock theory, T. Tsuchimochi, T. M. Henderson, G. E. Scuseria, and A. Savin, J. Chem. Phys. 133, 134108 (2010).
- 5. ROHF Theory Made Simple, T. Tsuchimochi and G. E. Scuseria, J. Chem. Phys. 133, 141102 (2010).
- 6. Constrained Active Space Unrestricted Mean-Field Methods for Controlling Spin-Contamination, T. Tsuchimochi and G. E. Scuseria, J. Chem. Phys. submitted

**Jan Phillip Solovej**, Department of Mathematics, University of Copenhagen, Denmark. *The Scott correction in different models of atoms and molecules*: The topic of this talk is the energy asymptotics of large atoms and molecules. I will discuss joint work with Ostergaard-Sorensen and Spitzer on relativistic corrections to the energy and recent joint work with Erdos and Fournais on corrections to the energy due to magnetic self-interactions. In both cases the leading order of the energy (as the atomic number gets large) is not affected by the corrections. It is given by the classical Thomas-Fermi energy. The corrections come in the next order: the Scott order.

**Viktor N. Staroverov**, Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7. *Solved and unsolved problems in the theory of model Kohn-Sham potentials*: Direct approximation of Kohn-Sham potentials is an intriguing alternative to the usual pursuit of density-functional approximations for the exchange-correlation (xc) energy. The two central issues of potential-driven DFT are inversion of functional differentiation (how to recover the energy functional from a given Kohn-Sham potential) and the problem of integrability (how to ensure that a directly approximated potential is a functional derivative of some functional). The inversion problem was solved by van Leeuwen and Baerends [Phys. Rev. A 51, 170 (1995)]. More recently [J. Chem. Phys. 133, 101104 (2010)], we found a way to construct integrable model potentials without knowing their parent functionals. Integrability matters more than is often assumed since non-integrable model potential of van Leeuwen and Baerends, numerous approximations to the optimized effective potential, the exchange potential of Becke and Johnson, and its various extensions) have limited use precisely because they are non-integrable. I will overview the recent progress in the methodology of potential-driven DFT and discuss the current challenges for the development of practical Kohn-Sham potential approximations.

Yan Alexander Wang, Department of Chemistry, University of British Columbia, Vancouver, Canada, yawang@chem.ubc.ca. *Functional Derivatives and Differentiability in Density-Functional Theory*: Based on Lindgren and Salomonsons analysis on Fréchet differentiability [Phys. Rev. A 67, 056501 (2003)], we showed a specific variational path along which the Fréchet derivative of the Levy-Lieb functional does not exist in the unnormalized density domain. This conclusion still holds even when the density is restricted within a normalized space. Furthermore, we extended our analysis to the Lieb functional and demonstrated that the Lieb functional is not Fréchet differentiable. Along our proposed variational path, the Gâteaux derivative of the Levy-Lieb functional or the Lieb functional takes a different form from the corresponding one along other more conventional variational paths. This fact prompted us to define a new class of unconventional density variations and inspired us to present a modified density variation domain to eliminate the problems associated with such unconventional density variations.

Aihui Zhou, LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China, Email: azhou@lsec.cc.ac.cn. *Finite Element Approximations of Nonlinear Eigenvalue Problems in Density Functional Models*: In this presentation, we will talk about finite element approximations of nonlinear eigenvalue problems in density

functional theory. We will present a priori and a posteriori error estimates of finite element approximations of both orbital-free type and Kohn-Sham density functional models. We will also show the convergence and complexity of adaptive finite element approximations and report some numerical results of finite element electronic structure calculations that support our theory. This presentation is based on some joint works with Huajie Chen, Xingao Gong, Lianhua He, and Zhang Yang.

#### **Participants**

Burke, Kieron (UC Irvine) Cances, Eric (ENPC and INRIA) Car, Roberto (Princeton University) Chen, Jingrun (University of California - Santa Barbara) Chen, Yakun (University of British Columbia) Ehrlacher, Virginie (Ecole des Ponts - ParisTech and INRIA) Ernzerhof, Matthias (University of Montreal) Esteban, Maria J. (CNRS & Universite de Paris-Dauphine) Friesecke, Gero (Technische Universitat Munich) Gao, Weiguo (Fudan University) Garcia-Cervera, Carlos (University of California, Santa Barbara) Gavini, Vikram (University of Michigan) Krasny, Robert (University of Michigan) Lahbabi, Salma (Université de Cergy) Lewin, Mathieu (CNRS / University of Cergy-Pontoise) Lin, Lin (Princeton University) Lopata, Kenneth (Pacific Northwest National Laboratory) Lu, Jianfeng (Courant Institute of Mathematical Sciences) Lu, Gang (California State University Northridge) Maday, Yvon (University Paris 6) Meza, Juan (Lawrence Berkeley National Laboratory) Ortner, Christoph (University of Warwick and University of Oxford) **Pask, John** (Lawrence Livermore National Laboratory) Prodan, Emil V. (Yeshiva University) Romaniello, Pina (Ecole Polytechnique) Salahub, Dennis (University of Calgary) Schneider, Reinhold (Technische Universitat Berlin (Germany)) Scuseria, Gustavo (Rice University) **Solovej, Jan Phillip** (University of Copenhagen) Staroverov, Viktor (University of Western Ontario) Wagner, Lucas (UC Irvine) Wang, Yan Alexander (University of British Columbia) Zhou, Aihui (Chinese Academy of Sciences)

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## **Chapter 4**

## Linear Algebraic Techniques in Combinatorics/Graph Theory (11w5033)

#### Jan 30 - Feb 04, 2011

**Organizer(s):** Hadi Kharaghani (University of Lethbridge), Saieed Akbari (Sharif University of Technology & Institute for Research in Fundamental Sciences (IPM), Tehran), Richard Brualdi (University of Wisconsin-Madison), Willem Haemers (Tilburg University), Behruz Tayfeh-Rezaie (Institute for Research in Fundamental Sciences (IPM)), Qing Xiang (University of Delaware)

#### **Overview**

Linear Algebra and Matrix Theory provide one of the most important tools–sometimes the only tool–in Combinatorics and Graph Theory. Even though the ideas used in applications of linear algebra to combinatorics may be very simple, the results obtained can be very strong and surprising. A famous instance is the Graham-Pollak theorem which asserts that if the complete graph of order n is partitioned into m complete bipartite subgraphs, then m is at least n-1 (n-1 arises naturally by recursively deleting a star at a vertex, but there are many other ways to achieve n-1). The only known proofs of this theorem use some form of linear algebra. How does linear algebra enter into this and other combinatorial problems?

Almost all combinatorial objects can be described by incidence matrices (e.g. combinatorial designs) or adjacency matrices (e.g. graphs and digraphs). Sometimes the Laplacian and Seidel matrices are also used. Therefore one basic approach is to investigate combinatorial objects by using linear algebraic parameters (rank, determinant, spectrum, etc.) of their corresponding matrices. Two of the great pioneers of this approach were H.J. Ryser and D.R. Fulkerson. Strong characterization and non-existence results can be obtained in this way. The application of linear algebra to combinatorics works in the reverse order as well. Many linear algebraic issues can be refined using combinatorial or graph-theoretic ideas. A classical instance of this is contained in the Perron-Frobenius theory of nonnegative matrices where use of an associated digraph gives more detailed information on the spectrum of the matrix. Another more recent, but now classical, instance is the use of an associated digraph to refine the classical eigenvalue inclusion region of Gershgorin.

Another classical instance of the use of linear algebra to get combinatorial information is the theorem of Bruck and Ryser which rules out the existence of finite projective planes of certain orders. A further instance is the Friendship Thoerem which states that a graph in which every pair of vertices have exactly one common neighbor is a bunch of triangles, glued together in one single vertex. The important class of highly structured graphs known as strongly regular (connected) graphs have a linear algebraic characterization: they are the graphs whose adjacency matrix have exactly three distinct eigenvalues. The Graham-Pollak theorem mentioned above can be further generalized to graphs in general giving a bound on the integer parameter m in terms of the adjacency matrix.

Sometimes the lines between linear algebra and combinatorics are blurred. A simple example is the Cayley-Hamilton theorem that asserts that a matrix satisfies its characteristic polynomial. This theorem can be formulated and proved as a theorem in graph theory. Sign-nonsingularity of a matrix, where nonsingularity depends only on the signs (+, -, 0) of its entries and not on its magnitudes, and the resulting theory and application to linear systems, is a both a linear algebraic issue and a combinatorial issue. The existence of Hadamard matrices of all orders 4m can be viewed as both a linear algebraic problem and a combinatorial design problem. Related to this basic combinatorial problem are bounds for the determinant of matrices of 1s and -1s. There are many more examples that can be given.

It seems to be the case and it has been conjectured that almost all graphs are determined by their spectrum (the adjacency spectrum as well as the Laplacian spectrum). This would mean that the spectrum can be used as a kind of fingerprint for a graph. Especially for large networks this is an interesting property which, for example, makes it possible to order these networks (in almost all cases) in a systematic way. In another direction it is shown that the null space of the incidence matrices of directed graphs, undirected graphs, and inclusion matrices of designs have correspondence with flows in graphs, zero-sum flows, and trades in Latin squares, respectively.

#### **Objectives of the Workshop**

The main objective in organizing this workshop was to bring together a broad representation of the large and diverse collection of researchers who have made substantial contributions using linear algebra techniques in combinatorics and graph theory, or using combinatorial and graph-theoretic ideas to investigate matrices. The expectation was that there would be considerable cross-fertilization of ideas leading to people learning new problems and new applications of linear algebra techniques, and that this would lead to new collaborations, insights, and breakthroughs. Recent successes in collaborations of this kind encouraged us in the belief that such a meeting could bring new perspectives on old problems and open up many channels of communication for future collaborative research. For young researchers in particular, it would be an excellent opportunity to see the wide scope of the subject and the many interesting directions that can be explored.

#### **Participants**

We feel that we were quite successful in enticing a strong and diverse group of participants from many different parts of the world. In addition to the organizers, the participants were:

Mahmud Akelbek (USA), Sejong Bang (S.Korea), Aart Blokhuis (The Netherlands), Steve Butler (USA), Bart De Bruyn (Belgium), Charles Colbourn (USA), Rob Craigen (Canada), Carlos Fonseca (Portugal), Shmuel Friedland (USA), Wolfgang Holzmann (Canada), Steve Kirkland (Ireland), Reza Khosrovshahi (Iran), Jack Koolen (S. Korea), Christian Krattenthaler (Austria), Esther Lamken (USA), Felix Lazebnik (USA), William Martin (USA), Seth Meyer (USA), Margarida Mitjana (Spain), Ali Mohammadian (Iran),

Bojan Mohar (Canada), Vladimir Nikiforov (USA), Juan Rada (Venezuela), Michael Schroeder (USA), Bryan Shader (USA), Azhvan Sheikh Ahmady (Canada), Doug Stinson (Canada), Hajime Tanaka (Japan), Paul Terwilliger (USA), Wei Wang (China), Steven Wang (Canada), Ian Wanless (Australia), Richard Wilson (USA), Yaokun Wu (China), Mieko Yamada (Japan),

#### Program

Many participants were very eager to speak in order that the other participants would learn of their recent work and have the opportunity to react to it and provide additional connections and references. As a result, we had a full program of talks. In spite of the full program, there was ample time at coffee breaks, lunches, dinners, and evenings for informal discussions and collaborative work. As usual Wednesday afternoon was free for enjoying Banff and its surroundings, and on Friday morning there was a lively problem session. On Tuesday night, about one-quarter of the workshop participants enjoyed the Karaoke night at one of the local Banff establishments.

The full program, as well as the problems posed in the problem session, are available on the BIRS website, so we only provide here a summary of the topics of the talks. Very broadly speaking, the talks were on the following topics, all connected in one way or another wih linear algebra and matrix theory.

- 1. distance-regular graphs and other combinatorial configurations
- 2. Hadamard matrices
- 3. hyperplanes in finite geometries
- 4. spectral graph theory
- 5. graph matching
- 6. permanents, determinants and pfaffians in enumerative combinatorics
- 7. testing a database for certain characteristics
- 8. nowhere zero flows in graphs
- 9. extremal graph theory
- 10. permutation arrays
- 11. difference sets, orthogonal arrays, and codes
- 12. Smith normal form and hypergraphs

#### **Participant Testimonials**

The most effective way to convey the great benefit that participants received from the workshop is through their own testimonials. Here we give a sample of what some of the workshop participants reported after the workshop.

- My work falls entirely within the domain of what I describe as "Combinatorial Linear Algebra". It is a rare opportunity for me to attend a meeting that so consciously pays attention to this most fertile intersection of fields. The collection of experts assembled at BIRS for this event was very impressive, and I was able to initiate a number of very helpful conversations regarding various lines of research, and I was afforded an opportunity to explain a new and exciting type of construction for certain matrices, which I and my collaborators have recently developed, to an audience uniquely equipped to understand its significance. This kind of meeting provides valuable fertilization for my work, of a sort that is not easily found elsewhere, not because I do not occasional cross paths with these same people, but because when I do it is often not in a context so focussed on this kind of exploration, and generally not in such a broad group of people attuned to studying this kind of problem. (Robert Craigen)
- It was a great meeting, with great people, in a singular place. BIRS contains excellent conditions for research in Mathematics. I had the possibility to update some recent results on my field(s) of interest and get several ideas for a future research. (Carlos Fonseca)
- I found Craigen's talk on Buston-Hadamard matrices offered an interesting avenue for further investigation. The fair number of talks on Laplacian matrices and energy of graphs broadened my understanding of this area and has perked my interest in it. Finally the problem session gave a number of leads for problems which may be useful to give to graduate students to work on. (Wolfgang Holzmann)
- I received some helpful comments after my talk, including three different people who provided some references to related work this sort of feedback will be quite valuable to me, as the research that I presented is a new area for me. Also, a new collaboration may emerge between myself and Juan Rada. After seeing his talk on energy for digraphs, I had some ideas as to how the problem might be addressed for tournaments, and I will correspond with Juan in the near future on that topic. (Steve Kirkland)
- I met several new people at this workshop. The talk of M. Mitjana made me realize that some of the research my student is doing is also useful for other people. For me the good point of this conference was that I met some old friends and the discussions I had with them really helped me to see where my next step in my research should be. Although this has no direct impact in the sense of a new paper or so, it was really helpful for me. (Jack Koolen)
- I enjoyed the Workshop a lot. I cannot claim that it led to new collaborations or new results. It was very instructive to see for me what is going on in fields that I am not so acquainted with. I was very glad to meet for the first time people (such as for instance Charles Colbourn, Felix Lazebnik, Ian Wanless) whose name I had known for long but had never met before. In the talks and in discussions I saw many inspiring problems. As I say, I cannot claim to be able to say something on them now, but I hope to do so at a later point. (Christian Krattenthaler)
- I had several very useful contacts, and they will result, hopefully, in future collaboration. Two participants decided to visit the University of Delaware this Spring to continue our discussions at the conference: W. Haemers (about chromatic number of Erdos-Renyi graph) and B. Shader (some linear hypergraph problems). I plan to continue some work I began with Vlado Nikiforov (on existence of special book-like configurations in graphs), and with Steven Wang concerning my conjecture on some class of permutation polynomials. It was very useful to meet with S. Akbari and other members of the group from Iran. Their research concerning the Alon-Tarsi conjecture was very interesting to me. We found several other common mathematical interests, exchanged some problems, and plan to continue communication. (Felix Lazebnik)
- More specifically, the discussions with some participants have given me new ideas that, I hope, will help to tackle problems that we have been dealing and we will possibly make progress in many of them.

Moreover, I have learn very recent results that I shall take into account in order to obtain new results. Finally, the last aspect I would like to emphasize is the benefit that represents to explain the own recent work to a such specialized audience and to collect their impressions. (Margarida Mitjana)

- Paul Terwilliger and I started work and made significant progress on the problem of characterizing the sign patterns of nilpotent tridiagonal matrices. (Bryan Shader)
- Thanks very much for organizing such a wonderful workshop. Indeed, I have made many new contacts and are interested in several problems presented in the workshop. The talks are diverse, but with the common practice of linear algebraic techniques. The length of talks are nice so that necessary backgrounds can be explained to general public. In particular, I become more interested in looking at some conjectures related to matrices over finite fields, which were discussed during the workshop. (Steven Wang)
- The workshop was a thoroughly worthwhile week for me. It allowed me to meet a number of big names in the field that had only ever been names on paper up to that point. In particular I was delighted to meet Friedland, who has done some of the most impressive work on permanents in the last few decades, and whose work has heavily influenced my own. I had some very interesting discussions and I learnt some useful results in the talk. To cap it all off, I was able to solve a problem that was posed on the first day (about existence of Latin retransmission permutation arrays). In time this will lead to a publication for me; and I believe it was also pleasing to Doug Stinson who posed the problem. Of course, the setting was just amazing. BIRS must be one of the most inspiring venues in the world (I can't think of anywhere that beats it). (Ian Wanless)
- I'd like to mention a few possible new collaborations after BIRS 11w5033. I talked with Professor Friedland about the graph isomorphsim problems and spectral characterization of graphs. He pointed out to me a paper of His in 1989 using Coherent Algebra for the purpose of graph isomorphism. So it's possible for us to make a collaboration to further study these relationship (Graph Isomorphsim, Spectral Characterization of Graphs and Cohentent Algebra); I discussed with Dr. Butler about the construction of graphs with the same generalized characteristic polynomial, which is not arised from GM-switching method. This could give some further resluts about my conjecture presented in the talk. I learned that Professor Steven Wang is an expert in Finite Field. Previously I have made some conjectures about the irreducibility of rational polynomials over rational fields. We decided to further communicate with each other to study these conjectures. (Wei Wang)
- I met Mieko Yamada from Japan the first time. I had read some of her papers on Hadamard matrices many years ago. So it was great to finally meet her and talk to her. Aart Blokhuis reminded us the Alon-Tarsi conjecture on even/odd Latin squares, and surveyed recent progress on the conjecture. Robert Craigen talked about his joint work with B. Compton and W. de Launney on constructions of Hadamard matrices, which are very interesting to me. (Qing Xiang)
- Prof. Xiang and I talked about the skew-Hadamard difference sets over elementary abelian groups. We
  also discussed about the Gauss sums and Jacobi sums over finite fields and Galois rings, and affirmed
  the importance of these concepts. We will discuss the applications of Gauss sums to difference sets and
  cyclotomy continuously after the workshop. I believe we could start new research. Prof. Craigen and I
  believed we could collaborate on the research of the generalized Hadamard matrices. The talk by Prof.
  Terwilliger gave the ideas to my research on association schemes over Galois rings. (Mieko Yamada)
- I enjoyed many wonderful talks there, either related to my research interest or out of my former research range. Especially, I learned from the workshop some progress on Erdos-Ko-Rado and on Alon-Tarsi, which are of much interest to some of my colleagues in Shanghai (Jun Wang, Jiayu Shao, Jiyou Li, etc.) and outside of Shanghai (Huajun Zhang, John Goldwasser), and I will surely forward what I learn here to them. (Yaokun Wu)

# Conclusion

In our opinion, and as confirmed by the testimonials of participants, the BIRS Workshop 11w5033 was a tremendous success. It was a stimulating week for participants with a substantial amount of information exchanged, and new contacts and collaborations made. A week spent at a BIRS workshop can have a large effect on the research of participants. It can lead to new perspectives and new ideas on one's research, and can lead to avenues of research that were not anticipated before. We believe that our workshop illustrates this very clearly. There is nothing in the world like BIRS. It's unique setting and organization is having a profound effect on the development of mathematics. We hope that we might organize another similar BIRS workshop in the not too distant future.

The following references are mainly confined to books and survey papers in the general area of the workshop.

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# Chapter 5

# **Ergodic Optimization (11w5039)**

Feb 06 - Feb 11, 2011

**Organizer(s):** Anthony Quas (University of Victoria), James Campbell (University of Memphis)

# **Overview of the Field**

The field is a relatively recently established subfield of ergodic theory, and has significant input from the two well-established areas of symbolic dynamics and Lagrangian dynamics. The large-scale picture of the field is that one is interested in optimizing potential functions over the (typically highly complex) class of invariant measures for a dynamical system. Tools that have been employed in this area come from convex analysis, statistical physics, probability theory and dynamic programming. The field also has both general aspects (in which the optimization is considered in the large on whole Banach spaces) and local aspects (in which the optimization is studied on individual functions). In the latter category, there has been input from physicists with numerical simulations suggesting that the optimizing measures are typically supported on periodic orbits. This should be contrasted with the situation typically found in the 'thermodynamic formalism' of ergodic theory, in which the measures picked out by variational principles tend to have wide support. Ergodic optimization may be viewed as the low temperature limit of thermodynamic formalism.

## **Recent Developments and Open Problems**

Recent developments in the field have been multi-faceted: there has been a general goal of establishing results showing that for a typical potential function, the optimizing measures are supported on periodic orbits. Until now, all results of this type have been established on separable Banach spaces of functions, whereas the principal goals have been to establish them for certain non-separable Banach spaces. In recent progress, a first non-separable Banach space with this property was identified. Another aspect that has been of considerable interest has been studying the maximizing measures obtained as limits of Gibbs measures as the temperature is reduced to 0. Recent work has identified natural examples in which this limiting process fails. Work is ongoing to relate this to physical processes. Other groups of researchers have used convex analysis and measures of spread coming from economics to identify whole classes of functions sharing common optimizing measures. This is particularly interesting as the measures that appear in this study are widely known in a variety of other contexts.

Each speaker included open problems as part of their lectures. Additionally we scheduled a problem session for the presentation of problems which may not have found their way into lectures. Here are some of those problems.

#### **Entropy of Nearest Neighbor SFT's**

**Definition:** Let X be a  $\mathbb{Z}^d$  nearest neighbor SFT with alphabet A, and multiple measures of maximal entropy. For such X, where  $d \ge 1$ , define

$$\alpha_d := \inf_X \{ (\log |A|) - h(X) \}$$

Ronnie Pavlov, in his talk, mentioned the following facts:  $\alpha_d > 0$  for all d,  $\alpha_1 = \log 2$ ,  $\alpha_2 < \log 2$ , and  $\alpha_{d+1} \le \alpha_d$  for all d. He asks if it is true, then, that  $\lim_{d\to\infty} \alpha_d = 0$ ?

Equivalently, one asks if there exist  $\mathbb{Z}^d$  nearest neighbor SFTs with multiple measures of maximal entropy and entropy arbitrarily close to the log of the alphabet size?

#### Some Questions Related to ×2-invariant Measures

The following were contributed by Oliver Jenkinson.

#### Continuous f with Lebesgue measure as the unique $\times 2$ -invariant f-maximizing measure

The following is Problem 3.9 in [1]

#### **Problem:**

Let  $T(x) = 2x \pmod{1}$ . Explicitly exhibit a continuous function  $f : [0,1] \to \mathbb{R}$  such that  $\int f(x) dx > \int f d\mu$  for all T-invariant probability measures  $\mu$  other than Lebesgue measure.

Some remarks:

- (a) The strict inequality is key; if the inequality were weak then a constant function would suffice.
- (b) It is known that such functions f exist (see [2, Cor. 1]).
- (c) By an "explicit" representation of f we have in mind some sort of series expansion, for example a Fourier expansion.
- (d) It is known that any such f cannot be too "regular"; for example f cannot be Hölder (see e.g. the discussion in [1, 2]). There are heuristic reasons (see [2]) for expecting such an f to be highly oscillatory.

Since periodic orbit measures are weak-\* dense in the set of T-invariant measures, the following weaker version of the above problem is perhaps no easier to solve.

#### **Problem:**

Let  $T(x) = 2x \pmod{1}$ . Explicitly exhibit a continuous function  $f : [0,1] \to \mathbb{R}$  such that  $\int f(x) dx > \frac{1}{n} \sum_{i=0}^{n-1} f\left(T^i(\frac{j}{2^n-1})\right)$  for all  $n \ge 1$  and  $0 \le j \le 2^n - 1$ .

#### Positive entropy uniquely maximizing measures for analytic functions?

Again, let  $T(x) = 2x \pmod{1}$ . It is known that there exist real analytic functions whose unique maximizing measure is strictly ergodic but non-periodic. Examples of such functions can be found within the one-parameter family  $f_{\theta}(x) = \cos 2\pi (x - \theta)$ : for certain values of  $\theta$  the  $f_{\theta}$ -maximizing measure is a Sturmian measure supported on a Cantor set. Non-periodic Sturmian measures are, in a sense, the closest to periodic among all non-periodic measures; for example the symbolic complexity of a non-periodic Sturmian orbit (which is a generic orbit for the corresponding Sturmian measure) is as small as it can be among non-periodic orbits. Non-periodic measures with higher complexity can also arise as maximizing measures for (higher degree) trigonometric polynomials; for example measures which are combinatorially equivalent to an interval exchange can occur. All these measures seem to have rather low symbolic complexity, however, so that the following question is open.

#### **Problem:**

If  $T(x) = 2x \pmod{1}$ , can a positive entropy T-invariant measure uniquely maximize a real analytic function f?

#### Sturmian measure with largest variance

Among ×2-invariant probability measures, it is known (see [3]) that Sturmian measures have the smallest variance (where variance denotes the quantity  $\int (x - \int x d\mu(x))^2 d\mu(x)$ ). More precisely, the variance of a Sturmian measure (around its mean) is strictly smaller than for all other invariant measures with the same mean value (i.e. barycentre). The variance of a Sturmian measure depends continuously on its parameter (or 'rotation number'), and the following is open (see [4]):

#### **Problem:**

Which Sturmian measure has largest variance?

We remark that symmetry considerations mean that if  $S_{\varrho}$  has largest variance then so does  $S_{1-\varrho}$ . Numerical experiment suggests that the relevant value of  $\varrho$  is approximately  $676/1761 \approx 0.383873$ .

#### **Zero Temperature Limits**

The following was submitted by Jean-René Chazottes (of the Centre de Physique Thorique, École Polytechnique) and Michael Hochman (Institute for Advanced Study, Princeton), who were not actually in conference but who recognized the importance of our meeting and the relevance to their work.

In a recent paper (Commun. Math. Phys. 297 (2010)), they exhibited Lipschitz potentials on the full shift  $\{0,1\}^{\mathbb{N}}$  such that the associated Gibbs measures fail to converge as the temperature goes to zero. In higher dimension, namely on the configuration space  $\{0,1\}^{\mathbb{Z}^d}$ ,  $d \ge 3$ , they showed that this non-convergence behavior can occur for the equilibrium states of finite-range interactions, that is, for locally constant potentials. Here are several open questions posed in that paper.

#### The one-dimensional case

In the previously mentioned paper they obtained the following result.

#### Theorem A:

There exist subshifts  $X \subseteq \{0,1\}^{\mathbb{N}}$  so that, for the Lipschitz potential  $\varphi_X(y) = -d(y,X)$ , the family  $\{\mu_{\beta\varphi}, \beta > 0\}$  does not converge (weak-\*) as  $\beta \to +\infty$ .

In this statement,  $d(\cdot, \cdot)$  is the usual distance on  $\{0, 1\}^{\mathbb{N}}$ . This theorem holds more generally for one-sided or two-sided mixing shifts of finite type.

#### **Topological dynamics of** X

Let  $\mu$  be an ergodic probability measure for some measurable transformation of a Borel space, and  $h(\mu) < \infty$ . By the Jewett-Krieger theorem there is a subshift X on at most  $h(\mu) + 1$  symbols whose unique shift-invariant measure  $\nu$  is isomorphic to  $\mu$  in the ergodic theory sense. For the potential  $\varphi_X$ , all accumulation points of  $\mu_{\beta\varphi}$  are invariant measures on X, so they all equal  $\nu$ ; thus  $\mu_{\beta\varphi} \to \nu$  as  $\beta \to +\infty$ . This shows that the zero-temperature limit of Gibbs measures can have arbitrary isomorphism type, subject to the finite entropy constraint, and raises the analogous question for divergent potentials:

#### Problem 1:

Given arbitrary ergodic measures  $\mu', \mu''$  of the same finite entropy, can one construct a Hölder potential  $\varphi$  whose Gibbs measures  $\mu_{\beta\varphi}$  have two ergodic accumulation points as  $\beta \to +\infty$ , isomorphic respectively to  $\mu', \mu''$ ?

#### Maximization of marginal entropy

Let  $\varphi$  be a Hölder potential and  $\mathcal{M}$  the set of invariant probability measures  $\mu$  for which  $\int \varphi d\mu$  is maximal. It is known that if  $\mu$  is an accumulation point of  $(\mu_{\beta\varphi})_{\beta>0}$  then  $\mu \in \mathcal{M}$  and furthermore  $\mu$  maximizes  $h(\mu)$  subject to this condition.

In the example constructed in the proof of Theorem A, the potential  $\varphi$  had two  $\varphi$ -maximizing ergodic measures  $\mu', \mu''$ , and the key property that we utilized was that their marginals at certain scales had sufficiently different entropies. In fact, the measure maximizing the marginal entropy on  $\{0, 1\}^n$  for certain n was alternately very close to  $\mu'$  and to  $\mu''$ .

It is an interesting question if such a connection between zero-temperature convergence and marginal entropy exists in general. Let  $\varphi$  be a Hölder potential, and for each n let  $\mathcal{M}_n^*$  denote the set of marginal distributions produced by restricting  $\mu \in \mathcal{M}$  to  $\{0,1\}^n$ . The entropy function  $H(\cdot)$  is strictly concave on  $\mathcal{M}_n^*$ , and therefore there is a unique  $\mu_n^* \in \mathcal{M}_n^*$  maximizing the entropy function. Let

$$\mathcal{M}_n = \{ \mu \in \mathcal{M} \, : \, \mu |_{\{0,1\}^n} = \mu_n^* \}.$$

This is the set of  $\varphi$ -maximizing measures which maximize entropy on *n*-blocks. Note that the diameter of  $\mathcal{M}_n$  tends to 0 as  $n \to \infty$  in any weak-\* compatible metric. Hence we can interpret  $\mathcal{M}_n \to \mu$  in the obvious way.

#### **Problem 2:**

Is the existence of a zero-temperature limit for  $\varphi$  equivalent to existence of  $\lim \mathcal{M}_n$ ? More generally, do  $(\mu_{\beta\varphi})_{\beta>0}$  and  $(\mathcal{M}_n)_{n>0}$  have the same accumulation points?

#### The multi-dimensional case

#### The case $d \ge 3$ :

Recall that a shift of finite type  $X \subseteq \{0,1\}^{\mathbb{Z}^3}$  is a subshift defined by a finite set L of patterns and the condition that  $x \in X$  if and only if no pattern from L appears in x. Given  $L \subseteq \{0,1\}^E$  one can define the finite-range interaction  $(\Phi_B)_{B \subset \mathbb{Z}^d, |B| < \infty}$  by

$$\Phi_E(x) = \begin{cases} -1/|E| & x|_E \in L\\ 0 & \text{otherwise} \end{cases}$$

and  $\Phi_B = 0$  for  $B \neq E$ ; the associated potential on  $\{0, 1\}^{\mathbb{Z}^d}$  is

$$\varphi_L(x) := \sum_{B \ni 0} \frac{1}{|B|} \Phi_B(x) = \begin{cases} -1 & x|_E \in L \\ 0 & \text{otherwise.} \end{cases}$$

Clearly an invariant measure  $\mu$  on  $\{0,1\}^{\mathbb{Z}^d}$  satisfies  $\int \varphi_L d\mu = 0$  if and only if  $\mu$  is supported on X; thus the shift-invariant ground states are precisely the shift invariant measures on X.

In the paper mentioned in the introduction we obtained the following result.

#### **Theorem B:**

For  $d \geq 3$  there exist locally constant (i.e. finite-range) potentials  $\varphi$  on  $\{0,1\}^{\mathbb{Z}^d}$  such that for any family  $(\mu_{\beta\varphi})_{\beta>0}$  in which  $\mu_{\beta\varphi}$  is an equilibrium state (i.e. a shift-invariant Gibbs state), the limit  $\lim_{\beta\to+\infty} \mu_{\beta\varphi}$  does not exist.

#### Comments.

The previous statement is rather subtle. If there were a unique Gibbs state for each  $\beta$  then there would be a unique choice for  $\mu_{\beta\varphi}$ , and the previous result could be formulated more transparently: there exist locally constant potentials such that  $\lim_{\beta\to+\infty} \mu_{\beta\varphi}$  does not exist. But we believe that in our example uniqueness does not hold at low temperatures.

Our result is about continuous families and does not contradict the fact that for each given family  $(\mu_{\beta\varphi})_{\beta>0}$ of equilibrium states, there always exists a subsequence  $(\beta_i)_{i\in\mathbb{N}}$  such that the limit  $\lim_{i\to\infty} \mu_{\beta_i\varphi}$  exists. This is due to compactness of the space of probability measures.

There is nothing new in the fact that one can choose *some* divergent family  $\beta \mapsto \mu_{\beta\varphi}$  of equilibrium states. Think *e.g.* of the Ising model below the critical temperature ( $\beta$  large enough): One can choose a family which alternates between the + and – phases. However it is also possible to choose families which converge to one of the ground states. Let us insist that in contrast to this kind of situation we prove the existence of examples where it is *not possible* to choose *any* family which converges to a ground state.

#### The case d = 2:

Let us say a few words about the limitations of the previous result. First, it seems likely that our examples support non-shift-invariant Gibbs states, i.e. Gibbs states which are not equilibrium states, and, furthermore, we do not know if the statement extends to them. Hence the requirement of shift-invariance. As for the

restriction  $d \ge 3$ , the method used in our construction, which produces a potential of the form  $\varphi_L$  above, does not work at present in d = 2.

#### **Problem 3:**

For  $d \ge 2$ , do there exist finite-range potentials on the *d*-lattice such that every family of Gibbs states  $\{\mu_{\beta\Phi}, \beta > 0\}$  fails to converge as  $\beta \to +\infty$ ?

# **Meeting Highlights**

The meeting featured some 13 lectures of a very high standard covering a wide range of topics in the area. The schedule allowed plenty of time for informal discussion between the participants and there was a good deal of lively discussion between talks. The participants included researchers at all ranks: from student to senior researcher.

The following lectures were given:

- M. Allahbakhshi, 'Measures of relative maximal entropy'
- V. Anagnostopoulou, 'First order stochastic dominance'
- G. Contreras, 'Maximizing measures and Lagrangian subactions'
- C. Gonzalez-Tokman, 'Approximating invariant densities of metastable systems'
- R. Iturriaga, 'Selection of a Hamilton Jacobi solution via a discount factor'
- O. Jenkinson, 'Ergodic Dominance'
- I. Morris, 'Joint spectral radius and its connection with ergodic optimisation'
- R. Pavlov, 'Shifts of finite type with nearly full entropy'
- M. Pollicott, 'Dynamical Zeta Functions'
- A. Quas, 'Rates of approximation of optimizing measures by periodic orbit measures'
- J. Siefken, 'Ergodic optimization and super-continuous functions'
- P. Thieullen, 'Rotation vector for minimizing configurations of the multi-dimensional Frenkel-Kontorova model'
- F. Vivaldi, 'Minimal modules of periodic orbits'

## **Outcome of the Meeting**

The meeting was very successful at presenting a broad spectrum of work related to the central topic. Many of the participants were meeting for the first time and there was a substantial impetus towards collaboration and future meetings. A number of the participants commenced initial discussions that show some promise of development into full collaborative work.

As usual, BIRS was a superb place to organize a meeting. Many participants were there for the first time. New and returning participants alike were eager to come to BIRS. From an organizational point of view, it was extremely smooth. Brenda's assistance on the ground was invaluable and friendly as ever.

# **Participants**

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# Chapter 6

# Advancing numerical methods for viscosity solutions and applications (11w5086)

# Feb 13 - Feb 18, 2011

**Organizer(s):** Roberto Ferretti (Universitá di Roma Tre, Dipartimento di Matematica), Maurizio Falcone (Universitá di Roma - La Sapienza), Ian Mitchell (University of British Columbia), Hongkai Zhao (University of California, Irvine)

Viscosity solutions are a well established analytical tool to treat highly nonlinear Partial Differential Equations. Following the emergence of an analytical theory, a number of numerical strategies have been studied, the interest in this field being both the development of efficient schemes and their use in real-world applications of the theory. The purpose of this workshop was precisely to collect together viscosity solution experts from applied mathematics, analysis and numerical methods as well as scientists and engineers researching related applications, so as to exchange and integrate ideas from these various fields.

The workshop has been co-sponsored by the research project and training network SADCO (see the homepage at http://itn-sadco.inria.fr/), which has provided travel funds for some participants, mainly doctoral and postdoc students. A further co-sponsorship has been provided by IMACS, who has agreed to publish a selection of papers from the workshop as a special issue of the journal Applied Numerical Mathematics.

The workshop has tried to give a reasonably complete and self-contained panorama of the current lines of research, also by means of some tutorial sessions, devoted to relevant recent advances in the field and especially directed to the younger portion of the audience.

## **Overview of the Field**

The typical problems addressed in the theory of viscosity solutions are nonlinear, first- and second-order Partial Differential Equations of either the stationary form

$$H(x, u, Du, D^{2}u) = 0 (6.1)$$

or the evolutive form

$$\begin{cases} u_t + H(x, u, Du, D^2 u) = 0, \\ u(x, 0) = u_0(x) \end{cases}$$
(6.2)

(where Du and  $D^2u$  stand for respectively the gradient and the Hessian of u), with suitable boundary conditions. A certain number of problems of interest in applications may be put in the form (6.1) or (6.2), and among others:

• The Dynamic Programming (or *Bellman*) equation for the value function of finite or infinite horizon optimal control problems (see [1]) in which

$$H(x, u, Du, D^{2}u) = \lambda u + \sup_{\alpha} \left[ -f(x, \alpha) \cdot Du - g(x, \alpha) \right]$$

Here,  $\lambda \ge 0$ ,  $f(x, \alpha)$  and  $g(x, \alpha)$  represent respectively the controlled dynamics and the running cost, and the Hessian matrix  $D^2u$  may appear in the case of stochastic control problems. A generalization to the case of differential games (the so-called *Isaacs* equation) is also possible;

• The equation of the Shape-from-Shading (SfS) problem, in which u(x) is the height of a lambertian surface which has irradiance I(x). In the classical model for the SfS (see [5]), u solves the stationary equation

$$|Du(x)| = \sqrt{\frac{1 - I(x)}{I(x)}};$$

• The equation of front propagation in *level set* models (see [13, 10]), in which

$$H(x, u, Du, D^2u) = c(x)|Du|$$

where a front at time t is represented as a level set of u(x, t), and c(x) represents its speed of propagation and may contain terms related to curvature (hence, to  $D^2u$ ) or to nonlocal properties. A classical example is provided by the choice

$$H(x, u, Du, D^{2}u) = -\operatorname{div}\left(\frac{Du}{|Du|}\right)|Du|$$

which corresponds to the level set model of the propagation by Mean Curvature.

The theory of viscosity solutions (see [1] for an extensive and self-contained treatment of the topic) is conceived to give a sound theoretical framework to equations like (6.1)–(6.2). Their analytical difficulties typically include strong nonlinearities, degeneracies, and the need for treating nonsmooth solutions in most relevant applications. In addition to such analytical complications, the application of viscosity solutions to the Dynamic Programming framework also requires working in a prohibitively high number of dimensions.

From a numerical viewpoint, the application of classical monotone schemes (upwind, Lax–Friedrichs) has been proposed from the very start of the theory. The first reference in this line is a work by Crandall and Lions [3], related to the numerical approximations of first-order HJ equations of the form

$$u_t + H(Du) = 0,$$

and inspired by the convergence theory of monotone schemes for conservation laws. This result has later been generalized in [2] to cover more general equations, including second-order equations like (6.1)–(6.2) with the only assumption of satisfying a comparison principle.

So far, the use of monotone schemes is supported by a stable and reliable theory, but has not proved efficient enough for the most challenging applications. On one hand, the low convergence rate requires a large number of nodes, and therefore a high computational complexity, as soon as a good accuracy is required. On the other hand, monotone schemes typically exhibit a highly viscous behaviour – this makes it difficult to locate the singularities of the solution, which are usually of interest in the applications (for example, they correspond to switching surfaces in dynamic programming equations). All such drawbacks are even more apparent when considering that some of the application we have in mind imply a high number of dimensions.

Hence, the search for more advanced and efficient techniques has become a key topic for applications. Among the main features of numerical techniques of interest for the field, we may list:

- a good cost-effectiveness, that is, a high convergence rate with respect to computational load;
- a good capability to approximate nonsmooth solutions, that is, a low numerical dispersion;
- the possibility to be implemented in high dimension with a reasonable complexity;
- a robust convergence theory.

We will examine in the sequel some of the techniques that have been proposed to answer these issues.

# **Recent Developments and Open Problems**

Taking into account the recent advances in the field, along with the research lines represented in the workshop, the organizers have chosen to give a special emphasis to some specific direction of work, and more precisely: Dynamic Programming control techniques, Discontinuous Galerkin schemes, Semi-Lagrangian schemes and fast solvers (Fast Sweeping, Fast Marching). Four tutorials have been organized on such topics, and this has allowed in particular the youngest portion of participants to fill possible gaps. Moreover, looking at the contributed talks, these four subjects have proved to be real state-of-the-art work lines.

We briefly review the state of related researches.

#### **Dynamic Programming**

Dynamic Programming approach to optimal control problems (which characterizes a control problem via the associated Bellman equation, see [1]) dates back to the 1950s and has been widely studied in the applied mathematical community since, but has always been considered an impractical method because of the so-called *curse of dimensionality*, the typically exponential increase in complexity at the increase of the dimension.

However, while the real-life, massive optimal control problems remain out of the reach, it is clear that the continuous growth in the performance of computers has widened the range of applicability of Dynamic Programming techniques. In addition to this *brute force* increase, last years have witnessed the development of more efficient numerical schemes, in terms of high-order discretizations, fast solvers, sparse grids and so forth.

A tutorial on the relationships between Optimal Control problems and Hamilton–Jacobi equations has been given by Ian Mitchell, who has also recalled the concept of viscosity solution and discussed some application to real-world problems, although in low state-space dimension.

#### **Discontinuous Galerkin schemes**

Among the various high–order techniques, Discontinuous Galerkin (DG) schemes have originally been proposed in the framework of linear hyperbolic equations [8], and after a certain number of generalizations, they have been given a stronger theoretical framework in the last decade. The application of DG methods to Hamilton–Jacobi equations has been first proposed in [6] and seems to be a promising line of research. One one hand, they share the high geometric flexibility of finite element methods, and on the other they are well-suited for problems with nonsmooth solutions. At the moment, their main drawback is computational complexity.

A tutorial on DG methods has been given by Fengyan Li, a reputed expert in the field, who has reviewed the main concepts of DG schemes, as well as their construction in the case of first-order Hamilton–Jacobi equations.

#### Semi-Lagrangian schemes

Semi-Lagrangian (SL) schemes have a long tradition (set up in the 60s-70s) in the fields of plasma physics and Numerical Weather Prediction (see [11]), but have also proved to be effective in approximating viscosity solutions (see [4] and the references therein).

The main advantage of this class of schemes is their capability to work at large time steps, at the obvious price of a higher complexity for a single step of the scheme. On the other hand, large time steps also imply a low numerical viscosity - a key feature when working with nonsmooth solutions. SL schemes also admit a very natural formulation when approximating Dynamic Programming problems.

A tutorial on SL schemes has been given by Roberto Ferretti, who has shown the principles of construction, along with the basic convergence theory, in the case of linear advection equations and first-order HJ equations.

#### **Fast solvers**

Starting from the original versions of the Fast Marching Method (FMM) and the Fast Sweeping Method (FSM), first proposed respectively by J. Tsitsiklis in [T] and by Zhao, Osher, Merriman and Kang in [14]

(see also the review paper [5]), the search for non-iterative solvers of static HJ equations has experienced a number of improvements and generalization in the last years, including nonhomogeneous, nonisotropic and nonmonotone propagation of the solution, as well as the use of unstructured meshes.

The tutorial on fast solvers has been split in two parts, respectively devoted to FM and to FS Methods, which have been given by Alexander Vladimirsky and by Hongkai Zhao. This has provided new material and discussion for the difficult, unsolved task of comparing the two techniques.

## **Presentation Highlights**

We give an overview of the talks presented at the workshop.

• M. Akian, Max–Plus algebra in the numerical solution of Hamilton–Jacobi and Isaacs Equations

A max-plus algebra approach to solve Hamilton–Jacobi and Isaacs equations is presented. First, the max-plus linearity of first order Hamilton–Jacobi equations allows one to construct approximations of their solutions by max-plus linear combinations, then use max-plus tools for their study. Second, monotone discretizations of stationary Isaacs equations yield to fixed point or spectral equations of dynamic programming operators of zero-sum, two player stochastic games.

Using Perron–Frobenius properties inspired by the max-plus linear special case, a policy iteration algorithm has been introduced for degenerate (multi-chain) equations. The talk shows how policy algorithms behave combined with multigrid methods, and how this combination asks max-plus questions.

• J.-D. Benamou, F. Collino, S. Marmorat, Local High Frequency wave content analysis

Given multi frequency domain wave data, the proposed new algorithm gives a pointwise estimate of the the number of rays, their slowness vectors and corresponding wavefront curvature. With time domain wave data and assuming the source wavelet is given, the method also estimates the traveltime. We present numerical results on synthetic data that demonstrate both the effectiveness and the robustness of the new method. Comparisons with more classical algorithms tends to show the superiority of the new method.

• Y. Cheng, O. Bokanowski, C.-W. Shu, Discontinuous Galerkin scheme for front propagation with obstacle

The talk considers front propagation problems in the presence of obstacles, modeled by

$$\min(u_t + H(x, \nabla u), \ u - g(x)) = 0,$$

where u is a level set function and g(x) is an obstacle function (Bokanowski, Forcadel and Zidani, SICON 2010). Following the lines of Cheng and Shu (JCP 2007), a direct Discontinuous Galerkin method for this Hamilton–Jacobi equation is proposed, for which in some special cases it is also possible to prove stability estimates for standard fully explicit RK DG schemes. Several numerical examples of front propagation are given to illustrate the efficiency of the method, and also the application of a narrow band approach is investigated.

#### • F. Camilli, D.Schieborn, Shortest paths and Hamilton-Jacobi equations on a network

This talk presents an extension of the theory of viscosity solutions to topological networks. Uniqueness, existence and approximation results for Hamilton-Jacobi equations of eikonal type are discussed. A prominent question in graph theory is how to efficiently detect shortest paths connecting a given vertex with prescribed source vertices in a weighted graph. A similar problem is studied, assuming that the running cost varies in a continuous way along the edges.

• E. Carlini, A Generalized Fast Marching Method on unstructured grids

Recently, a new version of the Fast Marching Method (called Generalized Fast Marching Method, GFMM) habeen proposed to treat the case of evolutive eikonal equations with speed that can change sign in time. In this talk, the extension of GFMM to unstructured grids is presented. The motivation for this work comes from several applications, in which methods to track interfaces are coupled with

other solvers (typically, finite elements or finite volumes) built on unstructured grids. A general convergence result based on the properties of the local solver is given, and some numerical tests are presented.

• S. Cacace, E. Cristiani, M. Falcone, *Two new Ordered Upwind Methods for Hamilton–Jacobi equa*tions

Two generalizations of the Fast Marching Method for the numerical solution of the eikonal equation are presented. The new methods are based on a semi-Lagrangian discretization and are suitable for Hamilton–Jacobi equations modeling monotonically advancing fronts, including anisotropic front propagation problems, Hamilton–Jacobi–Bellman and Hamilton–Jacobi–Isaacs equations. The algorithms are compared with classical Fast Marching and Fast Sweeping methods.

• N. Forcadel, Generalized Fast Marching Method and applications

The Fast Marching Method have been proposed by Sethian in 1996 to solve very efficiently front propagation problem when the front evolves in its normal direction with a positive speed depending only on space.

The goal of this presentation is to give a generalization of this algorithm when the normal velocity depends also on time and can change sign. It can be proved that the proposed algorithm is convergent and that the complexity is essentially the same as in the classical case.

Finally, some applications in dislocations dynamics and image segmentation are presented.

• F. Cagnetti, **D. Gomes**, H. Tran, *Adjoint methods for obstacle problems and weakly coupled systems of PDE* 

In this talk, some new results for obstacle problems and weakly coupled systems of PDE are presented. The adjoint method, recently introduced by L. C. Evans, is used to study obstacle problems, weakly coupled systems, cell problems for weakly coupled systems of Hamilton–Jacobi equations, and weakly coupled systems of obstacle type. In particular, new results about the speed of convergence of common approximation procedures are derived.

• O. Bokanowski, J. Garcke, M. Griebel, I. Klompmaker, A Semi-Lagrangian scheme using adaptive sparse grids for front propagation

Sparse grids are a technique for treating high-dimensional interpolation of functions without going through the typical exponential increase of complexity. This suggests that they could be a tool for applying SL schemes in higher dimensions.

The talk reviews the basic facts about sparse grid approximations, and presents the application of sparse grids to the construction of a SL scheme for both linear advection and eikonal propagation of fronts. The performances of the scheme are evaluated on a set on numerical tests, and open theoretical issues are discussed.

• J.-C. Nave, On some high-order, optimally local schemes for interface problems

The talk will present two schemes, one for the advection equation and the other for Poisson's equation with interface discontinuities. The peculiarity of these schemes is that they are local, but can achieve 4th order convergence (in the  $L^{\infty}$  norm). The basic idea hinges on the locality of Hermite basis, and that of the ghost fluid method. Some applications, as well as current thoughts on various extensions will be discussed.

• A. Oberman, Numerical methods for geometric elliptic Partial Differential Equations

Geometric Partial Differential Equations can be used to describe, manipulate and construct shapes based on intrinsic geometric properties such as curvatures, volumes, and geodesic lengths. They have proven useful in applications (such as Image Registration and Computer Animation) which require geometric manipulation of surfaces and volumes. A few important geometric PDEs which can be solved using a numerical method called Wide Stencil finite difference schemes will be discussed: Monge-Ampere, Convex Envelope, Infinity Laplace, Mean Curvature, and others.

Focusing in on the Monge-Ampere equation, it will be shown how naive schemes can work well for

smooth solutions, but break down in the singular case. A robust and efficient solver will be discussed, with a complexity comparable to solving the Laplace equation a few times.

• S. Serna, Hamilton-Jacobi equations with shocks arising from general Fokker–Planck equations: analysis and numerical approximation

A class of Hamilton–Jacobi equations whose solutions admit shocks is considered. This class of equations arise as the convective part of a general Fokker–Planck equation ruled by a nonnegative diffusion function that depends on the unknown and on its gradient. The main features of the solution of the Hamilton–Jacobi equations are reviewed and a suitable numerical scheme is proposed in order to approximate the solution in a consistent way with respect to the solution of the associated Fokker–Planck equation. The talk also presents a set of numerical results performed under different piecewise constant initial data with compact support for specific equations including the one- and two-dimensional relativistic Hamilton–Jacobi equation and the porous media Hamilton–Jacobi equation.

• W. Chen, Z. Clawson, and S. Kirov, R. Takei, A. Vladimirsky, *Optimal control with budget constraints and resets* 

Many realistic control problems involve multiple criteria for optimality and/or integral constraints on allowable controls. This can be conveniently modeled by introducing a budget for each secondary criterion/constraint. An augmented HJB equation is then solved on an expanded state space, and its discontinuous viscosity solution yields the value function for the primary criterion/cost. This formulation was previously used by Kumar & Vladimirsky to build a fast (non-iterative) method for problems in which the resources/budgets are monotone decreasing.

A more challenging case is addressed, in which the resources can be instantaneously renewed (& budgets can be "reset") upon entering a pre-specified subset of the state space. This leads to a hybrid control problem with more subtle causal properties of the value function. The problem is illustrated by finding (time-or-energy) optimal trajectories for a robot in a room with obstacles, constrained by the maximum contiguous time of visibility to a stationary enemy observer.

• S. Luo, Y. Yu, H. Zhao, A new approximation for effective Hamiltonians for homogenization of a class of Hamilton–Jacobi equations

This talk presents a new formulation to compute effective Hamiltonians for homogenization of a class of Hamilton–Jacobi equations. The formulation utilizes an observation made by Barron and Jensen about viscosity supersolutions of Hamilton–Jacobi equations. The key idea is how to link the effective Hamiltonian to a suitable effective equation. The main advantage of such a formulation is that only one auxiliary equation needs to be solved in order to compute the effective Hamiltonian  $\overline{H}(p)$  for all p. Error estimates and numerical examples are be presented.

• H. Zidani, Convergence result of a non-monotone scheme for HJB equations

The convergence of a non-monotone scheme for one-dimensional first order Hamilton–Jacobi–Bellman equations of the form

$$\begin{cases} v_t + \max_{\alpha} (f(x, \alpha)v_x) = 0\\ v(0, x) = v_0(x) \end{cases}$$

is presented. The scheme is based on the anti-diffusive method UltraBee. It is shown that, for general discontinuous initial data, a first-order convergence of the scheme towards the viscosity solution is achieved, in  $L^1$ -norm. The non-diffusive behavior of the scheme and its relevance are illustrated on several numerical examples.

### **Scientific Progress Made**

#### Latest advances of numerical techniques

The organizers have made an effort to bring together the most up-to-date trends in the numerical analysis of viscosity solutions. The meeting has confirmed that development and theoretical analysis of efficient

numerical schemes for viscosity solutions has had significant improvements in the last years, and in some cases (notably, Discontinuous Galerkin schemes and fast solvers) is likely to have further advances in the next future.

While most of the methodological work is carried out on academic test cases, a certain number of talks have presented numerical applications of less standard type and/or in higher dimension, which is encouraging for the application of advanced numerical techniques to real-world problems.

#### Interactions between various techniques

In order to address problems of interest for applications, it seems important that a careful mixing of different techniques could be implemented in practical computations. As a matter of fact, the interaction of various techniques has been exploited in many of the works presented. As an example, the application of fast methods has been studied in conjunction with different local solvers (monotone, Semi-Lagrangian, Discontinuous Galerkin), high dimensional techniques like sparse grids have been used in a Semi-Lagrangian framework, and so forth. This is an additional indication that the research is moving towards more challenging applications.

#### Key features and benchmark tests

A major obstacle to the use of viscosity solution approximation schemes in real-world problems - as in many parts of computational science - is that advanced algorithms are complex and hence difficult to implement, compare, and apply to specific problems. The organizers therefore held a discussion session on the final afternoon of the workshop to discuss the creation of a set of benchmark tests on which various algorithms could be implemented and compared. Such a suite of benchmarks can provide a variety of benefits to the community: a common basis for quantitative comparison of the strengths and weaknesses of specific approaches in publications, a common framework in which to teach and learn the variety of algorithms for newcomers to the field, a set of challenge problems important to application fields for which current schemes are unsuitable, etc. If algorithm designers are further willing to release their implementations of benchmark problems, then researchers from ! application fields will be able to adapt those algorithms to and test them on their problems much more easily. It is therefore hoped that a properly chosen set of benchmarks will both allow the field to grow more quickly and reach a broader audience. It has been agreed that the candidate benchmarks should contain some (or all) of the major difficulties encountered in this class of problems: inhomogeneous and/or anisotropic propagation of the solution, singularities and/or discontinuities in the solution, complex geometries, high dimensional setting, etc. It will also be useful for the candidates to have analytical solutions, or at least approximations determined by an alternative approach for validation and error analysis. Some benchmarks may be parameterized (in some way other than grid resolution) to permit studies of scaling behavior. The work has proved to be anything but trivial, but has raised great interest from participants and is still in progress.

## **Outcome of the Meeting**

Summarizing the scientific products of the workshop, it is worth to point out that:

• The meeting has gathered 31 researchers in the field of numerical methods for viscosity solutions:

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Benamou, Jean-David	INRIA Roquencourt
Bokanowski, Olivier	Université Paris-Diderot
Cacace, Simone	Sapienza – Universitá di Roma
Camilli, Fabio	Sapienza – Universitá di Roma
Carlini, Elisabetta	Sapienza – Universitá di Roma
Cristiani, Emiliano	Sapienza – Universitá di Roma
da Silva, Jorge Estrela	Instituto Superior de Engenharia do Porto
Falcone, Maurizio	Sapienza – Universitá di Roma
Ferretti, Roberto	Universitá di Roma Tre
Festa, Adriano	Sapienza – Universitá di Roma
Forcadel, Nicolas	CEREMADE – Université Paris-Dauphine
Giorgi, Tiziana	New Mexico State University
Gomes, Diogo	Instituto Superior Tecnico Lisboa
Guigue, Alexis	University of British Columbia
Kao, Chiuyen	Ohio State University
Klompmaker, Irene	TU Berlin
Li, Fengyan	Rensselaer Polytechnic Institute
Mecca, Roberto	Sapienza – Universitá di Roma
Mitchell, Ian	University of British Columbia
Nave, Jean-Christophe	McGill University
Oberman, Adam	Simon Fraser University
Rao, Zhiping	ENSTA ParisTech
Serna, Susana	Universitat Autonoma de Barcelona
Sethian, James	University of California, Berkeley
Smits, Robert	New Mexico State University
Tasso de Figueiredo Borges de Sousa, Joao	Universidade do Porto
Vladimirsky, Alexander	Cornell University
Yu, Yifeng	University of California, Irvine
Zhao, Hongkai	University of California, Irvine
Zidani, Hasnaa	ENSTA ParisTech and INRIA Saclay

including young doctoral and postdoc students.

- Four tutorials have been devoted to the main research lines represented at the workshop; this has provided a good introduction for the younger participants, as well as a chance to compare the various techniques.
- The talks have shown less and less academic numerical examples, along with an increasing trend to mix the various techniques in order to approach the most challenging applications.
- A round table has been allocated to a discussion about creating an established set of benchmark problems in the field of viscosity solutions, in a spirit similar to what has been done in Computational Fluid Dynamics. This is an ongoing work (Mitchell).
- Up to the writers' knowledge, at least a couple of other ongoing researches have been started among participants of the workshop, in particular one concerning dynamic programming on hybrid control problems (Ferretti, Zidani), and the other on Fast Marching Methods (Cacace, Carlini, Cristiani, Falcone, Vladimirsky).
- Due to the co-sponsorship that IMACS has given to this workshop, it is expected that some of the works presented at the workshop will be collected in a special issue of the journal Applied Numerical Mathematics.

# **Participants**

Akian, Marianne (INRIA Saclay–Ile-de-France and CMAP) Benamou, Jean-David (INRIA Roquencourt) Cacace, Simone (SAPIENZA - Universita' di Roma) Camilli, Fabio (Sapienza - Università di Roma) Carlini, Elisabetta (Università La Sapienza) Cristiani, Emiliano (Sapienza Università di Roma) da Silva, Jorge Estrela (Instituto Superior de Engenharia do Porto) Falcone, Maurizio (Università di Roma - La Sapienza) Ferretti, Roberto (Universita di Roma Tre, Dipartimento di Matematica) Festa, Adriano (Sapienza Universita' di Roma) Forcadel, Nicolas (CEREMADE Universit Paris-Dauphine) Giorgi, Tiziana (New Mexico State University) Gomes, Diogo (Instituto Superior Tecnico) Guigue, Alexis (University of British Columbia) Kao, Chiuven (Ohio State University) Klompmaker, Irene (TU Berlin) Li, Fengyan (Rensselaer Polytechnic Institute) Maurice-Bokanowski, Olivier (University Paris-Diderot) Mecca, Roberto (Sapienza Università di Roma) Mitchell, Ian (University of British Columbia) Nave, Jean-Christophe (McGill University) **Oberman, Adam** (Simon Fraser University) **Rao, Zhiping** (ENSTA ParisTech) Serna, Susana (Universitat Autonoma de Barcelona) Sethian, James (University of California, Berkeley) Smits, Robert (New Mexico State University) Tasso de Figueiredo Borges de Sousa, Joao (Universidade do Porto - Robotics and Systems Institute) Vladimirsky, Alexander (Cornell University) Yu, Yifeng (University of California Irvine - Department of Mathematics) Zhao, Hongkai (University of California, Irvine) Zidani, Hasnaa (ENSTA ParisTech & Inria Saclay)

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# Chapter 7

# Modelling and analysis of options for controlling persistent infectious diseases (11w5133)

# Feb 27 - Mar 04, 2011

**Organizer(s):** Jonathan Dushoff (McMaster University) David Earn (McMaster University) David Fisman (University of Toronto)

# Introduction

The 5-day BIRS workshop on *Modelling and analysis of options for controlling persistent infectious diseases* (28 February to 4 March 2011) addressed some of the key public health policy themes raised during the BIRS *Modelling the Impact of Policy Options during Public Health Crises* BIRS workshop in 2008,<sup>1</sup> and gathered an interdisciplinary mix of mathematical modellers, clinicians and public health officials to explore these themes in the context of endemic infectious diseases.

Endemic infectious diseases have caused high levels of mortality and morbidity in human populations for centuries, and efforts to control them have a mixed record of success; with spatial and temporal fluctuations and evolutionary adaptation making the diseases hard to eliminate. A number of infections (including polio, measles, mumps, rubella, whooping cough) have been drastically reduced in large parts of the world (typically by vaccination) but remain persistently endemic (or resurgent) in several areas. Other infections (including influenza and tuberculosis) have been controlled in some areas by public-health measures, but continue to cause widespread morbidity and mortality over large parts of the world. Still other infections (including influenza and HIV) continue to defy control through vaccination and public-health measures and cause morbidity and mortality throughout the world. The only endemic pathogen to have been eradicated by human efforts so far is smallpox.<sup>2</sup>

Mathematical models have contributed to the understanding and control of infectious diseases for over a

<sup>&</sup>lt;sup>1</sup>Brauer, F., Feng, Z., and Glasser, J. BIRS Workshop Report: *Modelling the Impact of Policy Options during Public Health Crises*, 27 July 1 August 2008.

<sup>&</sup>lt;sup>2</sup>Eradication is the reduction of an infectious disease's prevalence in the global host population to zero. Elimination refers either to the reduction of an infectious disease's prevalence in a regional population to zero, or to the reduction of the global prevalence to a negligible amount.

century and, with infectious diseases responsible for millions of deaths annually and their treatment and control imposing a significant economic burden, the need to develop efficacious models and to communicate the implications of these models to policy makers is as vital now as ever. Advances in knowledge and technology are creating new opportunities for progress: but many theoretical, clinical, practical and administrative challenges remain.

In gathering the group of mathematical modellers, clinicians and public health officials at the workshop, the organizers aimed to deepen mutual understanding of each communitys insights and needs, and explore new strategies for disease control. To facilitate this, each of the first four workshop days began with a lecture introducing one of four practical challenges: disease control priorities, endgame strategies, economic constraints, and human behavioural factors. Shorter talks and discussions followed; highlighting recent progress in response to the relevant challenge for specific diseases and the models and analyses underpinning this progress. The fifth day was dedicated to open discussion of the topics explored across the first four days.

An overarching goal was that the insights emerging during the workshop should be shared with the broader mathematical, scientific, public health, and lay communities and continue to stimulate and inform community dialogue beyond the workshop. The organizers are accomplishing this in both traditional and innovative ways. The traditional methods included posting conference videos and documents to the BIRS website, presentation of summary slides by participants to their home institutions, and the publication of papers in peer-reviewed journals: the innovative method is described in detail below.

# Mapping the BIRS workshop

A five-day workshop elicits a vibrant, multi-dimensional dialogue that is difficult to compress accurately into a short, linear summary, and experiential energy and focus among the participants that are difficult to sustain and share beyond the workshop.

To address these challenges in an innovative way, this, the workshop organizers are experimenting with a new kind of web-based, visual dialogue mapping tool (Debategraph) that enables the content and structure the groups conversations and thinking to be mapped collaboratively by the participants before, during and after the workshop and then shared, via the web, for other participants to explore and build upon the conversation.

Debategraph has been used in public policy projects by, amongst others *the White House, the UK Foreign Office, the European Commission and CNN*, and its use in the context of the BIRS workshop can be seen as part of the wider experiments underway with the open science movement. As noted in a recent Nature blog post:

"How we read, write, and communicate science is changing profoundly under the influence of new technologies. In several fields within and outside of computer science, models, tools and standards are being developed that aim to enhance, enable or entirely replace formerly ingrained forms of scientific communication. Scientists, publishers, and vendors in various disciplines are developing methods and tools to improve the process of creation, reviewing and/or editing of scientific content; working on technologies and techniques to interpret, visualize, or connect scientific knowledge more effectively; and formulating concepts, tools, standards, and techniques for sharing multimodal and research data. These developments are currently taking place in disparate and disconnected domains, including computational linguistics, bioinformatics, information science areas like the semantic web or web technologies in general, social sciences, and computer-human interface studies.<sup>3</sup>"

While the technology and thinking in this area remain nascent, the potential to engage interconnected networks of scientists, researchers and wider stakeholders in new kinds of transparent, systematic dialogue, practice and inquiry is tantalizing and the potential to shift the mode of discourse from the limited historical form and conventions of static, linear papers towards more open, dynamic and collaborative editable graphs of ideas and arguments is intriguing.

Debategraph is an early exemplar of the new family of tools that are starting to emerge in this domain, and Debategraphs adoption by policy makers and mass media organizations makes it an apt choice for the issues addressed by the BIRS workshop. The tools main characteristics, and the ways in which these characteristics were applied in the workshop are outlined below.

In essence, the map/graph building process in Debategraph involves four steps:

- breaking down the subject under discussion into discrete ideas;
- figuring out the relationships between those ideas;
- expressing the ideas and relationships visually; and
- reiterating steps 1-3 to improve the map as understanding and consensus develop.

Ideas are visualized as thought bubbles or boxes and relationships between ideas are visualized by directed arrows, with a distinctive colour scheme, reflecting types of ideas and types of relationships, layered across the visualization so that the implied structure and meaning of the network of ideas can be interpreted at a glance.

For example, Figure 7.2 shows the core set of building blocksIssues (orange) raised, Positions (blue) suggested in response to these Issues, and Supportive (green) and Opposing (red) Arguments advanced for and against the Positionsand Figure 7.3 illustrates how these building blocks have been applied in a small strand of the BIRS map:

In Figure 7.3, a question is asked about the remaining challenges to the eradication of polio. A potential challenge to the elimination of polio is proposed (that new monitoring methods will need to be developed to achieve eradication), and a reason is offered in support of this challenge (that the current signal from the paralytic disease will be lost). Videos, images, charts, tables, detailed text, documents, files citations and comments can be added to each idea, and ideas can be cross-linked to other ideas on the same or different maps. All members of the group can add new ideas and edit and rate existing ideas (with visual cues signalling which ideas have the strongest weight of support).

<sup>&</sup>lt;sup>3</sup>http://blogs.nature.com/eresearch/2011/07/04/towards-executable-journals

The ultimate aim is to weave all of the salient ideas, arguments, evidence and citations of which anyone in and beyond the group is aware into a single rich, transparent, dynamic structurein which each idea and argument is expressed just onceso that anyone can explore the resulting knowledge base quickly and gain a good sense of the key issues and the perceived merits of the potential responses. While many different ideas types and relationships are available in Debategraphincluding causality, consistency and formal logic the core dialogic triad described above (of Issues, Positions, and Supportive and Opposing Arguments) can be combined multiple times to build large, comprehensive maps (Figure 7.5).

As the map evolves, changes to the map are flagged to the community via email and RSS feeds and anyone who spots a gap and identifies a new idea can add the idea to the map immediately for the whole group to see.

In essence, by externalising and structuring thought in this mutable way, the maps begin to augment the individual and group ability to think through complex, interrelated issues; helping the participants and readers to overcome the cognitive constraints of short-term memory and sub-optimal group processes such as groupthink and homophilyand to do so in an often playful, creative and engaging way.

The maps allow individuals and groups to apply their minds to the full set of ideas rather than a partial subset, and by reasoning transparently and iteratively help the group to reason rigorously, with each idea always open to direct challenge and improvement. In much the same way as a mediator seeks to create a physical space in which conflict can be explored and resolved, the interactive maps provide a networked context in which the conflicting values and interests, of multiple stakeholders can be surfaced and addressed openly and in an explicitly reasoned way.

Sharing understanding in a structured and transparent form also helps each participant to see that his or her perspective has been heard and represented accurately in the appropriate context, which helps to build trust and ensure that the maps evolve towards a full and fair reflection of the subject under consideration.

Furthermore as each idea only has to be stated once openly on the map, the mapping process can be highly time-efficient compared to working with a large body of static documents (across which many ideas will typically be repeated many times). Group members can move quickly through the top-level structure of the map and identify both the specific strands that need their attention and the relationships of those strands to the rest of the material.

Finally, documenting the reasoning behind a teams thinking and decisions helps to bring greater clarity and accountability to the groups analysis, decision making, and actions, which, in turn helps the group and the wider community to identify and learn from any mistakes and to improve the decision making process over time.

## **Overview of the BIRS Workshop Discussions**

The map was displayed throughout the workshop on a second screen to the right of the main presentation screen Figure 7.7); with a visual facilitator, David Price (Debategraphs co-founder), mapping the presentations and group conversation as they unfolded. At the same time, group members with laptops were able to log-in, add to, edit, comment on, restructure and rate the ideas live as they were being discussed.

Across the duration of the workshop, the top level structure of the map evolved towards the form show in Figure 7.8, with a glossary, information sources and a cross-link to the workshop preparatory map accompanied by four main discursive branches: Diseases, Public Health Policy, Research Questions, and Lessons from Mathematical Modelling

The Disease branch of the map enables the participants and readers explore the workshop presentations and discussion by disease (Cholera, Clostridium Difficile, Dengue, HIV, Influenza, Lyme disease, Malaria, Measles, MRSA, Neglected Tropical Diseases, Pertussis, Polio, Rabies, Smallpox, Syphilis, TB, and the West Nile Virus), or by categories of disease (e.g., acute diseases, viral diseases, diseases with an environmental reservoir, diseases with pandemic potential, diseases spread by specific forms of transmission). The health policy issues addressed during the workshop included:

- Policy dynamics: What do policy makers want from modellers? Who are the key audiences for the messages from modellers? What role does the media play and how can modellers ensure that media communication is appropriate and effective? And how to overcome the current and detrimental disconnect between policy makers and modellers?.
- Economic issues: Externalities in public health; the need for, and benefits of, improving health-related infrastructure through investment; corruption and poor governance as drags on improvement of public health; ways to align human behaviour with the public good; the correlation between wealth and health; cost-effectiveness of various interventions; and the use of electronic prediction markets (such as the Iowa Electronic Health Markets, http://iehm.uiowa.edu/iehm/index.html) as alternative tool for public health surveillance.
- Control priorities: How to balance different control priorities (reduction of illness, reduction of death, prevention of spread, prevention of vaccine/drug escape); the potential utility of conjoint analysis as a tool for prioritisation; and the need for better data collection.
- Ethical Issues: health inequalities at a national and global scale; the trade-off between individual and population level interests; the social implications of switching from a policy strategy of elimination to one of disease management, and public health as a basic human right.
- Optimum strategies: Identifying whether an eradication, elimination or management strategy is pragmatic for a given disease and/or location, and the growing importance and utility of dynamically-crafted public health strategies
- Behavioural change: Whose behaviour should we be trying to change (e.g. people who are infected, susceptibles, public health officials, politicians, journalists) and how can we accomplish this behavioural change? Top down edicts from public health authorities may be counterproductivehow do we change peoples perception of what is valuable, empower them to find the answers for themselves, use social marketing tools used in other disciplines, etc.

The key research questions addressed by the workshop included:

- improving access to existing data sources (many of which are being collated at the International Infectious Disease Data Archive (IIDDA);
- the limitation of existing surveillance methods, and the desirability of involving modellers in the design and improvement of current surveillance and data gathering techniques;
- the potential utility of novel surveillance tools (such as Google Flu Trends);
- the challenges of modelling human behaviour (including the difficulty of untangling and pinpointing the behavioural component amid many variables and degrees of freedom);

- the degree to which models can provide insights into interactions between complex systems.g. disease systems, systems of governance, and multinational aid organizations that enhance the likelihood of successful disease control, and the need to avoid the temptation to always adopt a narrow disease-by-disease focus; and,
- whether the modelling and policy community is too focused on R0 in particularwhich policy makers like (as reducing the characteristics of disease to a single number makes it easier for policy makers to comprehend and communicate what is happening), and which mathematical epidemiologists like (because of the opportunities afforded to prove things about the threshold) and on quantitative prediction in general. Should modeling be rebranded as a toolbox for the management of uncertainty, rather as a source of reliable predictions?

Finally, the workshop participants thought it might be helpful, to help communicate the character and significance of the field to a wider audience, to identify some of the major contributions from mathematical modelling to field of public health so far; namely:

- Disease transmission thresholds: Infectious diseases need to create at least one case per case to persist in a population. This implies that a finite reduction in risk could lead to a disease going extinct at the population level, even if some or all individuals remain susceptible to some degree, a phenomenon known as herd immunity.
- Distribution of age at infection: Modelling has provided key insights into factors underlying the age
  distribution of infected individuals, and how this may change as an epidemic spreads or as risk factors
  change. Understanding this link has proved critical in particular for avoiding the possibility of perverse
  outcomes in public health interventions: an intervention that weakens but does not eliminate disease
  transmission will typically increase the average age of infected individuals; in some cases this can lead
  to greater total burden of disease.
- Heterogeneity / core groups: A small "core" group of disease transmitters may account for a large percentage of cases; with an 80/20 rule of thumb suggesting that 20% of the people in a community may contribute 80% of the contacts (disease, infection, susceptibility, etc.) and vice versa.
- Optimal strategies to manage resistance: Mathematical modelling has helped to identify optimal strategies for managing resistance. For example, the adoption of combination therapy for malaria.
- Snapshots and linear models may be dangerously misleading: Snapshots and linear models were, for a long time, the models of choice for public health officials; as they tend to be more accessible to the "common sense" understanding of non-mathematical policy stakeholders. However, natural systems are often better understoodand therefore offer a sounder basis for policy decisionsas dynamic, non-linear systems. For example, linear/snapshot models may miss the rebound/delayed effects arising from the elongation of inter-epidemic period and the build up of susceptibles during periods of lowered vaccination rates.
- Utility of modelling and simulation for planning: Mathematical modelling and simulation can provide a more effective basis for public health planning and decision making.

# **Continuing the BIRS Dialogue Online**

As noted earlier, one of the attractions of using web-based, collaboratively editable tools like Debategraph is that the dialogue and shared understanding can continue to build online after the workshop; both for the workshop attendees and for the wider public health stakeholders. Since the workshop concluded, the map has continued to growincluding material, for example, from the Gates Foundation and BIREME (a PAHO Specialized Center for Latin America) and now encompasses over a thousand ideas.

The full map, including all of the editing functionality, is embedded on the BIRS website here<sup>4</sup> and is freely available to embed on the blogs and websites of other interested organizations and readers of this report are welcome and encouraged to read and explore the map in depth, and to join the continuing dialogue there.

# **List of Participants**

Blumberg, Seth (NIH Fogarty / UCLA) Bolker, Ben (McMaster University) Boni, Maciej (Oxford University) Brown, Kevin (University of Toronto) Chan, Christina (University of Toronto) **Day, Troy** (Oueens University) Dushoff, Jonathan (McMaster University) Earn, David (McMaster University) Eichner, Martin (University of Tbingen) Eisenberg, Marisa (Ohio State University) Feng, Zhilan (Purdue University) Fisman, David (University of Toronto) Funk, Sebastian (Zoological Society of London) Glasser, John (US Centers for Disease Control and Prevention) Greer, Amy (Public Health Agency of Canada) He, DaiHai (McMaster University) Hempel, Karsten (McMaster University) Hill, Andrew (Self) Huppert, Amit (Gertner Institute for epidemiology and health policy research Sheba Medical Center) Hurford, Amy (York University/University of Toronto) Ke, Ruian (University of California, Los Angeles) Keegan, Lindsay (McMaster University) Krylova, Olga (McMaster University) Lindquist, Jennifer (University of Victoria) Loeb, Mark (McMaster University) Ma, Junling (University of Victoria) Mishra, Sharmistha (Imperial College) Moghadas, Seyed (Centre for Disease Modelling) Ng, Vicky (Centre for Public Helath and Zoonoses) Patocs, Audrey (McMaster University) Price, David (Debategraph) Sander, Beate (Ontario Agency for Health Protection and Promotion) Tien, Joe (Ohio State University) Tuite, Ashleigh (University of Toronto) van den Driessche, Pauline (University of Victoria) Worden, Lee (McMaster University) Yaari, Rami (Tel Aviv University) Yan, Ping (Public Health Agency of Canada)

<sup>58</sup> 

<sup>&</sup>lt;sup>4</sup>http://www.birs.ca/events/2011/5-day-workshops/11w5133/debategraph

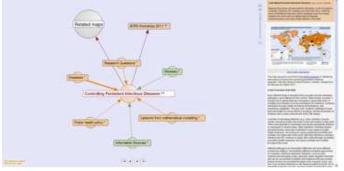
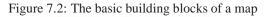


Figure 7.1: The BIRS Debategraph Controlling Persistent Infectious Diseases





# Figure 7.3: Exploring challenges to the eradication of Polio Challenges to Polio eradication? \* The effort to complete eradication of Polio has met with a number of challenges for which solutions are not readily available. $\hat{\mathbf{U}}$ New methods required to monitor Responds poliovirus circulation \* to New methods to monitor poliovirus circulation are increasingly necessary. Û Monitoring signal provided by paralytic Supports disease will be lost \* The signal provided by paralytic disease will be lost eventually.

Figure 7.4: Each idea can be articulated in depth

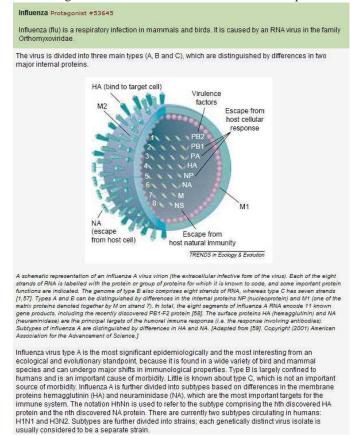
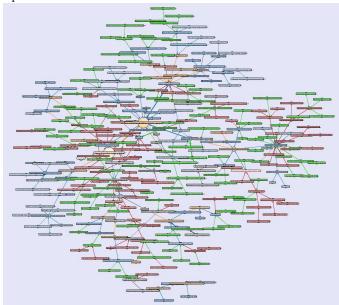


Figure 7.5: Large maps evolve from the combination and re-combination of small strands of arguments



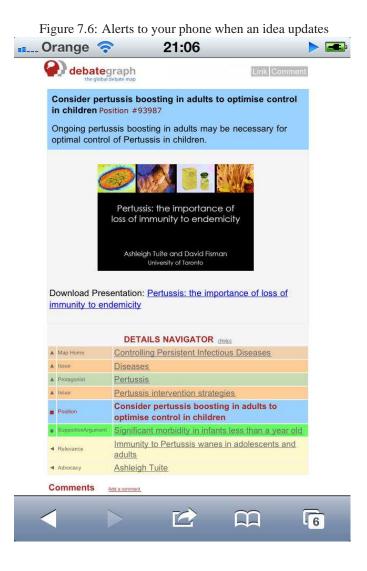


Figure 7.7: Mapping the discussion live during the workshop. David Price (right) builds and displays a map as David Earn talks. Other members contributed to the same map in real time during lectures.



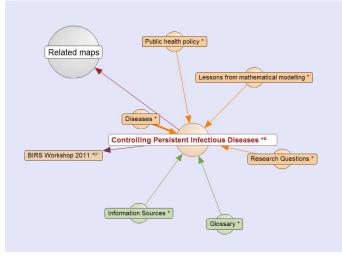


Figure 7.8: Top level issues addressed at the BIRS Workshop

Figure 7.9: Public Health Policy issues explored at the BIRS Workshop

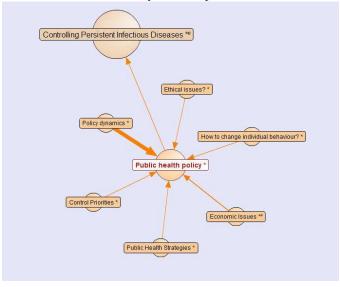
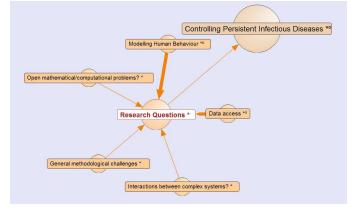


Figure 7.10: Research questions discussed at the BIRS Workshop



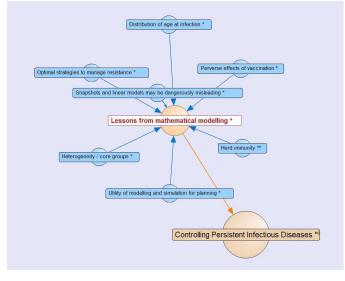


Figure 7.11: Key Lessons from Mathematical Modelling so far

Banff International Research Station for Mathematical Innovation and Discovery Publications Online Services Contact About BIRS Resources Programs Modelling and analysis of options for controlling persistent infectious diseases workshop Login Re debategraph Controlling Persistent Infect text Stream Finder Community He Share his may ind analysis or -, diseases" that was h - hruary to 4 Mar Add idea Diac uaa Cri nk Cite New map eld at t rch 201 ew of the field tention today is directed to the scourges ins, and methods for their control. There is set of agents that have managed to cau

Figure 7.12: Widening the Dialogue online after the BIRS workshop

# **Chapter 8**

# Sparse and Low Rank Approximation (11w5036)

# Mar 06 - Mar 11, 2011

**Organizer(s):** Gitta Kutyniok (Technische Universität Berlin) Holger Rauhut (University of Bonn) Joel Tropp (California Institute of Technology) Ozgur Yilmaz (University of British Columbia)

# **Overview of the Field**

Digital computers and their efficiency at processing data play a central role in our modern technology. Today, we use digital hardware in every aspect of our daily lives. Cell phones, digital cameras, MP3 players and DVD players are only a few examples where signals of interest, which are inherently analog, are acquired, converted to digital bit streams, stored in compressed form, and transmitted over noisy channels. In all these applications, the current demand is towards "higher-resolution" and "faster". In turn, the amounts of data we need to deal with is getting exceedingly large.

Recently, a new signal processing paradigm based on "sparsity" has emerged. This new paradigm exploits an empirical observation: many types of signals, e.g., audio, natural images, and video, can be well represented by "very few" elements of a suitable representation system. This fact has revolutionized data processing, and led to a rethinking about how to acquire various types of signals using a very limited amount of linear measurements. Consequently, this new paradigm has the potential to change the way we collect information about many types of signals.

One exciting development is the introduction of the method of Compressed Sensing [16, 7, 22, 36] which, for instance, led to the design of a single-pixel digital camera built at the Rice University, see http://dsp.rice.edu/cscamera. This research area is very new and hence various key research questions are still under investigation, and also the application of these techniques to, for instance, astronomical image and signal processing, radar imaging, wireless communication, and seismology is just in its beginning stage. Advancing research on these questions as well as studying the potential for diverse applications was a primary motivation for this workshop.

# **Mathematical Foundations**

The field of sparse and low-rank approximation is based on several mathematical ideas, and it has a variety of striking applications.

#### **Sparsity**

A function is *sparse* or *compressible* if it can be approximated by a short linear combination of basis functions drawn from a fixed collection. "Short" means that the number of basis functions needed is somewhat smaller than the ambient dimension of the function space. Compressible functions have less information than their dimension suggests. In many problems, the family of basis functions should describe the type of structures one hopes to find in the class of functions of interest; it may or may not form an orthogonal system.

Classical example A smooth function is well approximated by its lowest-order frequency components.

**Less classical example** A piecewise smooth function is well approximated by the most significant terms in its wavelet expansion.

Modern example Low-rank matrices can be expressed using a sum of a few rank-one matrices.

Sparsity is the main idea behind transform coding, the concept at the bottom of the JPEG scheme for image compression. Roughly, we transform an image into the discrete cosine domain; we retain only the terms in the expansion that have large coefficients; we store the few remaining coefficients. This operation achieves compression. To decompress, we apply the inverse discrete cosine transform to the compressed representation.

Another important perspective on sparsity is framed in terms of a linear inverse problem. Consider the system of linear equations

f = Ax

where f is the function of interest and A is a fixed matrix. The columns of A are the basis functions. We say that f has a sparse representation when the variable x is a sparse vector. In practice, of course, the equality is only approximate! But this situation arises often enough to base a field of research on it.

#### Algorithms that enforce sparsity

Given an observation of a function f, we would like to find a sparse (approximate) solution x to the linear inverse problem f = Ax. In general, this problem is computationally hard because it might require a combinatorial search. Remarkably, in certain situations, we can still accomplish this goal.

One approach is to solve a regularized inverse problem. Given an observed function f and a matrix A, solve [11, 16]

$$\min_{x \to 0} ||x||_1 \quad \text{subject to} \quad f = Ax.$$

In other words, instead of the classical  $\ell_2$  regularization, we use an  $\ell_1$  regularization instead, which has the effect of promoting sparsity in the solution.

The  $\ell_1$ -regularized optimization problem has a (trivial) closed-form solution when A is invertible. More generally, it can be solved using special-purpose convex optimization algorithms.

When the columns of A are roughly orthogonal, the solution to the  $\ell_1$ -minimization problem is close to the "true" sparse  $x^*$  for which  $f = Ax^*$ . We can quantify "roughly orthogonal" in several different ways, but the technical details are not that important here.

#### **Compressed sensing**

Consider a binary 0–1 vector  $x^*$  of length d with at most s entries equal to one. It is very inefficient to express this vector in the standard coordinate basis because it contains so many zeros. In fact, it only takes about  $s \log(d/s)$  bits to encode this vector (using run-length coding!).

The vector  $x^*$  is sparse in the sense that I described before because it can be represented efficiently in the standard basis. Is there some type of measurement that automatically sieves out the locations of the unit entries? In fact, the inner product between  $x^*$  and a random (say, Gaussian) vectors provides a lot of information about  $x^*$ .

Suppose that we could take measurements

$$f_i = \langle x^*, g_i \rangle, \quad i = 1, 2, ..., m$$

where  $g_i$  are independent, standard Gaussian random vectors. It turns out that, provided  $m > 2s \log(d/s)$ , the real-valued measurements  $f_1, ..., f_m$  contain all the information we need to (stably) reconstruct  $x^*$  [8, 17, 10].

How? Use tractable algorithms for sparse solution of linear inverse problems. We just need to find a sparse solution to f = Ax where the rows of A are the vectors  $g_1, ..., g_m$ . We can do this using  $\ell_1$  minimization. It turns out that the Gaussian matrix A has the property that the columns are "sufficiently orthogonal" to ensure that the true solution  $x^*$  is the unique min- $\ell_1$  solution of f = Ax.

## **Recent Developments and Open Problems**

While Gaussian random measurements are known to be optimal for compressive sensing they have the drawback of lacking a fast matrix vector multiply. Structured random measurement maps may overcome this computational bottleneck. Partial random Fourier matrices are known since the advent of compressive sensing to provide near optimal recovery guarantees. Recently, further types of structured random matrices were investigated. These include partial random circulant matrices [36, 37] (mentioned in the talk by Romberg), and time-frequency structured random matrices [34] (talk by Pfander). For both matrices the optimal expected recovery guaranties are so far open.

The extension of compressive sensing techniques to the recovery of low rank matrices is another recent development. A number of efficient recovery algorithms for this task have been developed over the last two years, including nuclear norm minimization [20, 39] (reported in the talk by Maryam Fazel), singular value thresholding [6], iteratively reweighted least squares [23], max norm minimization [30] (as presented by Nathan Srebro), and more. Also a number of theoretical results for low rank matrix recovery is available by now [39, 9, 38, 32] (talks by Maryam Fazel, Ben Recht), but many more developments can be expected, such as extensions to structured random measurement maps (initial insights were reported by Justin Romberg).

Ideas and techniques from compressive sensing were recently applied in new areas, which have not been the focus of research in compressive sensing in the beginning. The use of compressive sensing for quantization is investigated in the initial contributions [4, 27], and was reported at the workshop. Many open questions in this context remain, e.g., whether the use of efficient structured measurement maps is possible.

The Johnson-Lindenstrauss embedding represents a fundamental tool for dimensionality reduction, and is usually realized via random matrices. It was an early insight [3] that the fundamental concentration inequality leading to the Johnson-Lindenstrauss map, can also be used for proving the restricted isometry property, a fundamental concept in compressed sensing. It came as a recent surprise that also the converse is true: A matrix satisfying the restricted isometry property provides a Johnson-Lindenstrauss embedding after randomizing the column signs [29]. Eldar and Needell developed a variant of the Kaczmarz method for solving large linear systems, which exploits Johnson-Lindenstrauss maps [18]. In [21] a method for numerically solving dynamical systems in high dimensions using the Johnson-Lindenstrauss embedding was developed.

Manifold learning and processing is an increasingly important task with applications to machine learning, signal processing and more. In some cases, these manifolds are embedded into a very high dimensional space. Recently, investigations on the use of compressive measurement maps (such as Johnson-Lindenstrauss maps) in this context have been initiated (talks by Herman and Iwen). First results are promising, and many more development in this direction can be expected.

Recently, sparse approximation techniques were also applied for the numerical analysis of partial differential equations (PDEs) with random coefficients, as well as in parametric PDEs [13]. Here it can be shown that under certain conditions the solution to the parametric PDE as a function of the physical variable and parameter can be well-approximated by a sparse expansion in tensor product Legendre polynomials in the parameter, and with coefficient functions depending on the physical variable. The application of sparse approximation schemes seems promising, and moreover, this result leads to decay rates for greedy approaches in reduced basis methods [5]. Many more contributions in this direction are expected in the near future.

## **Presentation Highlights**

Reflecting the high-level of activity in the area, the workshop brought together world-experts from various areas of mathematics and engineering along with young researchers. Accordingly, nine talks were given

by junior researchers (one of them was a graduate student, the remaining eight were postdocs). Below, we categorize the presentations according to their specific focus.

#### **Compressed Sensing**

There were a large number of presentations that were on compressed sensing and its variations as well as implications of certain techniques developed in CS to other areas of mathematics.

#### Theory and algorithms for sparse recovery

*P. Boufounos* presented recent work in sparsity constrained optimization of arbitrary cost functions—as opposed to the quadratic cost functions of the usual sparse recovery algorithms— where he generalizes the Restricted Isometry Property (RIP) to a stability condition on the Hessian of the cost function. Furth ermore, Boufounos discussed the Gradient Support Pursuit (GraSP), an algorithm that generalizes known CS algorithms to perform sparsity constrained minimization of arbitrary cost functions.

*V. Temlyakov* considered greedy algorithms for sparse recovery, which constitute a viable alternative to  $\ell_1$  minimization in this context. He discussed so-called Lebesgue-type inequalities for greedy algorithms in Hilbert and Banach spaces.

*H. Mansour* studied weighted  $\ell_1$  minimization for signal construction from CS measurements when partial support information is available [26]. He proved that if the support estimate is more than % 50 accurate, then this alternative algorithm recovers the underlying sparse or compressible signal under weaker sufficient conditions than those for  $\ell_1$  minimization.

*V. Goyal* emphasized that most theoretical guarantees in sparse approximation are uniform over deterministic signal classes and consequently pessimistic. He proposed a Bayesian formulation based on the "replica method" from statistical physics [35]. Using this formulation, he presented an exact asymptotic analysis of many commonly-used decoders such as basis pursuit, lasso, linear estimation with thresholding, and zeronorm regularized estimation, which gives results that are more encouraging for compressed sensing than the usual uniform guarantees.

#### Mathematical and practical challenges in implementing compressed sensing

*R. Saab* showed that one can successfully employ "noise-shaping"  $\Sigma\Delta$  quantizers for compressed sensing. He proved that, by using appropriate Sobolev dual frames in the reconstruction,  $\Sigma\Delta$  quantizers utilize the inherent redundancy more efficiently than "any" round-off type quantization algorithm, at least in the case of Gaussian measurement matrices. Consequently,  $\Sigma\Delta$  quantizers outperform the round-off quantization schemes (generally referred to as memoryless scalar quantizers) in the compressed sensing setting [27].

*R. Baraniuk* considered 1-bit quantization for compressed sensing. He proposed the notion of a "Binary Stable Embedding", a property that ensures stable reconstruction from 1-bit measurements. Using this property, he presented some recovery guarantees for 1-bit compressed sensing [4]. In addition, he discussed algorithmic issues regarding 1-bit compressed sensing.

*Y. Eldar* reviewed her earlier work on "analog compressed sensing" which she calls "xampling". The goal in xampling is to build sub-Nyquist analog-to-digital converters. She then discussed how sub-Nyquist sampling of pulse streams can be used to identify linear time-varying systems and showed that sufficiently-underspread parametric linear systems, described by a finite set of delays and Doppler-shifts, are identifiable from a single observation as long as the time-bandwidth product of the input signal is proportional to the square of the total number of delay-Doppler pairs in the system [2].

*R. Calderbank* addressed two practical challenges: The first is a wireless uplink where mobile users in some geographic area need to register with a base station. The second is the distribution of information in a wireless sensor network. Inspired from compressed sensing and Reed-Muller codes, he presented a new deterministic framework for communication in wireless networks which can successfully address the above-mentioned challenges.

*T. Strohmer* used sparse MIMO Radar as a case study to analyze the potential benefits and pitfalls of compressive sensing, He noted that compressed sensing "finds itself caught between two extremes - the parametric and the non-parametric world". He noted that even though at first glance the benefits of Sparse

MIMO Radar seem obvious (robust with respect to noise, can detect weak targets), a careful analysis raises some challenging questions. He concluded that compressed sensing combines some of the strengths as well as some of the weaknesses of both the parametric and non-parametric methods.

A. Pezeshki discussed the sensitivity of compressed sensing to "basis mismatch", i.e., mismatch between the assumed and the actual models for sparsity. He presented some numerical examples, based on Fourier imaging, that demonstrate a significant dependence on the correct choice of the associated sparsity basis. He also presented theoretical results on how basis mismatch effects the "recovery error" that apply when a wide class of sparse recovery algorithms, including basis pursuit, are used [12].

#### Generalizations of compressed sensing

*M. Iwen* considered the problem of approximating low-dimensional manifolds in high-dimension using a small number of linear measurements, i.e., compressive measurements. He provided a simple reconstruction algorithm. He also obtained theoretical recovery guarantees.

*B. Recht* discussed a framework for "extending the catalog of objects and structures that can be recovered from partial information" [10]. He presented a family of algorithms—that are obtained in a convex optimization framework—for obtaining "sparse" approximations of these various objects and discussed general recovery guarantees and implementation schemes for these algorithms. While Recht's approach encompasses  $\ell_1$  minimization (compressed sensing) and nuclear-norm minimization (low rank matrix completion), it also shows that in various different problems an analogous approach can be adopted.

#### Mathematical results inspired by compressed sensing

*F. Krahmer* established a new connection between the Johnson-Lindenstrauss lemma (which is a central dimension-reduction result used in various computer science applications) and the restricted isometry property (RIP), a central concept in the theory of sparse recovery. Specifically, he proved that  $m \times N$  matrices satisfying the RIP of optimal order provide (via randomized column signs) optimal Johnson-Lindenstrauss embeddings up to a logarithmic factor in N. Krahmer's results yield the best known bounds on the necessary embedding dimension m for a wide class of structured random matrices, including partial Fourier and partial Hadamard matrices [29].

*D. Needell* considered the randomized Kaczmarz method that was recently proposed by Strohmer and Vershynin [40], who also shoved that this methods converges exponentially (in expectation). In her talk, Needell presented a modified version of the randomized Kaczmarz method (where at each iteration the optimal projection from a randomly chosen set is selected). She showed that this modified rate generally improves the convergence rate significantly. Furthermore, using dimension reduction methods based on Johnson-Lindenstrauss lemma, the run-time of the modified algorithm is on the same order as the run-time of the original version [18].

S. Foucart focused on two important problems on the geometry of finite-dimensional  $\ell_1$  spaces: estimation of Gelfand widths of their unit balls, and Kashin's orthogonal decomposition theorem. Using the theory of compressive sensing, he extended the known results to finite-dimensional  $\ell_p$  spaces ( $0 ) [25]. Furthermore, using compressed sensing methods, he obtained the lower estimate for the Gelfand width of <math>\ell_1^N$  in  $\ell_2^N$ .

#### **Sparse approximation**

*I. Daubechies* focused on a new mathematical theory for the empirical mode decomposition (EMD) algorithm. EMD is a heuristic technique that aims to decompose functions that have sparse expansions in terms of building blocks that can be viewed as locally harmonic functions with slowly varying amplitudes and phases that are well-separated in the time-frequency plane. Daubechies introduced a decomposition that "captures the flavor and philosophy of the EMD approach", however her method of constructing the components is different and uses the so-called "synchrosqueezed wavelet transform". She presented both theoretical results and applications of the algorithm [14].

J. Vybiral considered the problem of approximating a function  $f : \mathbb{R}^d \mapsto \mathbb{R}$  that is of the form f(x) = g(Ax) where A is a  $k \times d$  matrix with  $k \ll d$  from only a few values of f. Vybiral presented a randomized al-

gorithm and proved that (under some conditions on g and A) the algorithm produces a uniform approximation to f with high probability [24].

A. Cohen also discussed mathematical problems that involve functions of a very large number of variables. He focused on such problems in partial differential equations depending on parametric or stochastic variables where numerical difficulties arise due to the so-called "curse of dimensionality". Cohen explained how these difficulties may be handled in various contexts using the concepts of variable reduction and sparse approximation.

*S. Kunis* emphasized that sparse approximation is a powerful approach for handling high-dimensional problems, however he noted that it is critical that algorithms such as FFT need also be customized as to allow the use of sparsity to reduce the computational cost. To that end, he considered two generalizations of the FFT: a hyperbolic-cross FFT [15] and the so-called butterfly sparse FFT.

#### Low rank approximation

*M. Fazel* focused on theoretical recovery conditions for low rank matrices from (possibly noisy) linear measurements. She presented a framework that can be used to extend robust recovery results from vectors (as in the case of sparse recovery) to low-rank matrix recovery. She noted that this methodology is simple and leads to the tightest known sufficient conditions (e.g., in terms of the RIP of the measurement map) for low rank matrix recovery [32].

A. Agarwal discussed matrix decomposition problems where the goal is to recover from noisy observations matrices that can be decomposed as a sum of an (approximately) low rank matrix and a second matrix with some low dimensional structure. Agarwal proved a general theorem bounding the approximation error addressing the approximation obtained via a convex optimization problem that included nuclear norm minimization and an appropriate regularizer. Agarwal also used his results to study some special cases in the context of robust PCA [1].

*N. Srebro*'s talk was also on matrix recovery. Srebro focused on two forms of matrix regularization which constrain the norm of the factorization: the trace-norm (i.e., nuclear-norm) and the so-called max-norm (i.e.,  $\gamma_2 : \ell_1 \rightarrow \ell_{\infty}$  norm). Srebro discussed how these two norms relate to the rank and showed that simple low rank matrix completion guarantees can be obtained using these norms. Srebro also argued that the max-norm may be a better surrogate for the rank than the nuclear norm [30].

*J. Romberg* presented several architectures that use simple analog building blocks (vector-matrix multiply, modulators, filters, and ADCs) to implement different types of measurement schemes with "structured randomness". These sampling schemes allow us to take advantage of the (a priori unknown) correlation structure of the ensemble, which leads to a low rank matrix to be determined. Exploiting this fact reduces the total number of observations required to reconstruct the collection of signals.

#### **Applications in various disciplines**

*M. Fornasier* talked about a recent project where he combines various results on compressed sensing theory and algorithms, and learning functions in high-dimension to address problems related to learning, simulation, and control of particle systems, kinetic equations, and fluid dynamics models of interacting agents in high-dimension. He proposed an approach for the simulation of dynamical systems governed by functions of adjacency matrices in high-dimension by random projections via Johnson-Lindenstrauss embeddings, and recovery by compressed sensing techniques [21].

*M. Herman* presented results on denoising point cloud data using non-local techniques. His approach is grid-free, and thus preserves subtle geometric information in the data and thereby permits the identification of 3-dimensional structures in the point cloud. Herman successfully applied the techniques to LIDAR data to denoise objects of codimension 1 and 2 simultaneously.

A. Maleki's talk focused on a theoretical analysis of the nonlocal means algorithm, an image denoising method that has been successful in applications. Maleki presented results on the asymptotic risk analysis of this algorithm for images that are piecewise constant with a sharp edge discontinuity. He proved that the associated mean-square risk is suboptimal (and close to that of wavelet thresholding).

*F. Herrmann* addressed applications of compressed sensing to the full-waveform inversion problem in exploration seismology. He explained that the demand for higher quality imaging results in very large problem

sizes which is a fundamental obstacle. To address this problem, he proposed a dimension-reduction strategy based on compressed sensing and stochastic optimization [31].

*M. Sacchi*'s presentation was also on applications in exploration seismology focusing on industrial applications where the goal is to "reconstruct" 5-dimensional seismic data cubes from the observations (that are "incomplete" and noisy). He discussed reconstruction of large seismic volumes via rank reduction methods by posing the problem as a tensor completion problem.

*J.L. Starck* noted that the European Space Agency's PLANCK mission is designed to deliver full-sky coverage, low-noise level, high resolution temperature and polarisations maps. He reviewed some of the key problems of the PLANCK data analysis and presented how sparsity can be used to analyze such data set [33].

## Scientific Progress Made and Outcome of the Meeting

The meeting was very successful. Many participants mentioned to us that they greatly enjoyed the excellent talks, the fruitful discussions, the inspiring atmosphere at BIRS, and the neverending support of the BIRS staff.

Let us now briefly summarize the impact of our meeting.

• Initiation of communications between practitioners and mathematicians.

One main goal of our workshop was to invite people from very different areas, in particular, including practitioners who utilize methodologies from sparse and low rank approximation. This included researchers in the area of astronomical image and signal processing, radar imaging, wireless communication, and seismology. This BIRS workshop was a unique opportunity to initiate a fertile discussion between researchers from these areas and mathematicians. The talks by the practitioners indeed led to vivid debates; here we mention, in particular, the talk by Jean-Luc Starck on "Sparse analysis of the PLANCK cosmic microwave background data" and the talk by Richard Baraniuk on "1-bit Compressive Sensing and Binary Stable Embeddings"; as references see [33] and [4], respectively. We can report that these discussions led to several new collaborations between these two groups.

• Intensification of new directions in the field.

Various new directions both theoretical as well as applied were presented during talks, and vividly discussed afterwards. One main new direction in the field is matrix identification, which was the main focus of three talks. The general problem is to minimize the rank of a matrix subject to some general linear constraint, which has applications in various areas of high dimensional data processing. This direction is currently in its beginning stage and far more developments can be expected in the near future. As further directions, which are even more at the beginning stage, we exemplarily mention the high level analysis of linear inverse problems via convex geometry (Ben Recht) [10]. This workshop was hence a unique opportunity to discuss the most recent results and stimulate these directions.

• Discussion of methodologies.

Several talks made the audience sensitive to careful utilization of theoretically derived results in applications. One example was the discussion of the problem of basis mismatch in the talk by Ali Pezeshki (cf. [12]), in which he described the effect when the wrong sparsifying basis is chosen. Another talk which should be mentioned in this regard was given by Rayan Saab, see [27]. He discussed the sensitivity of Compressed Sensing to quantization, and provided one solution for this problem. Finally, the talk by Thomas Strohmer discussed various obstacles which have to be overcome to use sparse recovery methods for radar analysis; we refer to [28, 19]. These talks were very beneficial for the audience, in particular, for those not familiar with applications, making them sensitive to the needs of the practitioners.

• Introduction of young scientists.

Several of our participants were young, very promising scientists such as Felix Krahmer, Arian Maleki, and Rayan Saab. This workshop gave them an exceptional chance to present themselves and get in contact with the leading researchers in this area, and also to broaden their horizon. After the workshop, we

received excited feedbacks from this group, voicing the general opinion that this was a unique opportunity. Testimonial opinions are put on the BIRS webpage at http://www.birs.ca/events/2011/5-day-works

• Manifestation of the future direction of the field.

Since this workshop brought together the main leaders in the broad area of sparse and low rank approximations, it presented the possibility to debate and manifest the future directions of this field. Many intense discussions already took place right after most talks; in addition, we scheduled a general discussion session on the last day of the conference. Interesting open problems and possible future research directions came up. We therefore expect this workshop to have a signal effect which will significantly influence the research in this field in the future. As particular topics that came up in the discussion session we mention the following. In some practical recovery problems noise is added on the vector to be recovered. This poses severe problems in the application of compressed sensing, where in previous analysis the noise is assumed to be added to the measurement vector. It seems that methods have to be developed that are less sensitive to such type of noise (although it is presently not clear, whether this is possible at all). Furthermore, in the theoretical analysis of matrix completion more realistic probability models of selecting entries should be investigated. For instance, in applications to global positioning, usually only distance information on small distances is available. The near-optimal construction of deterministic compressed sensing matrices was discussed as well. While this remains a fundamental and important problem, no route to its solution could be identified in the discussion, which is certainly due to the hardness of the problem.

# **List of Participants**

Agarwal, Alekh (University of California Berkeley) Ayaz, Ulas (University of Bonn) Baraniuk, Richard (Rice University) Bodmann, Bernhard (University of Houston) Boufounos, Petros (Mitsubishi Electric Research Laboratories) Calderbank, Robert (Duke University) Casazza, Peter (University of Missouri) Cohen, Albert (Laboratoire Jacques-Louis Lions, Universite Pierre et Marie Curie) Daubechies, Ingrid (Duke University) Eldar, Yonina (Technion - Israel Institute of Technology) Fazel, Maryam (U Washington) Fornasier, Massimo (Austrian Academy of Sciences) Foucart, Simon (Universite Pierre et Marie Curie Paris) Goyal, Vivek (Massachusetts Institute of Technology) Herman, Matthew (UCLA) Herrmann, Felix (University of British Columbia) Huegel, Max (University of Bonn) Iwen, Mark (Duke University) Krahmer, Felix (University of Bonn) Kunis, Stefan (University of Osnabrueck) Kutyniok, Gitta (Technische UniversitLt Berlin) Maleki, Arian (Stanford University) Mansour, Hassan (University of British Columbia) Montanari, Andrea (Stanford University) Needell, Deanna (Stanford) Pezeshki, Ali (Colorado State University) **Pfander, Goetz** (Jacobs University) Rauhut, Holger (University of Bonn) Recht, Ben (University of Wisconsin) Romberg, Justin (Georgia Tech)

Saab, Rayan (University of British Columbia)
Sacchi, Mauricio (University of Alberta)
Srebro, Nathan (Toyota Technological Institute at Chicago)
Starck, Jean Luc (Service d'Astrophysique CEA/Saclay)
Strohmer, Thomas (University of California, Davis)
Temlyakov, Vladimir (University of South Carolina)
Tropp, Joel (California Institute of Technology)
van den Berg, Ewout (Stanford University)
Vybiral, Jan (RICAM Linz)
Ward, Rachel (Courant Institute)
Yilmaz, Ozgur (University of British Columbia)

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# **Chapter 9**

# Global/Local Conjectures in Representation Theory of Finite Groups (11w5008)

# Mar 13 - Mar 18, 2011

**Organizer(s):** Pham Huu Tiep (University of Arizona), Gunter Malle (Universitaet Kaiserslautern), Gabriel Navarro (University of Valencia)

# **Overview of the Field**

The Representation Theory of Finite Groups is a thriving subject, with many fascinating and deep open problems, and some recent successes. In 1963 Richard Brauer [5] formulated a list of deep conjectures about ordinary and modular representations of finite groups. These have lead to many new concepts and methods, but basically all of his main conjectures are still unsolved to the present day. A new development was opened up by the mathematician John McKay from Concordia University [17] in 1972 with an observation on degrees of characters for simple groups which was soon named the McKay conjecture and led to a wealth of difficult problems, relating global and local properties of finite groups, that also remain unproved. Profoundly significant are the Alperin Weight Conjecture formulated by J. Alperin [2] in 1986, and the structural explanation of some of the conjectures proposed by M. Broué [5]. These are usually called global/local conjectures, since they propose strong links between the representation theory of a finite group and that of certain of its local subgroups. We all gather that there should be a hidden theory explaining all these global/local phenomena, but yet such a theory still remains to be discovered.

Recently, considerable progress has been made in several directions. Firstly, there are now reductions to simple groups of the original McKay conjecture, the Alperin–McKay blockwise refinement and of the Alperin weight conjecture. Still, more and deeper knowledge of simple groups is needed in order to give a proof of these conjectures. Yet, for the first time the prospect of a complete proof of several of these fascinating conjectures seems in reach.

Another line of successes have been provided by proving some of these statements in some special cases. The difficulty of those give us a hint of the task ahead. For instance, Brauer's k(GV)-problem has only been solved after years of inspiring work of many mathematicians.

# **Recent Developments and Open Problems**

In the meeting, we concentrated on recent progress on the following famous and longstanding global/local conjectures.

#### The McKay Conjecture and refinements

The McKay conjecture is at the center of the representation and character theory of finite groups. It is the origin, together with the Alperin Weight Conjecture, of the more far-reaching Dade conjecture as well as of Broué's conjecture. If p is a prime and G is a finite group with Sylow p-subgroup  $P \le G$ , then the McKay conjecture asserts that

$$|\operatorname{Irr}_{p'}(G)| = |\operatorname{Irr}_{p'}(\mathbf{N}_G(P))|$$

where we denote by Irr(G) the set of irreducible complex characters of G and by  $Irr_{p'}(G)$  its subset consisting of characters having degree not divisible by p.

That is to say, fundamental information on the representation theory of G is encoded in some local subgroup of G, namely the Sylow normalizer.

In fact, J. McKay [17] made his conjecture only for G a simple group and for p = 2. It was Isaacs, in his landmark paper [10], who proved the conjecture for any prime p and any group of odd order. Some time later, J. Alperin [1] extended the statement to include Brauer blocks. This generalization is now known as the Alperin–McKay conjecture. T. Wolf [26] and E. C. Dade [7, 8], proved the conjecture for solvable groups. Various other classes of groups have also been considered.

Recently, M. Isaacs and G. Navarro [12], [19] discovered several refinements of the conjecture and these have contributed significantly to a further understanding of the problem. Yet another refinement is due to A. Turull [63] to include *p*-adic fields and Schur indices. Still more recently, Isaacs, G. Malle and Navarro [13] reduced the McKay conjecture to a question on simple groups. The latter has been solved for important families of simple groups by Malle and B. Späth [16], [23], relying heavily on the Deligne–Lusztig theory, and has led to interesting and difficult questions on automorphism groups of simple groups of Lie type. Ongoing work of M. Broué, P. Fong, and B. Srinivasan aims at proving the McKay conjecture and its recent refinements for finite reductive groups (in cross characteristic). The Isaacs–Malle–Navarro reduction raises the hope that a complete proof of the McKay conjecture may be possible in the not too distant future. This year, at the meeting, Späth has proposed a generalization of this reduction to the blockwise version, the Alperin–McKay conjecture [24].

#### The Alperin Weight Conjecture

If the McKay Conjecture counts characters of p'-degree, then the Alperin Weight Conjecture (AWC), as formulated by R. Knörr and G. R. Robinson [15], counts characters with maximal p-part, the so called defect zero characters. Specifically, a character  $\chi \in Irr(G)$  has defect zero if  $\chi(1)_p = |G|_p$ . Alperin's original formulation [2] is given by the formula

$$l(G) = \sum_{Q} z(\mathbf{N}_G(Q)/Q) \,,$$

where Q runs over representatives of conjugacy classes of p-subgroups in G; furthermore, z(X) is the number of defect zero characters of the group X, and l(G) is the number of p-regular classes of G. By using Möbius inversion, it is then possible to describe z(G) in terms of local subgroup information.

A strong form of AWC for  $\pi$ -separable groups was proved by Isaacs and Navarro in [11]. Quite recently, L. Puig [22] announced a reduction of AWC to a question on simple groups, and at the same time, Navarro and P. H. Tiep published another reduction to a statement for finite quasi-simple groups [21] which they verified for various classes of simple groups.

#### The Height Zero Conjecture

The Height Zero Conjecture, another famous problem on blocks, formulated by Brauer [5] in 1963, should lead to interesting questions on characters. If B is a p-block of a finite group with defect group D, then Brauer conjectured that all irreducible characters in B have height zero if and only if D is abelian. In particular, a positive solution would exhibit another connection between local and global invariants, providing, for example, an extremely simple method to detect from a group's character table whether its Sylow p-subgroup is abelian. The p-solvable case of the Height Zero Conjecture is an impressive theorem by D. Gluck and Wolf [9]. Interesting results on the Height Zero Conjecture include work of M. Murai [18], and of T. Berger

and Knörr [6]. But perhaps the most significant paper concerning this conjecture in recent years has been the solution of the Brauer's Height Zero Conjecture for 2-blocks of maximal defect by Navarro and Tiep [20]. At the conference, Malle announced work in progress with R. Kessar [14] which solves one direction of the Height Zero Conjecture relying on the above mentioned reduction theorem of Berger–Knörr. Also Tiep announced a very recent result of Navarro and him which would provide the first step towards a proof of the Brauer's Height Zero Conjecture for p-blocks of maximal defect for odd primes p.

#### The Broué Conjecture

The Alperin–McKay conjecture asserts that if B is a Brauer block of a finite group with b its First Main Theorem correspondent, then B and b have the same number of height zero characters. The block b is a uniquely determined block of the local subgroup  $N_G(D)$ , where D is the defect group of B.

Now, blocks are algebras, and Broué [5] conjectured that the algebras B and b have intimate structural connections that should imply the desired facts on height zero characters and much more. Currently, the Broué Conjecture is only stated for abelian defect group D, and it remains a challenge to find the correct formulation when the defect group is nonabelian. In 2008, J. Chuang and R. Rouquier [6] have given a proof of it for symmetric groups. At the conference, A. Evseev announced a refinement of the Broué Conjecture as well as the Alperin–McKay conjecture.

## **Presentation Highlights**

Definitely, one of the highlights was Späth's announcement of her reduction for the Alperin–McKay conjecture to simple groups. This goes along the lines of the Isaacs–Malle–Navarro reduction [13] for the McKay conjecture, as well as the recent Navarro–Tiep reduction [21] for the Alperin Weight Conjecture, and states that the Alperin–McKay conjecture holds for every *p*-block of every finite group, if every finite non-abelian simple group *S* satisfies a certain, *inductive Alperin–McKay* condition for the prime *p* (which is a collection of several statements to be verified for *S*). She also announced that this inductive Alperin–McKay condition is satisfied for the alternating groups  $Alt_n$  with  $n \ge 8$ , and for the simple groups of Lie type in their defining characteristic *p*.

Coming back to the McKay conjecture, recall that the Isaacs–Malle–Navarro reduction [13] for the McKay conjecture states that the McKay conjecture holds for the prime p for every finite group, if every finite non-abelian simple group S satisfies a certain, *inductive McKay* condition for the prime p. It is known that the inductive McKay condition holds for all alternating groups. It has now been partly proved by Brunat, another young participant of the workshop, and then in general by Späth, building on recent work of Maslowski that the inductive McKay condition holds for the simple groups of Lie type in the same characteristic p. Brunat gave a talk at the workshop about some steps of this proof.

With all the sporadic simple groups and the simple groups of Lie type with exceptional Schur multiplier already handled by Malle, the simple groups of Lie type in cross characteristic  $\ell \neq p$  are the remaining case on the way towards a complete proof of the McKay conjecture. Cabanes gave a talk about his recent joint work with Späth proving the inductive McKay condition for exceptional Lie-type groups of types  $G_2$ ,  ${}^3D_4$ ,  ${}^2F_4$ ,  $F_4$ , and  $E_8$ , showing how the bijections obtained by Malle [16] and Späth [23] could be chosen to be equivariant under outer automorphisms.

Broué gave an inspiring lecture about his recent work aiming at generalizing some basic tools of the representation theory of finite groups to arbitrary symmetric algebras, including Casimir element, induction-restriction functors, Higman's criterion, and character correspondences. It is expressed the hope that this approach will help explain various mysteries of many recent refinements of basic conjectures in modular representation theory.

One of the main tasks of the modular representation theory is to determine the *p*-blocks of finite (quasi-) simple groups. Malle gave a talk about his work in progress jointly with R. Kessar to classify the quasi-isolated blocks of finite exceptional groups of Lie type in bad characteristic. Together with previous results of many other mathematicians, this completes the aforementioned task. He also indicated how this important

work leads to nice consequences on the characterization of nilpotent blocks for quasi-simple groups, as well as on the completion of proof for the "if" direction of the Brauer Height Zero Conjecture.

The opening lecture of the workshop was given by M. Geck, who spoke about his very recent result on bounding the number of irreducible Brauer characters in any block of a finite group G of Lie type in cross characteristic by a constant depending only on the type of G. This in turns relies on recent deep work of G. Lusztig establishing the so-called cleanness of cuspidal character sheaves. Geck's result is expected to play a role in showing the inductive Alperin weight condition for groups of Lie type in their non-defining characteristic.

One of the key ingredients of the Gluck–Wolf proof [9] of the Brauer Height Zero Conjecture for the p-solvable groups and also of the Navarro–Tiep proof [20] of the Brauer Height Zero Conjecture for 2-blocks of maximal defect is provided by a result of Gluck and Wolf concerning a certain special situation in Clifford theory, which holds for all p-solvable groups and also holds when p = 2. In his talk at the conference Tiep announced and explained a very recent result of Navarro and him which generalizes the Gluck–Wolf theorem to odd primes p > 5.

Despite works of many mathematicians including recent work of J. Thompson, the structure of finite rational groups is still not well understood. An old conjecture in this area states that if G is rational then so are its Sylow 2-subgroups. So it was a big surprise that Navarro announced his recent joint work with Isaacs leading to a counterexample, a solvable group of order  $2^9 \cdot 3$ ) to this old conjecture! One could think *a posteriori* that one could discover this counterexample by searching the available database of groups of this kind of order. But as Navarro pointed out in his talk, it would take lots and lots of time to complete this search!

Somewhat related to this last topic, Gluck spoke about results concerning his recent conjecture that if a defect group D of a 2-block B of a finite group G is rational and satisfies  $D' \leq Z(D)$ , then all ordinary characters in B are 2-rational. In particular, he has proved his conjecture in the cases where G is solvable or if  $|D| \leq 8$ .

A new trend in modular representation theory centers around the idea of *categorification* to explore its connections with Lie theory, particularly through an action of a Lie algebra on the sum of the Grothendieck groups of representation categories of a sequence of groups or algebras, like the symmetric group  $\text{Sym}_n$  with  $n = 1, 2, \ldots$  B. Srinivasan gave a talk about her recent work concerning a similar situation where the Heisenberg algebra acts on the sum of the Grothendieck groups of the categories of  $\text{GL}_n(q)$ ,  $n = 1, 2, \ldots$  She showed in particular that this action is related to the Deligne–Lusztig functors.

An important problem in the modular representation theory is to understand the structure of a p-block with given defect groups D, for instance when D is small. At the workshop, S. Koshitani spoke about his recent joint work with R. Kessar and M. Linckelmann concerning the case when D is elementary abelian of order 8. In particular, they showed that the Alperin Weight Conjecture and a weak version of the Broué conjecture hold for such a 2-block. This is the first result of this type for arbitrary groups with given defect group in more than 30 years.

Another young participant, Kunugi, gave a talk about her joint work with H. Miyachi and Okyuama, in which they used Scott modules to prove the Morita equivalence between principal *p*-blocks of various general linear groups  $GL_n(q_i)$ , with  $q_i$ , i = 1, 2, two distinct prime powers. The case where the Sylow *p*-subgroups of  $GL_n(q_i)$  are abelian was known before, and confirmed the Broué conjecture in that case.

Yet another intriguing refinement of the Broué conjecture and (the Isaacs–Navarro refinement of) the McKay conjecture was announced by Evseev. He also showed that these latter refinements would imply the Alperin–McKay conjecture as well. In his talk he offered some evidence for these new conjectures.

C. Eaton's talk described the work of his Ph. D. student P. Ruengrot on a new block invariant — the group of all perfect isometries of the block. G. Hiß spoke about his joint work with N. Naehrig on some general set-up including p-modular Hecke algebras which would produce a bijection between simple modules in the head of a finite-dimensional module Y and simple modules in the socle of the endomorphism algebra of Y.

## Scientific Progress Made and Outcome of the Meeting

A main result of the meeting was to make clear that several old and famous conjectures in modular representation theory now seem in reach, like the McKay-conjecture, Alperin's weight conjecture and Brauer's height zero conjecture.

Aside from the officially scheduled talks, various informal discussions took place. One of them, which included about half of the participants of the meeting, concentrated on an assessment of the objectives to fulfill in checking the inductive conditions necessary for a proof of McKay's conjecture and Alperin's weight conjecture for all finite simple groups along with a tentative cast of the remaining tasks.

Numerous additional discussions led to further results; we reproduce some of the comments on these outcomes given by participants below. Following discussions of M. Geck, G. Malle and P.H. Tiep, it now seems reasonable to try a new attack on the basic set problem for all finite groups of Lie type in non-defining characteristic. This should play a role in an eventual verification of the inductive Alperin weight condition for these groups. Through this discussion, G. Navarro became interested in a reduction of the basic sets conjecture to simple groups.

Also, through discussions of M. Geck, G. Hiss and G. Malle, there is new progress on their programme to understand modular Harish-Chandra series in the non-linear prime case for finite classical groups.

Discussion of C. Eaton and S. Koshitani at this meeting resulted in a collaboration to investigate Alperin's weight conjecture and also Broue's abelian defect group conjecture for blocks with defect group of order  $p^2$ . S. Koshitani and B. Späth discussed much the Dade–Glauberman–Nagao correspondence, which plays an important role in the Navarro–Tiep reduction of the Alperin weight conjecture. They also discussed a recent preprint "About a minimal counterexample for the Alperin-McKay conjecture" by M. Murai related to Späth's reduction project. G. Hiss and S. Koshitani talked on Donovan's conjecture for groups with elementary abelian Sylow subgroup of order  $p^2$ , and on the classification problem of blocks of finite groups up to Morita equivalence under a mild hypothesis.

G. Navarro discussed and solved with B. Späth the problem of preservation of congruences in the Dade– Glauberman–Nagao correspondence for the reduction of the Alperin–McKay conjecture. This is expected to lead to a reduction of the Isaacs–Navarro refinement of the Alperin–McKay conjecture to simple groups. As a consequence of the talk of A. Evseev, G. Navarro was able to prove the Sylow self-normalizing case of Evseev's new conjecture for *p*-solvable groups.

M. Cabanes and B. Späth worked on their ongoing project to prove that the family of finite projective linear groups  $PSL_n(q)$  satisfies the inductive McKay condition, and investigated possibilities to generalize older results on McKay's conjecture towards the inductive Alperin–McKay condition. Späth and B. Srinivasan discussed Maslowski's recent Ph.D. thesis which provided the first half in the recent proof of the McKay conjecture for groups of Lie type in their defining characteristic and which is related to a project of Srinivasan to parametrize some semisimple conjugacy classes in certain classical groups.

M. Broué, P. Fong and B. Srinivasan continued work on their joint project concerning Dade's conjecture for groups of Lie type. P. Fong and B. Späth discussed a joint project, begun two years ago, on Harish-Chandra induction and Galois actions.

C. Eaton had a useful discussion with Kunugi on some unpublished work which resolved one of the questions posed in his talk. Also, he had the opportunity to continue his collaboration with Koshitani.

M. Cabanes also discussed very concrete points with B. Srinivasan about questions on Deligne–Lusztig constructions revisited by Bonnafé–Rouquier in a modular framework; he discussed irreducible characters of twisted group algebras with E. Dade, fusion in blocks with dihedral defect with C. Eaton.

During the discussions of A. Evseev, G. Malle, B. Späth and S. Koshitani, it was realized that it may be feasible (and easier than previously thought) to check the Evseev's refinement of the McKay conjecture in several new cases (e.g. for some groups of Lie type in non-defining characteristic).

In closing we would like to emphasize that all participants expressed the opinion that the meeting was very successful and stimulating for their research. They also underlined the fact that, due to the quite focussed topic and the informal atmosphere with the audience asking clarifying questions or making insightful comments, they profited much more from the individual talks than at most other conferences, with a broader theme.

As an example, we cite from a comment by B. Srinivasan: "In my view this was a very successful workshop. The participants were a judicious mix of senior, mid-level and junior researchers. I was able to learn from every lecture and have discussions with most of the participants [...] which led to new insights and ideas for my continuing research. It was also interesting to meet some of the junior participants for the first time and to learn what they are working on."

M. Cabanes told us: "The week in Banff was for me very fruitful. I had there an opportunity, unique in the past two years, of discussing subjects of interest to me with the best experts in the field. This was achieved through and around talks (including mine) but also by informal discussions occurring at all the moments in the day."

P. Fong told us: "Banff was a good meeting. The intimate setting gave a directness and immediacy to mathematical discussions. The talks ranged from the delicate and difficult nailing-down of individual cases for inductive proofs to bold, engaging questions such as Evseev's. We all went home with lots to think about."

D. Gluck commented: "I thought the conference was a nice blend of coherence and diversity."

And G. Hiß said: "I learned a lot form the talks give at the workshop, which all where excellent, without exception."

In all, this conference lived up to its promises of a quiet, inspiring and very comfortable place to make mathematics.

## **Participants**

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# Chapter 10

# Functor Calculus and Operads (11w5058)

# Mar 13 - Mar 18, 2011

**Organizer(s):** Nick Kuhn (University of Virginia), Michael Ching (University of Georgia), Victor Turchin (Kansas State University)

# Overview

The goal of this workshop was to bring together experts in the various forms of functor calculus, as well as the theory of operads, in order to discuss recent connections being made between these fields. The main areas covered were: (i) Goodwillie's homotopy calculus of functors, its structure, and relationship to the Whitehead Conjecture; (ii) embedding spaces as studied by the Goodwillie-Weiss manifold calculus and the actions of operads on such spaces; (iii) operads, especially the little-discs operads and Koszul duality; (iv) André-Quillen (co)homology, its applications, and its relation to homotopy calculus for functors of operadic algebras.

The workshop consisted of sixteen talks by researchers in these fields, with a focus on making connections between different topics and bringing to light some recent developments. Since the number of participants was limited by the fact that this was a half-workshop, we focused, for the most part, on inviting established researchers rather than graduate students and postdocs. The aim then was for new directions for future research to be explored.

# Background

#### **Homotopy Calculus**

The homotopy calculus of functors was developed by Goodwillie in the series of papers [G1, G2, G3]. For a functor F of to/from topological spaces or spectra, this theory systematically provides a sequence of approximations to F satisfying higher-order excision conditions. This sequence is known as the *Taylor tower* of F in reference to the analogy with ordinary Taylor series. The layers in this tower (i.e. the fibres of the maps between successive approximations) take a particularly simple form. Each layer is described by a single spectrum  $\partial_n F$  (the *n*th *derivative* of F) with an action of the symmetric group  $\Sigma_n$ , and the spectrum  $\partial_n F$ can often by computed.

The key example for the homotopy calculus seems to be the identity functor on based spaces. The Taylor tower for the identity functor converges at nilpotent spaces and the derivatives, and hence the layers, have been calculated by Johnson [J]. Arone and Mahowald [AM] used these calculations to give an explicit description of the *p*-local Taylor tower of the identity evaluated at a sphere. Their work also revealed interesting connections with chromatic homotopy theory, and new calculations of unstable  $v_n$ -periodic homotopy groups.

One way to understand homotopy calculus is as a tool for interpolating between stable and unstable homotopy theory. The layers of the tower are stable in the sense that their values on a space X depend only on the suspension spectrum of X. Piecing together the layers to form the tower then amounts to building in unstable data. One of the long-term question addressed by the workshop is how to understand the information needed to construct the entire tower from the layers which are relatively easy to describe.

The work of Arone-Mahowald [AM] and Arone-Dwyer [AD] has been highly influential in linking the homotopy calculus, especially for the identity functor, to other areas in homotopy theory. One topic that this workshop looked at in detail is the connection with the Whitehead Conjecture proved by Kuhn in [K1].

#### Manifold calculus and spaces of embeddings

The manifold calculus of Goodwillie and Weiss [W1, GW] concerns functors on the category of open subsets of a fixed manifold M and was developed primarily as a tool for studying spaces of embeddings of M in some other manifold N. The Taylor tower in this context interpolates between the space of embeddings  $\operatorname{Emb}(M, N)$  and the space of immersions  $\operatorname{Imm}(M, N)$ , which plays the role of the linear approximation to  $\operatorname{Emb}(M, N)$ . As in the case of the homotopy calculus the layers of the Taylor tower have a fairly simple form and for space of embeddings, these layers are related to the configuration spaces of points in N.

The question of convergence of the Taylor tower in the manifold calculus is an interesting one. The tower for the space  $\operatorname{Emb}(M, N)$  converges when  $\dim(N) - \dim(M) \ge 3$ . Note that this excludes the case of classical knots (i.e. embeddings of  $S^1$  in  $S^3$ ) but is effective for knots in dimensions 4 and higher. Considerable success has been had in applying the manifold calculus to calculate the homology of spaces of knots in higher codimension (see [LTV, ALTV, ALV]). For the classical case of knots in  $S^3$  the approach of Hatcher that exploits the structure of the group of diffeomorphisms preserving a knot turned out to be very fruitful. Based on this approach Budney introduced different operad actions [Bu1, Bu2] on the space of long knots in  $\mathbb{R}^3$  and showed that these actions are free. This almost completely determined the homotopy type of spaces of knots in  $\mathbb{R}^3$  and  $S^3$ .

#### **Operads and Koszul duality**

It has recently become apparent that the theory of operads plays a significant role in both the homotopy and manifold versions of the calculus of functors. The fact that the layers of the Taylor tower for embedding spaces are related to configuration spaces, makes it no surprise that there is a connection to the little disc operads. This connection was realized in a striking way by Sinha [S], who showed that the Taylor tower for the space of long knots in  $\mathbb{R}^m$  could be identified with the Tot-tower for a cosimplicial space associated with the little *m*-discs operad  $C_m$ . Sinha's models have been exploited in many ways. For example, Dwyer and Hess [DH] have shown that the knot spaces can be described as double-loopings of spaces of operad maps  $C_1 \rightarrow C_m$ .

It turns out that operads also play a significant role in the homotopy calculus. Ching showed in [C] that the derivatives (that is, the coefficient spectra that determine the layers in the Taylor tower) of the identity functor possess an operad structure and Arone and Ching [AC] showed that this operad naturally acts on the derivatives of other functors. A central role in this theory is played by Koszul duality for operads. In particular, the operad formed by the derivatives of the identity is Koszul dual to the cooperad formed by the derivatives of the functor  $\Sigma^{\infty}\Omega^{\infty}$  from spectra to spectra. This duality is a topological version of the rational Koszul duality between the Lie and commutative operads that lies at the heart of Quillen's models for rational homotopy theory [Q2].

#### André-Quillen homology and algebras over operads

The ideas of the calculus of functors are remarkably general and can easily be adapted to new contexts. For example, one can naturally describe analogues of the Taylor tower for functors on other categories. One of the most fruitful such generalizations is to functors of commutative S-algebras (that is,  $E_{\infty}$ -ring spectra).

Kuhn [K3] has used the Taylor tower of the identity functor on commutative S-algebras to study the Morava K-theory of infinite loop spaces. McCarthy, with various coauthors, has studied the Taylor tower of algebraic K-theory considered as a functor on the category of commutative S-algebras.

Recall that the homotopy calculus interpolates in some sense between stable and unstable homotopy theory. For commutative S-algebras, Basterra-Mandell [BM1] have shown that the notion of stable homotopy theory is essentially equivalent to topological André-Quillen homology (TAQ), that is, the derived functor of abelianization. It is therefore to be expected that a general theory of calculus for functors of commutative S-algebras will be closely related to TAQ and this relationship is clearly seen in the work of Kuhn and McCarthy.

Basterra-Mandell showed more generally that stabilization is given by Quillen homology for algebras over any suitable operad in the category of spectra (not just the commutative operad). This allows for a uniform approach to functor calculus for such categories of algebras. Given the extent to which various different operads already appear in the theory of calculus, this seems to be important.

# **Presentations on Current Work**

Here we give an overview of how the talks presented in the workshop relate to the main areas of study.

Several talks focused on the theoretical side of the homotopy calculus. **Greg Arone** described, in two talks, work on the problem of reconstructing the Taylor tower of a functor from its derivatives. His first talk described the action of the operad  $\partial_I$ , formed by the derivatives of the identity on based spaces, on the derivatives of any functor to or from the category of based spaces. His second talk concerned new work, also joint with Ching, that aims to describe all the remaining structure on the derivatives of a functor beyond these operad actions. This new structure is a coaction by a certain cotriple and such a coaction is sufficient to recover the entire Taylor tower of the functor.

**Eric Finster** gave towers of approximations for the suspension spectrum for a homotopy limit. These towers are inspired by the homotopy calculus and, for example, yield spectral sequences for calculating the stable homotopy or homology of such a limit.

**Brenda Johnson** reported on joint work with Kristine Bauer, Rosona Eldred and Randy McCarthy. Previous work of Johnson and McCarthy has produced alternative models of the Taylor tower of a pointed functor using a cotriple associated to the cross-effect construction. These models are equivalent to Goodwillie's for analytic functors. Johnson spoke here about a generalization of this previous work to Taylor towers in an unbased setting.

It has recently been conjectured that the Taylor tower of the identity functor on based spaces can be used to give a new proof of the Whitehead Conjecture (proved by Kuhn in [K1]). Two different approaches to this were presented at the workshop. **Mark Behrens** gave two talks related to this. He described a new perspective on the calculations of Arone-Mahowald, and then showed how this perspective can be used to produce a contracting homotopy for the Whitehead sequence, thus giving a new of the Conjecture. This work is described in [Be2]. **Bill Dwyer** described joint work with Greg Arone and Kathryn Lesh on another way to approach this.

**Ryan Budney** gave two talks: the first introducing the manifold calculus and its relationship with pseudoisotopy theory. In his second talk, he presented various operad actions on embedding spaces [Bu1, Bu2], in particular he described a new operad formed from 'splicing diagrams' that plays a central role.

**Michael Weiss** reported on joint work with Rui Reis on Pontryagin classes for topological vector bundles controlled by the cohomology of the group of homeomorphisms of  $\mathbb{R}^n$ . This work uses ideas from both the manifold calculus and Weiss's orthogonal calculus [W2].

Operads appeared in many of the talks at the workshop but they were studied in particular in talks by **Benoit Fresse** and **Pascal Lambrechts**. Fresse described the space of homotopy-automorphisms of the little 2-discs operads. Lambrects presented joint work with Ismar Volic on formality for little *N*-discs operads.

The other main collection of talks were on topological André-Quillen homology. **Kathryn Hess** gave a series of two talks introducing this topic, focusing on the generality of Quillen homology for algebras over arbitrary operads. She concluded by describing joint work with John Harper [HH] on Whitehead and Hurewicz-type Theorems for Quillen homology.

Mike Mandell described the structure of Quillen homology for operadic algebras in greater detail, making

Filling in for a last-minute withdrawal, **Dev Sinha** described recent detailed calculations in the cohomology of symmetric groups with relevance to operads.

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## Abstracts

#### Speaker: Gregory Arone (Virginia)

Title: Part 1: operads, modules and the chain rule

Abstract: Let F be a homotopy functor between the categories of pointed topological spaces or spectra. By the work of Goodwillie, the derivatives of F form a symmetric sequence of spectra  $\partial_* F$ . This symmetric sequence determines the homogeneous layers in the Taylor tower of F, but not the extensions in the tower. In these two talks we will explore the following question: what natural structure does  $\partial_* F$  possess, beyond being a symmetric sequence? Our ultimate goal is to describe a structure that is sufficient to recover the Taylor tower of F from the derivatives. Such a description could be considered an extension of Goodwillie's classification of homogeneous functors to a classification of Taylor towers.

By a theorem of Ching, the derivatives of the identity functor form an operad. In the first talk we will see that the derivatives of a general functor form a bimodule (or a right/left module, depending on the source and target categories of the functor) over this operad. Koszul duality for operads plays an interesting role in the proof. As an application we will show that the module structure on derivatives is exactly what one needs to write down a chain rule for the calculus of functors.

#### Title: Part 2: beyond the module structure

Abstract: The (bi)module structure on derivatives is not sufficient to recover the Taylor tower of a functor. In the second talk we will refine the structure as follows. We will see that there is a naturally defined comonad on the category of (bi)-modules over the derivatives of the identity functor, and that the derivatives of a functor are a coalgebra over this comonad. From this coalgebra structure one can, in principle, reconstruct the Taylor tower of a functor. Thus this coalgebra structure seems to give a complete description of the structure possessed by the derivatives of a functor.

We give an explicit description (as explicit as permitted by our current understanding) of the structure possessed by the derivatives of functors from Spectra to Spectra, from Spaces to Spectra and from Spaces to Spaces. An interesting example is the functor  $X \mapsto \Sigma^{\infty} \Omega^{\infty}(E \wedge X)$ . Here E is a fixed spectrum, and the functor can be thought as a functor from either the category of Spaces or Spectra to the category of Spectra. The derivatives of this functor are given by the sequence  $E, E^{\wedge 2}, \ldots, E^{\wedge n}, \ldots$ . The fact that this sequence is the sequence of derivatives of a functor seems to tell us something about the structure possessed by spectra in general. In particular it tells us that spectra possess a natural structure of a restricted algebra over the Lie operad (an observation first made by Bill Dwyer).

#### Speaker: Mark Behrens (MIT)

#### Title: Survey of the Goodwillie tower of the identity I

Abstract: The Goodwillie tower of the identity functor from spaces to spaces is a powerful tool for understanding unstable homotopy from the stable point of view. I will describe the derivatives of this functor, which were studied by Johnson and Arone-Mahowald. I will also explain the Arone-Mahowald computation of the homology of the layers of the tower evaluated on spheres. These layers were shown by Arone-Dwyer to be equivalent to stunted versions of the L(k) spectra studied by Kuhn, Mitchell, Priddy, and others.

Associated to the Goodwillie tower is a spectral sequence which computes the unstable homotopy groups of a space from the stable homotopy groups of the layers. I will explain consequences for unstable  $v_k$ -periodic homotopy discovered by Arone and Mahowald. I will also discuss relations with the EHP sequence at the prime 2. Specifically, differentials in the Goodwillie spectral sequence can often be computed in terms of Hopf invariants, and differentials in the EHP sequence can often be computed in terms of attaching maps in the L(k)-spectra.

#### Title: Survey of the Goodwillie tower of the identity II

Abstract: I will recall Ching's operad structure on the derivatives of the identity. Coupled with operadic structures recently discovered by Arone-Ching, this gives an action of a certain algebra of Dyer-Lashof-like operations on the layers of the Goodwillie tower of any functor from spaces to spaces. Specializing to the case of functors concentrated in degrees n and 2n, we will derive a formula for the homological behavior of the k-invariant of the associated Goodwillie tower.

The 2-primary Goodwillie tower of  $S^1$  is closely related to the Whitehead conjecture (a.k.a. Kuhn's theorem). Work of Arone-Dwyer-Lesh shows that the k-invariants in the tower for  $S^1$  deloop to give candidates for a contracting homotopy to Kuhn's Kahn-Priddy sequence, and conjectured this was indeed the case. The homological formulas for k-invariants will be used to compute these delooped k-invariants, verifying the conjecture (Arone-Dwyer-Lesh have simultaneously developed a different proof of their conjecture.)

#### Speaker: Ryan Budney (Victoria)

#### Title: A primer on concordance or pseudoisotopy

Abstract: I'll describe the context for concordance and pseudoisotopy, the Morlet Disjunction lemma, the pre-80's work on the subject. Tom's dissertation, and his work with Weiss and Klein on The Embedding Calculus, up to around Dev Sinha's early work on the embeddings.

#### Title: Manifold embeddings and operads

Abstract: This talk will be about "where we are and where we're going", describing recent work of Sinha, Salvatore, Turchin, Arone, Lambrechts, Dwyer and Hess on rational homotopy-type and iterated loop-space

structures on embedding spaces. I'll also talk about other operads that act on embedding spaces and how they might fit into what is known.

#### Speaker: Bill Dwyer (Notre Dame)

#### Title: Symmetric powers vs. the calculus filtration

Abstract: The talk will discuss ideas which shed light on the relationship between the (increasing) filtration of the Eilenberg-MacLane spectrum  $H\mathbb{Z} = SP^{\infty}(S^0)$  by the symmetric power spectra  $SP^n(S^0)$ , and the (decreasing) filtration of the circle  $S^1$  by the Goodwillie tower of the identity functor. Figuring in the picture is a peculiar object which is both simplicial and cosimplicial, and, in either guise, is both trivial and is not. Many Bredon (co)homology spectral sequences collapse, and the circle does double duty as the sphere  $S^1$  and as the Eilenberg-MacLane space  $K(\mathbb{Z}, 1)$ . Kuhn's Theorem (the Whitehead Conjecture) is in the background.

#### Speaker: Eric Finster (EPFL)

#### Title: The Goodwillie tower for homotopy limits

Abstract: In view of the many fruitful applications of the Goodwillie Calculus to the study of mapping spaces of various types, a natural question is the extent to which similar techniques can be applied to the study of their twisted cousins, that is, to spaces of sections. Homotopy theorists have two closely related convenient ways of modeling a space of this type: as the totalization of a cosimplicial space or as the homotopy limit of a diagram. These two models are essentially equivalent to each other in the sense that every homotopy limit can be realized as the total space of its cosimplicial replacement, and conversely, the total space of a fibrant cosimplicial space is equivalent to its homotopy limit when viewed as a diagram over  $\Delta$ .

One advantage of a cosimplicial model, however, is that it comes with a canonical filtration, the totalization tower. Applying a generalized homology theory to the totalization tower yields the Bousfield-Kan spectral sequence, which under favorable conditions allows one to compute homological invariants of the associated total space. Viewed in another light, the Bousfield-Kan spectral sequence can be seen as a canonical filtration of the spectrum  $\Sigma^{\infty}$  Tot  $\mathcal{X}$  and we can discuss convergence in these terms: we say the Bousfield-Kan spectral sequence is convergent when the natural family of maps

$$\{\Sigma^{\infty}\operatorname{Tot}_{n}\mathcal{X}\}_{n\in\mathbb{N}}\longrightarrow \{\operatorname{Tot}_{n}\Sigma^{\infty}\mathcal{X}\}_{n\in\mathbb{N}}$$

constitutes a pro-equivalence of spectra from the constant tower at  $\Sigma^{\infty}$  Tot  $\mathcal{X}$  to the totalization tower of the cosimplicial spectrum  $\Sigma^{\infty}\mathcal{X}$ .

Homotopy limits, on the other hand, might be said to have a slight conceptual advantage in that they correspond nicely with our geometric intuition. Taking K to be a simplicial set, a diagram  $F : \Delta K \to S$  indexed by the simplex category of K can be thought of as a presheaf of spaces on K, and its homotopy limit as the space of global sections, which we will here denote by  $\operatorname{holim}_K F$ .

In this lecture, we present a stable filtration

$$\Sigma^{\infty} \operatorname{holim}_{K} F \to \operatorname{holim}_{P_{n}K} \Sigma^{\infty} F_{n}$$

which plays the role of the Goodwillie tower for homotopy limits, generalizing Arone's model for  $\Sigma^{\infty} \operatorname{Map}(K, X)$ when X is the common value of a constant functor F. After outlining the basic construction, we discuss convergence issues, examine its relationship to the Bousfield-Kan spectral sequence, and provide examples.

#### Speaker: Benoit Fresse (Lille)

#### Title: Homotopy automorphisms of $E_2$ -operads and Grothendieck-Teichmüller groups

Abstract: The notion of  $E_2$ -operad usually refers to a topological operad which is weakly equivalent to Boardman-Vogt' operad of little 2-cubes C<sub>2</sub>. This structure is used to model operations acting on 2-fold loop spaces. The structure of an  $E_2$ -operad is also used in simplicial and in differential graded algebra in order to model a first level of homotopy commutative structures.

In the algebraic setting, one considers the singular chain complex of the operad of little 2-cubes  $Sing_{\bullet}(C_2)$ , which defines an operad in simplicial cocommutative coalgebras. For our purpose, we form a dual structure  $Sing^{\bullet}(C_2)$ , which is a cooperad in cosimplicial commutative algebras. In what follows, we prefer to adopt the terminology of cosimplicial commutative Hopf cooperad (also commonly used in the literature) for the category of cooperads in cosimplicial commutative algebras and we use the notation  $cHopf \mathcal{O}p_1^c$  to refer to

this category. The first objective of this talk is to explain that the category  $cHopf \mathcal{O}p_1^c$  gives a faithful algebraic model for the rational homotopy category of operads (assuming that  $\mathbb{Q}$  is our ground ring). In the case of little 2-cubes, we will prove that the application of a space-like functor to a fibrant replacement of  $Sing^{\bullet}(C_2)$  yields a topological operad  $(C_2)_{\mathbb{Q}}^{\wedge}$  such that  $\pi_*(C_2)_{\mathbb{Q}}^{\wedge} = 0$  for \* > 1 and  $\pi_1(C_2)_{\mathbb{Q}}^{\wedge}$  is the rational prounipotent completion (the Malcev completion) of the fundamental group of  $C_2$ .

Our main goal is to determine the homotopy of the space of homotopy automorphisms  $\operatorname{haut}_{\mathcal{T}op\mathcal{O}p}(C_2)^{\wedge}_{\mathbb{Q}}$  associated to this topological operad  $(C_2)^{\wedge}_{\mathbb{Q}}$ . Formally, we have a simplicial function space  $\operatorname{Map}_{\mathcal{T}op\mathcal{O}p}(\mathsf{P},\mathsf{P})$  associated to any topological operad P. The space of homotopy automorphisms  $\operatorname{haut}_{\mathcal{T}op\mathcal{O}p}(\mathsf{P},\mathsf{P})$  consists of the connected components of  $\operatorname{Map}_{\mathcal{T}op\mathcal{O}p}(\mathsf{P},\mathsf{P})$  which are attached to homotopy equivalences of operads  $\phi : \mathsf{P} \xrightarrow{\sim} \mathsf{P}$ . Basically, we can also identify  $\pi_0(\operatorname{haut}_{\mathcal{T}op\mathcal{O}p}(\mathsf{P}))$  with the group of homotopy classes of these operad homotopy equivalences  $\phi : \mathsf{P} \xrightarrow{\sim} \mathsf{P}$ . Actually, the construction of  $\operatorname{haut}_{\mathcal{T}op\mathcal{O}p}(\mathsf{P})$  makes sense if P is cofibrant as an operad only. Therefore, we tacitly apply the definition to a cofibrant replacement of P when the operad P is not itself cofibrant.

For basic reasons, we are mostly interested in a subspace  $\operatorname{haut}_{\mathcal{T}op\mathcal{O}p}^{1}(\mathsf{C}_{2})^{\wedge}_{\mathbb{Q}} \subset \operatorname{haut}_{\mathcal{T}op\mathcal{O}p}^{1}(\mathsf{C}_{2})^{\wedge}_{\mathbb{Q}}$ , formed by restricting ourselves to the connected components of operad homotopy equivalences inducing the identity in homology. The operad  $(\mathsf{C}_{2})^{\wedge}_{\mathbb{Q}}$ , which has no homotopy in degree  $* \neq 1$ , has a simple categorical model yielded by the Malcev completion of the operad of colored braid groupoids. The prounipotent version of the Grothendieck-Teichmüller group  $GT(\mathbb{Q})$ , defined by Drinfeld, can be identified with the group of automorphisms of this operad in groupoids. Accordingly, we can form a group morphism

$$\eta: GT(\mathbb{Q}) \to \pi_0(\operatorname{haut}_{\mathcal{T}op\mathcal{O}p}(\mathsf{C}_2)^{\wedge}_{\mathbb{Q}}),$$

which is obviously injective (use fundamental groupoids). For our purpose, we consider a group  $GT^1(\mathbb{Q}) \subset GT(\mathbb{Q})$ , formed by removing a central factor  $\mathbb{Q}^{\times}$  in  $GT(\mathbb{Q})$ . Our main result asserts:

Theorem. We have

$$\pi_*(\operatorname{haut}_{\mathcal{T}op\mathcal{O}p}((\mathsf{C}_2)^{\wedge}_{\mathbb{Q}}) = \begin{cases} GT^1(\mathbb{Q}), & \text{if } * = 0, \\ 0, & \text{otherwise} \end{cases}$$

Most of the talk will be devoted to the formulation of this theorem. The remaining time will be used to give an outline of the proof. In brief, our arguments rely on a study of the deformation complex of  $Sing^{\bullet}(C_2)$  in the category of cosimplicial Hopf cooperads.

#### Speaker: Kathryn Hess (EPFL)

Title: *What is André-Quillen (co)homology and why is it important?* Abstract: In this talk I will first describe classical André-Quillen homology, which was invented, essentially simultaneously, by Michel André and by Dan Quillen in the late 1960's. Quillen defined a very general homology theory, calculated as derived functors of abelienization, for objects in any category with all finite limits and enough projectives; special cases include both singular homology of spaces and (reduced) homology of groups. The Quillen homology of commutative rings is called *André-Quillen homology*.

I'll present Quillen's homology theory in the general setting and sketch proofs of its important elementary properties: the transitvity long exact sequence, invariance under base change and a sort of additivity. I'll then describe briefly the particular cases of commutative rings and of associative algebras.

In the late 1990's, Maria Basterra defined *topological André-Quillen cohomology (TAQ)* of commutative ring spectra and proved that homotopical analogues of the transitvity long exact sequence and invariance under base change held for this new theory. I will describe the construction of TAQ and explain why it is of interest to stable homotopy theorists. In particular, any connective, commutative ring spectrum admits a Postnikov tower decomposition, where the k-invariants correspond to classes in TAQ. Also, as shown by Basterra and Mike Mandell, TAQ is universal, in the sense that every cohomology theory of  $E_{\infty}$ -ring spectra is TAQ with appropriate coefficients. Finally, as an aide to computation, I will state Mandell's theorem relating André-Quillen homology of  $E_{\infty}$ -simplicial algebras and of commutative ring spectra to that of  $E_{\infty}$ -differential graded algebras.

In the second part of this talk, I will briefly survey applications of André-Quillen (co)homology. In particular I will describe the role of André-Quillen homology in Haynes Miller's proof of the Sullivan conjecture. I will then sketch Bousfield's proof that André-Quillen homology is the natural home of obstructions to realizing a morphism  $H_*(K; \mathbb{F}_p) \to H_*(L; \mathbb{F}_p)$  of cocommutative coalgebras with compatible Steenrod algebra

structure as a map of spaces, as well as its generalization by Paul Goerss and Mike Hopkins, where  $H_*(-;\mathbb{F}_p)$  is replaced by  $E_*$  for any commutative ring spectrum satisfying the Adams conditions and the commutative operad by any operad in spectra. If time permits, I will also talk about work of Natàlia Castellana, Juan Crespo and Jérôme Scherer on finite generation of mod p cohomology over the Steenrod algebra, in which André-Quille homology played an important role.

#### Title: André-Quillen homology and towers

Abstract: This second talk will be more closely related to the theme of this workshop, as I will describe various towers related to (André-)Quillen homology that are, at the very least, highly analogous to the towers of Goodwillie calculus.

I will begin by presenting work of Nick Kuhn, who, for any commutative ring spectrum R, constructed a filtration of  $\operatorname{TAQ}(R)$  such that the filtration quotients look just like the fibers of stages of a Goodwillie tower. The filtration gives rise, for any field  $\mathbb{F}$ , to a spectral sequence converging to  $H^*(\operatorname{TAQ}(R);\mathbb{F})$ , which Kuhn applied to computing  $\operatorname{TAQ}(R)$  for  $R = \Sigma^{\infty} S^1_+, \Sigma^{\infty} \mathbb{Z}/2_+$ , and  $D(S^1_+)$ , where D denotes the Spanier-Whitehead dual.

Let X be spectrum, and let  $\mathbb{P}X$  denote the free commutative ring spectrum generated by X. To elucidate the relationship between  $K(n)_*(\mathbb{P}X)$  and  $K(n)_*(\Omega^{\infty}X)$ , Kuhn constructed and studied the André-Quillen tower of an augmented, commutative R-algebra (in spectra) A, which is the Goodwillie tower of the identity functor on the category of R-algebras, evaluated on A. Its limit is essentially an I-adic completion of A, where I is the augmentation ideal of A. I will present Kuhn's results on properties of the André-Quillen tower, such as when it converges and its relation with localization.

I will conclude by talking about joint work with John Harper on a homotopy completion tower interpolating between Quillen homology and homotopy completion of algebras in symmetric spectra over a general operad  $\mathcal{O}$ , which generalizes Kuhn's André-Quillen tower. Our understanding of this homotopy completion tower enabled us to prove that, under reasonable conditions on the operad  $\mathcal{O}$ , if an  $\mathcal{O}$ -algebra map induces a weak equivalence on Quillen homology, then it also induces a weak equivalence on homotopy completions. Moreover, under mild connectivity conditions, an  $\mathcal{O}$ -algebra X is weakly equivalent to its homotopy completion, i.e., the homotopy completion tower for X converges to X. As almost immediate corollaries, we obtained Whitehead and Hurewicz theorems for Quillen homology. We have also established a Serre-type finiteness theorem for Quillen homology: under reasonable cofibrancy and connectivity conditions on the operad  $\mathcal{O}$ , if the homotopy groups of each level of the operad are finitely generated, then finiteness (respectively, finite generation) of the Quillen homology groups of an  $\mathcal{O}$ -algebra implies finiteness (respectively, finite generation) of its homotopy groups.

#### Speaker: Brenda Johnson (Union)

#### Title: Cross-effects, cotriples and calculus: an update

Abstract: In a series of papers published between 1998 and 2004, Randy McCarthy and I developed an analogue of Goodwillie's calculus of homotopy functors in an abelian setting using cross effects and cotriples. For functors  $F : \mathcal{A} \to \mathcal{B}$  where  $\mathcal{A}$  is a pointed category with finite coproducts and  $\mathcal{B}$  is an abelian category, the (n + 1)st cross effect  $cr_{n+1}F$  is a symmetric functor of n + 1 variables first used by Eilenberg and Mac Lane. The functor  $cr_{n+1}$  and the diagonal functor  $\Delta^*$  form an adjoint pair between the categories of functors from  $\mathcal{A}$  to  $\mathcal{B}$  and functors from  $\mathcal{A}^{\times n+1}$  to  $\mathcal{B}$  which in turn yields a cotriple  $\perp_{n+1} = \Delta^* \circ cr_{n+1}$  on the category of functors from  $\mathcal{A}$  to  $\mathcal{B}$ . For  $F : \mathcal{A} \to \mathcal{B}$  the cotriple produces an augmented simplicial object  $\perp_{n+1}^{*+1} F \to F$  whose homotopy cofiber gives us a functor  $\Gamma_n F := \text{cofiber}(\perp_{n+1}^{*+1} F \to F)$ . These  $\Gamma_n F$  can be assembled into a tower of functors  $\cdots \to \Gamma_{n+1}F \to \Gamma_n F \to \dots \Gamma_1 F \to \Gamma_0 F$ . The *n*th term in this tower,  $\Gamma_n F$ , is a degree *n* functor, i.e., its (n + 1)st cross effect is quasi-isomorphic to 0. This is a weaker condition than the *n*-excisive condition satisfied by the terms in Goodwillie's Taylor tower of a homotopy functor. In his thesis, Andrew Mauer-Oats extended this cotriple tower construction to endofunctors of the category of based spaces. He also proved that when F is a functor that commutes with geometric realization,  $\Gamma_n F \simeq P_n F$ , the *n*th term in Goodwillie's Taylor tower of the functor F.

In this talk I will discuss recent work with K. Bauer, R. Eldred, and R. McCarthy to extend these ideas to a more general context. We work with functors  $F : C_f \to D$  where C and D are simplicial model categories,  $f : A \to B$  is a morphism in  $C, C_f$  is the full subcategory of objects  $A \to X \to B$  that factor the morphism f, and D is stable. In this setting, the functors  $cr_{n+1}$  and  $\Delta^*$  only form an adjoint pair up to homotopy. Mauer-Oats handled this problem for spaces by using combinatorial techniques to show directly that  $\perp_{n+1}$  is a cotriple. In the current work, we identify two adjoint pairs whose composition yields  $\perp_{n+1}$  as its associated cotriple. With this, the construction of the tower

$$\dots \Gamma_{n+1}^f F \to \Gamma_n^f F \to \dots \Gamma_1^f F \to \Gamma_0^f F$$

proceeds much as it did in the abelian case. The *n*th term is now a functor that is *n*-excisive relative to *f*, that is, it takes strongly cocartesian (n + 1)-cubes of objects built by using the morphism *f* to cartesian diagrams. When *F* commutes with realizations, we generalize Mauer-Oats' results, showing that  $\Gamma_n^f F$  is *n*-excisive and  $P_n F$  and  $\Gamma_n^f F$  are weakly equivalent functors. More generally, for an arbitrary  $F : C_f \to \mathcal{D}$  (that does not necessarily commute with realizations) evaluation at the initial object *A* in  $C_f$  yields a weak equivalence  $\Gamma_n^f F(A) \simeq P_n F(A)$ .

#### Speaker: Pascal Lambrechts (Louvain-la-Neuve)

#### Title: Formality of the little N-disks operad

Abstract: This is joint work with Ismar Volic. The little N-disk operad is an important object in functor calculus, notably in the manifold calculus of embeddings of a manifold into a vector space. Since the work of Fred Cohen in the 1970's, the homology of this operad is well known to be a (generalized) Poisson operad. In the paper "Operads, motives and deformation quantization", M. Kontsevich stated and sketched the proof that this operad is formal. This means that there exists a zigzag of quasi-isomorphims of operads connecting the chains on the little disks operad with its homology (with coefficients in the field of real numbers). The special case of operads of little two-dimensional disks this has been proved by Tamarkin.

In this talk we will explain the proof of the formality of this operad. The main idea of the proof is to build a certain graph-complex and to show 1) that it is quasi-isomorphic to the chains of the little disks operad, thanks to a construction which is called the Kontsevich configuration integral; 2) that it is also quasi-isomorphic to its homology, which is proved by a simple algebraic argument. In order to properly interpret the integral we will replace the little disks operad by an equivalent one, namelythe operad of configuration spaces compactified la Fulton-MacPherson. We will recall some interesting geometry of this operad.

Actually the formality result is more precise than initially stated by Kontsevich: (i) formality holds in the category of CDGA's, which encode rational homotopy type; (ii) we consider that the little disk operad has an operation in arity 0; (iii) some relative version of the operad holds.

An important technical point in the proof is that we need to use a variant of deRham theory for semialgebraic sets instead of smooth manifolds. We probably will not have the time to explain this subtelity. There is also a cyclic version of formality for the framed little 2-disks operad proved by J. Giansiracusa and P. Salvatore

#### Speaker: Mike Mandell (Indiana)

#### Title: Quillen Cohomology of Operadic Algebras and Obstruction Theory

Abstract: Quillen defined homology in terms of abelianization. For operadic algebras Quillen homology is the derived functor of indecomposibles, and the bar duality (or "derived Koszul duality") construction provides a model for the Quillen homology. The k-invariants of Postnikov towers for algebras over an operad O lie in the Quillen cohomology groups, and this leads to an obstruction theory for O-algebra structures and O-algebra maps. I will discuss my recent paper with Maria Basterra where we apply this obstruction theory to show that BP is an  $E_4$  ring spectrum.

#### Speaker: Michael Weiss (Aberdeen)

Title: Smooth maps to the plane and Pontryagin classes

Abstract: This is joint work with Rui Reis.

The long-term goal is to prove that the Pontryagin classes in the 4i-dimensional rational cohomology of BTOP(n), due to Novikov and Thom, satisfy the standard relations that we expect from Pontryagin classes of vector bundles, for example: vanishing when i > 2n. Here TOP(n) is the topological group of homeomorphisms from  $\mathbb{R}^n$  to itself. It is not difficult to recast this as a problem in orthogonal calculus, for the functor  $V \mapsto BTOP(V)$  from real vector spaces with inner product to based spaces. Throwing in smoothing theory as well, one can recast it as a problem about spaces of regular (nonsingular) smooth maps from  $D^n \times D^2 \to D^2$ , extending the standard projection on the boundary. Imitating the parametrized Morse theory of Cerf and K Igusa, we investigate these spaces of regular maps by thinking of them as being contained in spaces of smooth maps to the plane with only moderate singularities. Then we need homotopy formulae for spaces of smooth maps with only moderate singularities. This leads us to Vassiliev's discriminant method. We reformulate that as a method for proving theorems in manifold calculus (formerly "embedding calculus"). The reformulation gives us some generalizations, allowing us to impose good behavior conditions not just on singularities in the source,  $D^n \times D^2$ , but also on singularity sets in the target,  $D^2$ . That gives us a lot to play with. We hope it is enough.

# **Participants**

Arone, Greg (Univ. Virginia) Basterra, Maria (University of New Hampshire, Durham) **Bauer, Kristine** (University of Calgary) Behrens, Mark (Massachusetts Institute of Technology) Budney, Ryan (University of Victoria) Ching, Michael (University of Georgia) Dwyer, William (Notre Dame University) Finster, Eric (Ecole Polytechnique Fédérale de Lausanne) Fresse, Benoit (Université Lille 1 - Sciences et Technologies) Harper, John (Ecole Polytechnique Fédérale de Lausanne) Hess, Kathryn (Ecole Polytechnique Fédérale de Lausanne) Johnson, Brenda (Union College) Kuhn, Nick (University of Virginia) Lambrechts, Pascal (Universite de Louvain) Lesh, Kathryn (Union College) Mandell, Michael A. (Indiana University) Miller, Haynes (Massachusetts Institute of Technology) Salvatore, Paolo (Univ. of Rome Tor Vergata) Sinha, Dev (University of Oregon) Turchin, Victor (Kansas State University) Weiss, Michael (University of Aberdeen)

# Chapter 11

# Stochastic Multiscale Methods: Bridging the Gap Between Mathematical Analysis and Scientific and Engineering Applications (11w5120)

# Mar 27 - Apr 01, 2011

**Organizer(s):** Guillaume Bal (Columbia University) Roger Ghanem (University of Southern California) Wing Liu (Northwestern University) George Papanicolaou (Stanford University) Boris Rozovsky (Brown University)

# **Overview**

Issues of uncertainty quantification, model validation, and optimization under uncertainty have taken center stage in many areas of science and engineering. Likewise, multiscale modeling and computing capabilities are becoming the standard against which model-based predictions are gauged. It thus behooves the scientific community, at this juncture, to elucidate the mathematical foundation of stochastic multiscale concepts so as to ensure a steady evolution of scientific capabilities as engines of economical growth societal wellbeing.

Exchanging information across scales is one of the most significant challenges in multiscale modeling and simulation. By necessity, and naturally within a multiscale context, information is truncated as it is presented to a coarser scale, and is enriched as it traverses the opposite path. Information is lost and corrupted as it is, respectively, upscaled and downscaled. Mitigating these errors can be set on rigorous ground through a probabilistic description of information, whence finite-dimensional approximations of measures provides an analytical path for describing the coarsening and refining of information. Stochastic analysis, therefore, provides a rational context for the analysis of multiscale methods.

This Workshop was designed to cement a dialog between mathematicians, mechanicians, and computational scientists that will lay the foundation for an accelerated growth in stochastic multiscale methods. Thirty colleagues from academia and US national laboratories and research funding agencies participated in the Workshop, including 6 graduate students, and participants from USA, Canada, France, Belgium, England and Saudi Arabia.

While accommodations at Banff were generously covered by a BIRS grant, travel expenses for the organizers and the graduate students were covered by an NSF grant.

The Workshop featured 18 hour-long talks, spread over four days, with open discussion throughout the meeting and specially in the evenings.

Stochastic Multiscale Methods: Bridging the Gap Between Mathematical Analysis and Scientific and Engineering Applications

# **Summary of Presentations**

Paul Newton talk was entitled "Metastatic progression via biased random walks on a cancer network" in which he described procedures for developing a Markov Chain (MC) model for the progression of cancer in the lung. A 50-dimensional state of the MC is obtained from a network characterization of the lung, and associated stationary transition probabilities are estimated from a dataset containing 3827 data points. The mean first passage time on metastasis is obtained through Monte Carlo sampling and used to identify trajectories of metastasis progression.

In his talk entitled "An elliptic inverse problem arising in groundwater flow," Andrew Stuart described an adaptation of Bayesian parameter estimation to stochastic processes. In the process, he described the extension of Bayes theorem to infinite dimensions. Further, using Polynomial Chaos representation of the posterior, an efficient sampling algorithm is developed that is competitive with MCMC procedures.

Howman Owhadi described optimal uncertainty quantification in a talk entitled "Bridging scales with incomplete information Optimal Uncertainty Quantification." Driven by the need to carry out analytical certification with limited data and poorly understood model, he presented a mathematical construction that provides optimal bounds on tail probabilities. The construction is based on concentration inequalities and McDiarmid's inequality and reduces the problem to the product of convex linear combinations of Dirac masses over a lattice. The fundamental ideas were demonstrated on a hypervelocity impact problem.

Wing Kam Liu, in his talk "Bridging of the Scales, Multiscale Modeling & Simulation of Uncertain Archetype Motion," described a new perspective on material modeling involving building blocks. These socalled "archetypes" are associated with behaviors on a variety of scales, as needed for the problem at hand. In addition to describing the practical relevance and reach of this new "science of material" the presentation described how the physical postulates of material motion can be adapted to these archetypes, resulting in governing equations that are intrinsically multiscale, and the possible sources of uncertainty associated with the new representations.

In her talk entitled "Stochastic Multiscale Analysis and Design," Wei Chen picked-up where Wing Kam Liu left and explained how the adaptation of the archetype theory to the concurrent optimization of hierarchical materials and product designs across multiple scales. She emphasized the significance of design specification to the delineation of uncertainty, and the importance of accounting for modeling errors.

Sergey Lototsky described "Mean-preserving stochastic renormalization of differential equations." By introducing Wick products into stochastic differential equations, the form of these equations is simplified, permitting the use of usual calculus instead of Ito calculus.

Habib Najm described the "Analysis of uncertain dynamical network models." Motivated by the network structure of many physical problems, the critical need for model reduction, and the significant uncertainties in both the original and reduced models, he discussed a coupling between polynomial chaos expansions and singular perturbation-like analysis. A spectral analysis of the discrete system of equations resulting from the stochastic Galerkin projection is thus analyzed, and stability properties of the underlying stochastic physical system are investigated.

Jim Nolen's presentation on "Importance sampling for random elliptic equations," was about the use of importance sampling to compute statistics of the solutions to a (elliptic) PDE with random coefficients. In the context of a Monte Carlo simulation to compute the statistics, one wants to minimize the number of samples needed for accurate statistical estimation, since generating each sample is an expensive computation (solving a PDE). An importance sampling scheme was described based on linearization and asymptotic analysis of the map from coefficients to solution.

In his talk "Kinetic limits and imaging models for waves in random media," Olivier Pinaud described methods for imaging inclusions buried in a random medium from detector measurements. The focus was on a regime where the interaction between the wave and the medium is strong. After reviewing relevant scales and some standard mathematical results associated with this problem, a new approach based on a transport problem was proposed. Numerical examples were used to provide an interpretation and shed light on the mathematical statements.

In his talk "Variance reduction and multiscale FEM for random media", Frédéric Legoll presents efficient yet accurate numerical approaches for characterizing random media that capitalize on an assumed random perturbation around a periodic mean. For strongly stochastic materials, a variance reduction approach is proposed, while for weakly random materials, specialized approaches are also described that take advantage

of multiscale and homogenization approaches.

In her talk "Noise sensitivities in systems with delays and multiple time scales," Rachel Kuske described the effect of delays and multiple time scales on the dynamics of nonlinear systems. Dynamical systems with delayed feedback often exhibit complex oscillations that are significantly affected by stochastic fluctuations, particularly if multiple time scales are present. Then transients ignored in the deterministic system can dominate the long range behavior. The approaches described capture the effects of noise and delay in the contexts of piecewise smooth systems, nonlinearities, and discontinuities.

Wenjia Jing talked about "Fluctuation in random homogenization: motivations, corrector theory, and algorithm test." He introduced a corrector theory that provides an estimate for the fluctuations around the homogenized solution with significant implications to inverse problems. For elliptic equations with random multiscale potentials, a systematic corrector theory was developed that clearly depend on the regularity of Green's function and correlation range of the underlying random field.

Maarten Arnst presented a talk entitled "Dimension reduction and measure transformation in stochastic multiphysics modeling," described the possibility and significance of affecting a transformation of probability measures as information is exchanged between models in a multiphysics problem. Issues of convergence and embedded quadrature were also discussed.

Youssef Marzouk discussed "Multiscale and map-based methods for statistical inference in inverse problems." Specifically, methods for characterizing the mapping between the prior and posterior random variables are presented.

In his talk, "Adaptive Multi-Level Monte Carlo Simulation," Raul Tempone generalizes a multilevel Forward Euler Monte Carlo method introduced in [1] for the approximation of expected values depending on the solution to an Ito stochastic differential equation. Previous work proposed and analyzed a Forward Euler Multilevel Monte Carlo method based on a hierarchy of uniform time discretizations and control variates to reduce the computational effort required by a standard, single level, Forward Euler Monte Carlo method. The present work introduces and analyzes an adaptive hierarchy of non-uniform time discretizations, generated by adaptive algorithms. These adaptive algorithms apply either deterministic time steps or stochastic time steps and are based on adjoint weighted a posteriori error expansions. Under sufficient regularity conditions, both in the present analysis and numerical results, which include one case with singular drift and one with stopped diffusion, significant savings in the computational cost were observed.

Alireza Doostan's talk, "On sparse approximation techniques for uncertainty propagation", described the adaptation of LASSO techniques to the characterization of the solution of partial differential equations with stochastic coefficients. Significant savings both in terms of representation effort and computational effort are described.

In his talk entitled "tP-CKM: Bayesian continuum closure evaluation from stochastic microdynamics," Sorin Mitran considers a generic problem of great significance in polymer flows and several biological applications. The problem exhibits dependence of the continuum scale on microconfigurations that are themselves affected by boundary conditions imposed on the continuum. The physics is specified at the microscale which is stochastic and does not equilibrate quickly. The approach involves predictions at the continuum scale (assumed to be true), through a hierarchical Bayesian formalism across scales (microscale and kinetic scale). Adaptation of the formalism to advanced computational platforms, including GPUs, is also discussed.

Finally, Sonjoy Das talked about an "An energy based stochastic mapping between high and low fidelity models." In this talk a framework and algorithms were described to develop stochastic coarse scale models that encapsulate errors stemming from upscaling from a deterministic fine scale.

## **Summary of the Breakout Sessions**

Discussion sessions were held each evening, kicking off for a few hours at one of the classrooms. This section presents a synthesis of those discussions.

#### Synergies between UQ and Multiscale

There are clear synergies between multiscale physical behavior and mathematical analysis on one hand, and uncertainty quantification on the other hand. Indeed crossing scales entails shedding or interpolating for Stochastic Multiscale Methods: Bridging the Gap Between Mathematical Analysis and Scientific and Engineering Applications

information, while uncertainty in behavior is often due to omissions in coupling to subscale information (physical processes or measurements). This tight linkage can be described as follows:

- 1. multiscale provides possible physical context for uncertainty.
- 2. scales cannot be all well characterized, even with access to higher performance computing resources. Uncertainty analysis is thus needed to represent irrecoverable information.
- 3. the implications of multiscale uncertainties have to be described in the context of specific predictions (on specific quantities of interest) and specific decisions, with well defined objectives functions.

### **Typical Applications**

While it was recognized that multiscale and uncertainty analyses are ubiquitous in science, engineering and the physical world, an attempt was made to delineate the scope of relevance of multiscale processes as captured by the Workshop participants. The following (incomplete) list was produced, and thought to reflect many current areas in science where synergetic advances in uncertainty quantification and multiscale analysis is likely to lead to significant mathematical, scientific, and technological breakthroughs.

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interacting multiscale systems (so-	subsurface flows including carbon sequestra-
cial/infrastructures)	tion and nuclear repository ( QoI are fracture,
	failure, extremes) and environmental remedi-
	ation (percolation, homogenized limits).
power grid: fault analysis on huge systems	materials science: homogenized systems,
	fracture, failure, design, meta materials, dam-
	age.
complex fluids	regulatory finance
turbulence	interfaces
weather and geophysical processes (eg. Ice)	climate
biological processes (cellular, biomechanics,	
etc)	

#### **Components of a Multiscale System and Associated b Challenges**

Some features of a coherent stochastic multiscale system emerged following a number of discussions to include (1) Characterization, (2) Computing, (3) Probabilistic Modeling, (4) Validation, (5) Scientific Discovery, and (6) Decision & Design.

A description of any of these features seems to be strongly dependent on an identification of the quantity (or quantities) of interest. Under, Characterization, measurements of the same phenomenon at different scales was deemed significant in order to understand the structure of statistical dependence between the different scales. This in turn requires developing models of sensors. It is clear that a combination of statistical and physics-based understanding would be critical at this stage. Hierarchical models, including hierarchical Bayesian models were mentioned as significant for addressing some of these challenges. Computing is clearly a critical driver of research for both multiscale and uncertainty quantification. It plays a role in uncertainty quantification, and in integration of analyses across scales. Mathematical challenges related to computing pertain essentially to convergence, error estimation, and numerical efficiency. It was felt that Probabilistic Modeling is a key component for both formulating a well-posed problem (that does not violate physical premises or mathematical hypotheses), a useful problem (that acknowledges the quantity of interest) and an optimal problem (that packages available evidence appropriately). The issue of Validation was deemed critical for the multiscale problems. In particular, the validation of single-scale simulations, cross-scale exchange, and coupled multiscale simulations seem to each be important and challenging in its own right. There are conceptual, statistical, and physical aspects to each of these pieces. The issue of Scientific Discovery was identified as an important contribution of both multiscale and uncertainty analyses. The discovery of emergent behaviors from multiscale couplings, and from interaction of fluctuating parameters is a clear path for discovering behaviors and issues not measurable in a deterministic or single-scale setting.

This highlights the value of numerical explorations without the imperative of a clear quantity of interest. Alternatively, one could try to formulate quantities of interest that are consistent with the purpose of scientific discovery. Finally, it was also felt that in most cases, understanding the ultimate purpose of a numerical simulation, whether **Decision or Design**, is paramount for developing acceptable probabilistic models and ascertaining the value of multiscale enrichment.

#### **Some Mathematical Challenges**

We had a long discussion on reduced order models (ROM), including reductions within a single-scale and within a multiple scale context.

Some issues that were discussed:

- 1. Reduced order models (ROM) must be tested against mathematically provable limits.
- 2. ROM must be adapted to achievable data modalities.
- 3. Characterize the combined uncertainty in cross-scaling/model reduction.
- 4. statistical/logical/mathematical/computational relations between data from across scales.
- 5. does prediction of individual specimen behavior make sense ? if not, what are limits on prediction ? how can multiscale push those limits ?
- 6. Bayesian paradigm revisited: what is our prior information, and what is the mathematical structure available to compute the likelihood in a multiscale context, with data and uncertainty at every scale and junction.
- 7. curse of dimensionality.
  - minimnum-maximum spanning sets in high dimensions.
  - low rank tensor approximation and sparse approximation.
  - connection to reality (are observable really high-dimensional ?)
- 8. mathematical formulations and analysis of uncertainty propagation.
  - analysis on tensor spaces.
  - verification and error analysis.
- 9. inference from limited data.
- 10. validation of key concepts including upscaling.
- 11. sufficiency of data for subscale reconstruction.
- 12. upscaling as a physical process and as an information exchange process.
- 13. to what extent can subscale be constrained by coarse scale ?
- 14. constrain mathematical models with multiscale features.
- 15. algorithms/ computation: model-based simulations and statistical computing.
- 16. stochastic programming for multiscale problems.
- 17. constraining inference with multiscale information and practical considerations (too little data, incomplete models).
- 18. design-informed separation of scales.

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## **Grand Challenges**

A small number of grand challenges were identified as generically relevant across all applications and which are likely to spawn new physics and mathematics. These are stated as follows:

- Define multiscale data needed to be sufficiently predictive for a given QoI
- Quantify credibility of multiscale coupling and information passing
- Understand implications of information fusion from multiple scales with varying levels of confidence
- Develop benchmark problems to drive research.

# **List of Participants**

Arendt, Paul (Northwestern University) Arnst, Maarten (University of Southern California) **Bal. Guillaume** (Columbia University) Bellis, Cedric (Columbia University) Chen, Wei (Northwestern) Comboul, Maud (University of Southern California) Das, Sonjoy (SUNY - Buffalo) **Doostan, Alireza** (University of Colorado) Ghanem, Roger (University of Southern California) Greene, Steven (Northwestern) Guilleminot, Johann (Universite Paris-Est) Jing, Wenjia (Columbia University) Kuske, Rachel (University of British Columbia) Legoll, Frederic (Ecole Nationale des Ponts et Chaussees LAMI) Liu, Wing (Northwestern University) Lototsky, Sergey (University of Southern California) Marzouk, Youssef (Massachusetts Institute of Technology) Mehrez, Loujaine (Katholieke Universiteit Leuven (KU Leuven)) Mitran, Sorin (University of North Carolina) Monard, Francois (Columbia University) Najm, Habib (Sandia National Laboratories) Newton, Paul (University of Southern California) Nolen, James (Duke University) Owhadi, Houman (California Institute of Technology) Phipps, Eric (Sandia National Laboratories) Pinaud, Olivier (Columbia University / Université Lyon 1) Prudhomme, Serge (UT Austin) Red-Horse, John (Sandia National Laboratories) Stargel, David (AFOSR) Stuart, Andrew (Warwick University) Tempone, Raul (KAUST) von Schwerin, Erik (KAUST)

# Chapter 12

# Geometric flows in mathematics and physics (11w5010)

# Apr 17 - Apr 22, 2011

**Organizer(s):** Mauro Carfora (University of Pavia) Zindine Djadli (Institut Fourier, Université Grenoble 1) Gerhard Huisken (Max-Planck-Institute for Gravitational Physics) Lei Ni (University of California, San Diego) Eric Woolgar (University of Alberta)

# **Overview of the Field**

Few, if any, fields of mathematics have experienced the success that geometric analysis since it emerged as a field of its own about 35 years ago, having formed at the nexus of PDEs, Riemannian geometry, and related fields such as Kähler geometry, general relativity, and applied mathematics. Soon after, the study of geometric flow equations commenced in earnest and has since become one of the most fruitful areas of geometric analysis. Examples of problems that have been solved through the study of geometric flows include the Poincaré conjecture, the Thurston geometrization conjecture, the Penrose conjecture, the differentiable sphere theorem, and the *n*-dimensional Rauch-Hamilton spherical space forms conjecture.

Geometric analysis has always owed much to physics. For example, the positive energy conjecture of general relativity stimulated Schoen and Yau to produce their geometric analysis proof. Conversely, physics has gained much from geometric analysis, an example of this being provided by Yau's proof of the Calabi conjecture, making possible the use of Calabi-Yau manifolds in string theory phenomenology. It is therefore natural for physicists to search for ways to exploit the mathematical progress made in geometric flow equations, and natural as well for mathematicians to use physics as a source for new problems to solve using geomtric flows. There have been a series of meetings in recent years, typically consisting mostly of mathematicians together with a smaller number of physicists, who gather together to discuss progress in the field and possble new applications. One such meeting was a workshop held at BIRS in 2008. The meeting was highly successful, so this motivated us to hold another BIRS workshop on the topic in 2011.

In the last three years, new themes have emerged in the subject. Traditionally, Ricci flow has been applied to Riemannian metrics on closed manifolds (i.e., compact manifolds that have no boundary). This endeavour has continued to have new successes, a recent one being the Brendle-Schoen proof of the differentiable sphere theorem. However, Ricci flow on noncompact manifolds is becoming more important. A large group in France, gathered about Gérard Besson at Grenoble, has been working on this, hoping to apply the results to the classification problem for open 3-manifolds. Furthermore, if one imposes that the metric should obey asymptotic fall-off conditions of certain types (prime examples being asymptotically flat metrics and conformally compactifiable metrics), then the Ricci flow of these metrics has applications to physics. The asymptotically flat problem was studied a few years ago by Oliynyk-Woolgar and Dai-Ma, but the confor-

Figueras-Pau-Wiseman. The Ricci flow on manifolds-with-boundary is proving to be an even more difficult problem. We have a satisfactory theory only when the boundary is totally geodesic, in which case the manifold can be "doubled", reducing the problem to the compact manifold case.

Numerics are emerging as an area of interest for geometric flows. Mean curvature flow has many practical applications which have driven numerical work using this flow. However, for Ricci flow, there has not yet been much numerical work, btu that can be expected to change. On the last day of the workshop, a discussion session was held on the topic of numerical Ricci flows. Two questions come to mind: What are the Ricci flow problems that will motivate numerical investigations? And how do we overcome the computational challenges that these problems would pose?

### **Presentation Highlights**

#### Peter Topping: Instantaneously complete Ricci flows

Peter Topping spoke on joint work with G Giesen on Ricci flows which are complete for all  $t \in (0, T)$  and  $x \in \mathbb{R}^2$ , but are such that either curvature becomes unbounded as  $t \searrow 0$  or the metric becomes incomplete when extended back to t = 0. There is a general existence theorem for this flow for "initial data" (in the above sense) given on a Riemann surface, with the flowing metric being complete at all positive times. Topping was also able to give a formula for the maximal existence time of the flow in terms of the volume of the initial data surface. If the initial metric is conformally equivalent to a complete hyperbolic metric H, then the flow actually  $C^0$ -converges to H at least as fast as 1/t.

### Gérard Besson: Natural maps, differential rigidity, and Ricci and scalar curvature.

In this talk, Besson posed the question of when a degree 1 map from one closed smooth *n*-manifold Y to another X is homotopic to a diffeomorphism. He disucssed a result of Bessières, Besson, Courtois, and Gallot that when g is a metric on Y with  $\operatorname{Ric}(g) \ge -(n-1)g$  and  $g_0$  is a hyperbolic metric on X, then there is an  $\epsilon$  depending only on the dimension and diameter of X such that f is homotopic to a diffeomorphsim whenever  $\operatorname{vol}(X, g_0) \le \operatorname{vol}(Y, g) \le (1 + \epsilon) \operatorname{vol}(X, g_0)$ . The proof works by constructing "natural maps"  $Y_k \to X$  that converge to an isometry, so that X is the Gromov-Hausdorff limit of a sequence of manifolds obeying a lower bound on Ricci curvature. Thus X and  $Y_k$  are diffeomorphic (for large k) by a theorem of Cheeger and Colding.

### Philippe G LeFloch: Weakly regular $T^2$ -symmetric spacetimes.

This talk discussed a weak formulation of the Cauchy initial value problems for the spacetime Einstein equations Ric = 0. The problem is to find weak solutions from rough initial data exhibiting  $T^2$ -symmetry. LeFloch argues that the initial data constraints and Einstein evolution equations for the Cauch y problem in the weak  $T^2$ -symmetric setting can be formulated in the sense of distributions and solved accordingly.

### Gerhard Dziuk: Computation of geometric flows

This talk concerned numerical methods for geometric PDEs on surfaces, including moving surfaces, and on applications. One begins by discretizing the surface, for example by approximating the surface by a piecewise polynomial surface which can then be described by n-simplices defined by a grid of a certain spacing h (e.g., for piecewise linear approximation, use polynomials of degree 1). Then one can develop a discrete version

of the mean curvature vector. The most simple approach fails to give a good approximation to the true mean curvature vector and to the Willmore energy of a 2-sphere in  $\mathbb{R}^3$ , but this can be greatly improved through the use of Ritz projection. The speaker gave explicit numerical examples of evolution of certain surfaces under this discrete Willmore flow. The talk ended with some discussion of a discretization of Ricci curvature, based on a suggestion of G Huisken, which may prove suitable for discrete Ricci flow in higher dimensions and without symmetry.

### Felix Schulze: On short time existence of the network flow.

This was a report on joint work of the speaker with T. Ilmanen and A. Neves on how to prove the existence of an embedded, regular network moving by curve shortening flow in the plane, starting from a nonregular initial network.

Here a regular network consists of smooth, embedded line segments such that

at each endpoint, if not infinity, there are three arcs meeting under a 120 degree angle. In the nonregular case, an arbitrary number of line segments are allowed to meet at an endpoint, without an angle condition. The proof relies on gluing in appropriately scaled self-similarly expanding solutions and a new monotonicity formula, together with a local regularity result for such evolving networks.

This short time existence result also has applications in extending such a flow of networks through singularities.

### Reto Müller: Central blow-ups of Ricci flow singularities.

Scaling invariance properties of the heat equation motivated Hamilton to presume that singularities of the Ricci flow should be modeled by nontrivial

gradient shrinking solitons. Perelman's W-entropy monotonicity strengthens this conjecture, showing that for any central blow-up sequence the shrinking

soliton equation is approached in a weighted  $L^2$ -sense. Moreover, a similar

solution equation is approached in a weighted  $L^-$ -sense. Moreover, a simila

(but more hidden) indication follows from the monotonicity of Perelman's

reduced volume functional.

After explaining these motivations, the speaker demonstrated how Hamilton's conjecture can be proved in the case of Type I Ricci flows. This was joint work of the speaker with Joerg Enders and Peter Topping. Then he described possible extensions (in low dimensions) to the general case and presented partial results obtained with collaborators Robert Haslhofer and Carlo Mantegazza.

### Eric Bahuaud: Ricci flow of smooth asymptotically hyperbolic metrics.

This was the first of two talks on the interesting topic of Ricci flow of asymptotically hyperbolic (i.e., conformally compactifiable) metrics. The speaker described his proof that, given a smoothly conformally compact metric, there is a short time solution to the Ricci flow evolving from the given metric that remains smoothly conformally compact. Similar results were also obtained in independent work reported by Shi below. The speaker applied recent results of Schnürer, Schulze, and Simon to prove a stability result for conformally compact metrics sufficiently close to the hyperbolic metric. The speaker described his recent joint work with Jie Qing and his PhD student Jie Wu. They investigated the behaviour of normalized Ricci flow whose initial metric is epsilon-Einstein on a complete, noncompact Riemannian manifold. They show that a under nondegeneracy condition on the initial metric the solution to the normalized Ricci flow exists for all time and converges exponentially fast to some Einstein metric. In accord with Bahuaud's result described above, they were able to show that if the initial metric can be conformally compactified then the conformal structure of the boundary-at-infinity is preserved by normalized Ricci flow. Furthermore, the limit is a conformally compact Einstein metric.

#### Robert Haslhofer: A mass decreasing flow in dimension three.

After reviewing the relationship between Perelman's energy-functional, the stability of Ricci-flat spaces, and the ADM mass from general relativity, the speaker introduced a mass-decreasing flow for asymptotically flat

three-manifolds with nonnegative scalar curvature. This flow is defined by

iterating a suitable Ricci flow with surgery and conformal rescalings and

has a number of nice properties. In particular, wormholes pinch off and

nontrivial spherical space forms bubble off in finite time. Moreover, a

noncompact variant of Perelman's energy-functional is monotone along the

flow. The long time behaviour seems to be quite delicate to analyze, but the speaker conjectured that the flow always squeezes out all the initial mass. He can prove this under an *a priori* assumption relating the ADM-mass and the

Perelman energy.

#### Artem Pulemotov: A mass decreasing flow in dimension three.

A very important issue for Ricci flow is the choice of appropriate boundary conditions for the flow on compact manifolds-with-boundary. To be useful, such boundary conditions would have to produce some degree of control over the flow of curvature through a boundary. However, (short time) existence and well-posedness ought to require that the boundary conditions should be not worse than first differential order in the metric, so any control of curvature through the boundary would have to follow rather indirectly from conditions on, say, the induced metric and extrinsic curvature. One can attempt the DeTurck approach, in which case a natural boundary condition would be to set the DeTurck vector field to be either zero or perhaps just tangent to the boundary. However, it is not entirely clear that this condition will yield existence (and, though the speaker did not raise it in the talk, it is not at all clear that it would then produce a useful degree of curvature control).

The speaker instead attempts to work directly with the Ricci flow without DeTurck vector field. Then the number and type of boundary conditions that one can impose is unclear, since the principal symbol of the operator that defines this flow has nontrivial kernel. The speaker is able to show existence of solutions under the boundary condition that the mean curvature be held constant. The question of what additional conditions to impose to obtain uniqueness and well-posedness remains open.

The Ricci flow with boundary has many applications. Among them, the speaker noted

the regularization of Riemannina metrics and the numerical work on phase transitions in quantum gravity of Headrick and Wiseman.

### Joakim Arnlind: Poisson algebraic geometry of Kähler submanifolds.

A Poisson algebra is an algebra with skew bracket that obeys the Jacobi identity and the identity  $\{ab, c\} = a\{b, c\} + \{a, c\}b$ . This talk described joint work of the speaker with J Hoppe and G Huisken. They want to know which geometric quantities can be written as algebraic expressions in the Poisson algebra of functions on an embedded surface. The answer, apparently, is "almost everything". They studied that the differential geometry of almost Kähler submanifolds and formulated this in terms of the Poisson structure induced by the inverse of the Kähler form. More precisely, the submanifold relations, such as Gauss' and Weingarten's

equations (as well as many other objects), can be expressed as Poisson brackets of the embedding coordinates. It is then natural to ask the following question: Are there abstract Poisson algebras for which such equations hold? They answer this question by introducing Kähler-Poisson algebras and show that an affine connection can be defined, fulfilling all the desired symmetries and relations; e.g., the Bianchi identities. Furthermore, as an illustration of the new concepts they are able to derive algebraic versions of some well known theorems in differential geometry. In particular, they prove that Schur's lemma holds and that a lower bound on the Ricci curvature induces a bound on the eigenvalues of the Laplace operator. It will be very interesting to see how far this approach can be pushed.

#### Jingyi Chen: Lagrangian mean curvature flow for entire graphs.

Chen reported on his joint work with Albert Chau and Yu Yuan. They prove longtime existence and estimates for solutions to a fully nonlinear parabolic equation  $\frac{\partial u}{\partial t} = \sum_i \arctan \lambda_i$ , where the  $\lambda_i$  are the eigenvalues of the Hessian  $\nabla \nabla u$ , for  $C^{1,1}$  initial data  $u_0$  subject to one of two conditions. These conditions are that either  $u_0$  is convex or the Hessian of  $u_0$  obeys  $-(1 + \delta)I \leq \nabla \nabla u_0 \leq (1 + \delta)I$  for some  $\delta$  that depends on the dimension. They also show that a supercritical condition on the Lagrangian phase is preserved under evolution by this equation.

#### Maria Buzano: Homogeneous Ricci flow.

Let (M, g) be a Riemannian manifold of dimension n and let g(t),  $t \in [0, T)$  be a Ricci flow on M with initial metric g. An important property of the Ricci flow is that it preserves symmetries of the initial metric g. It is then natural to investigate the Ricci flow on Riemannian manifolds which admit a transitive action by a closed group G of isometries. These are called homogeneous Riemannian manifolds. They are diffeomorphic to quotients G/K, where K is the isotropy group of a point in M with respect to the G-action. On this kind of space, we can restrict attention to those Riemannian metrics which are invariant under the action of G. This invariance is then preserved under the Ricci flow.

The speaker considers the Ricci flow on compact homogeneous spaces of the following type. Let G/K be a compact homogeneous space, with G compact and connected and K a closed connected subgroup of G such that G/K is effective. Suppose that there exists an intermediate Lie group H, with G > H > K, such that H/K is isotropy irreducible and every G-invariant Riemannian metric on G/K is obtained from a fixed Riemannian submersion  $H/K \to G/K \to G/H$ , by

rescaling the metric on the fibre and the base. In particular, these include the

case of compact homogeneous spaces G/K with two isotropy irreducible inequivalent summands and such that K is not maximal in G. Such homogeneous spaces are interesting because they include many examples of compact homogeneous

spaces which do not admit any invariant Einstein metric. The lowest dimensional

non-existence example is the 12-dimensional manifold SU(4) = SU(2) found by Wang and Ziller. Subsequently, Böhm and Kerr have shown that

this is the least dimensional example of a compact homogeneous space which

does not carry any G-invariant Einstein metric. Note that this example is of the type described above.

More non-existence examples can be obtained from the following fact. On a compact manifold, Einstein metrics are characterised variationally as the critical points of the Hilbert action. Hence, G/K does not carry any G-invariant Einstein metric if the traceless Ricci tensor restricted to one of the isotypical summands of the isotropy representation is positive definite for all G-invariant Riemannian metrics. By a theorem of Böhm, this implies that G/K is of the type described above, yielding many new examples of compact homogeneous spaces which do not carry any invariant Einstein metric. On the homogeneous spaces considered here, the speaker is able to show that the Ricci flow always develops a type I singularity in finite time. In particular, two possible behaviours can occur. Either the whole space shrinks to a point in finite time or the fibre H = K in the above Riemannian submersion shrinks to a point in

finite time and the total space G/K converges in the Hausdorff-Gromov topology

to the base space G = H. Moreover, the first behaviour can happen only if

G = K admits G-invariant Einstein metrics. However, there is always an open

subset of initial conditions such that the Ricci flow develops the second kind of

behaviour. It would be interesting to rule out type II singularities in the homogeneous case and investigate the Ricci flow in the case where K is a

maximal subgroup of G, at least in the two isotropy summands case.

#### Brett Kotschwar: Ricci flow and the holonomy group.

The speaker described his proof that the restricted holonomy group of a complete smooth solution to the Ricci flow of uniformly bounded curvature cannot

spontaneously contract in finite time. It follows then from an earlier

result of Hamilton that the holonomy group is exactly preserved by the

equation. In particular, a solution to Ricci flow may be Kähler or locally

reducible (as a product) at some time in the evolution only if the same is true at all previous times.

The problem can be reduced to one of backwards uniqueness for a certain system

satisfying coupled parabolic and ordinary differential inequalities via the

interpretation of the evolution equations in terms of the natural Lie bracket on two-forms. The backwards uniqueness of this system then follows from a earlier general result of the speaker. As the (Carleman-type) estimates responsible for this result measure — and, in principle, limit — the rate at which the

curvature operator can asymptotically "acquire" null directions, there is hope that these estimates (or improvements thereof) may have application in future work on analysis up to and including the singular time.

### Fuquan Fang: Ricci flow on 4-manifolds and Seiberg-Witten equations.

The speaker described his work with Zhang and Zhang over the last several years on the Ricci flow of both closed and noncompact 4-manifolds. The idea is to try to classify the asymptotic behaviour of immortal (fixed-volume normalized) Ricci flows on such manifolds, as has been done for 3-manifolds. Working with the normalized flow on a closed 4-manifold, the speaker and his collaborators have shown that the flow either collapses in the Cheeger-Gromov sense, subconverges to a Ricci soliton, or subconverges in the pointed Gromov-Hausdorff sense to a finite collection of complete (noncompact) negative Einstein metrics. They further prove that closed 4-manifolds admitting an immortal normalized Ricci flow either have a positive rank *F*-structure, admit a shrinking Ricci soliton, or satisfy the Hitchin-Thorpe inequality  $2\chi(M) \ge 3|\tau(M)|$ , for  $\chi(M)$  the Euler invariant of *M* and  $\tau(M)$  the signature. If the Yamabe invariant is  $\sigma(M) \le 0$  this inequality can be strengthened to  $2\chi(M) - 3|\tau(M)| \ge \frac{1}{96\pi^2}\sigma^2(M)$ . A corollary is that the Euler characteristic is  $\ge 0$  and vanishes iff the solution collapses along a subsequence of times.

The collaborators can find similar results by assuming that the Seiberg-Witten equations can be solved on the 4-manifold, giving a nontrivial Seiberg-Witten invariant (which counts generic irreducible solutions of these equations). If this invariant is nonzero and if |Ric[g(t)]| < const along the flow, then they obtain  $\chi(M) \geq 3\tau(M)$ .

The speaker also considered the case of finite-volume noncompact manifolds. These can also be studied with the fixed-volume normalized Ricci flow. Immortal solutions then either collapse along a subsequence or subconverge to a collection of complete negative Einstein manifolds; the shrinking solitons never occur.

#### Miles Simon: Expanding solitons with non-negative curvature operator coming out of cones.

The speaker described joint work that he did with Felix Schulze. They show that a Ricci flow of any complete Riemannian manifold without boundary with bounded non-negative curvature operator and asymptotic volume ratio  $\lim_{r\to\infty} \frac{\operatorname{vol}(M^n)}{r^n} \neq 0$  exists for all time and has constant asymptotic volume ratio.

They show that there is a limit solution, obtained by scaling down this solution at a fixed point in space, which is an expanding soliton coming out of the asymptotic cone at spatial infinity.

### Tobias Lamm: Geometric flows with rough initial data.

Given a flow problem  $\frac{\partial u}{\partial t} = F(x, t, u, Du, D^2u)$ , the speaker asks the question, "What are the right assumptions on the initial data  $u_0(x) = u(x, 0)$  to get well-posedness?" He is able to show the existence of a global unique and analytic solution for the mean curvature flow and the Willmore flow of entire graphs for Lipschitz initial data with small Lipschitz norm. He also shows the existence of a global unique and analytic solution to the Ricci-DeTurck flow on Euclidean space for bounded initial metrics which are close to the Euclidean metric in  $L^{\infty}$  and to the harmonic map flow for initial maps whose image is contained in a small geodesic ball.

#### Sylvain Maillot: Ricci flow with surgery and applications to open 3-manifolds.

The speaker discussed his joint work with L Bessières and G Besson, some of which is still in progress. Applications of Ricci flow with surgery include Perelman's proof of Thurston's geometrization conjecture and Coda Marques's result on connectedness of spaces of metrics of positive scalar curvature. The speaker discussed extensions of this work to noncompact manifolds. One goal is a Ricci flow proof of the geometrization conjecture in the noncompact, finite volume case, a result originally proved by Thurston using other methods. The finite volume restriction allows the use of the fixed-volume normalized Ricci flow. This would provided a unified approach to geometrization of closed manifolds and of compact manifolds with non-empty boundary comprised of a union of torii.

The speaker posed a conjecture that would generalize a result of Codá Marques for closed manifolds: that for a noncompact manifold M with sifficiently simple topology, the space of complete metrics on M with scalar curvature having a positive minimum should be path-connected.

### Numerical Ricci Flow Discussion Group

The Friday morning session was given over to a group discussion of numerical geometric flows. The main idea was to find mathematical problems that could be addressed by numerical Ricci flow, to anticipate the technical issues that might arise, and to begin to define an approach.

The session was surprisingly well attended, considering it was informal and was on the last morning of the workshop. At least two thirds of the participants were in attendance.

One of the problems suggested to the group is the long-standing problem of constructing an explicit nontrivial metric on a Calabi-Yau manifold. This requires real dimension 4, but is most interesting in real dimension 6, so it is something of a challenge numerically (though there has been some work in dimension 4 already). In a more general setting, Ricci flow might not converge to an Einstein metric, for the same reason that applies to any "relaxation method". Namely, the linearized flow is governed in this case by the Lichnerowicz Laplacian of the Einstein metric, which may contain a negative (i.e., repulsive) mode. However, an advantage is that Kähler Ricci flow is known to converge exponentially to a Kähler-Einstein metric.

Maria Buzano proposed a different problem, which is the study of possible Type II singularities in the flow of manifold of low cohomogeneity that are not rotationally symmetric. Then the computer no longer has to deal with a high-dimensional spatial grid. Gerhard Dziuk pointed out that because the problem involves evolution close to a singularity, during the flow the time step will have to be reduced near the region of singularity formation as the singularity forms Multi-grid methods will have to be employed. The question arose as to whether there might be a computationally efficient way to do this. Miles Simon pointed out the Perelman's pseudolocality theorem gives a technique to predict the change in curvature over a spatial region during for an interval of time. This may be just the tool necessary to allow for the development of an efficient multi-grid code to study singularities in Ricci flow.

### **List of Participants**

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## Chapter 13

# **Algebraic Graph Theory (11w5119)**

### Apr 24 - Apr 29, 2011

**Organizer(s):** Chris Godsil (University of Waterloo) Michael Newman (University of Ottawa)

### **Overview of the Field**

Algebraic graph theory comprises both the study of algebraic objects arising in connection with graphs, for example, automorphism groups of graphs along with the use of algebraic tools to establish interesting properties of combinatorial objects. One of the oldest themes in the area is the investigation of the relation between properties of a graph and the spectrum of its adjacency matrix. A central topic and important source of tools is the theory of association schemes. An association scheme is, roughly speaking, a collection of graphs on a common vertex set which fit together in a highly regular fashion. These arise regularly in connection with extremal structures: such structures often have an unexpected degree of regularity and, because of this, often give rise to an association scheme. This in turn leads to a semisimple commutative algebra and the representation theory of this algebra provides useful restrictions on the underlying combinatorial object. Thus in coding theory we look for codes that are as large as possible, since such codes are most effective in transmitting information over noisy channels. The theory of association schemes provides the most effective means for determining just how large is actually possible; this theory rests on Delsarte's thesis [4], which showed how to use schemes to translate the problem into a question that be solved by linear programming.

### **Recent Developments and Open Problems**

Brouwer, Haemers and Cioabă have recently shown how information on the spectrum of a graph can be used to proved that certain classes of graphs must contain perfect matchings.
Brouwer and others have also investigated the connectivity of strongly-regular and distance-regular graphs. This is an old question, but much remains to be done. Recently Brouwer and Koolen [2] proved that the vertex connectivity of a distance-regular graph is equal to its valency. Haemers and Van Dam have worked on extensively on the question of which graphs are characterized by the spectrum of their adjacency matrix. They consider both general graphs and special classes, such as distance-regular graphs. One very significant and unexpected outcome of this work was the

construction, by Koolen and Van Dam [10], of a new family of distance-regular graphs with the same parameters as the Grassmann graphs. (The vertices of these graphs are the k-dimensional subspaces of a vector space of dimension v over the finite field GF(q); two vertices are adjacent if their intersection has dimension  $k_1$ . The graphs are q-analog of the Johnson graphs, which play a role in design theory.) These graphs showed that the widely held belief that we knew all distance-ular

regular

graphs of "large diameter" was false, and they indicate that the

classification of distance-regular graphs will be more complex (and more interesting?) than we expected.

Association schemes have long been applied to problems in extremal set theory and coding theory. In his (very) recent thesis, Vanhove [14] has demonstrated that they can also provide many interesting results in finite geometry.

Recent work by Schrijver

and others [13] showed how schemes could used in combination with semidefinite programming to provide significant improvements to the best known bounds. However these methods are difficult to use, we do not yet have a feel for we might most usefully apply them and their underlying theory is imperfectly understood.

Work in Quantum Information theory is leading to a wide range of questions which can be successfully studied using ideas and tools from Algebraic Graph Theory.

Methods from finite geometry provide the most effective means of constructing

mutually unbiased bases, which play a role in quantum information theory and in

certain cryptographic protocols. One important question is to determine the maximum size

of a set of mutually unbiased bases in *d*-dimensional complex space. If *d* is a prime power the geometric methods just mentioned provide sets of size d + 1, which is the largest possible. But if *d* is twice an odd integer then in most cases no set larger than three has been found. Whether larger sets exist is an important open problem.

### **Presentation Highlights**

The talks mostly fitted into one of four areas, which we discuss separately.

### Spectra

Willem Haemers spoke on universal adjacency matrices with only two distinct eigenvalues.

Such matrices are linear combinations of I, J, D and A (where D is the diagonal matrix of vertex degrees and A the usual adjacency matrix). Any matrix usually considered in spectral graph theory has this form, but Willem is considering these matrices in general. His talk focussed on the graphs for which some universal adjacency matrix has only two eigenvalues. With Omidi he has proved that such a graph must either be strong (its Seidel matrix has only two eigenvalues) or it has exactly two different vertex degrees and the subgraph induced by the vertices of a given degree must be regular.

Brouwer formulated a conjecture on the minimum size of a subset S of the vertices of a strongly-regular graph X such that no component of  $X \setminus S$  was a single vertex.

Cioabă spoke on his recent work with Jack Koolen on this conjecture. They proved that it is false, and there are four infinite families of counterexamples.

### **Physics**

As noted above, algebraic graph theory has many applications and potential applications to problems in quantum computing, although the connection has become apparent only very recently. A number of talks were related to this connection.

One important problem in quantum computing is whether there is a quantum algorithm for the graph isomorphism problem that would be faster than the classical approaches.

Currently the situation is quite open. Martin Roetteler's talk described recent work [1] on this problem. For our workshop's viewpoint, one surprising feature is that the work made use of the Bose-Mesner algebra of a related association scheme; this connection had not been made before. Severini discussed quantum applications of what is known as the Lovász theta-function of a graph. This function can be viewed as an eigenvalue bound and is closely related to both the LP bound of Delsarte and the Delsarte-Hoffman bound on the size of an independent set in a regular graph. Severini's work shows that Lovász's theta-function provides a bound on the capacity of a certain channel arising in quantum communication theory Work in quantum information theory has lead to interest in complex Hadamard matrices ---these are  $d \times d$  complex matrices H such that all entries of H have the same absolute value and  $HH^* = dI$ . Both Chan and Szöllősi dealt with these in their talks. Aidan Roy spoke on complex spherical designs. Real spherical designs were much studied by Seidel and his coworkers, because of their many applications in combinatorics and other areas. The complex case languished because there were no apparent applications, but now we have learnt that these manifest themselves in quantum information theory under acronyms such as MUBs and SIC-POVMs. Roy's talk focussed on a recent 45 page paper with Suda [12], where (among other things) they showed that extremal complex designs gave rise to association schemes. One feature of this work is that the matrices in their schemes are not symmetric, which is surprising because we have very few interesting examples of non-symmetric schemes that do not arise as conjugacy class schemes of finite groups.

### **Extremal Set Theory**

Coherent configurations are a non-commutative extension of association schemes. They have played a significant role in work on the graph isomorphism problem but, in comparison with association schemes, they have provided much less information about interesting extremal structures. The work presented by Hobart and Williford may improve matters, since they have been able to extend and use some of the standard bounds from the theory of schemes. Delsarte [4] showed how association schemes could be used to derive linear programs, whose values provided strong upper bounds on the size of codes. Association schemes have both a combinatorial structure and an algebraic structure and these two structures are in some sense dual to one another. In Delsarte's work, both the combinatorial and the algebraic structure had a natural linear ordering (the schemes are both metric and cometric) and this played an important role in his work. Martin explained how this linearity constraint could be relaxed. This work is important since it could lead to new bounds, and also provide a better understanding of duality. One of Rick Wilson's many important contributions to combinatorics was his use of association schemes to prove a sharp form of the Erdős-Ko-Rado theorem [15]. The Erdős-Ko-Rado theorem itself ([5])

can certainly be called a seminal result, and by now there are many analogs and extensions of it which have

been derived by a range of methods. More recently it has been realized that most of these extensions can be derived in a very natural way using the theory of association schemes.

Karen Meagher presented recent joint work (with Godsil, and with Spiga, [8, 11]) on the case where the subsets in

the Erdős-Ko-Rado theorem are replaced by permutations. It has long been known that there is an interesting association scheme on permutations, but this scheme is much less manageable than the schemes used by Delsarte and, prior to the work presented by Meagher, no useful combinatorial information had been obtained from it.

Chowdhury presented her recent work on a conjecture of Frankl and Füredi. This concerns families  $\mathcal{F}$  of *m*-subsets of a set X such that any two distinct elements of have exactly

 $\lambda$  elements in common. Frankl and Füredi conjectured that the  $m\mbox{-sets}$  in any such family

contain at least  $\binom{m}{2}$  pairs of elements of X. Chowdhury verified this conjecture in a

number of cases; she used classical combinatorial techniques and it remains to see whether algebraic methods can yield any leverage in problems of this type.

### **Finite Geometry**

Eric Moorhouse spoke on questions concerning automorphism groups of projective planes, focussing on connections between the finite and infinite case. Thus for a group acting on a finite plane, the number of orbits on points must be equal to the number of orbits on lines. It is not known if this must be true for planes of infinite order. Is there an infinite plane such that for each positive integer k, the automorphism group has only finitely many orbits on k-tuples? This question is open even for k = 4. Simeon Ball considered the structure of subsets S of a k-dimensional vector space over a field of order qsuch that each d-subset of S is a basis. The canonical examples arise by adding a point at infinity to the point set of a rational normal curve. These sets arise in coding theory as maximum distance separable codes and in matroid theory, in the study of the representability of uniform matroids (to mention just two applications). It is conjectured that, if  $k \le q-1$ then  $|S| \le q+1$  unless q is even and k=3 or k=q-1, in which case  $|S| \le q+2$ . Simeon presented a proof of this theorem when q is a prime and commented on the general case. He developed a connection to Segre's classical characterization of conics in planes of odd order, as sets of q + 1 points such that no three are collinear. There are many analogs between finite geometry and extremal set theory; questions about the geometry of subspaces can often be viewed as q-analogs of questions in extremal set theory. So the EKR-problem, which concerns characterizations of intersecting families of k-subsets of a fixed set, leads naturally to a study of intersecting families of k-subspaces of a finite vector space. In terms of association schemes this means we move from the Johnson scheme to the Grassmann scheme. This is fairly well understood, with the basic results obtained by Frankl and Wilson [6]. But in finite geometry, polar spaces form an important topic. Roughly speaking the object here is to study the families of subspaces that are isotropic relative to some form, for example the subspaces that lie on a smooth quadric. In group theoretic terms we are now dealing with symplectic, orthogonal and unitary groups. There are related association schemes on the isotropic subspaces of maximum dimension. Vanhove spoke on important work from his Ph. D. thesis, where he investigated the appropriate versions of the EKR problem in these schemes.

### **Outcome of the Meeting**

It is too early to offer much in the way of concrete evidence of impact. Matt DeVos

observed that a conjecture of Brouwer on the vertex connectivity of graphs in an association scheme was wrong, in a quite simple way. This indicates that the question is more complex than expected, and quite possibly more interesting. That this observation was made testifies to the scope of the meeting.

On a broader level, one of the successes of the meeting was the wide variety of seemingly disparate topics that were able to come together; the ideas of algebraic graph theory touch a number of things that would at first glance seem neither algebraic nor graph theoretical. There was a lively interaction between researchers from different domains.

The proportion of post-docs and graduate students was relatively high. This had a positive impact on the level of excitement and interaction at the meeting. The combination of expert and beginning researchers created a lively atmosphere for mathematical discussion.

### **List of Participants**

Ahmadi, Bahman (University of Regina) Alinaghipour, Fatemeh (University of Regina) Ball, Simeon (Universitat Politcnica de Catalunya) Butler. Steve (UCLA) Chan, Ada (York University) Chowdhury, Ameera (University of California San Diego) Cioaba, Sebastian (University of Delaware) DeVos, Matt (Simon Fraser University) Farr, Graham (Monash University) Godsil, Chris (University of Waterloo) Gosselin, Shonda (University of Winnipeg) Gottshall, Alyssa (Worcester Polytechnic Institute) Greenfield, Kara (Worcester Polytechnic Institute) Guo, Krystal (University of Waterloo) Haemers, Willem (Tilburg University) Hobart, Sylvia (University of Wyoming) Kharaghani, Hadi (University of Lethbridge) Lee, Jae-Ho (University of Wisconsin-Madison) Mancinska, Laura (University of Waterloo/Institute for Quantum Computing) Martin, William (Worcester Polytechnic Institute) Meagher, Karen (University of Regina) Moorhouse, Eric (University of Wyoming) Morgan, Kerri (The University of Melbourne) Mullin, Natalie (University of Waterloo) Newman, Michael (University of Ottawa) **Ozols, Maris** (Institute for Quantum Computing) Purdy, Alison (University of Regina) Rahnamai Barghi, Amir (K. N. Toosi University of Technology) Roberson, David (University of Waterloo) Roetteler, Martin (NEC Laboratories America) Rooney, Brendan (University of Waterloo) Roy, Aidan (University of Waterloo) Sankey, Alyssa (University of New Brunswick) Severini, Simone (University College London) Szollosi, Ferenc (Central European University) Vanhove, Frederic (Universiteit Gent) Williford, Jason (University of Wyoming) Wilson, Richard (California Institute of Technology) Worwawannotai, Chalermpong (University of Wisconsin) Young, Michael (Iowa State University)

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## Chapter 14

# Organized tropical convection and large-scale circulation: Theory, modeling, and observations (11w5047)

### May 01 - May 06, 2011

**Organizer(s):** Boualem Khouider (University of Victoria) Andrew J. Majda (New York University) Chidong Zhang (U Miami)

### Overview

The tropical circulation workshop brought together 33 specialists in the field of tropical convection and largescale circulation from North America and Australia, with various backgrounds, including mathematicians, physicists, and meteorologists. It brought together a spectrum of scientists and mathematicians with a good balance between early career faculty/scientists and very senior researchers. There were five students and post docs.

Each morning started with a session of two to three 30-minute-long focussed talks, to give an overview on the state-of-the-art a specific topic. This was followed by a panel discussion on that specific topic to elaborate further and initiate a brain-storming of the topic of the day. The afternoon started with a session of 5 to 6 15-minute talks of more traditional research-type. It was then followed by and interactive open discussion session. The discussion often revolved around one or more the topics related during the 15-minute talks. The panels consisted of a chair (one of the organizers, who will present the topic and direct the discussion) and up to 5 expert panellists. The audience and especially the young students and postdocs were encouraged to participate by asking questions and making comments. The interactive sessions were free-format open discussion to stimulate spontaneous interventions.

### **Workshop Objectives**

Despite the recent advancement in theory, observation, and modeling to improve our ability of understanding, simulating, and predicting tropical organized convective systems, many fundamental issues need to be fully addressed:

1. Given the observed self-similarity in convective development, what mechanisms distinguish the generation of tropical perturbations of different scales and propagating speeds (e.g., the MJO vs. convectively coupled Kelvin wave)??

- 2. How does the convective multiscale interaction occur in conjunction with convective interaction with the environment (e.g., moisture)??
- 3. What is the untapped potential and limitation of cumulus parameterization in weather and climate models in representing tropical organized multiscale convective systems and their interaction with the large-scale dynamics and thermodynamics? ?
- 4. How can new theoretical insights guide innovative data analysis on tropical organized multiscale convective systems and their interaction with the large scales, especially in the context of the new generation of satellite observations (e.g., TRMM, A-Train) and field campaigns in the near future? ?
- 5. How can new observations and numerical simulations inspire more theoretical ideas??
- 6. How should innovative numerical experiments be designed to test new ideas from theories and observations?

The dynamics of organized multiscale convective systems in the tropics presents one of the most challenging problems in contemporary dynamical meteorology. Its expedited progress requires new developments in applied mathematics, fluid mechanics, scientific computing, observations, statistical physics, and cross-fertilizing between all these fields.

Tropical meteorology has experienced some fundamental advances in recent years, both theoretical and observational (due in large measure to significant improvements in satellite databases). However the sparseness of in situ data, in both space and time, limits their applicability and calls for the development of new statistical and applied math tools and expertise from cross disciplines for their analysis. Higher resolution coverage with radars, balloons and ship-borne data is still not feasible to the extent of the tropics. Thus, targeted field campaigns motivated by theoretical work are highly desirable. The improvement of operational models in the tropics passes both through theories and intuitions gained from the effective analysis of the observational records. There is an immediate need for new developments in the theoretical and modeling aspects of tropical meteorology. The workshop has focused on the following topics:

- Vertical structure and self-similarity of large scale tropical convective systems?
- Effects of the MJO on monsoon dynamics and rainfall?
- MJO initiation and tropical extra-tropical teleconnections ?
- Atmosphere-Ocean coupling and the MJO ?
- Climate predictability and data assimilation in the tropics.

### **Workshop Sessions and Discussions**

### Day 1, Morning: Tropical convection, Synergy between theory and observations

The meeting was opened by a presentation by Mitch Moncrieff of NCAR on convective organization and intersection of weather and climate. Moncrieff argued for the multiscale representation of convection in climate and weather forecast models. He demonstrated that the intersection between weather and climate spans a wide range of time scales involving processes such as the diurnal and the seasonal cycles of solar heating. The diurnal cycle forces mesoscale convective systems that in turn influence synoptic and planetary scale waves such as the Madden Julian oscillation while the seasonal cycle which triggers monsoons has a direct impact on synoptic scale convectively coupled waves and the MJO. The known two-way interactions between the synoptic and planetary scale waves and mesoscale convective systems are well represented in neither weather-forecast nor climate models. According to Moncrieff, mesoscale systems are absent in present

climate models but they are well represented in cloud resolving modeling (CRM) and, to some extent, numerical weather prediction (NWP) models. He argued for the representation of the upscale energy transport by organized convection as well as for the control of convection by the large scales. Through various examples of numerically simulated mesoscale convective systems, he showed as an example how the large-scale shear can influence the organization of convection at such scales. He argued against the old paradigm of convection being interpreted as one small scale isolated phenomenon and for a multi-type convection phenomena occurring on wide spectrum of scales that interact with each other.

Sam Stechmann of U. of Wisconsin followed by a talk on multiscale theories and models for the MJO. He introduced the concept of multiscale cloud which refers to clusters and superclusters of cloudy cells that are observed to propagate in the tropics and are responsible for the largest portion of rainfall in the tropics. Starting with the more general theory of equatorial wave dynamics, he introduced a new theoretical model for the MJO as an oscillatory and neutrally stable mode that is best represented by the interaction between the planetary scale low-level moisture and precipitation. Because of its neutral stability, it is called the MJO skeleton. The MJO mode is sustained by synoptic and meso-scale convective systems that provide the necessary upscale transport of energy, reminiscent of the multi-type convection paradigm seen in Moncrieffs talk.

Katherine Staub from Susquehanna University then reported on the outstanding notion of MJO initiation. She begin by asking some fundamental questions as why the MJO is often initiated in the Indian Ocean and how MJO events can be identified accurately in observational data. For the latter, two main tools exist, namely, the space-time filtering introduced by Wheeler and Kiladis and real-time multivariate MJO (RMM) index of Wheeler and Hendon. She gave some pros and cons for both methods. She argued that RMM is dominated by wind anomalies and ORL (which is a surrogate of precipitation) doesnt seem to contribute. As such it may lead to false alerts as she demonstrated through various examples. She concludes that since MJO is primary driven by convection this latter issue should be always taken into account when making MJO diagnostics.

#### Panel Discussion #1: The upcoming CINDY/DYNAMO field program

The panel consisting of Zhang (chair), Johnson, Jakob, Schumacker, and Stechmann were asked the following question. How can theory help set up observation goals and how can observation best help feedback to the theory?

Johnson: Should target the diurnal cycle. Hovmuller diagrams of the MJO already demonstrated the influence of diurnal cycle variability of convection. This is indeed consistent with Moncrieffs earlier talk.

Schumacher: Need radars with different wavelengths to measure various cloud types (precipitating and non-precipitating) and polarimetry (or dual polarization) to get cloud microphysics measurements.

Jakob: Convective parametrization problem should be addressed. New observations are needed to build new stochastic paramtrizations.

Stechmann: How background state affects CCWs and mesoscale CSs needs to be addressed. Theories exist but observations are very diffuse when it comes to this matter. Moisture convergence and shear are both important for the selection of cloud types.

The audience more or less agreed that congestus cloud preconditions the environment for deep convection and stratiform clouds are a follow up of deep convection. But the fundamental question about what triggers congestus clouds still remained.

It has been suggested that traditional statistical data analysis could not address this questions. Majda warned about the use of EOFs that can be very misleading. It was then agreed that DYNAMO could address key dynamical triggers that EOFs maybe missing. Jakob then added that existing reanalysis products are bad for wind convergence, especially, for vertical structure of the divergence field. It was mentioned that according to some work done by Rossow and co-workers, the MJO is basically present at all time in terms of the moisture field but the question as when it intensifies and precipitates remains This is in some sense consistent with the neutrally stable (moisture-precipitation) mode presented by Stechmann.

It was argued that moisture tendency is mostly controlled by vertical advection while congestus detrainment plays a secondary role. Can new observations be used to address this issue?

### Day 1, Afternoon

The afternoon of Day 1 started by two 15-minute talks by Courtney Schumacher (Texas A&M) and Christian Jakob (Monash, Australia). Jacob reported on the convection parameterization problem and on how new observations could help design or calibre existing stochastic multicloud parametrization. It was suggested that existing notion of cloud regimes observed at various scales could be used as guidelines. There should be a distinction between small and large scale parametrization. What variable should be measured for the design of future stochastic parameterizations? Does large vertical velocity control the mean and standard deviation of the stochastic convection or rather their ratio does? Is convection a Poisson process as it was suggested previously? Schumachers talk was on stratiform rain formation and co-existence of various cloud types. She noticed however some geographical variations in the intensity of the various types of convection. Congestus heating is very weak over land and over the Atlantic Ocean it is very shallow. Stratiform rain is higher over the ocean than over land. Using a TWP-ICE radar network, she demonstrated the existence of three regimes of convection: Strong convection, suppressed convection, and easterly convection.

This was then followed by two 15-minute talks by George Kiladis and Juliana Dias of NOAA. Kiladis lectured on principal modes of tropical variability and Juliana Dias exposed a new method for identifying convectively coupled waves. Kiladis showed through a judicious use of EOF analysis the spectrum of tropical waves, which can effectively capture the continium nature of the MRG and n=0 EIG branch near k=0, where eastward and westward moving MRG waves are divided. He showed examples of MRG waves that are meridionally tilted, which first move westward then progressively northward. Dias started by relating some problems with traditional Hovemuller diagrams of Tb, for example, in capturing spectrally filtered Kelvin waves. Instead, she suggests using contiguous cloudy regions (CCRs, which are traditionally used for mesoscale systems) in order to capture well the tails of the distribution. She used Radon transformation to separate zonally propagating CCRs whose peaks are associated with propagating waves.

### Open Discussion #1: MJO initiation versus MJO intensification

The main driving question is weather initiation of convection, on a large enough scale (in the Dynamo experiment for example), implies the initiation of an MJO event? Perhaps, it is necessary but not sufficient. Also what mechanisms allow such triggering of large scale convection in first place?

Possibilities:

- 1. Dry MJO mode: Is there an extra-tropical mode that excites and intensifies a moisture mode (as in the Majda-Stechmann skeleton MJO model).
- 2. Stochastic initiation.
- 3. Successive versus primary MJO events. It is argued that some MJO events are triggered by the remains of previous MJO events while sometimes MJO seem to start independently of others.
- 4. Formation of wave packets of mesoscale systems favoured by a sheared environment or by the succession of cold pools.
- 5. Persistence of dry pre-onset region, which in some sense related to the existence of a moisture mode, mentioned earlier in the day.

### Day 2, Morning: Models

The second day was dedicated to models and modeling issues related to the general circulation and clouds. The morning session consisted of three 30-minute talks delivered by Dargan Frierson (U. Washington), David Randall (U. Colorado), and Philip Austin (U. British Columbia).

Frierson is interested in the use of idealized climate models to study specific climatic processes. He described the northward shifting of the ITCZ (the region of intensive convection in the tropical belt) due to global warming and the compensating effect of cooling by aerosols. He suggested that the ITCZ shifting is due to the balanced structure of the forcing by solar heating and longwave cooling. Frierson noted that humans actually contribute to both effects through namely the release to the atmosphere of greenhouse gases and aerosols, respectively. He suggested that the likely shifting of the ITCZ would cause a dramatic change

in the climate system. He pointed out that the very complex-traditional climate models as opposed to his simplified model (which is carefully tuned to the problem) fail to capture accurately the ITCZ. So such change in our climate would not be predicted accurately by current operational GCMs.

David Randalls talk was on qualifying the limits of convection parameterization. He started by saying that the main issue with the conventional cumulus parameterization is the lack of scale separation between the convective scales and the large scale circulation that we aim to represent by these models. He argued that with current climate models, higher resolution doesnt necessarily mean better forecast because the sample size (of clouds) becomes smaller and the quasi-equilibrium assumption breaks down. Instead, one should consider non-equilibrium or stochastic closure assumptions. He then demonstrated through direct numerical simulations using a 256x256 km domain that the lag between the forcing and precipitation response depends on the period of the forcing and the standard deviation depends on the domain size and argued that these are good metric for stochastic parameterization of convection though he questioned whether such a stochastic behaviour can be also seen in observation. He concluded by suggesting that super-parameterization (clouds are represented by numerical model that is run in parallel within each grid-cell of the GCM) is some kind of stochastic parameterization after all, which in some sense explains its own success.

Austin described a new methodology for statistical analysis of large-eddy simulation of shallow cumulus clouds. He motivated his study by the uncertainties in entrainment and detrainment of the mass flux in GCMs. His algorithmic approach tracks cloudy parcels as they ascend and descend and uses various interpolation techniques to measure mixing of dynamics and thermodynamics quantities. He demonstrated the methodology for two case studies of shallow cumulus over land (ARM) and over the ocean (BOMEX). His findings suggested that cloud area controls future properties of the parcels and provides core protection, cloud entrainment is proportional to area and is controlled by large eddies while detrainment is driven by mixing of dry air.

### Panel discussion #2: Climate Models

The models panel consisted of 4 panellists (Austin, Frierson, Kiladis, and Randall) and a chair (Khouider). First the following issues were identified to be important:

- New generation of climate models highly advanced in terms of scientific computing;
- Tendency for unified frameworks: Seamless modeling, etc.
- Super-parameterization v.s. global CRMs and the future of coarse resolution GCMs.
- Convection parametrization problem is still open.
- How to use observations in the parameterization process?
- Phenomenological/process driven models.
- Quantitative validation of statistical features.
- Data driven parameterizations. Is it possible to gather enough data from obs? What kind of data should one use? What data are available and waht data are good enough? Could numerical simulations help? What is the equivalent of DNS in the climate community? LES? What are the key issues/processes that can be quantified by such models?
- Convection parameterization v.s. organized convection parametrization: The multicloud/self-similarity paradigm.
- Representation of mesoscale systems.
- Stratiform anvils and associated downdrafts.
- Congestus clouds: what role do they play? How are they different from deep clouds? Are they represented in current GCMs? Are they parametrizable? (Are they functions of the large scale variable/variables?) Is moisture convergence the cause or the effect? Is there a connection with the 0oC layer?

- Role of shallow cumulus? Do we understand its associated turbulence?
- Stochastic models
- Uncorrelated random noise v.s. multi-scale correlated (both in time and space) Markov chain type models.
- What calls for stochastic modelling? Grid resolution v.s. separation/non-separation of scales? Nature of the problem?
- What kind of processes is intrinsically stochastic? Turbulent entrainment v.s. triggering? Conceived as add-ons to preexisting (deterministic) parametrizations. Can we do better?
- How about stochastic super-parametrization?
- If the future is for global CRMs and superparameterization: Aren't we to some extent shifting the problem to smaller scales ... to cloud microphysics? (Another buzzword). More so for LES. Are the interactions between cloud physics and small scale eddies understood? How complex is this problem? Can stochastic models help at such small scales?

The panel noted that current GCMs do not capture well the vertical structure of C.C.Ws. Kiladis showed some slides relating of some of his earlier work where various models were compared against observation that confirmed this statement. It then argued that simple models that take into account the morphology of tropical clouds capture well the vertical structure and Khouider gave a brief explanation on the board of the Khouider-Majda multicloud model. It is also noted that there are more complex models that capture the vertical structure such as the Lagragian-Overturning Model of Haertel (presented later in the afternoon).

### Day 2, Afternoon

The Tuesday afternoon session started with five 15-minute talks by Khairtoudinov (CUNY), G. Zhang (SCRIPT), Y. Frenkel (NYU), M. Waite (Waterloo), and W. Boos (Yale).

Haertel presented a new global circulation model based on the Lagrangian tracking of fluid parcels. The fluid parcels are advected by the ambient velocity and allowed to switch vertical position whenever there is an instability. The method which is originally designed for the ocean circulation and is called a Lagrangian overturning model. Despite the crudeness of the model, which uses a limited number of parcels (of a 500 km) to represent the whole atmosphere, it captures well some surrogate of the Madden Julian Oscillation with many realistic features.

Khairtoudinov gave a lecture on his new results using the multiscale modeling framework (MMF) model. He used both 2d and 3d simulations to address the issue of the transition from shallow to deep convection. He first recalled that the super-parametrization framework already demonstrated a huge success by being the first model to simulate a realistic MJO and when the model (SPCAM) is coupled to the ocean it produced the full sprectrum of convectively coupled waves. He then looked at the sensitivity of MJO simulations to external and internal factors. He demonstrated that moisture is key and when stratiform heating is shut off the MJO becomes a Kelvin wave. A key question remains unanswered however. Why is ocean coupling so important for the full spectrum of convective coupled waves?

Zhangs talk was on convection parameterization and tropical climate. His main contribution is to address differences between ealrier so-called CAPE closure parameterizations and recent CAPE-tendency parameterization. He demonstrated that the new closure improves the Hadley and Walker circulations. Zhang noted that some other feature are also improved with the CAPE tendency closure such as the atmospheric response to ENSO and the MJO in terms of Hovmuller diagram representation. Curiously, when the shallow convection is turned off the MJO disappears in the model.

Frenkel discussed some numerical simulations using the stochastic multicoud model of Khouider et al. as a paradigm example to improve the variability of organized tropical convection. He showed that the stochasticization of convection in the model not only improves the variability of the waves but it also improves their physical and dynamical structure. Intriguingly, he showed an example of simulation results that looked impressively similar to those shown by detailed cloud resolving simulations (which is thousands if not millions of times more expansive in terms of computational complexity) obtained by Grabowski and co-worker with the same episodic bursts of convective events.

M. Waite presented CRM simulations of the transition from shallow to deep convection through moistening by congestus detrainment. He showed that prior to the transition to deep convection congestus clouds from sporadically and detrain in the middle troposphere depositing a substantial among of moisture that help precondition the environment for deep convection. It is demonstrated through various sensitivity tests that three dimensional turbulent mixing of moisture plays a major role in delaying the transition to deep convection and in moistening the environment through congestus detrainment. It is also established that while temperature mixing is also important it plays a secondary role.

Booss talk was about the investigation of the monsoon variability through an axisymmetric modeling framework. His framework is based on a model Hadley circulation using the one baroclinic mode-QTCM model. He conjectured that a second baroclinic mode is not necessary for monsoon dynamics unlike convectively coupled waves.

#### Open discussion session #2: Super-parameterization and MJO super-rotation

The discussion was led by Majda who described his recent work in Xing et al. 2009 where they showed the success of super-parameterization strategies, in two different shear regimes: A strong shear that allows organized convection and a weak shear where chaotic convection persists. They particularly demonstrated the feasibility of sparse space-time super-parameterization. The discussed that reported on how a hierarchy of models could be put in synergy and help understand better various aspects of the climate modeling problem, including global CRMs, super-parameterization GCMs, Coarse resolution GCMs, idealized GCMs, and analytical/asymptotic models.

The discussion then followed on the MJO super-rotation, which has been noticed in various idealized simulations and demonstrated in asymptotic models. It has been asked whether global warming will lead to stronger MJO and thus to supper-rotating, i.e, equatorial westerly, mean wind. At the present times the mean wind in the tropics is very weak and is mainly easterly. Various research directions to address this issue have been suggested regarding the MJO: change in frequency of the propagation signal, sensitivity to seasonal variability, and evidence of super-rotation in observations.

### Day 3: Data assimilation and predictability

There were three talks in this session: M. Wheeler (Australian Weather Bureau), W. W. Tung (Perdue), and J. Harlim (NC State). Wheeler reported on the MJO prediction for improving weather forecast skill over Australia. Using the RRM index in a T47 ocean-coupled model, he showed that compared to a statistical benchmark model, the numerical model that is conditioned to the MJO phases had a better skill overall and the skill of the ensemble mean is better than the mean skill of each individual member. She particularly demonstrated the sensitivity of the skill to the initial MJO phase. He also showed that strong MJOs resulted in better forecast-skill than weak MJO cases.

Tungs talk was on intrinsic predictability of the MJO. The main issue she was interested in is how to separate chaotic dynamics from observational noise. She started by recalling that in current state-of-the-art, the MJO predictability doesnt exceed 30 days. She then presented and adaptive denoising algorithm based on spline interpolation. She used the Lorenz 63 model with an artificial noise added as an example to illustrate her methodology. She then applied it to the case of the MJO index EOF 1. The chaotic dynamics were captured by the adaptive denoising algorithm and the MJO skill was improved to 50 days.

Harlim presented some applied math tools for tropical data assimilation. He started by giving a short tutorial on the theory of data assimilation. The main difficulty in the tropical weather prediction problem, according to Harlim, is due to the lack of scale separation and balanced dynamics for the large scales. He was interested in the general problem of model error quantification in complex dynamical systems for which is he presented an online model error estimation strategy. His strategy is based on a mock dynamical equation for parameter evolution consisting of a stochastic differential equation. He tested his model in a two-layer QG model (Smith et al.) in two distinct regimes: open jet and blocked circulations.

### Panel discussion #3: Predictability and data assimilation for the tropics

Panellists: Tung, Wheeler, Harlim, Chair: Majda. The hardcore problem thats been largely discussed is the design of radical strategies for stiff-turbulent systems. There was also discussion about the use of a benchmark model for various climate models. The Canadian climate model (CCCma) in particular has been identified as one with a large ensemble spread, which is apparently a good thing for data assimilation.

### Day 4, Morning: Theory

The Thursday morning session started with a series of short talks by J. Biello (UC Davis), J. Frederikson (CSIRO, Australia), L. Smith (U Wisconsin), and W. Shubert (Colorado State). Biello presented a multiscale asymptotic model for the meso/planetary scale interactions through gravity waves in the deep tropics. His model is based on the Majda-Klein IPESD theory and on the new findings by Dolaptchiv of a planetary scale pressure balance. He is interested in the modulation of the ITCZ convection by planetary scale gravity waves and to develop a tropical wave theory with matching condition to mid-latitudes. He started by deriving the MEWTG equations and then showed some numerical simulation using the asymptotic model of large scale gravity waves that tend to homogenize the zonal wind.

Frederiksons talk was about extra-tropical initiation of the MJO. He started with the barotropic-baroclinic vorticity equations and the thermodynamic equations in a mean shear and mean potential temperature basic state. The tropical-extratropical model exhibits wave solutions consistent of all the classical equatorially trapped wave-modes and an MJO mode but no WIG waves. Stronger basic states seem to lead to a stronger MJO mode and extra-tropical disturbances result in an MJO mode response but no Kelvin wave response. Consistently, the MJO mode has a significant barotropic component. He suggested that the MJO mode is related to the classical barotropic-baroclinic instability, which seems to move to the tropics and reduces the moist static stability.

Smith presented a 3D Bousinesq model for the hurricane embryo. To emphasize the role of hot towers in cyclogenesis, she considered a Boussinesq fluid with a small Froude number with a condensational heating. The gaol is to compare numerical simulation of the full Bousinesq system that support gravity waves with a simplified model obtained earlier by Majda et al. She also studied the sensitivity of the hot tower to the low-level shear.

Shuberts talk was on the derivation of new long wave approximations that does not distort the Rossby waves. His strategy consists of rewriting the linearized equatorial beta-plane primitive equations in Riemann invariants and then partitioning the solution into a Kelvin and a non-Kelvin parts. He then introduced a new functional that he called the Ripa-Moura potential for the non-Kelvin part which satisfies a certain master equation. A new long-wave model was then obtained by neglecting second order derivative terms in the Ripa-Moura potential. The new model filter out the inertio-gravity waves just like the classical long-wave equations but they retain an accurate Rossby spectrum.

### Panel Discussion #4: Theory

The panel on theory consisted of three panellists (Moncrieff, Frederiksen, Biello) and a chair (Majda). Frederikson commented on the possibility that extra-tropical modes such as the PNA and AO may play some major role in the extra-tropical initiation of the MJO. Smith explained the importance of parallel v.s. perpendicular shear in the transport of momentum from convective to larger scales. She also commented on the possible role of gravity waves in dynamics of hot towers, so important for the hurricane embryo. According to Moncrieff, some aquaplanet inter-comparison studies are necessary in order to understand how climate person (??) with respect to some specific physical mechanisms. He also pointed out that there are some studies done for the case of momentum transport in parallel shears.

### Day 4, Afternoon

There were three talks by R. Johnson (Colorado), S. Sessions (New Mexico), and S. Tulich (NOAA). Johnsons talk was on various aspects of observed MJO events. He pointed out over the Indian Ocean the role of atmospheric humidity is key and should be addressed by the DYNAMO program. He suggested that an SST–surface wind map should be very informative as air generally flows from cold to warm water. In YOTC MJO,

however, he noticed an eastward extension of the MJO. He also noted that the mixed layer variability may play a role in MJO dynamics. The stratiform/deep convection ratio seems to be another important variable; MISMO reported 26-27% of stratiform rain while it is a bout 40% in TOGA CORE. Sometimes stratiform rain doesnt lag deep convection (in MISMO). However, a major issue is that the MISMO result is mostly a reanalysis product and some of these discrepancies maybe an artifact of the underlying models.

This session was interested in incorporating some observational data into WTG simulations of tropical convection while Tulich reported on convectively coupled gravity waves and their interaction with the diurnal cycle. Later in the day there was an informal discussion on satellite observations. There is huge flux of data arriving from the sky and people are wondering what is the best way to extract the maximum out of it. The data mining problem has arrived.

A concluding discussion was held on Friday morning. The following points were mentioned as additional points to what were covered earlier in the workshop.

- Mechanisms for initiation of deep convection. Importance of low-level moisture as a necessary condition for deep convection under normal conditions. Low-level moistening by detrainment is not sufficient. Low-level heating maybe key but need to be addressed by observations.
- 2. Concept of gross-moist static stability: there is no observation evidence for it.
- 3. Modeling studies to address scale interaction issue. Wave and convection interaction.
- 4. Convective momentum transport.
- 5. Extra-tropical influence although somehow covered in the MJO initiation.
- 6. Surface evaporation.
- 7. Cloud radiation.

### **List of Participants**

Ajayamohan, R. S. (Environment Canada) Austin, Phillip (UBC) **Biello, Joseph** (UC Davis) Boos, William (Yale) De La Chevrotiere, Michele (University of Victoria) **Dias, Juliana** (NOAA) Frederiksen, Jorgen (CSIRO) Frenkel, Yevgeniy (New York University) Frierson, Dargan (University of Washington) Haertel, Patrick (Yale University) Harlim, John (North Carolina State) Jakob, Christian (Monash University) Johnson, Richard (Colorado State U.) Khairoutdinov, Marat (Stony Brook University) Khouider, Boualem (University of Victoria) Kiladis, George (National Atmospheric and Oceanic Administration) Majda, Andrew J. (New York University) Moncrieff, Mitchell (NCAR) Muraki, David (Simon Fraser University) Randall, David (Colorado State University) Remmel, Mark (U.C. Davis) Schubert, Wayne (Colorado State University) Schumacher, Courtney (Texas A&M) Sessions, Sharon (New Mexico Tech.) Smith, Leslie (University of Wisconsin)

Stechmann, Samuel (University of Wisconsin-Madison)
Straub, Katherine (Susquehanna University)
Tulich, Stefan (NOAA)
Tung, Wen-Wen (Perdue University)
Waite, Michael (University of Waterloo)
Wheeler, Matthew (Centre for Australian Weather and Climate Research)
Zhang, Chidong (U Miami)
Zhang, Guang (Scripps Institution of Oceanography)

## Chapter 15

# Number Theory and Physics at the Crossroads (11w5001)

### May 08 - May 13, 2011

**Organizer(s):** Victor Batyrev (Universität Tübingen) Charles Doran (University of Alberta) Sergei Gukov (California Institute of Technology) Noriko Yui (Queen's University) Don Zagier (Max-Planck Institut für Mathematik Bonn)

This is the fifth gathering of this series of workshops in the interface of number theory and string theory. The first one was held at the Fields Institute in 2001. The subsequent workshops were all held at BIRS, and this one was the fourth BIRS workshop. The workshop met from May 8th to May 13th for five days. Altogether 40 mathematicians (number theorists and geometers) and physicists (string theorists) converged at BIRS for the five-days' scientific endeavors. About half of the participants were familiar faces, while the other half were new participants. There were 24 one-hour talks, and our typical working day started at 9:30am and ended at 9:30pm. Indeed we worked very hard, and the workshop was a huge success!

This fourth workshop was partially dedicated to Don Zagier on the occasion of his completing the first life cycle and reaching the 60 years of age.

This series of workshops has been getting very prominent in the community and attracted more applications than the workshop could accommodate.

There was overwhelming urge from the participants to organize a five-day workshop in two or three years time at BIRS. We are indeed planning to submit a proposal for the next BIRS workshop in due course.

### **Overview of the Field**

One of the most significant discoveries in the last two decades in the theoretical physics is, arguably, string theory and mirror symmetry. Spectacular discoveries in string theory have inspired many new developments in mathematics. However, mathematicians and physicists have been living in the parallel universes, and evidently there have been very little interactions between the two sets of researchers, with some exceptions.

The original purpose of organizing this series of workshops was to promote and enhance communications between the two camps. This series of workshops brought together researchers to BIRS in number theory, algebraic/arithmetic/differential/symplectic/toric geometry, and physics (string theory) whose common interests were/are centered around modular forms, but not restricted to it. At the fourth workshop, we witnessed very active and intensive interactions of both camps from early mornings to late nights. These interactions proved to be very futile and fruitful, and each workshop at BIRS brought the two camps closer and closer. At the end of workshops, we all felt that all things modular have came together at BIRS from both sides: number theory and physics (in particular, string theory). At the end of the workshop, all participants felt that both camps have finally crossed boundaries and established relatively comfortable rapport.

The Proceedings of the 2003 BIRS workshop in this series entitled "Calabi–Yau Varieties and Mirror Symmetry" (eds. N. Yui et al.) has been published as "Mirror Symmetry V" in Studies in Advanced Mathematics Series from American Mathematical Society and International Press (2006). Since the 2003 workshop, many articles dealing with subjects in the interface of number theory, geometry and physics (string theory) have appeared, and time has come to have a mathematical journal devoted to articles in this area. Thus, in 2007, the new journal "Communications in Number Theory and Physics" (CNTP) was launched from International Press with editors-in-chief: R. Dijkgraaf, D. Kazdhan, M. Kontsevich and S.-T. Yau. The journal has been publishing excellent articles, providing a venue for dissemination of results in this interface well into the future. The journal has proved to be an enormous success. Many participants of this series of workshops have published articles, and many have served as referees for the journal.

For quite while now, we have witnessed that modular forms, quasi-modular forms and automorphic forms play central roles in many areas of physics, e.g., quantum field theory, conformal field theory, black holes, mirror symmetry, *F*-theory, and 4D gauge theory. Most prominently, generating functions counting the number of curves on Calabi–Yau manifolds (e.g., Gromov–Witten invariants), elliptic genera/partition functions of conformal field theory, and generating functions in 4D gauge theory are all characterized by some kinds of modular forms (classical modular forms, quasi-modular forms, mock modular forms, Jacobi forms, Siegel modular forms. etc.)

Physical duality symmetries relate special limits of the various consistent string theories (Types I, II, Heterotic string and their cousins, including F-theory) one to another. By comparing the mathematical descriptions of these theories, one reveals often quite deep and unexpected mathematical conjectures. The best known string duality to mathematicians, Type IIA/IIB duality also called *mirror symmetry*, has inspired many new developments in algebraic and arithmetic geometry, number theory, toric geometry, Riemann surface theory, and infinite dimensional Lie algebras. Other string dualities such as Heterotic/Type II duality and F-Theory/Heterotic string duality have also, more recently, led to series of mathematical conjectures (and results), many involving elliptic curves, K3 surfaces, modular forms of one variable, and Siegel modular forms.

The principal theme of this workshop was centered around modular forms in the broadest sense, though not restricted to it. Many types of modular forms enter the physics scenes, and one of the main goals of the field is to understand conceptually "why" modular forms appear often in physics landscapes.

### **Recent Developments and Open Problems**

Since the last BIRS workshop in 2008, we have seen some new developments: a number of problems have been solved. Many, though not all, articles have been published in the Communication in Number Theory and Physics Volume 3 (2009) and Volume 4 (2010). Some sample results are listed below.

(A) Topological quantum field theory.

• The article of Dimofte, Gukov, Lenells and Zagier [3] developed several new methods for computing all-loop partition functions in perturbative Chern–Simons theory with complex gauge group  $G_{\mathbf{C}}$ . A notion of "arithmetic topological quantum field theory" was introduced and a conjecture (with supporting evidence) was formulated that  $SL(2, \mathbf{C})$  Chern–Simons theory is an example of such a theory.

(B) Hodge structures and renormalization in physics.

• The article of Bloch and Kreimer [1] observed that the renormalization of Feynman amplitudes in physics is closely related to the theory of limiting mixed Hodge structures in Mathematics. Using Hodge theory, the Feynmann amplitudes are studied and classified, and the renormalization problem is reduced to the study of logarithmically divergent projective integrals. This paper has opened the floodgates and subsequently many articles on graph hypersurfaces and Feynman integrals have been published, for instance, [2].

(C) Elliptic genera, mock modular forms and Jacobi forms, and moonshine.

• The theory of mock modular forms are used to study elliptic genera of hyperKähler manifolds in terms of the representations of  $\mathcal{N} = 4$  supercomformal algebra. For instance, the article of T. Eguchi and K. Hikami [6] obtained the exact formula for the Fourier coefficients of the elliptic genus for K3 surfaces, which counts the number of non-BPS representations. For three-dimensional cases, Jacobi forms are considered instead of mock modular forms.

• Subsequently, Eguchi, Ooguri and Tachikawa [7], they pointed out that the elliptic genus of the K3 surface has a natural decomposition in terms of dimensions of irreducible representations of the Mathieu group  $M_{24}$ . The reason is still a mystery. The recent article of Miranda Cheng [3] gave further evidence for this connection studying the elliptic genus of K3 surfaces twisted by some symplectic automorphisms. This gave a new "moonshine" for  $M_{24}$ .

Understanding the monstrous moonshine in connection with string theory is and will be a major open problem.

(D) The modularity of the Galois representations arising from Calabi–Yau varieties over Q.

• The modularity of rigid Calai–Yau threefolds over  $\mathbf{Q}$  has been established in Gouvêa and Yui [8]. These are 2-dimensional Galois representations, and proof is built on the resolution of the Serre conjectures by Khare–Wintenberger [10] and Kisin [11] on the modularity of 2-dimensional residual Galois representations. The result is that the Galois representation associated to a rigid Calabi–Yau threefold over  $\mathbf{Q}$  is equivalent to a Galois representation of a modular form of weight 4.

• For the modularity of higher (> 2) dimensional Galois representations arising from Calabi–Yau varieties over  $\mathbf{Q}$ , the article of Livné–Schütt–Yui [12] has established the (motivic) modularity of 16 K3 surfaces defined over  $\mathbf{Q}$  with non-symplectic group actions acting trivially on algebraic cycles (these K3 surfaces are studied by Vorontsov, Nikulin and Kondo). The Galois representations have dimension between 2 and 20 excluding 8 and 14. The main results are that these K3 surfaces are dominated by Fermat surfaces and thus of CM type. The modularity of the Galois representations is established by automorphic induction process.

The modularity of higher dimensional Galois representations arising from Calabi–Yau varieties remains an open problem. This is regarded as a concrete realization of the Langlands Program.

(E) The modularity of families of Calabi-Yau varieties.

Contrary to the modularity questions discussed in (**D**), the objects here are families of Calabi–Yau varieties, e.g., one-parameter families of K3 surfaces, or families of Calabi–Yau threefolds parametrized by Shimura varieties.

• Consider families of K3 surfaces which are lattice polarized by lattices of large ranks. Clingher and Doran [4] classified lattice polarized K3 surfaces by the rank 17 lattice  $H \oplus E_8 \oplus E_7$ , and described the coarse moduli space and the inverse of the period map in terms of Siegel modular forms, i.e., Eisenstein series  $E_4$ ,  $E_6$  of weight 4 and 6 and Igusa cusp forms of weight 10 and 12.

• The paper of Hashimoto and Terasoma [9] studied the period map of the family  $\{\mathcal{X}_t\}$  with  $t = (t_0, t_1) \in \mathbf{P}^1$  of quartic family of K3 surfaces defined by  $\mathcal{X}_t : x_1 + \dots + x_5 = t_0(x_1^4 + \dots + x_5^4) + t_1(x_1^2 + \dots + x_5^2)^2 = 0$  in  $\mathbf{P}^4$  with homogeneous coordinates  $(x_1 : \dots : x_5)$ . This family admits a symplectic group action by the symmetric group  $S_5$ . The Picard number of a generic fiber is equal to 19. The inverse of the period map was constructed using automorphic forms of one variable. They use different method from that of Clingher and Doran. In fact, automorphic forms are constructed as the pull-backs of the fourth power of theta constants of genus 2.

(F) Non-existence of mirror Calabi-Yau threefolds.

• The mirror principle states that given a Calabi–Yau threefold X, there exists a Calabi–Yau threefold Y, the mirror of X, with  $h^{1,1}(X) = h^{2,1}(Y)$  and  $h^{2,1}(X) = h^{1,1}(Y)$ . A further refinement is that the variation of Hodge structures on the third cohomology group in the deformations of X is related, in specific way, to the Kähler cone in the second cohomology group of the deformation of Y. The expected relation between deformations of X and the Kähler cone of Y requires that there exist boundary points in the (complex structure) moduli space of X where the variation of Hodge structures on the  $H^3$  has maximal unipotent monodromy. Recently, Rohde [13] found examples of families which do not admit such boundary points. Examples of families of these Calabi–Yau threefolds are product type  $S \times E$  where S is a K3 surface and E an elliptic curve, equipped with automorphisms of order 3, and are of CM type. The moduli spaces of these families of Calabi–Yau threefolds are Shimura varieties. For these families, the mirror symmetry principle fails.

Is there any modification of mirror symmetry principle to accommodate these examples?

### **Presentation Highlights**

There are new recent developments in the field, many of which are reported at the workshop, but have not yet been published. We had a very diverse spectrum of talks and topics at this workshop more so than the previous workshops. Topics of lectures ranged from various aspects of modular forms, Calabi–Yau differential equations, wall-crossings formulas, Donaldson–Thomas invariants, topological strings and Gromov–Witten invariants, Eynard–Orantin recursion formulas, holomorphic anomaly equations, mirror symmetry, among others. Subject area of interest might be classified into not clearly disjoint sets of the following subjects:

(a) (Classical) Modular forms, quasimodular forms, vector-valued modular forms, mock modular forms, Igusa, Siegel, Hilbert, and Jacobi modular forms.

(b) Moduli spaces of Calabi-Yau varieties, Hodge theory.

- (c) Mirror symmetry and modular forms.
- (d) Topological string theory, Gromov-Witten invariants, Eynard-Orantin recursion formulas.

(e) Feynman integrals, quantum field theory and modular forms.

- (f) Conformal field theory and modular forms.
- (g) Holomorphic anomaly equations.
- (h) Calabi-Yau Differential equations.
- (i) Wall-crossing formula, Donaldson-Thomas invariants.
- (j) New kinds of moonshine.
- (k) Other topics in the interface of number theory and physics not covered above.

There were essentially no talks devoted to mock modular forms, nor to multiple zeta-values. Also the modularity of Galois representations arising from Calabi–Yau varieties defined over  $\mathbf{Q}$  was not covered in this workshop.

Here are some highlights of the talks. For detailed descriptions of these talks, the reader is referred to the section 6 "Abstracts of Talks Presented at the Workshop" below.

• V. Bouchard talked about the "remodelling conjecture" which asserts that the generating functions of Gromov–Witten invariants of a toric Calabi–Yau threefold X are completely determined in terms of topological recursion. The topological recursion considered in this talk was the Eynard–Orantin recursion, and it was applied to the complex curve  $\Sigma$  mirror to X. The full free energies  $F_g$  was computed including the constant term, and the result was that the constant terms computed through the Eynard–Orantin recursion are precisely those of Gromov–Witten theory. This established the remodelling conjecture for the full free energies including the constant term.

• F. Brown talked about modular forms in quantum field theory. He defined Feynman integrals associated to graph hypersurfaces, and then related Feynman integrals to the theory of motives. Kontsevich conjectured in 1997 that the point counting functions of graph hypersurfaces over a finite field  $\mathbf{F}_q$  ( $q = p^n$ ) are (quasi) polynomials in q. A counter-example was given to the Kontsevich conjecture that the counting functions are given modulo  $pq^2$  by modular form arising from a singular K3 surface associated to the modular form of weight 3, i.e., the eta-product  $(\eta(q)\eta(q^7))^3$ . Also, counterexamples to several conjectures in mathematics and physics (e.g., Kontsevich's conjecture that the Euler characteristic of graph hypersurfaces are mixed Hodge–Tate type) were also presented.

• **R.** Song introduced a new holomorphic system of differential equations, called the tautological system, which govern the period integrals of Calabi–Yau hypersurfaces in a partial flag variety. The construction is an imitation of the GKZ system for toric Calabi–Yau hypersurfaces, and indeed the new system coincides with the GKZ in toric Calabi–Yau case.

• D. Morrison gave interpretations from physics points of view to lattice polarized K3 surfaces of large Picard rank  $18 - \ell$  with  $\ell \in \{0, 1, 2\}$  (e.g., the rank 17 case was discussed earlier by Clingher, and also by Kerr). Dreams (Plans) were (1) to determine normal forms for equations of elliptically fibered K3 surfaces, (2) to understand family over  $\Gamma \setminus O(2, 18)/O(2) \times O(18)$  by  $\Gamma$ -modular forms, and (3) to establish dictionary between physics of monodromy and mathematics of monodromy. Two examples (*F*-theory compactification in IIB theory in 10 dimensions, and heterotic-string on  $T^k \times \mathbf{R}^{1,9-k}$  at large radius) were discussed.

• M. Mulase discussed mathematics and geometry behind the Eynard–Orantin topological recursion formula in random matrix theory. An attempt was made to answer the question "what does the E–O formula calculate?" The Eynard–Orantin type topological recursion formula was calculated for the canonical Euclidean volume of the combinatorial moduli space of pointed smooth algebraic curves. The recursion comes from the edge removal operation on the space of ribbon graphs. As an application, a new proof was given for the Kontsevich constants for the ratio of the Euclidean and the symplectic volumes of the moduli space of curves.

• **B. Szendroi** presented refined Donaldon–Thomas (DT) theory. DT theory is the enumerative theory of sheaves on Calabi–Yau threefolds. It is used, for instance, to calculate Gromov–Witten invariants. It also counts D-branes. A *q*-refinement of DT theory was suggested by works of physicists. This talk reported on a recent computation on refined DT theory using motivic invariants of Kontsevich–Soibelman, and of Behrend–Bryan–Szendroi.

• J. Walcher presented his work in progress on *New normal functions for Calabi-Yau threefolds*. The basic principle of classical mirror symmetry is the correspondence between enumerative geometry (Gromov–Witten theory, A-model) and complex algebraic geometry (variation of Hodge structure, B-model). A few years ago, it was understood that this correspondence can also be applied in the context of D-branes, linking enumerative geometry of Lagrangian submanifolds with algebraic cycles. In this context, the A-model was understood first, and the B-model slightly later. There are then a few cases in which the correspondence can be formulated as a theorem. In most cases studied now, however, the B-model is much more powerful, and the A-model is lacking, due mostly to the lack of methods of constructing suitable Lagrangian submanifolds.

Thus, the theme of the talk was the computation of analytic (Hodge theoretic) invariants of algebraic cycles, specifically normal functions for codimension 2 cycles on families of Calabi-Yau threefolds, and their interpretation via mirror symmetry as generating functions of enumerative invariants. He started with a review of the case in which a theorem has been proven (together with D. Morrison as far as B-model is concerned, and with Pandharipande and Solomon for the A-model)- the enumerative geometry of real rational curves on the quintic as mirror to a special family of conics on the mirror quintic. He then described the generalizations that have been obtained, by various collaborations. Firstly to the class of 14 one-parameter hypergeometric Calabi-Yau differential equations (in the terminology of Almqvist, Enckevort, van Straten, Zudilin), and their inhomogeneous extensions. 10 of the 14 work as for the quintic, the remaining 4 do not seem to admit the similar hypergeometric extension. He then described further hypergeometric extensions (using points of order 3 and 4 instead of 2), as well as a number of non-hypergeometric extensions (such as Pfaffian Calabi-Yaus studied by Shimizu-Suzuki). He summarized his work on multi-parameter models. He ended with a return to the mirror quintic. The main novelty of the most recent calculations are two results of arithmetic flavor: Firstly, the Ooguri-Vafa multi-cover formula in general involves a di-logarithm twisted by a Dirichlet character (tentatively styled a D-logarithm). Secondly, in a way anticipated by Kerr and collaborators, the expansion of the normal function in the large complex structure degeneration limit in general involves an algebraic number field, even if the cycle itself is defined over the integers. This has potentially profound implications for the enumerative geometry.

Talks by Ruifang Song on *Picard–Fuchs system of Calabi–Yau complete intersections in partial flag varieties*, and by Balazs Szendroi on *Motivic Donaldson–Thomas theory of some ocal Calabi–Yau threefolds* were video-taped for dissemination to wider audience.

### **Scientific Progress Made**

Many of the participants have been collaborating in joint projects, and BIRS offered an ideal environment to pursue their joint projects. Also some new collaborations were initiated at this meeting. It is expected that results of these scientific endeavors will be reported in the next meeting at BIRS.

The most noteworthy progress of the workshop might be that mathematicians and physicists finally felt at ease with each other trying to understand problems in the interface of number theory (modular forms), geometry (Hodge theory), and physics (string theory), combining expertise from both camps.

### **Outcome of the Meeting**

The meeting was a huge success. It has encouraged further communications among mathematicians and physicists who share common interests on subjects in the interface of mathematics and string theory. Many participants mentioned that they liked the informal and friendly atmosphere of the workshop, which contributed to the success of the workshop. Indeed mathematicians (resp. physicists) benefited tremendously from face to face discussions with physicists (resp. mathematicians). Audience were encouraged to ask questions to speakers during their talks, and indeed there were lots of questions! With many interesting talks, workshop was very intense and exhaustive. Everybody has learned something new from attending the workshop. There are number of joint continuing projects and/or some new projects were originated at this workshop. Participants are encouraged to submit their articles for publication in "Communications in Number Theory and Physics (CNTP)".

There was a strong desire among participants to have the next workshop in this series at BIRS in two (or three) years time.

### Abstracts of Talks Presented at the Meeting

### Speaker: M. Ballard (UPenn, Math.)

## Title: Matrix factorization categories for complete intersections with applications to Orlov spectra of triangulated categories

Abstract: We provide a description of the category of singularities of a (graded) complete intersection in terms of a category that is a natural extension of category of matrix factorizations. This description utilizes work of L. Positselski on derived categories of curved differential graded algebras. In the style of T. Dyckerhoff, we give an analogous description of the dg-category of functors between the category of singularities of two (graded) complete intersection singularities. This allows us to compute the Hochschild cohomology of such categories. We also use these descriptions to prove that the Rouquier dimensions of the derived categories of a coherent sheaves on the self-product of the Fermat elliptic curve and on a closely associated K3 surface are two. This verifies a conjecture of Orlov in these cases. This is joint work with D. Favero and L. Katzarkov.

#### Speaker: F. Brown (Jussieu, Math.)

### Title: Modular forms in quantum field theory

Abstract: In perturbative Quantum Field theory, physical predictions are obtained by computing the Feynman integrals associated to the graphs in the theory. These integrals are periods of the complement of a certain hypersurface associated to each graph, and, at least in low orders, are expressible in terms of the Riemann zeta function.

In the first part of the talk I will give an overview of recent work relating Feynman amplitudes to the theory of motives, and in the second part I will report on joint work with Oliver Schnetz in which we find a range of examples of graph hypersurfaces which are modular. This unexpected discovery disproves a certain number of conjectures about the arithmetic nature of graph hypersurfaces.

### Speaker: M. Bogner (Mainz, Math.)

### Title : Symplectically rigid monodromy tuples induced by fourth order differential Calabi–Yau operators

Abstract: We classify all  $Sp_4(\mathbf{C})$ -rigid, quasi-unipotent monodromy tuples having a maximally unipotent element and show that all of them can be constructed via tensor- and Hadamard-products of rank one tuples. Furthermore, we translate those constructions to the level of differential operators and investigate whether such a monodromy tuple is induced by a fourth order differential Calabi–Yau operator. We also obtain closed formulae for special solutions of those operators. This is joint work with Stefan Reiter.

### Speaker: V. Bouchard (Alberta, Math.)

### Title: The geometry of mirror curves

Abstract: According to the "remodeling conjecture", the generating functions of Gromov–Witten invariants of toric Calabi–Yau threefolds are fully determined in terms of a topological recursion. At the root of the recursion is the geometry of the corresponding mirror curves. In this talk I will describe the geometry of mirror curves and the remodeling conjecture, focusing on the fate of "constant terms". In particular, I will explain how the "pair of pants" decomposition of mirror curves plays a role in the topological recursion, in

mirror analogy to the topological vertex formalism on the Gromov–Witten side. This is joint work with Piotr Sulkowski.

### Speaker: A. Clingher (Missouri–St. Louis, Math.)

### Title: On a Family of K3 Surfaces of Picard Rank 16

Abstract: I will report on a classification for the K3 surfaces polarized by the lattice H + E7 + E7. In terms of periods, the moduli space of these objects is a quotient of a four-dimensional bounded symmetric domain of type IV. Explicit normal forms will be presented, as well as a discussion of modular forms associated to this family.

### Speaker: S. Galkin (IMPU, Math.)

### Title: Fano and Mathieu

Abstract: There is a correspondence between G-Fano threefolds and conjugacy classes in Mathieu group  $M_{24}$ . Construction of cusp-forms from conjugacy classes in Mathieu group is well-known. It is less known that A-model on G-Fano threefolds also naturally produce modular forms. Why these two lists of modular forms are so similar is yet another moonshine.

#### Speaker: T. Gannon (Alberta, Math.)

### Title : Vector-valued automorphic forms and the Riemann-Hilbert problem

Abstract: In this talk I'll sketch the basic theory of vector-valued automorphic forms for arbitrary finiteindex subgroups of any genus-zero Fuchsian group of the first kind, and arbitrary representation and arbitrary weight. I'll describe the analogues here of Grothendieck's Theorem, Riemann–Roch, Serre duality, etc and show they can be sharpened into effective tools (e.g. for finding dimensions and basis vectors). A crucial role is played by Fuchsian differential equations. I'll focus on the most familiar case of  $SL(2, \mathbb{Z})$ , where there are plenty of direct applications to physics, geometry and algebra. This is joint work with Peter Bantay.

### Speaker: P. Gunnells (UMass, Math.)

#### Title: Metaplectic Whittaker functions and lattice models

Abstract: Whittaker functions are special functions on algebraic groups that play an important role in number theory and representation theory. Just as the usual exponential function is the basic ingredient for Fourier expansions, Whittaker functions provide the special functions needed to do nonabelian harmonic analysis in the theory of automorphic forms.

In this talk we will discuss the structure of spherical Whittaker functions on finite covers of GL(n) over padic fields (i.e. metaplectic groups). We will show how such functions are related to certain two-dimensional lattice models from statistical physics. In particular, we will show that metaplectic Whittaker functions can be described using partition functions attached to six-vertex lattice models. We will define and give examples of all the relevant objects.

This is joint work with Ben Brubaker, Dan Bump, Gautam Chinta, and Sol Friedberg.

### Speaker: S. Hosono (Tokyo, Math.)

### Title: Mirror symmetry and projective geometry of Reye congruences

Abstract: A line congruence is a congruence of lines given by a variety in Grassmannian G(2, n + 1). Reye congruence is a line congruence defined by a linear system of quadrics on  $\mathbf{P}^n$ , and for n = 3 it's relation to Enriques surfaces is a well-studied subject in projective geometry.

In this talk, we will consider the Reye congruence for n = 4, where we naturally come to a Calabi–Yau three fold X, (called generalized Reye congruence in [Oliva,1994]). We make a sutable mirror family to X by Batyrev–Borisov construction supplemented by a  $\mathbb{Z}_2$  quotient. We will then observe that there appear two different large complex structure limits in the complex structure moduli space. We identify one of them with the mirror to the Reye congruence X and for the other we find a new Calabi–Yau threefold Y, which we construct as the double cover of a determinantal quintic in  $\mathbb{P}^4$  branched over a curve of genus 26 and degree 20. By using mirror symmetry, we will calculate the BPS numbers for both X and Y. It is observed that some of them have nice explanations as the numbers of curves on X and Y. It is conjectured that X and Y are derived equivalent although they are not birational. We announce a proof of this fact briefly, referring to a paper which will appear soon.

References:

[1] S. Hosono and H. Takagi, "Mirror symmetry and projective geometry of Reye congruences I", arXiv:1101.2746v1[mathAG].

[2] S.Hosono and H. Takagi, "Mirror symmetry and projective geometry of Reye congruences II – Derived equivalence".

### Speaker: M. Kerr (Washington University St. Louis, Math.)

### Title: On isotrivial families of K3 surfaces

Abstract: We describe an explicit construction of K3-fibered Calabi–Yau threefolds, together with their period mappings into appropriate Mumford-Tate domains. This is joint work with A. Clingher and C. Doran, and based on their modular families of M-polarized K3 surfaces. Part of the talk will review their construction as well as the analogous story for elliptically-fibered K3's.

### Speaker: A. Klemm (Bonn, Physics)

### Title : Omega backgrounds and generalized holomorphic anomaly equation

Abstract: We derive an anomaly equation which incorporates the general Omega background in the B-model. We discuss applications to topological string theory on Calabi–Yau backgrounds and N = 2 gauge theory with (massive) flavors. Using geometric engineering on the Enriques Calabi–Yau we derive Seiberg–Witten curves for the conformal cases, which are compatible with Nekrasovs partition function.

### Speaker: J. Manschot (CEA, Physics)

### Title: The Betti numbers of moduli spaces of sheaves on the projective plane

Abstract: Electric-magnetic duality of gauge theory implies modular properties for generating functions of invariants of moduli spaces of sheaves. I'll explain the computation of the generating functions of Betti numbers of moduli spaces of sheaves with rank 1, 2 and 3 on the projective plane in terms of indefinite theta functions. The main ingredients are wall-crossing and the blow-up formula.

### Speaker: D. Morrison (UC Santa Barbara, Math. & Physics)

### Title: K3 surfaces, modular forms, and non-geometric heterotic compactifications

Abstract: Type IIB string theory has an  $SL(2, \mathbb{Z})$  symmetry and a complex scalar field  $\tau$  valued in the upper half plane, on which  $SL(2, \mathbb{Z})$  acts by fractional linear transformations; this naturally suggests building models in which  $\tau$  is allowed to vary. Although the  $SL(2, \mathbb{Z})$ -invariant function  $j(\tau)$  can reveal some of the structures of these models, for their full construction and study we need  $SL(2, \mathbb{Z})$  modular forms, particularly the Eisenstein series  $E_4(\tau)$  and  $E_6(\tau)$  and the corresponding Weierstrass equations. The Weierstrass equations can also be analyzed in algebraic geometry via the theory of elliptic curves. This approach leads to the "F-theory" compactifications of type IIB theory.

Similarly, the heterotic string compactified on  $T^2$  has a large discrete symmetry group  $SO(2, 18; \mathbb{Z})$ , which acts on the scalars in the theory in a natural way; there have been a number of attempts to construct models in which these scalars are allowed to vary by using  $SO(2, 18; \mathbb{Z})$ -invariant functions. In our new work, we give (in principle) a more complete construction of these models, using  $SO(2, 18; \mathbb{Z})$ -modular forms analogous to the Eisenstein series. In practice, we restrict to special cases in which either there are no Wilson lines – and  $SO(2, 2; \mathbb{Z})$  symmetry – or there is a single Wilson line – and  $SO(2, 3; \mathbb{Z})$  symmetry. In those cases, the modular forms can be analyzed in detail and there turns out to be a precise theory of K3 surfaces with prescribed singularities which corresponds to the structure of the modular forms. Using these two approaches – modular forms on the one hand, and the algebraic geometry of the K3 surfaces on the other hand – we can construct non-geometric compactifications of the heterotic theory.

This is a report on two joint projects: one with McOrist and Sethi and the other with Malmendier.

#### Speaker: H. Movasati (IMPA, Math.)

### Title: Mirror quintic Calabi-Yau modular forms

Abstract: In this talk we first reintroduce the classical (quasi) modular forms using algebraic de Rham cohomology of elliptic curves and the corresponding Gauss–Manin connections. We then apply the same ideas to the one parameter family of mirror quintic Calabi–Yau threefolds and we get a new (quasi) modular form theory generated by seven series algebraically independent over the field of complex numbers. The modular group is the monodromy group of such a family and it is generated by two explicit matrices in the four dimensional symplectic group with integer coefficients. The automorphy factor in this case has image inside an algebraic group of dimension six which is generated by two multiplicative and four additive subgroups. We present the functional equation of such (quasi) modular forms, however, we emphasis that the characterization of such functions in the algebraic geometric context and through polynomial ordinary differential equations is much more convenient for calculations. At the end we present some conjectures following some similar statements in the case of elliptic curves and classical modular forms. The talk is based on the following articles which can be found in my homepage:

- (1) Quasi-modular forms attached to elliptic curves, I, Lecture notes at Besse, France 2010
- (2) Eisenstein type series for Calabi-Yau varieties, Nuclear Physics B, 847, 2011, 460-484.
- (3) Quasi-modular forms attached to Hodge structures, Preprint.

### Speaker: M. Mulase (UC Davis, Math.)

Title: A topological recursion in B-model as the Laplace transform of a combinatorial equation

Abstract: The topological recursion formula discovered by Eynard and Orantin in random matrix theory has been applied to Gromov–Witten theory by string theorists (Bouchard, Klemm, Marino, and Pasquetti), and has produced an effective conjectural formula that calculates both open and closed Gromov–Witten invariants of toric Calabi–Yau threefolds. Recently some special cases of this conjecture have been solved by mathematicians. In this talk, the key idea of these mathematical work, the Laplace transform playing the role of the mirror symmetry transformation, will be explained. This talk is based on my joint papers with Chapman, Eynard, Penkava, Safnuk, and Zhang.

### Speaker: **B. Pioline** (LPTHE, Jussieu, Physics)

### Title: Automorphy in hypermultiplet moduli spaces

Abstract: The hypermultiplet moduli space in type II string theories compactified on a Calabi–Yau threefold provides a unifying framework for Gromov–Witten invariants (worldsheet instantons), Donaldson– Thomas invariants (D-instantons) with a new type of invariants (NS5-instantons). String dualities require that this moduli space should be invariant under  $SL(2, \mathbb{Z})$ , or larger arithmetic groups obtained by combining  $SL(2, \mathbb{Z})$  with monodromies and large gauge transformations. I will review recent progress in understanding quantum corrections to the perturbative moduli space metric consistently with these automorphic symmetries.

### Speaker: J. C. Rohde (Hamburg, Math.)

### Title: Maximal automorphisms of Calabi-Yau manifolds versus maximally unipotent monodromy

Abstract: Let X denote a Calabi–Yau 3-manifold. Moreover let p denote the period map of the  $F^2$  bundle in the variation of Hodge structures of weight 3 of the local universal deformation of X. There are examples of Calabi–Yau 3-manifolds X satisfying that p is constant. In the case of these examples X cannot be a fiber of a maximal family of Calabi–Yau 3-manifolds with maximally unipotent monodromy. This contradicts the assumptions of a classical formulation of the mirror symmetry conjecture. Almost all known examples of this kind arise from the observation that the  $F^2$  bundle is an eigenspace of the non-trivial action of an automorphism of order 3 or 4 of the local universal deformation over its base space. Moreover the associated period domain is a complex ball containing a dense set of complex multiplication points in all known examples of this kind.

### Speaker: A. Sebbar (Ottawa, Math.)

### Title: On the critical points of modular forms

Abstract: In this talk, we study the critical points of modular forms. In particular, we prove that for each modular form f for a discrete group G, its derivative f' has infinitely many non-equivalent zeros, and all, but a finite number, are simple. Applications will also be provided.

#### Speaker: **R. Song** (Harvard, Math.)

### Title: The Picard-Fuchs systems of Calabi-Yau complete intersections in partial flag varieties

Abstract: We introduce a system of differential equations associated to a smooth algebraic variety X with the action of a complex Lie group G and an ample G-linearized line bundle L on X. Assuming G acts on X with finitely many orbits, we show that this system is holonomic (in particular, its solutions form a locally constant sheaf of finite rank over a Zariski open dense subset). This construction recovers the GKZ systems when X is a toric variety. When  $G = SL_n$ , X = G/P where P is a parabolic subgroup of G and  $L = K_X^{-1}$ , we get a holonomic system of differential equations to which period integrals on Calabi–Yau hypersurfaces in X are solutions. This can also be generalized to the case of Calabi–Yau complete intersections in X. This is based on a joint work with Bong H. Lian and S.-T. Yau.

#### Speaker: J. Stienstra (Utrecht, Math.)

#### Title: Dimer models and hypergeometric systems

Abstract: This talk will be an updated review of the relation between dimer models and hypergeometric systems. First the definition of a dimer model will be given and illustrated with nice pictures. Then it will be

shown how these pictures contain the equations for toric compactifications. Finally there will be comments on what this might tell about hypergeometric systems.

### Speaker: B. Szendroi (Oxford, Math.)

### Title: Motivic DT theory of some local Calabi-Yau threefolds

Abstract: Donaldson-Thomas theory is the enumerative theory of sheaves on Calabi–Yau threefolds, or more generally objects in CY3 categories. Work of Nekrasov and Hollowood–Iqbal–Kozcaz–Vafa suggested a *q*-refinement of this theory. This was realized mathematically using motivic invariants by Kontsevich–Soibelman and Behrend–Bryan–Szendroi, with closely related work done also by Dimofte–Gukov.

We aim to explain this theory, and a recent computation of the motivic invariants on the resolved conifold geometry, in all chambers of the space of stability conditions. This is joint work with Andrew Morrison, Sergey Mozgovoy and Kentaro Nagao.

### Speaker: R. Rodriguez-Villegas (Texas-Austin, Math.)

### Title: The A-polynomial at q = 1, the dilogarithm and the asymptotics of q-series

Abstract: I will discuss an approach to the value at q = 1 of the A-polynomial of a general quiver. (This polynomial counts the number of absolutely irreducible representations of the quiver over  $F_q$ .) The truncations of a formula of Hua for these polynomials yield q-series of the form

$$\sum_m q^{Q(m)} x^m / (q)_m$$

where Q is a quadratic form and m runs over a lattice. The asymptotics of this series as q approaches 1 is then related to a truncated form (conjecturally polynomial) of the A-polynomial at q = 1.

Speaker: J. Walcher (McGill, Math. & Physics)

Title: New Normal Functions for Calabi-Yau Threefolds

Abstract: The expansion of normal functions associated with families of algebraic cycles on Calabi–Yau threefolds around the large complex structure point has been given enumerative interpretation via mirror symmetry. This is an update on the most recent calculations, which exhibit several new interesting features.

### Speaker: U. Whitcher (Harvey Mudd, Math.)

### Title: K3 Surfaces with $S_4$ Symmetry

Abstract: Hypersurfaces in toric varieties offer a rich source of examples of K3 surfaces and Calabi–Yau varieties. We use a toric residue map to study variation of complex structure for families of K3 hypersurfaces with a high degree of symmetry. This talk describes joint work with Dagan Karp, Jacob Lewis, and two Harvey Mudd College undergraduates, Daniel Moore and Dmitri Skjorshammer.

### List of Participants

Ballard, Matthew (University of Wisconsin) Batyrev, Victor (Universität Tübingen) Bogner, Micheal (University of Mainz) Bouchard, Vincent (University of Alberta) Brown, Francis (CNRS, Institut Mathematiques de Jussieu) Carnahan, Scott (IPMU, University of Tokyo) Clingher, Adrian (University of Missouri-St.Louis) **Dimofte, Tudor** (Institute for Advanced Study) Doran, Charles (University of Alberta) Friedrich, Roland (Humboldt-Universität zu Berlin) Galkin, Sergey (University of Tokyo) Gannon, Terry (University of Alberta) Gukov, Sergei (California Institute of Technology) Gunnells, Paul (University of Massachusetts Amherst) Harder, Andrew (University of Alberta) Hosono, Shinobu (University of Tokyo, Graduate School of Mathematical Sciences) Keller, Christoph (California Institute of Technology)

Kerr, Matt (Washington University in St. Louis) Klemm, Albrecht (University of Bonn) Lewis, Jacob (University of Vienna) Maier, Robert (University of Arizona) Manschot, Jan (CEA/Saclay) Morrison, David (University of California Santa Barbara) Movasati, Hossein (IMPA - Instituto de Matematica Pura e Aplicada) Mulase, Motohico (University of California, Davis) Neitzke, Andy (University of Texas at Austin) Novoseltsev, Andrey (University of Alberta) Pioline, Boris (CNRS and Universite Pierre et Marie Curie - Paris 6) Rodriguez Villegas, Fernando (University of Texas at Austin) Rohde, Jan Christian (University Hamburg) Sebbar, Abdellah (University of Ottawa) Shapiro, Ilya (University of Waterloo) **Song, Ruifang** (Harvard University) **Stienstra, Jan** (Utrecht University) Szendroi, Balazs (Oxford University) van Straten, Duco (Johannes Gutenberg-Universitie) Walcher, Johannes (McGill University) Whitcher, Ursula (University of Wisconsin) Yui, Noriko (Queen's University) Zagier, Don (Max-Planck Institut für Mathematik Bonn)

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# Chapter 16

# Harmonic Analysis in Convex Geometry (11w5034)

# May 15 - May 20, 2011

**Organizer(s):** Alexander Koldobsky (University of Missouri) Dmitry Ryabogin (Kent State University) Vladyslav Yaskin (University of Alberta) Artem Zvavitch (Kent State University)

## A short overview of the field

Convex geometry is an old subject that can be traced at least to Archimedes. The problems are usually very easy to formulate, nevertheless, the methods and approaches to these "easy" problems are very diverse, different from one problem to another, and sometimes to solve the problem one has to use the ideas from Topology, Analysis, Differential Geometry and even Ergodic Theory. The diversity and the mixture of methods are not the only reasons why people are still interested in Convexity. Other reasons are that completely new methods keep coming into play, and as a result new applications are discovered.

Harmonic Analysis methods are among them. Despite the fact that the Fourier coefficients and Parseval identity were first used by Hurwitz more than a century ago in the solution of the isoperimetric problem, the methods of Harmonic Analysis received a new breath only at the end of the last century, when they were applied to problems related to sections and projections of Convex bodies. In particular, the method of the Fourier transform of distributions were applied to the solution of celebrated Busemann-Petty problem, Shephard problem, the problem of the local characterization of zonoids, and to many other problems.

The use of harmonic analysis in the study of problems in convex geometry has been recently becoming more and more standard. Behind each class of bodies in question (such as zonoids, intersection bodies, centroid bodies, etc.) there are certain objects from Harmonic Analysis. The study of the underlying properties of these objects leads to an understanding of the properties of the associated bodies in question.

## **Presentation Highlights**

The topics of the workshop included harmonic analysis on the sphere and special classes of bodies, theory of valuations, discrete geometry and tomography, probability and random matrices, quantum information theory, and Mahler conjecture.

We start the description with a harmonic analysis type result proved by Paul Goodey in his joint work with Wolfgang Weil. They studied certain properties of the operators on the sphere and their applications to geometric problems. To formulate the results we introduce some definitions. A linear operator  $T: C^{\infty}(S^{n-1}) \to C^{\infty}(S^{n-1})$  is said to be standard if it is linear, continuous, bijective and intertwining.

T has the local positivity property, if T satisfies:

(LP) If  $f \in C^{\infty}(S^{n-1})$  is a function such that, for each  $x \in S^{n-1}$ , there is  $\epsilon = \epsilon(x) > 0$  and a function  $g = g_{x,\epsilon} \in C^{\infty}(S^{n-1}), g \ge 0$ , with Tf = Tg on the (open)  $\epsilon$ -neighborhood  $U_{\epsilon}(x)$  of x, then it follows that  $f \ge 0$ .

T has the equatorial positivity property, if the following holds:

(EP) If  $f \in C^{\infty}(S^{n-1})$  is a function such that, for each  $x \in S^{n-1}$ , there is  $\epsilon = \epsilon(x) > 0$  and a function  $g = g_{x,\epsilon} \in C^{\infty}(S^{n-1}), g \ge 0$ , with Tf = Tg on the (open)  $\epsilon$ -neighborhood  $U_{\epsilon}(x^{\perp})$  of  $x^{\perp}$ , then it follows that  $f \ge 0$ .

Furthermore, T has the local support property, if:

(LS) For every  $f \in C^{\infty}(S^{n-1})$ , we have supp  $f \subset \text{supp } Tf$  or supp  $f \subset \text{supp } Tf^*$ , where  $f^*$  is the reflection of f in the origin.

T has the equatorial support property, if:

(ES) For  $f \in C^{\infty}(S^{n-1})$  with supp  $Tf \subset U_{\epsilon}(x)$ ,  $\epsilon > 0$ ,  $x \in S^{n-1}$ , we have supp  $f \subset U_{\epsilon}(x^{\perp})$ . Goodey and Weill prove the following results.

**Theorem 16.0.1** A standard operator T on  $C^{\infty}(S^{n-1})$  has the local positivity property, if and only if it has the local support property.

**Theorem 16.0.2** A standard operator T on  $C^{\infty}(S^{n-1})$  has the equatorial positivity property, if and only if *it has the equatorial support property.* 

The importance of these theorems is in the description of the phenomenon lying behind the local / equatorial characterization of zonoids and intersection bodies. As an application, the authors also obtain local and equatorial characterizations of  $L_p$ -intersection bodies, mean section bodies, and their associated spherical transforms.

Gabriel Maresch presented his joint work with Franz Schuster on The Sine Transform of Isotropic Measures.

Recall that a non-negative finite Borel measure  $\mu$  on the unit sphere  $S^{n-1}$  is said to be isotropic if for all  $x \in \mathbb{R}^n$ ,

$$||x||_2 = \int_{S^{n-1}} \langle x, u \rangle^2 d\mu(u)$$

The sine transform  $S\mu$  of a finite Borel measure  $\mu$  on  $S^{n-1}$  is the continuous function defined by

$$(\mathcal{S}\mu)(x) = \int_{S^{n-1}} \|x\| u^{\perp} \|d\mu(u), \quad x \in \mathbb{R}^n$$

The latter defines a norm on  $\mathbb{R}^n$  whose unit ball is denoted by  $S^*_{\mu}$  and its polar by  $S_{\mu}$ . Let  $\kappa_n$  denote the volume of the Euclidean unit ball in  $\mathbb{R}^n$  and define

$$\alpha_n := \frac{n(n-1)^{2n}}{\Gamma(n)^{1/(n-1)}}, \text{ and } \gamma_n := \frac{(n-1)\kappa_{n-1}^2}{\kappa_{n-2}\kappa_n}.$$

Their main result is

**Theorem 16.0.3** If  $\mu$  is an even isotropic measure on  $S^{n-1}$ , then

1)

$$\frac{\kappa_n}{\gamma_n^n} \le V(S_\mu^*) \le \frac{\kappa_n \gamma_n^n}{\alpha_n},$$

with equality on the left if and only if  $\mu$  is normalized Lebesgue measure. 2)

$$\frac{\kappa_n \alpha_n}{\gamma_n^n} \le V(S_\mu) \le \kappa_n \gamma_n^n,$$

with equality on the right if and only if  $\mu$  is normalized Lebesgue measure.

Rolf Schneider gave a talk on zonoids with isotropic generating measures, based on a joint work with Daniel Hug.

A convex body  $Z \subset \mathbb{R}^n$  is a zonoid if its support function has a representation

$$h(Z,u) = \int_{S^{n-1}} |\langle u,v\rangle| \mu(dv), \qquad u \in \mathbb{R}^n,$$

with an even, finite Borel measure  $\mu$  on the unit sphere  $S^{n-1}$ .

They proved

**Theorem 16.0.4** If  $j \in \{1, ..., n\}$  and if  $Z_1, ..., Z_j \subset \mathbb{R}^n$  are zonoids with isotropic generating measures, then

$$V(Z_1, ..., Z_j; B_2^n[n-j]) \ge 2^j \kappa_{n-j}.$$

For j = 1, the latter inequality holds with equality. For  $j \ge 2$ , equality holds if and only if  $Z_1 = \cdots = Z_j$  is a cube of side length 2.

As a corollary, they obtained

**Theorem 16.0.5** Let  $Z \subset \mathbb{R}^n$  be a zonoid with isotropic generating measure  $\mu$ . If  $j \in \{1, ..., n\}$ , then

$$V_j(Z) \ge 2^j \binom{n}{j}.$$

For j = 1, the latter inequality holds with equality. For  $j \ge 2$ , equality holds if and only if Z is a cube of side length 2.

A few talks at the workshop were devoted to the theory of valuations.

Let  $\mathcal{K}^n$  be the set of convex bodies in an *n*-dimensional Euclidean vector space V and let A be an abelian semigroup. A function  $\phi : \mathcal{K}^n \to A$  is called a valuation if

$$\phi(K) + \phi(L) = \phi(K \cup L) + \phi(K \cap L)$$

whenever  $K, L, K \cup L \in \mathcal{K}^n$ .

Valuations on convex bodies have been actively studied. A famous classical result in this area is Hadwigers classification of rigid motion invariant real valued continuous valuations as linear combinations of the intrinsic volumes. Among many applications, this result gives an effortless proof of the famous Principal Kinematic Formula from integral geometry.

In his talk, Franz Schuster presented a joint work with Semyon Alesker and Andreas Bernig where they obtained the decomposition of the space of continuous and translation invariant valuations into a sum of SO(n) irreducible subspaces. To describe their result, we will recall some definitions and notation.

A valuation  $\phi$  is called translation invariant if  $\phi(K+x) = \phi(K)$  for all  $x \in V$  and  $K \in \mathcal{K}^n$  and  $\phi$  is said to have degree i if  $\phi(tK) = t^i \phi(K)$  for all  $K \in \mathcal{K}^n$  and t > 0. We call  $\phi$  even if  $\phi(-K) = \phi(K)$  and odd if  $\phi(-K) = -\phi(K)$  for all  $K \in \mathcal{K}^n$ . We denote by Val the vector space of all continuous translation invariant complex valued valuations and we write  $\operatorname{Val}_i^{\pm}$  for its subspace of all valuations of degree i and even/odd parity. An important result by McMullen is that

$$\operatorname{Val} = \bigoplus_{0 \le i \le n} \operatorname{Val}_i^+ \oplus \operatorname{Val}_i^-.$$

We need the following basic fact from the representation theory of the group SO(n): The isomorphism classes of irreducible representations of SO(n) are parametrized by their highest weights, namely sequences of integers  $(\lambda_1, \lambda_2, ...,$ 

 $\lambda_{\lfloor n/2 \rfloor}$ ) such that

$$\begin{cases} \lambda_1 \ge \lambda_2 \ge \dots \ge \lambda_{\lfloor n/2 \rfloor} \ge 0, & n \text{ odd,} \\ \lambda_1 \ge \lambda_2 \ge \dots \ge \lambda_{n/2-1} \ge |\lambda_{n/2}|, & n \text{ even.} \end{cases}$$

The natural action of the group SO(n) on the space Val is given by

$$(\theta\phi)(K) = \phi(\theta^{-1}K), \qquad \theta \in SO(n), \ \phi \in Val.$$

The authors prove the following decomposition of the space Val into irreducible SO(n)-modules.

**Theorem 16.0.6** Let  $0 \le i \le n$ . The space  $\operatorname{Val}_i$  is the direct sum of the irreducible representations of  $\operatorname{SO}(n)$  with highest weights  $(\lambda_1, \lambda_2, ..., \lambda_{\lfloor n/2 \rfloor})$  precisely satisfying the following additional conditions: (i)  $\lambda_j = 0$  for  $j > \min\{i, n - i\}$ ;

(ii)  $|\lambda_j| \neq 1$  for  $1 \leq j \leq \lfloor n/2 \rfloor$ ; (iii)  $|\lambda_2| \leq 2$ . In particular, under the action of SO(n) the space Val<sub>i</sub> is multiplicity free.

They give also give applications of this theorem to geometric inequalities.

Judit Abardia presented her joint work with Andreas Bernig on projection bodies in complex vector spaces.

Let V be a real vector space of dimension n, and Let K be a convex body in V. The projection body of K is denoted by  $\Pi K$  and is defined by its support function:

$$h_{\Pi K}(u) = \operatorname{vol}_{n-1}(K|u^{\perp}) = \frac{n}{2}V(K, ..., K, [-u, u]), \qquad u \in S^{n-1}$$

**Theorem 16.0.7** Let W be a complex vector space of complex dimension  $m, m \ge 3$ . If the operator  $Z : \mathcal{K}(W) \to \mathcal{K}(W)$  is

1) translation invariant, 2)  $SL(W, \mathbb{C})$ -contravariant, 3) continuous Minkowski valuation, then  $Z = \Pi_C$ , where  $C \in \mathbb{C}$  is a convex body and

$$h(\Pi_C K, u) = V(K, ..., K, Cu), \qquad u \in S^{2m-1},$$

 $Cu = \{ cu : c \in C \subset \mathbb{C} \}.$ 

is

The converse also holds for every  $C \in \mathcal{K}(\mathbb{C})$ .

This is a complex version of the result, proved earlier by Monika Ludwig: If an operator  $Z : \mathcal{K}^n \to \mathcal{K}^n$ 

translation invariant,
 SL(V, R)-contravariant,
 continuous Minkowski valuation,
 then Z = cΠ, c ∈ ℝ<sup>+</sup>.

The dual notion of the projection body is the intersection body. It was introduced by E. Lutwak in 1988 and played a crucial role in the solution to the Busemann-Petty problem. Let K be a star body in  $\mathbb{R}^n$ . Its intersection body IK is the star body whose radial function is given by

$$\rho_{IK}(\xi) = \operatorname{vol}_{n-1}(K \cap \xi^{\perp}), \qquad \xi \in S^{n-1}.$$

If K is origin-symmetric and convex, then Busemann's theorem asserts that IK is also convex. However, this is not true without the symmetry assumption on K.

Mathieu Meyer jointly with Shlomo Reisner introduced the notion of the convex intersection body CI(L) of L. It is defined by its radial function

$$\rho_{CI(L)}(u) = \min_{z \in P_u(L^{*g(L)})} \operatorname{vol}_{n-1} \left( \left[ P_u(L^{*g(L)}) \right]^{*z} \right).$$

In this formula, g(L) is the centroid of L,  $P_u$  denotes the orthogonal projection from  $\mathbb{R}^n$  onto  $u^{\perp}$ , and if  $E \subset \mathbb{R}^n$  is an affine subspace,  $M \subset E$  and  $z \in E$ ,

$$M^{*z} = \{ y \in E; \langle y - z, x - z \rangle \le 1 \text{ for every } x \in M \}.$$

They prove that the body CI(L) obtained from this construction is actually convex!

If K is symmetric and convex, then IK is convex. But what can we say about IK if K is merely a star body?

Jaegil Kim presented his work (joint with V. Yaskin and A. Zvavitch), where they extend Busemann's theorem to p-convex bodies. Recall that given a star body K and  $p \in (0, 1]$ , we say that K is p-convex if, for all  $x, y \in \mathbb{R}^n$ ,

$$||x+y||_{K}^{p} \le ||x||_{K}^{p} + ||y||_{K}^{p}$$

or, equivalently  $t^{1/p}x + (1-t)^{1/p}y \in K$  whenever x and y are in K and  $t \in (0,1)$ .

**Theorem 16.0.8** Let K be a p-convex symmetric body in  $\mathbb{R}^n$  for  $p \in (0,1]$ . Then the intersection body IK of K is q-convex for every  $q \leq [(1/p-1)(n-1)+1]^{-1}$ .

The sharpness of this result, its generalizations to some general measure spaces with log-concave or *s*-concave measures, as well as other geometric implications were also discussed.

Hermann König presented a joint work with Alexander Koldobsky "On the maximal measure of sections of the *n*-cube".

They study the analogues of Ball's cube slicing theorem for the Gaussian measure and more general measures.

Let  $h: [-1,1] \to \mathbb{R}_{>0}$  be even and in  $C^1$ . Then

$$d\mu_h(s) := \prod_{j=1}^n h(s_j) ds_j / \left( \int_{-1}^1 h(r) dr \right)^n, \quad s = (s_j)_{j=1}^n \in B_\infty^n,$$

defines a probability measure on the *n*-cube  $B_{\infty}^n$ . For  $a \in S^{n-1}$  let

$$A(a,h) := \mu_h \{ x \in B^n_\infty | \langle x, a \rangle = 0 \}$$

be the (n-1)-dimensional measure of the central section orthogonal to a. For  $k \in \{1, ..., n\}$ , let

$$f_k := \frac{1}{\sqrt{k}} (\underbrace{1, \dots, 1}_k, 0, \dots, 0) \in S^{n-1}.$$

**Theorem 16.0.9** Let  $h : [-1,1] \to \mathbb{R}_{>0}$  be even and in  $C^3$  with  $h' \le 0$ ,  $h'' \le 0$ ,  $h''' \ge 0$  on [0,1] and  $h(0) \le \frac{3}{2}h(1)$ . Suppose further that

$$\pi\left(\int_0^1 r^2 h(r)dr\right)\left(\int_0^1 h(r)^2 dr\right)^2 \ge \left(\int_0^1 h(r)dr\right)^5.$$

Consider

$$d\mu_h(s) := \prod_{j=1}^n h(s_j) ds_j / \left( \int_{-1}^1 h(r) dr \right)^n, \quad s = (s_j)_{j=1}^n \in B_\infty^n$$

Let  $a = (a_j)_{j=1}^n \in S^{n-1}$  with  $a_1 \ge \dots \ge a_n \ge 0$ . Then, if  $a_1 \le 1/\sqrt{2}$ ,  $A(a,h) \le A(f_2,h)$ .

This theorem applied to the Gaussian measure gives

**Corollary 16.0.10** For  $\lambda > 0$  consider the Gaussian measure with  $h(r) = exp(-\lambda r^2)$ ,

$$d\mu(s) = \exp(-\lambda \|s\|_2^2) ds / \left(\int_{-1}^1 \exp(-\lambda r^2) dr\right)^n, s \in B_\infty^n.$$

Then for  $\lambda \leq 0.196262$  and  $a_1 \leq 1/\sqrt{2}$ ,

$$A(a,h) \le A(f_2,h),$$

while for  $\lambda > 0.196263$  and large n,

Alex Iosevich and Eric Grinberg presented their results in discrete geometry and tomography.

Alex Iosevich spoke about distribution of lattice points near families of convex surfaces. He used the operator bounds for generalized Radon transforms to obtain lattice point bounds previously approached using hands on number theoretic methods.

Eric Grinberg presented his joint results with David Feldman.

In the standard mathematical model of tomography, an unknown function in Euclidean space is to be recovered from data regarding its integrals over certain families of lines, planes, etc. The treatment of this problem involves both the geometry of the collection of lines, planes etc., and the analysis of function spaces that model the data. Grinberg and Feldman replaced the Euclidean space by an affine or projective space over a finite field, so as to focus the recovery and inversion problem on the collection lines involved. They also gave a series of properties of the Radon transform in this context culminating in a Gelfand-style admissibility theorem, which characterizes minimal sets of lines whose x-rays determine a function.

Several speakers presented their results on probability and random matrices.

Rafal Latala talked about the tail inequalities for order statistics of log-concave vectors and their applications. He presented the new tail estimates for order statistics of isotropic log-concave vectors and showed how they may be applied to derive deviation inequalities for lr norms and norms of projections of such vectors. Part of the talk was based on his joint work with Radoslaw Adamczak, Alexander Litvak, Alain Pajor and Nicole Tomczak-Jaegermann.

Mark Rudelson studied the following question: to which extent the spectral and geometric properties of the row product of independent random matrices resemble those properties for a matrix with independent random entries, (the row product of K matrices of size d by n as a  $d^K$  by n matrix, whose rows are entry-wise products of rows of these matrices). In particular, he showed that while the general volume ratio property does not hold for these matrices, it still holds in case of a cross-polytope.

Peter Pivovarov presented his joint work with G. Paouris on the rearrangements and Isoperimetric Inequalities. They studied the rearrangement inequalities and their use in isoperimetric problems for convex bodies and classes of measures.

Let  $\mathcal{P}_{[n]}$  be the class of probability measures on  $\mathbb{R}^n$ , absolutely continuous with respect to Lebesgue measure.

For  $N \ge n, x_1, ..., x_N \in \mathbb{R}^n$ , consider the  $n \times N$  matrix  $[x_1...x_N]$ . If  $C \subset \mathbb{R}^N$  is a convex body, then

$$[x_1...x_N]C = \left\{\sum_{i=1}^N c_i x_i : (c_i) \in C\right\} \subset \mathbb{R}^n.$$

#### Theorem 16.0.11 Suppose

1)  $N \ge n$  and  $\mu_1, ..., \mu_N \in \mathcal{P}_{[n]}; f_i = \frac{d\mu_i}{dx};$ 2)  $C \subset \mathbb{R}^N$  is a convex body. Set

$$\mathcal{F}_C(f_1, \dots, f_N) = \int_{\mathbb{R}^n} \dots \int_{\mathbb{R}^n} \operatorname{vol}([x_1 \dots x_N]C) \prod_{i=1}^N f_i(x_i) dx_n \dots dx_1.$$

If  $||f_i||_{\infty} \leq 1$  for i = 1, ..., N, then

$$\mathcal{F}_C(f_1,...,f_N) > \mathcal{F}_C(\mathbb{I}_{D_n},...,\mathbb{I}_{D_n}),$$

where  $D_n \subset \mathbb{R}^n$  is the Euclidean ball of volume one.

There were two talks on the quantum information theory. This theory is now one of the most active fields in science since the prospect of building quantum computers becomes more and more concrete.

Elisabeth Werner spoke about her joint results with S. Szarek and K. Zyczkowski. They investigated the nested subsets of a convex body formed by the set of trace preserving, positive maps acting on density matrices of a fixed size. Working with the measure induced by the Hilbert-Schmidt distance they derived asymptotically tight bounds for the volumes of these sets.

Deping Ye gave a talk about his joint results with G. Aubrun and S. Szarek. He discussed the problem of the detecting quantum entanglement, which is a central problem in the quantum information theory. First discovered by Einstein-Podolsky-Rosen in 1935, quantum entanglement serves as fundamental and key ingredients for many objects in quantum information, such as, quantum algorithms, quantum key distributions, and quantum teleportation.

A quantum state  $\rho$  on the N dimensional system  $\mathcal{H}_N$  may be identified as a density matrix, i.e., an  $N \times N$ positive semi-definite matrix with trace 1. It can be obtained by partial tracing over the K dimensional environmental system  $\mathcal{H}_K H$ ; namely,  $\rho = M M^{\dagger}$  where M is a  $N \times K$  (complex) matrix and  $M^{\dagger}$  denotes its complex conjugate. Deping presented the recent progress on estimating the threshold K, such that a random induced quantum state being separable and/or entangled.

The vast majority of the participants were interested in problems related to duality. The duality problems discuss the relations between the properties of a given convex body K, and the properties of its polar  $K^*$ . In particular, many questions about sections and projections of convex bodies fall into this category. Several conjectures stipulate that a direct duality connection between projections and sections, if found, would lead to a significant progress in the area of convex geometry.

Mahler conjecture, asking for the minimum, among all convex K, of the volume product  $vol_n(K)vol_n(K^*)$ is, in a way, a step to resolve the mystery. Despite many important partial results, the problem is still open in dimensions 3 and higher.

At the workshop, several participants reviewed the known results related to the conjecture. Carsten Schütt explained that the minimum of the volume product may not be reached for the body having a positive curvature at a point. Yehoram Gordon presented a proof of the functional version of the above result. The approach was extensively discussed by a group of participants.

An interest has been expressed in discrete versions of results related to duality and volumes of polytopes. Shlomo Reisner discussed the relations of the volume product of polygons, and presented a method that allows to prove the following result: the volume product of polygons in  $\mathbb{R}^2$  with at most n vertices is bounded from above by the volume product of regular polygons with *n* vertices.

A classical bound on the minimum of the volume product, given by Mahler himself in the two-dimensional case, is based on a beautiful procedure of "erasing vertices". The analogue of this idea in the three (and higher)-dimensional space is not known, and it would be very interesting to understand the structure of "neighbouring" polytopes that has the same vertices plus(minus) one additional vertex. Viktor Vigh gave a talk on on the sewing construction of polytopes, which allows one to construct a wide variety of neighbourly polytopes that are not necessarily cyclic. He also presented some new results on the sewing construction and, as a corollary, a fast algorithm for sewing in practice.

There were other results on lattice polytopes. Ivan Soprunov explained how the bound on the number of interior lattice points of a lattice polytope P, in terms of the volume of P, is related to zeroes of polynomial systems.

David Alonso-Gutiérrez gave a talk on the factorization of Sobolev inequalities through classes of functions, based on a joint work with J. Bastero and J. Bernués.

For  $1 \leq p < \infty$  and a function  $f : \mathbb{R}^n \to \mathbb{R}$ , define

$$||f||_{\infty,p} = \left(\int_0^\infty (f^{**}(t) - f^*(t))^p \frac{dt}{t^{p/n}}\right)^{1/p}$$

where  $f^*$  is the decreasing rearrangement of f, and  $f^{**}$  is the Hardy transform of  $f^*$  defined by  $f^{**}(t) =$  $\frac{1}{t} \int_0^t f^*(s) ds.$ Let

$$\mathcal{E}_p^+(f) := \frac{2^{1/p}}{I_p} \left( \int_{S^{n-1}} \|D_u^+ f\|_p^{-n} du \right)^{-1/n},$$

where  $D_u^+ f := \max\{\langle \nabla f(x), u \rangle, 0\}$ , and  $I_p^p := \int_{S^{n-1}} |u_1|^p du$ .

The authors use tools from classical real analysis and recent advances in convex geometry to establish the correct relation between  $\mathcal{E}_p^+(f)$  and  $||f||_{\infty,p}$ .

**Theorem 16.0.12** Let 
$$1 \le p < \infty$$
 and  $\frac{1}{q} = \frac{1}{p} - \frac{1}{n}$ ,  $q \in (-\infty, -n) \cup \left[\frac{n}{n-1}, \infty\right]$ . Then  
$$\mathcal{E}_p^+(f) \ge \left(1 - \frac{1}{q}\right) n\omega_n^{1/n} \|f\|_{\infty,p}, \qquad \forall f \in W^{1,p}(\mathbb{R}^n).$$

Moreover the constant is sharp.

Igor Rivin talked about the "limit" convex sets of finite volume in hyperbolic space. He indicated some results on the dimension (Minkowski and Hausdorff) of such sets, and gave some geometric corollaries. He also presented an analogue of Dvoretzky's Theorem in the context of Hyperbolic Geometry.

# Outcome of the meeting

The meeting was very successful, we were lucky to bring together mathematicians from many countries and many research areas, such as harmonic analysis, theory of valuations, discrete geometry and tomography, probability and random matrices, quantum information theory. Besides the leading scientists, we also had 14 graduate students and recent PhDs participating in the workshop. The friendly atmosphere created during the workshop helped many participants not only to identify the promising ways to attack the old problems but also to get acquainted with many open new ones.

# **List of Participants**

Abardia, Judit (Frankfurt University) Alfonseca-Cubero, Maria de los Angeles (North Dakota State University) Alonso-Gutierrez, David (University of Alberta) Berck, Gautier (Polytechnic Institute of NYU) Dann, Susanna (Louisiana State University) Fish, Alexander (University of Wisconsin) Goodey, Paul (University of Oklahoma) Gordon, Yehoram (Technion) Grinberg, Eric (University of Massachusetts Boston) Iosevich, Alex (University of Rochester) Kim, Jaegil (Kent State University) Koenig, Hermann (Universitaet Kiel) Latala, Rafal (University of Warsaw) Maresch, Gabriel (Vienna University of Technology) Meyer, Mathieu (Université Paris-Est Marne-la-Vallée) Pivovarov, Peter (University of Missouri) Reisner, Shlomo (University of Haifa) Reitzner, Matthias (University of Osnabrueck) Rivasplata, Omar (University of Alberta) **Rivin, Igor** (Institute for Advanced Study) Rudelson, Mark (University of Michigan, Ann Arbor) Ryabogin, Dmitry (Kent State University) Schneider, Rolf (University of Freiburg) Schuett, Carsten (Christian-Albrechts-Universitaet) Schuster, Franz (Vienna University of Technology) Soprunov, Ivan (Cleveland State University)

Stancu, Alina (Concordia University)
Szarek, Stanislaw (Case Western Reserve University)
Taschuk, Steven (University of Alberta)
Vigh, Viktor (University of Calgary)
Vitale, Rick (University of Connecticut)
Wannerer, Thomas (TU Wien)
Weberndorfer, Manuel (Vienna University of Technology)
Weil, Wolfgang (Universitaet Karlsruhe)
Werner, Elisabeth (Case Western Reserve University)
Yaskin, Vladyslav (University of Alberta)
Ye, Deping (Carleton University)
Zvavitch, Artem (Kent State University)

# Chapter 17

# Interactions between contact symplectic topology and gauge theory in dimensions 3 and 4 (11w5085)

# Mar 20 - Mar 25, 2011

**Organizer(s):** Denis Auroux (University of California, Berkeley) Hans U. Boden (Mc-Master University) Olivier Collin (Université du Quebec à Montréal) John Etnyre (Georgia Institute of Technology)

# Introduction

This workshop focussed on interactions between contact and symplectic geometry, gauge theory, and lowdimensional topology. Each of these subjects is an active area of current research and interactions between them have led to breakthroughs on long standing problems. Our workshop was a follow-up to the BIRS events *Interactions of geometry and topology in low dimensions* from March of 2007 and *Interactions of Geometry and Topology in dimensions 3 and 4* from March 2009. Because the fields are progressing at a rapid pace, there were many new and interesting results presented at the workshop and new projects were initiated at the workshop as well.

Participants were selected from among the world experts in these areas. The organizers made an effort to balance interest between the different research areas and to ensure that the most important current trends were well represented. There was a good mixture of well-established researchers (Honda, Lisca, Matic, Mrowka, Stern) and younger talented mathematicians (Hom, Lekili, Ma'u, Vela-Vick, Vertesi, Zarev). This stimulated many lively discussions and enabled a rich exchange of ideas in all directions.

# **Overview of the Field**

Over the last several decades it has become clear that the topology of manifolds in low-dimensions is subtly and beautifully intertwined with diverse flavors of geometry, like hyperbolic, symplectic and contact, as well as ideas from physics, such as gauge theories and mirror symmetry. Collaborations among people working in these diverse areas has exploded over the last few years resulting in the solutions to venerable conjectures in topology as well as the birth of entire new sub-fields and perspectives in these areas. Highlights of some of the more spectacular recent results include the characterization of which 3-manifolds admit a symplectic structure when crossed with  $S^1$ , the Heegaard-Floer characterization of fibered knots, the proof of Property P for nontrivial knots in  $S^3$ , the solution to the Weinstein conjecture (and generalizations of it) and a deepening of our understanding of exotic smooth and symplectic structures on 4-manifolds. Critical tools in these developments are invariants inspired by gauge theories and topological quantum field theories. These invariants – Donaldson-Floer, Seiberg-Witten, Ozsváth-Szabó, Khovanov homology and Embedded contact homology to name a few – have intriguing relations among them, and a better understanding of these will lead to significant progress not only in topology but also in contact and symplectic geometry and physics. An even more promising direction is the interplay between these invariants and more constructive approaches to low-dimensional manifolds – open book decompositions of contact 3-manifolds, symplectic fillings, Lefschetz fibrations, knot surgery constructions among many others. This interaction between powerful invariants and constructive methods is more than ever one of the driving forces in this subject. Below we will survey some of the most active branches of low-dimensional topology, thereby outlining natural directions and objectives for the workshop.

**Unification of invariants:** Recently there has been much progress in showing various invariants defined in starkly different ways actually compute the same thing. This has allowed for many striking results. For example, as Taubes and Hutchings have made progress identifying Seiberg-Witten Floer theory with Embedded Contact Homology, Taubes has managed to spin these ideas into a proof of the much studied Weinstein Conjecture in dimension 3: for any compact oriented 3-manifold M and  $\alpha$  a contact 1-form on M, the vector field that generates the kernel of the 2-form  $d\alpha$  has at least one closed integral curve. Further developments have allowed for extensions and refinements of the Weinstein conjecture and it appears we are on the cusp of identifying the two theories. The ramifications of such a convergence of theories are as yet unknown but given the spectacular results following from progress on this program, one expects great things. For instance, progress on Pidstrigatch and Tyurin's program to prove the Witten conjecture relating instanton Floer homology with Seiberg-Witten Floer homology has led to the solution of the famous conjecture that all non trivial knots in  $S^3$  have Property P: that is that non trivial surgery yields a manifold with non trivial fundamental group. Another exciting, spectacular, and very recent instance of unification of invariants is the work in progress of Kutluhan, Lee and Taubes relating Embedded Contact homology to Heegaard-Floer homology.

Another current trend in the area is the understanding of the relationship between the various invariants of Floer type for knots and 3-manifolds and Khovanov homology. Khovanov homology was constructed as a categorification of the Jones polynomial of knots and its nature is very algebraic and combinatorial. Ozsváth and Szabó derived a spectral sequence whose  $E^2$  term is a suitable variant of Khovanov's homology for a link, converging to the Heegaard Floer homology of the double branched cover of the link. The progress accomplished on combinatorial Heegaard-Floer homology has already enabled Manolescu and Ozsváth to explore further the relationship between the two theories, through the notion of homological thinness. There are good reasons to believe that this will be an active area of research for the coming years, as this should also be related to the link invariant constructed by Seidel and Smith using the the symplectic geometry of nilpotent slices. In another direction, Kronheimer and Mrowka have established an intriguing relationship between the khovanov (co)homology and the knot instanton Floer homology, again via a spectral sequence, and their new work builds on their foundational results on singular instanton connections over 4-manifolds and has application to answering affirmatively the question whether Khovanov homology detects the unknot. (The answer to the same question with the Jones polynomial is not known.)

**Developing computation techniques:** Most of the topological invariants arising from gauge theory and contact / symplectic topology rely extensively on analytical tools, which makes explicit computations particularly difficult since information about spaces of solutions to such PDE problems is scarce. In the past few years there has been dramatic progress in combinatorial approaches to Ozsváth-Szabó theory as well as Contact Homology. Indeed, the problem of combinatorially constructing Heegaard-Floer groups without resorting to counting pseudo-holomorphic curves has taken a very promising turn as knot Floer homology was given a purely combinatorial interpretation by Manolescu, Ozsváth and Sarkar. This has already led to progress in the classification of transverse knots in contact manifolds as well as work by Ng on bounds for the Thurston-Bennequin invariant of Legendrian knots. It is expected that the theory will progress greatly over the course of the next few years thanks to the combinatorial set-up. Moreover, Bourgeois, Ekholm and Eliashberg have constructed an exact sequence that allows one to compute the contact homology of a contact manifold obtained from "Legendrian surgery" on another one. This construction is particularly "simple" in dimension 3 where there is essentially an algorithm for writing down the contact homology of a contact 3-

manifold obtained from Legendrian surgery on a Legendrian knot. With recent progress on the classification of Legendrian knots in various knots types this could yield a flood of information about contact 3-manifolds.

The recent work of Lipshitz, Ozsváth and Thurston has opened a whole new direction by extending Heegaard-Floer homology to the case of 3-manifolds with boundary. Among other applications, this allows one to compute Heegaard-Floer homology by decomposing a 3-manifold into a sequence of elementary cobordisms between oriented surfaces.

Exploiting interactions between constructions and invariants: The emergence of invariants of embeddings from contact homology is also one of the promising avenues of research in the area. Given a manifold embedded in Euclidean space, one can look at its unit conormal bundle in the unit cotangent bundle of Euclidean space to get a Legendrian submanifold. Computing the contact homology of this Legendrian gives an invariant of the original embedding. Ekholm, Etnyre, Ng and Sullivan have recently rigorously computed this invariant for knots in 3-space and shown it is equal to a very powerful combinatorial invariant defined by Ng. This invariant has surprising connections with many classical invariants of knots and seems quite strong. Exploring this new invariant of knots and extending it to other situations should be a fruitful line of research for years to come. Moreover, contact homology is only the tip of the iceberg of Symplectic Field Theory (SFT). This theory, introduced by Eliashberg, Givental and Hofer, has been an inspirational and driving force in symplectic geometry for over a decade now, and recent advances in its rigorous definition suggest that a precise formulation of the relative version should emerge in the coming years. It appears there will still be much work to do to extract computable and meaningful pieces that one can use in applications. In the end though, it is expected that the theory will be invaluable in symplectic and contact geometry and will provide more invariants, not only for Legendrian knots in contact 3-manifolds and Lagrangian cobordisms between them, but also for topological knots by considering the conormal construction mentioned above. Evidence for this comes from Abouzaid's recent demonstration that the symplectic geometry of cotangent bundles can be used to distinguish exotic smooth structures on spheres of high dimension. Can such ideas be exploited in dimension 4 to attack the smooth Poincaré conjecture?

In one dimension higher, one of the driving questions in 4-dimensional topology is the smooth Poincaré conjecture and its symplectic analog. It is rather unbelievable that topologists still don't know how many smooth structures there are on the 4-sphere or the complex projective 2-space, and which admit symplectic structures. There has recently been a burst of activity in this area. Michael Freedman, Robert Gompf, Scott Morrison, and Kevin Walker have shown how to use Khovanov homology to get an obstruction to specific handle decompositions of homotopy 4-spheres being the actual 4-sphere (that is this obstruction could identify a counterexample to the smooth Poincaré conjecture, if it exists!). After this work Selman Akbulut and Robert Gompf showed that many potential counterexamples to the Poincaré conjecture are actually the standard sphere. Another approach to such problems is to try to build exotic smooth structures on "smaller and smaller" 4-manifolds. After Freedman and Donaldson's work in the early 1980's the problem for  $CP^2 \#_n \overline{CP^2}$  could be handled for n = 9, After Kotschick, who handled the case n = 8, there was little progress made until J. Park's breakthrough a few years ago. There has since been a flurry of activity on existence of exotic smooth structures on small symplectic 4-manifolds by different teams of researchers (Akhmedov-Park, Baldridge-Kirk, and Fintushel-Stern-Park). The advances are made by exploiting a certain tension between constructions and invariants. Using clever new cut-and-paste constructions such as knot and rim surgery, together with an intimate understanding of their effect on invariants such as the Seiberg-Witten invariants, one can often deduce the presence of several (generally infinitely many) exotic smooth structures. The constructions ideally involve modifying the 4-manifold so as to alter the invariants without destroying the symplectic structure or homeomorphism type. This requires one to perform surgeries along particularly well-chosen surfaces embedded in the 4-manifold. It is reasonable to expect further progress on this important problem for some additional small symplectic 4-manifolds (e.g.  $\mathbb{CP}^2$ ,  $\mathbb{CP}^2 \# \overline{\mathbb{CP}^2}$ , or  $S^2 \times S^2$ ) via the various approaches that have been developed and the continued influence of the powerful 4-manifold invariants arising from gauge theory and symplectic geometry.

**Contact structures on 3-manifolds and Heegaard-Floer theory:** The existence of tight contact structures on 3-manifolds has been an important subject of investigation for a long time and, since the year 2000, significant progress has been made in our understanding of which 3-manifolds admit tight contact structures. This fundamental question has potential applications not only to contact geometry but also low-dimensional topol-

ogy and dynamics. It also illustrates very well the natural interactions between the invariants described above and constructive methods. After many incremental steps by several mathematicians, Lisca and Stipsicz have completely classified which Seifert fibered 3-manifolds admit a tight contact structure. Their approach relies heavily on Heegaard-Floer homology through a non-vanishing criterion for the contact invariant of Ozsváth and Szabó for Seifert fibred manifolds. On the other hand, geometric methods reminiscent of the theory of normal surfaces of Haken and Kneser have led Colin, Giroux and Honda to general results such as: (1) Every 3-manifold has only finitely many homotopy classes of 2-plane fields which carry tight contact structures. (2) Every closed atoroidal 3-manifold carries finitely many isotopy classes of tight contact structures. One of the outstanding and fundamental questions here is the understanding of tight contact structures on hyperbolic 3-manifolds. Work of Kazez, Honda and Matić has led to a characterization of tight 3-manifolds in terms of right-veering diffeomorphisms, a step which should make calculations in contact homology and Heegaard Floer homology manageable, but thus far the condition of a manifold being hyperbolic has not been properly understood in this context. It is hoped that the current wide-ranging technology will help elucidate the problem of tight structures on 3-manifolds.

## **Highlights from the Workshop**

A variety of geometric approaches to low-dimensional topology were represented, and several high-profile recent results in the field were featured prominently in the workshop. Here are a few key recent developments that were presented at the workshop: relations between Seiberg-Witten Floer homology and Heegaard-Floer homology, relations between various invariants of knots and of Legendrian/transverse knots, combinatorial approaches to computing Heegaard-Floer invariants and applications to various homology theories to low-dimensional topology and specifically knot/link theory.

Recently, two groups of researchers have been pursuing two different approaches to identifying Seiberg-Witten Floer homology and Heegaard-Floer homology. There is considerable interest in relating these theories on both theoretical and practical grounds, as each theory has its strengths in terms of computability and applicability. One group working on this problem, Cagatay Kutluhan, Yi-Jen Lee, and Clifford Taubes, was represented at the workshop by Kutluhan and Lee; Kutluhan gave a talk on their program to identify the two invariants [KLTI, KLTII, KLTIII]. The other group, Vincent Colin, Paolo Ghiggini and Ko Honda, were represented at the workshop by Ghiggini and Honda. They both gave talks outlining their approach to this correspondence [CGHI, CGHII].

Lenny Ng discussed joint work with Tobias Ekholm, John Etnyre and Michael Sullivan, about a new invariant of transverse knots that arose out of knot contact homology [EENS, 25]. These new invariants seem particularly strong but very difficult to work with. Specifically they can distinguish most known pairs of transverse knots that have Legendrian approximations with small grid number. It was clear from the talk that much of the power of these invariants is still hidden away in the complicated algebras that describe knot contact homology, but many hints at how to extract information were discussed.

Jen Hom described an invariant associated to the knot Floer complex and used it to define a new smooth concordance homomorphism [8]. Applications include a formula for the tau invariant of iterated cables, better bounds (in many cases) on the 4-ball genus than tau alone, and a new infinite family of smoothly independent topologically slice knots.

Ciprian Manolescu gave a talk on a program, joint with Peter Ozsváth and Dylan Thurston, to combinatorially compute the Heegaard-Floer invariants of 3- and 4-manifolds. The 3-manifold work was discussed in the paper [MOT], but the 4-manifold work has yet to appear. The algorithm Manolescu described is based on presenting the manifolds in terms of links in  $S^3$ , and then using grid diagrams to represent the links. To compute the invariants, one uses certain positive domains on the grid, which can be encoded into "formal complex structures".

There has been little work involving contact structures on open 3–manifolds, with two notable exceptions being [E] and [T]. In his talk, Shea Vela-Vick discussed joint work with John Etnyre and Rumen Zarev defining an invariant of contact structures on open manifolds and showed that for a knot complement this new invariant corresponds to the minus version of Heegaard-Floer homology. This invariant along with the work in [T] opens to door to the exploration of contact structures on open 3–manifolds. In addition it provides new insight into the relation between sutured Heegaard-Floer theory and knot Heegaard-Floer theory and

illustrates the important but mysterious role contact geometry seems to play in Heegaard-Floer theory.

# **Featured Talks**

What follows is a list of the 21 one-hour talks featured at the workshop. The central themes were (some talks fit into more than one theme):

- Twisted Alexander Polynomials. (Talks 1, 19)
- Floer Theory. (Talks 15, 21)
- Heegaard-Floer, Seiberg-Witten and/or Khovanov homology and applications. (*Talks 5, 6, 8, 9, 11, 17, 18*)
- Relations between homology theories. (Talks 2, 3, 4, 7)
- Knots, invariants, concordance. (Talks 1, 5, 6, 12, 13, 18, 20)
- Mapping class groups and contact structures. (Talks 10, 16)
- 4-dimensional manifolds and invariants. (Talks 9, 14, 19)

Below is a detailed list of speakers, titles, and brief descriptions of their talks.

- 1. **Stefan Friedl** (University of Cologne) *Twisted Alexander polynomials of hyperbolic knots* Given a hyperbolic knot we study the twisted Alexander polynomial as a function on the character variety and corresponding to the discrete and faithful representation. In particular we will discuss formal properties of such polynomials and their relation to fiberedness, chirality, the volume and the knot genus. This is based on joint work with Nathan Dunfield, Nicholas Jackson, Taehee Kim and Takahiro Kitayama.
- 2. Paolo Ghiggini (CNRS Laboratoire Jean Leray) From HF to ECH via open book decompositions I
- 3. **Ko Honda** (University of Southern California) *From HF to ECH via open book decompositions II* This is a series of two talks aimed at showing an isomorphism between the hat-versions of Heegaard-Floer homology (*HF*) and of embedded contact homology (*ECH*). Heegaard-Floer homology, defined by Ozsváth and Szabó, is constructed from a Heegaard splitting of a three manifold and embedded contact homology, defined by Hutchings and Taubes, is constructed from a contact form.

In our proof of HF=ECH we use open book decompositions as interpolating objects between Heegaard splittings and contact forms. The first step in the proof is to reduce the computation of both  $\widehat{HF}$  and ECH to complexes defined from the page and the monodromy of the open book. Then we construct chain maps between these modified HF and ECH complexes by counting pseudo-holomorphic maps in suitably defined symplectic cobordisms. Finally we prove that the maps induced in homology are inverse of each other by degenerating the cobordisms and performing a relative Gromov-Witten computation. This is a joint work with Vincent Colin.

In Part 1 we will explain how adapt the *ECH* complex to an open book decomposition. In Part 2 we will explain the construction of the chain maps between  $\widehat{HF}$  and  $\widehat{ECH}$ .

- 4. Eli Grigsby (Boston College) On Khovanov-Seidel quiver algebras and bordered Floer homology I will discuss a relationship between Khovanov- and Heegaard Floer-type homology theories for braids. Specifically, I will explain how the bordered Floer homology bimodule associated to the doublebranched cover of a braid is related to a similar bimodule defined by Khovanov and Seidel. This is joint work with Denis Auroux and Stephan Wehrli.
- 5. Matt Hedden (Michigan State University) Unlink detection and the Khovanov module Kronheimer and Mrowka recently showed that Khovanov homology detects the unknot. Their proof does not obviously extend to show that Khovanov homology detects unlinks of more than one component, and one could reasonably question whether it actually does (the Jones polynomial, for instance,

does not detect unlinks with multiple components). In this talk, I'll discuss how to use a spectral sequence of Ozsvath and Szabo in conjunction with Kronheimer and Mrowka's result to settle the question (in the affirmative). This project is joint with Yi Ni, and had its birth at the Banff workshop two years ago.

6. Jen Hom (University of Pennsylvania) Concordance and the knot Floer complex

We will use the knot Floer complex, in particular the invariant epsilon, to define a new smooth concordance homomorphism. Applications include a formula for tau of iterated cables, better bounds (in many cases) on the 4-ball genus than tau alone, and a new infinite family of smoothly independent topologically slice knots. We will also discuss various algebraic properties of this construction, including a total ordering, a "much greater than" relation, and a filtration.

- Cagatay Kutluhan (Columbia University) Heegaard Floer meets Seiberg–Witten Recently Yi-Jen Lee, Clifford Taubes, and I have announced a proof of the conjectured isomorphisms between Heegaard Floer and Seiberg–Witten Floer homology groups of a 3-manifold. The purpose of this talk is to outline our construction of these isomorphisms.
- 8. Tye Lidman (UCLA) Heegaard Floer Homology and Triple Cup Products

We use the recent link surgery formula of Manolescu and Ozsváth as well as the theory of surgery equivalence of three-manifolds due to Cochran, Gerges, and Orr to relate Heegaard Floer homology to the cup product structure for a closed oriented three-manifold. In particular, we give a complete calculation of the infinity flavor of Heegaard Floer homology for torsion  $Spin^c$  structures with mod 2 coefficients. This establishes an isomorphism with Mark's cup homology, mod 2, a homology theory defined solely using the triple cup product form.

9. Ciprian Manolescu (UCLA) A step-by-step algorithm to compute 3- and 4- manifold invariants I will describe an algorithm for computing the Heegaard Floer invariants of three- and four-manifolds (modulo 2). The algorithm is based on presenting the manifolds in terms of links in  $S^3$ , and then using grid diagrams to represent the links. To compute the invariants, one uses certain positive domains on the grid, which can be encoded into "formal complex structures". One needs to check that all formal complex structures on the grid are homotopic - this is known to be true for certain grids called sparse,

and conjectured to hold in general. The talk is based on joint work with P. Ozsvath and D. Thurston.

10. Dan Margalit (Georgia Institute of Technology) Combinatorics of Torelli groups

The Torelli group of a surface is the subgroup of the mapping class group consisting of elements that act trivially on the homology of the surface. One interesting subgroup of the Torelli group is the set of elements commuting with some hyperelliptic involution. It has been conjectured that this subgroup is generated by Dehn twists. I will present some progress on this conjecture. A key ingredient is a new proof that the Torelli group is generated by bounding pair maps. This is joint work with Tara Brendle and Allen Hatcher.

11. Tom Mrowka (Massachusetts Institute of Technology) Filtrations on Singular Instanton Knot Homology

This talk will discuss two filtrations that arise on Singular Instanton Knot Homology that refine the spectral sequence beginning with Khovanov homology and converging to the Singular Instanton Knot Homology. This is joint work with Peter Kronheimer.

12. Lenny Ng (Duke University) Transverse homology and its properties

After a brief summary of knot contact homology and some of its properties, I'll describe how a contact structure induces filtrations on the underlying complex that yield an invariant of transverse knots, transverse homology (joint with Tobias Ekholm, John Etnyre, and Michael Sullivan). I'll try to provide some perspective on the mysterious nature of this invariant, with emphasis on its general behavior and comparison to previously developed transverse invariants. If time permits, I'll discuss how transverse homology might produce a new Bennequin-type bound on self-linking number.

13. Brendan Owens (University of Glasgow) Alternating links and rational balls

For a slice knot K in the 3-sphere it is well known that the double branched cover  $Y_K$  bounds a smooth

rational homology 4-ball. Paolo Lisca has shown that this condition is sufficient to determine sliceness for 2-bridge knots, and that this generalizes to 2-bridge links. I will discuss the problem of determining whether  $Y_L$  bounds a rational ball when L is an alternating link.

#### 14. Jongil Park (Seoul National University) A classification of numerical Campedelli surfaces

In order to classify complex surfaces of general type with  $p_q = 0$  and  $K^2 = 2$  (such surfaces are usually called numerical Campedelli surfaces), it seems to be natural to classify them first up to their topological types. It has been known by M. Reid and G. Xiao that the algebraic fundamental group  $\pi_{alg}$  of a numerical Campedelli surface is a finite group of order  $\leq 9$ . Furthermore the topological fundamental groups  $\pi_1$  for any numerical Campedelli surfaces are also of order  $\leq 9$  in as far as they have been determined. Hence it is a natural conjecture that  $|\pi_1| \leq 9$  for all numerical Campedelli surfaces. Conversely one may ask whether every group of order  $\leq 9$  occurs as the topological fundamental group or as the algebraic fundamental group of a numerical Campedelli surface. It has been proved that the dihedral groups  $D_3$  of order 6 or  $D_4$  of order 8 cannot be fundamental groups of numerical Campedelli surfaces. Furthermore, it has also been known that all other groups of order  $\leq 9$ , except  $D_3, D_4, \mathbb{Z}/4\mathbb{Z}, \mathbb{Z}/6\mathbb{Z}$ , occur as the topological fundamental groups of numerical Campedelli surfaces. Unlike the case of topological fundamental group, there is also a known numerical Campedelli surface with  $H_1 = \mathbb{Z}/6\mathbb{Z}$  (in fact  $\pi_{alg} = \mathbb{Z}/6\mathbb{Z}$ ). Therefore all abelian groups of order  $\leq 9 \operatorname{except} \mathbb{Z}/4\mathbb{Z}$  occur as the first homology groups (and algebraic fundamental groups) of numerical Campedelli surfaces. Nevertheless, the question on the existence of numerical Campedelli surfaces with a given topological type was completely open for  $\mathbb{Z}/4\mathbb{Z}$ . Recently Heesang Park, Dongsoo Shin and myself constructed a new minimal complex surface of general type with  $p_g = 0, K^2 = 2$  and  $H_1 = \mathbb{Z}/4\mathbb{Z}$  (in fact  $\pi_{alg} = \mathbb{Z}/4\mathbb{Z}$ ) using a rational blow-down surgery and a Q-Gorenstein smoothing theory, so that the existence question for numerical Campedelli surfaces with all possible algebraic fundamental groups are settled down. In this talk I'd like to review how to construct such a numerical Campedelli surface.

#### 15. Tim Perutz (University of Texas-Austin) The Fukaya category of the punctured 2-torus

In effect, Heegaard Floer theory takes place invokes the Fukaya category of the g-fold symmetric product of a genus g surface, with a filtration arising from a basepoint. The structure of this category is non-trivial to describe even in the genus-one case, and that is the subject of this talk. The filtered Fukaya category of the torus is generated by two circles, but it carries an interesting A-infinity structure. We use Hochschild cohomology to show that A-infinity structures on the relevant algebra are classified by two parameters in the ground ring. An Ext-algebra of two sheaves on a Weierstrass cubic curve carries an A-infinity structure of the right sort, and the coefficients  $g_2$  and  $g_3$  of the curve can be identified with our two parameters. In this way, the Fukaya category of the punctured torus (the "HF-hat" category) embeds into the dg category of perfect complexes on some cubic curve - in fact, a nodal cubic. Is this a hint of a theory mirror to Heegaard Floer cohomology? This is joint work with Yanki Lekili.

16. **Olga Plamenevskaya** (State University of New York at Stony Brook) *Planar open books, monodromy factorization and symplectic fillings* 

A theorem of Wendl says that if a contact structure admits a planar open book  $(S, \phi)$ , all its Stein fillings arise from factorizations of the *given* monodromy  $\phi$  as a product of positive Dehn twists. To obtain applications of this result, we develop combinatorial techniques to study positive monodromy factorizations in the planar case. As a corollary, we classify symplectic fillings for all contact structures on L(p,1), and detect non-fillability of certain contact structures on Seifert fibered spaces. (joint with J. Van Horn- Morris.)

- 17. **Dylan Thurston** (Barnard College, Columbia University) *Heegaard Floer homology is natural* The easiest statement of invariance for Heegaard Floer homology gives an isomorphism class of groups for each 3-manifold. Can this be improved (like ordinary homology) to give an actual group, rather than an isomorphism class? We show that *HF* homology does associate a group to a based 3-manifold, giving, for instance, an action of the based mapping class group. In the proof, there is one new move on Heegaard diagrams that had not been previously checked.
- 18. David Shea Vela-Vick (Columbia University) Contact geometry and Heegaard Floer invariants for noncompact 3-manifolds

I plan to discuss a method for defining Heegaard Floer invariants for 3-manifolds. The construction is inspired by contact geometry and has several interesting immediate applications to the study of tight contact structures on noncompact 3-manifolds. In this talk, I'll focus on one basic examples and indicate how one defines a contact invariant which can be used to give an alternate proof of James Tripp's classification of tight, minimally twisting contact structures on the open solid torus. This is joint work with John B. Etnyre and Rumen Zarev.

19. **Stefano Vidussi** (University of California Riverside) *Refined adjunction inequalities for 4-manifolds* with a circle action

Given a smooth 4-manifold M, there is an estimate on the minimal genus among representatives of a class of  $H_2(M)$  in terms of an adjunction inequality involving Seiberg-Witten basic classes. In spite of the importance of such inequality in various problems (e.g. the solution of Thom Conjecture) it is known that in general such inequality is not sharp. In particular, in 1998, Peter Kronheimer proved that such inequality can be sharpened for 4-manifolds of the form  $S^1 \times N^3$  using the Thurston norm of N. It is not clear how to extend Kronheimer's approach to other classes of manifolds.

Here we discuss how, using an approach that is quite different from Kronheimer's, we can recast and extend such result to 4-manifolds that are circle bundles over a 3-manifold whose fundamental group satisfies certain group-theoretic properties. More specifically, this group must be virtually RFRS; for example in the case of Haken hyperbolic manifolds (with  $b_1 > 1$ ) this is a consequence of Dani Wise's program. The talk is based on joint work with Stefan Friedl.

20. Liam Watson (UCLA) Decayed knots and L-spaces

This talk introduces the notion of a decayed knot, a property derived from the left-orderability of the fundamental group of the knot. Decayed knots (1) have sufficiently positive surgeries with non-left-orderable fundamental group and (2) admit decayed cables, for sufficiently positive cabling parameters. This behaviour closely mirrors the behaviour of L-space surgeries on knots in the three-sphere. Indeed, known examples of decayed knots are L-spaces knots. This is joint work with Adam Clay.

21. **Katrin Wehrheim** (Massachusetts Institute of Technology) Quilted Floer homology - transversality and applications

I can briefly state a new, improved, and actually proven transversality for quilted Floer homology. From there, I can explain two recent applications: a) SU(n) invariants for 3-manifolds with a homotopy class of maps to  $S^1$ ; which use a version of Cerf theory for Morse functions to  $S^1$  with connected fibers. b) calculation of Floer homology for the Chekanov-Polterovich torus in  $S^2 \times S^2$ ; which uses strip shrinking for immersed geometric composition and a weak removal of singularity for figure eight bubbles.

# **Scientific Progress Made**

The workshop brought together leading experts from several different areas, and this sparked much scientific interaction. There were many very interesting talks proposed, and in making up the final schedule, the organizers tried to allow sufficient time for informal scientific discussions in order to facilitate interactions between the subject areas. This was accomplished by scheduling enough break time throughout the talk timetable and some longer breaks during the day to encourage as much informal open-ended discussions as possible. The evenings provided collaborating teams of researchers time to meet and discuss their research projects.

There were a number of new results that were proved at the workshop or whose proof was stimulated by conversations held during the workshop. Some of these came out of long-term collaborative projects, others from newly formed collaborations, and some came from ideas stimulated by talks and other interactions at the workshop.

Recently, using the language of Heegaard Floer knot homology two invariants were defined for Legendrian knots. One — the so called *grid invariant* — in the standard contact 3-sphere defined by Ozsvath, Szabo and Thurston [OST] in the combinatorial settings of knot Floer homology, and the other by Lisca, Ozsvath, Stipsicz and Szabo [LOSS] — known as the LOSS invariant — in knot Floer homology for a general contact 3-manifold. Both of them also give an invariant of transverse knots, in fact they were the first such invariants. The definitions of these invariants are quite different, but it has been conjectured since their initial definition that they are indeed the same. During the conference John A. Baldwin and David Shea Vela-Vick, and Vera Vértesi, completed a program showing that the above two definitions give the same invariant in the standard contact 3-sphere. The ideas formulated at BIRS further led to an alternate definition of these invariants which is more natural from the perspective of transverse knot theory. The approach is to give a new characterization of the invariants for transverse braids as the bottommost elements with respect to the filtration of knot Floer homology given by the axis. This work in still in progress, but is at a very promising stage. Discussing this work with John Etnyre, Etnyre revealed a program he and a student Bulent Tosun had to also establish the equivalence of these invariants. This approach involved generalizing the notion of grids to all 3-manifolds and seeing how both the grid and LOSS invariants fit into this picture. Prompted by discussions at the workshop Etnyre pushed this program forward and now believes it is close to fruition. The two different approaches by the two different groups promise new insight into these important new invariants and it is clear the BIRS workshop was key to the rapid progress on both programs.

Recently John Etnyre, Shea Vela-Vick and Rumen Zarev had defined a "limit homology" for knots using a sequence of sutured manifolds and maps between their sutured Heegaard-Floer homology. They also defined a new invariant of transverse knots in this new homology. They had previously conjectured the equivalence of this homology theory and  $HFK^-$  as well as the transverse invariant and the LOSS invariant. At BIRS, they showed that the transverse invariant does agree with the LOSS invariant under an appropriate identification of the limit groups with the minus version of knot Floer homology. This work gives a completely new perspective on not only the LOSS invariant but the minus Heegaard-Floer groups for knots as well. There are already plans to generalize this to open 3-manifolds and initiate a study of contact structures on open 3-manifolds.

Lenny Ng started a project at BIRS with Dylan Thurston, after Thurston's talk on naturality mentioned above. Applying the naturality results in Heegaard Floer theory to the grid transverse invariant in *HFK*, they believe they can strengthen the invariant. So far it appears they can distinguish some of the Birman-Menasco transverse knots using these techniques. This is quite interesting as these examples have so far resisted all previous attempts to try to distinguish them with invariants. Ng and Thurston are also exploring a transverse version of the mapping class group.

During the BIRS workshop Matthew Hedden and Olga Plamenevskaya completed the work on their paper [HP]. The environment of BIRS turned out to be incredibly productive for Hedden and Plamenevskaya, who were able to make substantial progress and significantly strengthen their results. The paper studies contact invariants associated to rational open books and uses them to verify tightness of contact structures on manifolds obtained by surgery on bindings of open books. They were granted permission to stay at BIRS for two extra days before the workshop; this extra time allowed them to prove a theorem. Moreover, another important lemma for the paper arose from conversations Plamenevskaya had with other workshop participants, specifically John Etnyre and Jeremy Van Horn-Morris. In addition, a chance conversation between Hedden and Van Horn-Morris at breakfast inspired a simple proof that the open book with trivial monodromy is characterized by the knot Floer homology of its binding. The ideas involved may prove useful for a variety of "botany" type questions.

During the workshop, Tom Mrowka and Nikolai Saveliev got to work on their index theorem project (their third collaborator on this, Danny Ruberman, was unfortunately not present), and while at BIRS, they managed to finish it up, and a preprint has posted to the arxiv shortly after the meeting [MRS].

Ciprian Manolescu and Dylan Thurston used the time at the BIRS workshop to work on a final version of their paper [MOT] that they have written with Peter Ozsváth.

Many participants also reported starting new projects, but they are at a more preliminary state than those mentioned above. For example Tye Lidman and Liam Watson began a project pertaining to the leftorderability of graph manifold integer homology spheres. This involves and was inspired by the results mentioned in Watson's talk that related left-orderability to Heegaard Floer homology. In another example Cagatay Kutluhan mentioned conversations with Jeremy Van Horn-Morris and Gordana Matic during the BIRS workshop, indicated an application of his construction, with Yi-Jen Lee and Cliff Taubes, of the isomorphism between Heegaard Floer and Seiberg-Witten Floer homologies to symplectic filling obstructions. The expectation is to be able to prove new results about such obstructions. After the workshop in Banff, Kutluhan started working on a project based on this expectation. There were numerous other such anecdotes as well as mentions of longtime collaborators finding time to further ongoing work (notably, the workshop was a valuable opportunity for collaborators on different continents, such as Stephan Friedl and Stefano Vidussi, to get together). Lastly, the workshop was an ideal opportunity for strong young researchers to talk with more established mathematicians. In one such example, Jonathan Williams specifically noted how important conversations with Katrin Wehrheim and Tim Perutz were to his research program. In another such example, Jonathan Yazinski discussed some ideas he has for constructing exotic smooth structures on various small 4-manifolds with Jongil Park, Ron Stern and Rafael Torres. In one case, Ron Stern was able to explain to explain why the construction would not lead to the desired conclusion, namely an exotic smooth structure on  $CP^2 \# \overline{CP}^2$ . In another case, Rafael Torres and Jonathan Yazinski worked together on an approach for modifying "numerical" constructions of algebraic surfaces to produce exotic 4-manifolds.

# **List of Participants**

Auroux, Denis (University of California, Berkeley) Baker, Ken (University of Miami) Baldwin, John (Princeton University) Boden, Hans U. (McMaster University) Collin, Olivier (Université du Quebec à Montréal) Etnyre, John (Georgia Institute of Technology) Friedl, Stefan (University of Cologne) Ghiggini, Paolo (CNRS - Laboratoire Jean Leray (Nantes)) Grigsby, Julia Elisenda (Boston College) Hedden, Matthew (Michigan State University) Hom, Jen (University of Pennsylvania) Honda, Ko (University Southern California) Kutluhan, Cagatay (Harvard University) Lee, Yi-Jen (Purdue University) Lekili, Yanki (University of Cambridge) Licata, Joan (Stanford University) Lidman, Tye (UCLA) Lisca, Paolo (University of Pisa) Ma'u, Sikimeti (MSRI/Barnard) Manolescu, Ciprian (UCLA) Margalit, Dan (Georgia Institute of Technology) Matic, Gordana (University of Georgia) Mrowka, Tom (Massachusetts Institute of Technology) Ng, Lenny (Duke University) Owens, Brendan (University of Glasgow) Park, Jongil (Seoul National University) Perutz, Tim (University of Texas-Austin) Plamenevskaya, Olga (State University of New York at Stony Brook) Saveliev, Nikolai (University of Miami) Sivek, Steven (MIT) Stern, Ronald (University of California, Irvine) Thurston, Dylan (Barnard College, Columbia University) Torres, Rafael (Oxford University) Van Horn-Morris, Jeremy (AIM) Vela-Vick, David Shea (Columbia University) Vertesi, Vera (MIT) Vidussi, Stefano (University of California Riverside) Watson, Liam (UCLA) Wehrheim, Katrin (Massachusetts Institute of Technology) Williams, Jonathan (University of California Berkeley)

Yazinski, Jonathan (McMaster University) Zarev, Rumen (University of California, Berkeley)

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# Chapter 18

# **Algebraic Combinatorixx (11w5025)**

# May 22 - May 27, 2011

**Organizer(s):** Georgia Benkart (University of Wisconsin - Madison) Stephanie van Willigenburg (University of British Columbia) Monica Vazirani (University of California, Davis)

# **Overview of the Field**

Algebraic combinatorics is a broad discipline with substantial connections to many areas of mathematics and physics such as representation theory, algebraic geometry, number theory, knot theory, mathematical biology, statistical mechanics, symmetric functions, invariant theory, and quantum computing. These connections are reflected in the topics that were featured at the workshop:

#### I. Combinatorics of Representations

- (i) representations of groups and algebras
- (ii) combinatorial objects that arise in the study of representations such as crystal bases, Littelmann paths, tableaux, quivers, Littlewood-Richardson coefficients, knots and tangles, and alternating sign matrices

#### **II. Geometry and Combinatorics**

- (i) Schubert varieties, Grassmannians, cluster algebras, and tropical geometry
- (ii) simplicial complexes, polytopes, discrete Morse theory, Whitney stratification, phylogenetic trees
- (iii) reflection and braid groups and hyperplane arrangements

#### **III. Combinatorial Functions**

- (i) symmetric functions such as group characters, Schur functions, Schur *P*-functions, *k*-Schur functions, and Macdonald polynomials (both symmetric and nonsymmetric)
- (ii) quasisymmetric functions, combinatorial Hopf algebras, and noncommutative Schur functions,
- (iii) Kazhdan-Lusztig polynomials.

The topics are interconnected and the workshop focused on many interesting, open problems. Among them:

(a) study the composition poset that arises from considering quasisymmetric functions and find a tower of algebras connected with it;

- (b) provide a straightforward combinatorial description for Kazhdan-Lusztig polynomials; and
- (c) give a combinatorial interpretation for the Kronecker product of Schur functions.

The answers would impact representation theory, algebraic geometry, mathematical physics, and computer science.

## **Goals of the Workshop**

The workshop brought together forty-two senior and junior female mathematicians to collaborate on cuttingedge research problems in algebraic combinatorics and related fields and to forge mentoring networks, with the long-term goal of increasing and strengthening the participation of women in mathematics.

The workshop also had a major mentoring component. Almost two-thirds of the participants were earlycareer (pre-tenure or recently tenured) women faculty members, postdoctoral fellows, or graduate students.

## Format

The program for the workshop consisted of seven 45-minute survey lectures on the latest research developments, which were given by more established researchers, and twelve 25-minute shorter research talks. In addition, eleven participants presented posters and gave a brief 2-3 minute preview of their poster before it was displayed. Roughly half the time was spent working in smaller groups organized according to research interests, where actual research problems were discussed. Groups gave brief daily updates to the entire workshop audience on the topics and problems they had worked on and posed open questions. As a result, there was much collaboration and discussion. At the end of the workshop, the groups presented reports (which are attached below). During two of the evenings there were panel discussions on building the tools to succeed: from professional development to work-life balance. BIRS Scientific Director, Professor Nassif Ghoussoub, and chair of the BIRS Board of DIrectors, Attorney Karen Prentice, visited during the workshop, spoke with participants, and led them on a tour of the new TransCanada PipeLines Pavillion scheduled to open in the fall.

## **Participants**

Before submitting a formal proposal to BIRS, the organizers sent out a description of the proposed workshop to women working in algebraic combinatorics to gauge interest. Within 24 hours, the organizers had received positive responses from over half of the women contacted, and within less than a week's time, they had heard from all but two. Some of the women offered to prepare reading lists and to help apply for grants.

To encourage more participation from early-career mathematicians and from those working at smaller colleges, the organizers advertised for applications in various venues including the Association for Women in Mathematics newsletter and website, through the Canadian Mathematical Society and its Women in Mathematics Committee, and by sending out announcements to several combinatorics email lists and to mathematics departments across the U.S. The response was overwhelming. Less than a third of the junior-level mathematicians who applied could be accommodated. The majority of the workshop participants were quite junior (26 of the 42 participants received their doctoral degrees after 2001 or are currently enrolled as graduate students).

### **Group Research Projects and Scientific Progress**

#### Group I: Alternating Sign Matrices, Crystal Bases, and Tableaux

*Members:* Julie Beier, Angèle Hamel, Gizem Karaali, Anne Schilling, and Jessica Striker. After the first day Sophie Morier-Genoud and Karola Meszaros also participated.

The group spent most of its time on two separate projects related to common themes that interested the whole group. The first project attempted to interpret the poset of alternating sign matrices as a modified

crystal graph. The second project aimed to compute the order of the promotion map on hooks. At this time they have a conjecture for the latter and some computational evidence that supports it. In the former project, too, the group has made some progress. The group is excited about these two questions and is continuing to work on them together.

#### Group II: k-Derangements and the Sandpile Problem

*Members*: Hélène Barcelo, Camillia Smith Barnes, Heather Dye, Susanna Fishel, Kristina Garrett, Kathryn Nyman, Bridget Tenner

The group began the week investigating k-derangements and eventually turned its attention to the Sandpile Problem.

A *k*-derangement is a permutation in  $S_n$  such that the induced permutation on the set of all unordered *k*-tuples leaves no *k*-tuple fixed. A permutation  $\sigma \in S_n$  is a *k*-derangement if and only if the cycle decomposition of  $\sigma$  does not contain a set of cycles whose lengths partition *k*.

The group found a recursive formula for the number of 2-derangements in  $S_n$  and used this to verify an existing exponential generating function (A. Fraticelli, Missouri State REU 2009). However, finding a closed form for the number of 2-derangements of n requires counting partitions which avoid subpartitions, and this turns out to be very difficult.

A sandpile is a partition  $\lambda = (\lambda_1, ..., \lambda_t)$  represented by its Ferrers shape. The group studied the following operation on sandpiles: a grain of sand can "fall" from column *i* to column *i* + 1 provided  $\lambda_i - \lambda_{i+1} \ge 2$ . This Sandpile Model induces a directed graph on the set of partitions of *n*: place an edge from  $\mu$  to  $\lambda$  if  $\lambda$  arises from a grain of sand falling in  $\mu$ . Note that this graph is generally not connected. A partition in which no "sand" can fall further is a *fixed point* (a sink of the graph), and a partition which could not have arisen from a dynamic operation on any previous partition is a *garden of eden* (a source).

The group raised the following questions about the Sandpile Problem and made progress on several of them.

- 1. How many partitions are both fixed points and gardens of eden?
- 2. The directed sandpile graph is contained in the (non-graded) dominance poset,  $\mathcal{D}_n$  and as such is a poset itself. Is this sandpile poset graded?
- 3. Given a fixed point, can we determine its connected component?
- 4. What are the equivalent questions for the more generalized models? (Jumping Pile, Ice Pile, Theta Model, etc.)

Partitions which are both fixed points and gardens of eden were easily characterized. The group is now working on recursive formulas, and enumerating these "fixed gardens" may be possible with generating functions. They believe they can describe the covering relations in  $\mathcal{D}_n$  which do not survive in the sandpile subposet, and that the resulting connected sandpile components are graded. Finally, they suspect that the connected components are obtained as follows. Take a highest-ranked fixed point and its upper order ideal. This ideal corresponds to one of the graph components. Removing this ideal and repeating this process with the remaining partitions would give the next component, and so on, until all components have been recovered.

The group plan is to collect and then disseminate our individual notes in mid to late June. The group hopes to meet via video conferencing later in the summer to continue work on these questions with an eye on extending the theory to the models mentioned above (Jumping Pile, Ice Pile, Theta Model, etc.).

#### **Group III: Symmetric and Quasisymmetric Functions**

*Members:* Christine Bessenrodt, Soojin Cho, Huilan Li, Sarah Mason, Vidya Venkateswaran, Stephanie van Willigenburg, Martha Yip, Meesue Yoo

The group investigated quasisymmetric and Schur *P*-functions. For a composition  $\alpha$ , *F* is said to be a composition tableau of shape  $\alpha$  if it has  $\alpha_i$  cells in the *i*-th row from the top, and the diagram is filled with positive integers such that the following three conditions are satisfied:

1. left-most column is strictly increasing from top to bottom

#### Algebraic Combinatorixx

- 2. rows are weakly decreasing from left to right
- 3. triple rule: supplement F by adding enough cells with zero valued entries to the end of each row so that the resulting supplemented tableaux,  $\hat{F}$ , is of rectangular shape  $l \times m$ . Then for  $1 \le i < j \le l$ ,  $2 \le k \le m$ ,

$$\left(\hat{F}(j,k) \neq 0 \text{ and } \hat{F}(j,k) \geq \hat{F}(i,k)\right) \Rightarrow \hat{F}(j,k) > \hat{F}(i,k-1).$$

Then the quasisymmetric Schur function [8] indexed by a composition  $\alpha$  is defined to be

$$\mathcal{S}_{\alpha} = \sum_{\substack{F \text{ a composition} \\ \text{tableaux of} \\ \text{shape } \alpha}} x^{F}.$$

where  $x^F = \prod x_i^{\# i}$ . These functions refine the Schur functions indexed by partitions  $\lambda$  as follows:

$$s_{\lambda} = \sum_{\tilde{\alpha} = \lambda} \mathcal{S}_{\alpha}.$$
(18.1)

The Schur *P*-function is defined by

$$P_{\lambda} = \sum_{T} 2^{-l(\lambda) + b(T)} x^{T},$$

where T are certain SSYTx of shape  $\lambda$ , b(T) is the number of positions where *i* occurs in a given column but not in the next column, and  $\lambda$  is a strict partition (see [9]).

**Research Collaboration:** The group investigated the following natural question: just as Schur functions decompose into quasisymmetric Schur functions, as given in [8], is it possible to decompose the Schur *P*-functions into a sum of quasisymmetric Schur *P*-functions? The group was able to answer this question in the affirmative and will study several other aspects of these quasisymmetric Schur *P*-functions. In particular, they would like to express these functions in other bases, find a Pieri rule, and see if there is a representation-theoretic interpretation.

#### Group IV: Diagram Algebras and the Representation Theory of the QSYM Poset

Members: Georgia Benkart, Christine Bessenrodt, Maud Devisscher, Rosa Orellana, Alison Parker, Monica Vazirani

Group discussions focused on two problems. The first, which was inspired by Kronecker products for symmetric groups, explored the following question. Given two diagram algebras  $A_k$  and  $A_\ell$  of the same kind (perhaps both Temperley-Lieb algebras or both partition algebras or both Brauer algebras), and an irreducible module  $M_k$  and  $M_\ell$  for each, determine the decomposition for the induced module

$$\operatorname{Ind}_{A_k \times A_\ell}^{A_{k+\ell}} M_k \boxtimes M_\ell$$

as a module for  $A_{k+\ell}$  in the generic semisimple case and the structure of the induced module in the nongeneric case. The second problem the group discussed involved the composition poset that arose from considering quasisymmetric functions. The group viewed this poset as the labels for the irreducible modules of a tower of algebras in the same spirit as Young's lattice of partitions is the poset corresponding to irreducible modules of the symmetric groups  $S_k$  (or their group algebras in characteristic 0). They computed what might be dimensions for these algebras. At first the numbers seemed to be matching with the number of connected planar maps with k edges, but the numbers diverged starting with compositions of 6. Paths in the poset correspond to certain tableaux. If  $p_{\alpha}$  is the number of paths from the unique composition of 0 to a given composition  $\alpha$ , and if  $\tilde{\alpha}$  is the partition corresponding to  $\alpha$ , then  $\sum_{\alpha:\tilde{\alpha}=\lambda} p_{\alpha} = \dim S^{\lambda}$ , where  $S^{\lambda}$  is the Specht module labelled by  $\lambda$ . It is an interesting problem to look for patterns in these path numbers and for a possible analogue of the hook length formula.

#### Group V: Möbius Function of the QSYM Poset

Members: Heather Dye, Patricia Hersh, Karola Meszaros, Bridget Tenner, Lauren Williams

The group studied an analogue of Young's lattice, determining the Möbius function and homotopy type of each interval. The posets considered were recently introduced by Christine Bessenrodt, Kurt Luoto, and Stephanie van Willigenburg [2] in their development of a Pieri Rule for noncommutative symmetric functions (NSYM). A composition v covers a composition u in this poset if multiplication of the composition u by a single box yields a positive combination of compositions in which v appears with a positive coefficient. The group became interested in the question of how strong an analogy exists between these posets and the Pieri Rule poset for traditional symmetric functions, namely Young's lattice.

Unlike Young's lattice, these new posets are not distributive lattices, are not lattices, and in fact are not shellable (or even Cohen-Macaulay). Nonetheless, the group proved that each interval is homotopy equivalent to a ball or sphere using lexicographic discrete Morse functions. This implies that the Möbius function of each interval is 0, 1 or -1, something these posets do have in common with Young's lattice (where again each interval is homotopy equivalent to a ball or a sphere).

Another result shown during the workshop was a closed form description of which pairs of elements u, v satisfy u less than or equal to v. The previous description by [2] was of the covering relations, and did not make apparent which pairs u, v would be comparable. Further collaboration on a closely related poset, one giving the Pieri Rule for quasisymmetric functions is planned for the near future. Ongoing group work involves collecting Möbius function data using Stembridge's posets software package. The group expects to complete a paper this summer with an analysis of the NSYM poset, and hopefully also the QSYM poset.

In a different direction, two members of the group (Patricia Hersh and Lauren Williams) also continued work in their ongoing collaboration to determine the homeomorphism type of the totally nonnegative part of the Grassmannian. In particular, they identified further properties of reduced expressions for permutations that are needed to extend to the setting of Postnikov's plabic graphs, and made definite progress towards the proofs. They also analyzed fibers over 0-cells in Postnikov's map from a polytope of plabic graphs to the totally nonnegative part of the Grassmannian. The time at BIRS provided a good opportunity for them to make further headway on this fairly involved project.

#### **Group VI: Chip Firing**

Members: Melody Chan, Caroline Klivans, Megan Owen, Josephine Yu

A chip firing game consists of a graph with its vertices labelled by integers, which can be thought of as the number of chips allocated to that vertex, along with a distinguished vertex called the *bank*. A vertex *fires* by sending one chip to each of its neighbouring vertices. Two group members, Josephine Yu and Caroline Klivans, were already interested in different variations of the chip firing game, so they first presented their work, and then the group focused on a generalization of the chip firing game to a higher dimensional complex, instead of a graph.

Josephine Yu told the group about a variant of the chip firing game, in which the underlying graph has lengths on its edges, and the definition of chip firing moves is expanded to make them equivalent to the set of *tropical rational functions* on that metric graph [7]. In this scenario, the set of all chip firing moves that makes a chip configuration non-negative forms a *tropical linear system* or *tropical module*. The set of all such functions also forms a cell complex.

Caroline Klivans explained the *dollar game*, in which the bank is the only vertex allowed a negative value and can only fire when no other vertex can fire. A chip configuration is *stable* when only the bank can fire, *recurrent* when there exists some sequence of fires that bring the configuration back to this starting one, and *critical* when it is both stable and recurrent. The set of critical configurations is particularly interesting, because it forms a finite Abelian group, called the *critical group* (or *sandpile group* or *Picard group*), which is isomorphic to the quotient group of  $\mathbb{Z}^{n-1}$  modulo the reduced Laplacian. Using this definition of the critical group, it is possible to generalize these results to higher dimensional simplicial complexes [6]. However, in this context, the original meaning of a critical configuration is lost.

The group spent the remaining group time trying to figure out a combinatorial definition of a critical configuration in this higher dimensional setting. In particular, to bridge the two perspectives, they tried to generalize the idea of tropical rational functions on a graph to tropical rational functions on a simplicial

complex.

#### Group VII: Flag Homology Spheres and the Gamma Vector

Members: Margaret Bayer, Margaret Readdy, Michelle Wachs

The group used Gal's conjecture as a starting point for their discussions. Recall that for an *n*-dimensional simplicial complex with its *h*-vector encoded as the polynomial  $h(t) = h_0 + h_1 t + \cdots + h_n t^n$ , the gamma vector  $\gamma = (\gamma_0, \ldots, \gamma_n)$  is defined by the change of basis formula

$$h(t) = \sum_{i=0}^{n} \gamma_i \cdot t^i (1+t)^{n-2i}.$$

In 2005 Gal conjectured that for flag homology spheres the entries of the  $\gamma$ -vector are nonnegative. There are five questions the group is pursuing.

- 1. Which *h*-vectors occur from flag homology spheres? A special case is to first study simplicial polytopes whose Stanley-Reisner ring has its face ideal generated by squarefree degree 2 monomials.
- 2. It is known that flag homology spheres occur from the operations of taking the barycentric subdivision of a flag homology sphere or by barycentrically subdividing an edge of a flag homology sphere. Do these two operations capture all flag homology spheres?
- 3. Given a  $\gamma$ -vector with entries  $\gamma_i \ge 0$ , i = 0, ..., n, construct a poset whose order complex has that  $\gamma$ -vector.
- 4. Given a flag homology sphere not arising from the order complex of a poset, is there another poset construction or generalization of the order complex construction?
- 5. It is known that substituting  $\mathbf{cv} = \mathbf{1}$  and  $\mathbf{dv} = \mathbf{2t}$  into the cd-index of an Eulerian poset P recaptures the gamma vector of the order complex of P. Purtill showed the coefficients of the cd-index of the face lattice of the n-simplex and the n-cube enumerate the "cd-variation" of André and signed André polynomials. Do the resulting coefficients of the  $\gamma$ -vector in these two cases have meaning?

#### **Group VIII: Quantum Schubert Calculus**

*Members:* Elizabeth Beazley, Anna Bertiger, Nicole Lemire, Anne Shepler, Kelli Talaska, Julianna Tymoczko The group studied a problem in quantum Schubert calculus. The goal was to better understand the quantum cohomology ring of G/B for groups G of all types. The tools available are using the isomorphism

$$QH^*(G/B) \simeq H^*(G/B) \otimes_{\mathbb{Z}} \mathbb{Z}[q_1, \dots, q_r]$$

and the fact that  $H^*(G/B)$  has a basis of the Schubert classes, indexed by the Weyl group of G. The big open problem in quantum Schubert calculus is to find the closed formulas for the numbers  $c_{u,v}^w$  and monomials  $q^d = q_1^{d_1} \cdots q_r^{d_r}$  such that

$$\sigma_u * \sigma_v = \sum_{d,w} c^w_{u,v} q^d \sigma_w$$

Postnikov has provided a combinatorial formula for all the monomials  $q^d$  that appear with nonzero coefficient in any product  $\sigma_u * \sigma_v$  in terms of certain admissible paths in the quantum Bruhat graph in type A. Since  $QH^*(G/B)$  is isomorphic to  $\mathbb{Z}[q_1, \ldots, q_r][x_1, \ldots, x_r]/I_q^W$  where  $I_q^W$  is the ring of invariants under the action of the Weyl group W, the key was to define an explicit quantum Pieri rule. This week, the group produced a conjectural type-free quantum Pieri rule, from which a type-free admissibility condition and hence a closed combinatorial formula for the monomials  $q^d$  can easily be derived. Their conjecture matches the known formulas when specialized to type A, and the group's next step will be to test the conjecture in other types and then either modify or prove the conjecture. In future work, they would consider the case of G/P for an arbitrary parabolic subgroup P.

# **Outcome of the Meeting**

The organizers were inspired to propose this workshop after the highly successful "Connections for Women Workshop on Combinatorial Representation Theory and Representations of Finite Groups and Related Topics" at the Mathematical Sciences Research Institute in January 2008 and the "WIN" (Women in Numbers) Workshop at BIRS in November 2008. Both programs highlighted accomplishments of women researchers while introducing younger participants to role models, potential mentors and collaborators, and important problems in the field. We expect the momentum generated by "Algebraic Combinatorixx" to have long-lasting effects far beyond the 5-day meeting just as the "WIN" activities have continued since the time of their 2008 BIRS meeting and include a conference proceedings, special sessions at national and sectional AMS meetings, and continued collaboration. As yet another indication of the successful impact of "WIN" as well as the continued need, "WIN2: Women in Numbers 2" was among the 48 workshops chosen (out of 142 proposed) to be held at BIRS in 2011.

The long-term benefits of the Algebraic Combinatorixx workshop are expected to be an increase in the participation of women in research activities related to algebraic combinatorics and related fields, a research network of potential collaborators, and visibility and connectivity for younger researchers especially those at smaller colleges or isolated in departments not having a strong research presence in combinatorics. Given that almost two-thirds of the participants will have received their PhDs after 2001, they (and their experiences at this workshop) will play a critical role in shaping the field for a long time to come.

## **Testimonials**

The following quotes are taken from testimonials from workshop participants. Some participants comment on the mentoring component of the workshop; others mention the high level of talks; and others stress the importance of the working groups and successful research projects started while at BIRS.

The BIRS workshop greatly impacted my research. In general, over the past year I have wanted to begin a successful collaborative mathematical project in algebraic combinatorics, with an aim of broadening the scope of my active research beyond the immediate sphere of my thesis. Geographical and financial constraints make forging such collaborations difficult, and I am incredibly indebted to the organizers for helping to make this professional goal a reality during the BIRS workshop. In particular, there was a new project that I was interested in working on, for which I did not feel as though I was individually equipped with the requisite background. I proposed this problem to my designated research group, we generated a conjecture which would solve the problem, and we currently have a working draft of a joint paper. Of the four other group members, three of the four are individuals with whom I likely would not have had a chance to collaborate otherwise, and whose energy and expertise were vital to the movement of the project. My group members will certainly remain important contacts for me, and without the workshop several of these professional relationships would not have been made. Moreover, given more time at the workshop, I am confident that one or two additional collaborations might have begun, both with people in and outside of my designated working group. —

The participation in the workshop was an amazing experience. The quality of the talks was exceptional, and the discussion between talks was very lively; I met many mathematicians (in particular younger ones) whom I hadn't known before. The 'research in teams' initiated by the organizers will probably lead to a joint paper with members of the team; it was a fruitful discussion on quasisymmetric analogs of Schur P-functions which both are among my current research interests (apart from the organizer Steph van Willigenburg I had not met any other member of the team before). A talk of one of the principal speakers (Anne Schilling) on the rather new topic of k-Schur functions together with direct exchange on her data on k-Schur functions already led to a conjecture on the determinants of the corresponding tables and a refined one on the invariants; this is closely related to my own work on character tables of the symmetric groups. We have exchanged emails after the meeting and will keep in touch on these questions. A poster and short presentation by a younger participant (Kelli Talaska) on determinants for special graphs led to an exchange on determinants and invariants for paths in certain quiver algebras, where formulae of a similar structure occurred in work of mine; it is not clear yet

what can be learned from this observation. Also, data on the composition poset appearing in work with Steph van Willigenburg and collaborators were discussed also with Georgia Benkart; here, the question is whether the data helps in finding an algebra that is connected with the composition data. —

This was, by far, the best conference I have ever been to. Everything was organised as to maximize interactions between (junior and senior) participants. And it worked brilliantly! I have come back with several new research projects with new collaborators. More specifically, I have started a project with Rosa Orellana on the restriction/induction rules for the Partition algebra (and other diagram algebras). This should give a new approach to the longstanding problem of describing the Kronecker product of Schur functions. With my "working group" at the conference (Benkart, Vazirani, Parker, Orellana), we have started investigating possible representation theoretic interpretations of the quasi-Schur functions introduced by van Willigenburg, Mason, Bessenrodt and al. and we plan to continue this work in the coming months. Following my talk at the conference, I have also had very useful discussions with Georgia Benkart, who suggested new directions for my own work, such as investigating the representation theory of the derragement algebra, and the relationship between the decomposition of tensor space for the orthosymplectic super Lie algebra and the Brauer algebra. I would also like to mention another aspect of the conference which (indirectly) influences my research as well. I did not know there were so many women in this field. I usually only meet a few at conferences. And many of them face the same challenge of juggling research and family life. I felt really encouraged hearing about other (more senior) people's stories and sharing experiences. ----

Participation in the BIRS workshop Algebraic Combinatorixx led to new research ideas, new research collaborations, and meeting new people. This was a fantastic workshop, well scheduled to really take advantage of being at BIRS. We had many interesting talks, but also plenty of time dedicated to small working groups. This workshop had a secondary theme beyond the research topic. It was an all women's workshop and time was set aside for panel discussions and general group discussion of the issues and difficulties facing women in mathematics. I truly appreciate BIRS supporting this additional aspect of the workshop. It is hard to describe the need and positive effect such gatherings have for female mathematicians. Among other things, I was "re-charged" to come home and face the challenges that arose while I was away. —

I found this conference to be well-organised with a surprisingly refreshing format. The organisers decided to have more expository talks - from which one learns more anyhow and fewer talks in general in order to put an emphasis on group discussions. My particular group was a good mix of people from different backgrounds and stages in their career. Our group started a project in a area that is new to all of us but for which our common background allowed us to discuss. I learned quite a lot from these discussions as well as from the talks. We hope that a paper (at least one) will result from this collaboration and are in the process of working further on it. This collaboration most likely would not have started up without this conference. Although this workshop did not personally affect my job prospects as I am tenured, it was a valuable opportunity for mentoring as most of the participants were in the early stages of their career. I had some doubts about the all-woman format before attending, but was pleasantly surprised on how the whole thing worked out. I would say that it was one of the most effective workshops that I have attended and the organisers are to be congratulated. —

The workshop impacted my current research. In our group, we worked on quasi-symmetric Schur *P*-functions. We conjectured the formula for that and plan to work on more problems related to quasi-symmetric Schur *P*-functions. We hope to write a paper together. In this workshop I worked with some professor from Korea. This was the first time I could collaborate a Mathematician from a such far place. The workshop affected my job prospects. The other participants told us that women in Math usually are more productive as age grows. —

This was the best conference I have ever attended. The mathematics was superb, and I have started (at least) two new collaborative projects as a result. Additionally, the opportunity for panels and other discussions about women's issues in academia/mathematics was very valuable. I hope we can do this again!!! —

I generally do not like to rank events, but I must confess that if I was asked what is the best math workshop you ever attended, this would be it! I am so thankful for the opportunity you gave us to learn about some of the "hot topics" in combinatorics, as well as for this unique occasion to start new and exciting collaborations. I felt revived, and so much energised. I am so thankful that there are so generous and thoughtful people such as yourselves. Your services to the combintorics as well as the combinatorixx communities are immense! Let me know if you would need help for the next one! —

This was a fantastic workshop. The scholarship was outstanding. The focus on professional development was at an exceptionally high level. The research that I began during that workshop has continued with a dedication that I have never experienced in a research group this large, or from research arising out of an impromptu discussion. The professional contacts that I made and solidified promise to be exceedingly useful, both to my research and career more broadly (mine as well as theirs, I hope). The organizers are to be commended for the time, energy, and thoughtfulness that they put into this conference. I hope that BIRS will support more workshops of this form—I can only imagine the scientific impact if every research area had a group of organizers who could bring together women in their discipline this effectively. —

Every time I have the opportunity to attend BIRS I have an outstanding experience. This workshop was no exception. The opportunity to meet a wide range of women algebraic combinatorialists led to my making many new valuable contacts across the globe. Furthermore the breadth of talks and high quality of exposition meant that I cemented a number of concepts and deepened my knowledge of many more. The poster sessions for graduate students helped them to bring their research to the attention of many senior mathematicians, and the panels gave much valuable insight to life in academia for all participants. One of the most amazing aspects of the workshop was the collaboration groups, which brought together researchers of similar interests in groups to discuss open problems. By the end of the workshop at least four papers were originated (my group included), with the amenities that BIRS provides being crucial to the success of these projects: breakout rooms to work in, the library for resources, the lounge for continuing discussions late into the night, the mealtimes for swapping ideas with other groups. As an organizer, I was thrilled to hear from a number of participants that this was the best conference they had \*ever\* attended, and that BIRS was a fundamental contributor to this.

# **Future Plans**

We expect to maintain a web site and mailing list so that communication and collaboration can continue far beyond the five days of the workshop. Many of the groups continue to work on the projects begun at BIRS and several papers are expected to result from these collaborative efforts. Plans were discussed for possible future meetings and for subsets of the participants to meet in research groups either via teleconferencing or by research visits.

# Acknowledgments

We acknowledge with gratitude the hospitality of the Banff International Research Station and wonderful assistance from its staff and the funding received from National Science Foundation grant #DMS-1101740.

# **List of Participants**

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# Chapter 19

# KAM theory and Geometric Integration (11w5132)

# Jun 05 - Jun 10, 2011

**Organizer(s):** Walter Craig (McMaster University) Erwan Faou (Ecole Normale Superieure de Cachan Bretagne) Benoit Grebert (Universite de Nantes, France)

## **Overview of the Field**

The main goal of this meeting was to bring together people working on the qualitative behavior of solutions of Hamiltonian systems (ordinary differential equations and partial differential equation) both from the theoretical and numerical points of view.

The motivation for this workshop came from some recent developments both from the theoretical and numerical sides done essentially on the qualitative analysis of Hamiltonian Partial differential equations, of highly oscillatory systems. The principal equations of mathematical physics, whether it is quantum mechanics, Bose – Einstein condensates, molecular dynamics, ocean waves, the *n*-body problem of celestial mechanics, or Einstein's equations in general relativity, are in fact Hamiltonian dynamical systems when viewed in the proper coordinates. This implies many important dynamical features such as energy and volume preservation, conservation of adiabatic invariants over long time, and existence of periodic orbits. In the particular case of PDEs, major advances have been recently made in this *qualitative* long time analysis and this is a very active field of research (see for instance [3, 20, 2, 8] and the references therein).

The numerical simulation of such systems - and in particular the qualitative behavior of numerical schemes - is of major importance from the point of view of the applications (molecular dynamics and drug design, wave propagations, etc...). In this direction, the *Geometric numerical integration* theory (see for instance [17, 21] in the finite dimensional case (*i.e.* for ordinary Hamiltonian differential equations as appearing in classical mechanics) has now reached a very good level of maturity and some situations are completely understood. For example the use of a *symplectic numerical integrator* applied to a Hamiltonian system ensures the existence of a *modified energy*. However this very important result known as *backward error analysis* cannot be applied directly to Hamiltonian Partial differential equations or highly oscillatory systems where the presence of high frequencies can lead to instabilities.

These observations lend weight to the mathematical point of view that the topics of dynamical systems and nonlinear partial differential equations should be considered to be cousins, and have a lot in common. In particular this point of view has lead to the consideration of the global behavior of orbits of a Hamiltonian PDE in an appropriate phase space, the pursuit of the mathematical technology of normal forms, the study of stable orbits and KAM tori, possibly of infinite dimension, and a number of results analogous to Nekhoroshev stability and Arnold diffusion. Over the past decade there has been a number of important contributions to this point of view from a theoretical standpoint.

On the other hand, it is a very important direction of research to adapt the point of view of Hamiltonian dynamics to numerical simulations of (at least some of) the physical phenomena mentioned above. Some major past achievements include developments of symplectic numerical integrator routines, and their use in fluid mechanics and large scale particle dynamics computations. The focus of this workshop at BIRS was to bring the Hamiltonian PDE and the scientific computing communities together, to reflect on future common directions of research, to encourage the development of numerical methods to effectively model the evolution of continuum systems possessing infinitely many degrees of freedom, and to communicate the most up-to-date theoretical and numerical research.

# Workshop organization

The talks given during the workshop have reflected the mixed nature of the audience. We have tried to schedule theoretical and numerical talks every day, rather that having full sessions dedicated to one particular topic.

Most of the participants played the game, and tried to make survey talks explaining the particular problems and difficulties they encounter in their work, rather that focusing on specific technical difficulties and feats. We refer to the appendix for the abstract of the talks given during the workshop.

Dividing now the talks into "theoretical" and "numerical", we can group them as follows:

#### Theoretical talks

- Dario Bambusi (Univ. Milano) Asymptotic stability of solitary waves in dispersive equations
- Mohammed Lemou (CNRS & Univ. Rennes) Orbital Stability of Spherical Galactic Models
- Stephen Gustafson (Univ. Vancouver) Global symmetric Schrödinger maps
- Laurent Thomann (Univ. Nantes) Resonant dynamics for the quintic non linear Schrödinger equation
- Thomas Kappeler (Univ. Zürich) NLS & KAM
- Yannick Sire (Univ. Marseille) KAM theory for whiskered tori on lattices
- Rafael de la Llave (Univ. Texas) An a-posteriori KAM theorem for whiskered tori for some ill-posed Hamiltonian PDE
- Philippe Guyenne (Univ. Delaware) A Hamiltonian higher-order NLS equation for surface gravity waves
- Renato Calleja (Univ. McGill) KAM theory for dissipative systems: from rigorous results to numerics

#### Numerical talks

- Ernst Hairer (Univ. Geneva) Modulated Fourier expansions
- Chus Sanz-Serna (Univ. Valladolid) Numerical mathematics and the method of averaging
- Florian Méhats (Univ. Rennes) Stroboscopic averaging for highly oscillating nonlinear Schrödinger equations
- Zaijiu Shang (Acad. Sci. Beijing) Numerical Stability of Hamiltonian Systems by Symplectic Integration
- Carles Simó (Universitat de Barcelona) Jet transport and applications
- Melvin Leok (Univ. California at San Diego) General Techniques for Constructing Variational Integrators
- Weizhu Bao (Univ. Singapore) Modeling, analysis and simulation for degenerate dipolar quantum gas

- Fleur McDonald (Massey Univ.) Travelling Wave Solutions for Multisymplectic Discretisations of Wave Equations
- Alexander Ostermann (Univ. Innsbruck) Meshfree integration of evolution equations

Of course, some talks were already made of mixed theoretical/numerical results: either by presenting very theoretical aspects of geometric integrators (modulated Fourier theory, stroboscopic averaging), or by showing numerical simulations to illustrate theoretical results (water-wave equations for instance).

Concerning the management of the sessions, the organizers were particularly satisfied by the discussions raised after almost every talks. It always opened very interesting and stimulating conversations, often concerning possible new scientific links, for instance between numerical averaging, backward error analysis and Nekhoroshev estimates in the finite dimensional case, or the analogy between rigid body integrators and the Schrödinger map equation, and on the notion of numerical integration of periodic or quasi periodic solutions to Hamiltonian PDEs (solitary waves, resonant systems).

# Highlights

We would like to emphasize some recurrent themes that appeared in our discussions. Essentially, they can be divided into two directions.

#### • Can geometric integrators yield to theoretical advances?

Let us recall that a *geometric integrator* (see for instance [17, 21]) is a numerical method that tries to reproduce the qualitative behavior of a dynamical system rather than approximating precisely one single trajectory. This is of particular importance for Hamiltonian systems for which the long time behavior of solutions is driven by the existence of invariants (the Hamiltonian energy, adiabatic invariant in highly oscillatory systems) or the presence of resonances. In the finite dimensional case, the well known *backward error analysis* theory (see [17, Chapter IX] and the references therein) shows that the numerical discrete trajectory associated with a *symplectic integrator* applied to a Hamiltonian system can be interpreted as the exact continuous solution of a *modified* Hamiltonian system, over very long time. This results implies that the long time evolution observed on the computer is NOT the exact solution of the Hamiltonian system.

What can we learn from numerics? Extensive simulation has now become a powerful tool to analyze the qualitative behavior of dynamical systems, particularly in infinite dimension (Partial differential equations). But the transfer from numerical observations to new mathematical proofs for the exact system has to be made very carefully, based on the fact that the observed qualitative behavior is made on the modified Hamiltonian which may include extra resonance phenomenons of on the other hand regularization effects. This is particularly the case for Hamiltonian PDEs where the space discretization induces by nature a regularization in the high frequencies.

Many works remain to be done in this direction. To be helpful from the theoretical point of view, the analysis of the geometric integrators has to be performed at the highest level from the mathematical analysis point of view.

#### What makes geometric integrators work?

As we have seen above, geometric integrators can be considered as a tool for finding new nonlinear phenomenons. On the other hand, many recent studies on nonlinear Hamiltonian PDEs can be used to derive new geometric integrators, or can help in the understanding of the capacities and limits of traditional numerical methods widely used in applied mathematics. For example the reproduction of stability phenomenons for solitary waves in Hamiltonian PDEs is not guaranteed by the simple use of symplectic methods, and the understanding of the continuous stability mechanisms (particularly for high regularity perturbation) could lead to invent new stable integrators which might not belong to the standard class of numerical integrators in general situations. Another example is given by the Schrödinger map equation whose particular symplectic structure might require the invention of new efficient numerical integrators.

More generally, the understanding of the long time behavior of numerical integrators cannot be dissociated from the most recent advances in nonlinear PDEs. For example in the case of the integrable nonlinear Schrödinger equation in dimension one, a natural question would be to analyze the possible preservation of the integrable nature of the equation by numerical schemes (existence of numerical Lax pairs?).

Another very important issue in the long time simulation of dynamical systems is the influence on round-off errors, which might lead to wrong conclusion when trying to study the chaotic nature of a dynamical system over long time. Try to overcome this difficulty is a very difficult question appearing in the long time simulation of the solar system in astronomy, but which is also present in fluid simulations or in quantum mechanics.

In a similar way, the numerical discretization of three-dimensional Bose-Einstein condensates is an ongoing high-performance computing challenge which is closely related to topical questions on the Gross-pitaevskii equations, Hermite polynomials and sparse approximations of Hamiltonian PDEs. This is a hot topic that should know many advanced in the next years both from the theoretical and numerical point of view.

Finally, the delicate question of numerical resonance has been addressed many times, as it is always difficult to separate the resonant effects induced by the continuous system from the resonances created by the discretization itself (discrete time step, aliasing, etc..). Taking into account these effects is surely a crucial step to invent new efficient integrators, or at least to have a good idea of the domain of validity of classical integrators.

# Conclusion

Organizing such a mixed workshop between two different community always constitutes a challenge both for the organizers and the participants. We hope that the participants took benefit in many discussions with mathematicians from another community during the whole week. This surely brought participants to new possible interactions. The BIRS was a perfect place for organizing such a meeting, and we hope that we will be able to organize again such meeting in some next future.

# Appendix: Abstracts of the talks

#### Speaker: Weizhu Bao (National University of Singapore)

#### Title: Modeling, analysis and simulation for degenerate dipolar quantum gas

Abstract: In this talk, I will present our recent work on mathematical models, asymptotic analysis and numerical simulation for degenerate dipolar quantum gas. As preparatory steps, I begin with the three-dimensional Gross-Pitaevskii equation with a long-range dipolar interaction potential which is used to model the degenerate dipolar quantum gas and reformulate it as a Gross-Pitaevskii-Poisson type system by decoupling the two-body dipolar interaction potential which is highly singular into short-range (or local) and long-range interactions (or repulsive and attractive interactions). Based on this new mathematical formulation, we prove rigorously existence and uniqueness as well as nonexistence of the ground states, and discuss the existence of global weak solution and finite time blowup of the dynamics in different parameter regimes of dipolar quantum gas. In addition, a backward Euler sine pseudospectral method is presented for computing the ground states and a time-splitting sine pseudospectral method is proposed for computing the dynamics of dipolar BECs. Due to the adaption of new mathematical formulation, our new numerical methods avoid evaluating integrals with high singularity and thus they are more efficient and accurate than those numerical methods currently used in the literatures for solving the problem. In addition, new mathematical formulations in twodimensions and one dimension for dipolar quantum gas are obtained when the external trapping potential is highly confined in one or two directions. Numerical results are presented to confirm our analytical results and demonstrate the efficiency and accuracy of our numerical methods. Some interesting physical phenomena are discussed too.

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#### Speaker: Dario Bambusi (University of Milano)

Title: Asymptotic stability of solitary waves in dispersive equations.

Abstract: We consider the subcritical Hamiltonian NLS in  $\mathbb{R}^3$ ; it is well known that under suitable assumptions on the nonlinearity it admits a family of travelling solitary waves which are orbitally stable. We prove that generically they are asymptotically stable.

The result was known when the Floquet spectrum of the soliton has no non trivial eigenvalues. It is here extended to the general case.

The proof (which is developed in an abstract framework) is based on the combination of Hamiltonian and dispersive techniques. The main technical difficulties one has to face are related to the fact that the generators of the symmetry are unbounded operators. This obliges to develop Marsden-Weinstein reduction theory when the group action is only continuous and normal form theory when the generating vector field is not smooth. This also causes some difficulties for dispersive estimates. Such difficulties are solved using recent results by Parelman and Beceanu on Strichartz estimates for time dependent potentials.

#### Speaker: Renato Calleja (University of Delaware)

#### Title: A numerically accessible criterion for the breakdown of quasi-periodic solutions

Abstract: We formulate and justify rigorously a numerically efficient criterion for the computation of the analyticity breakdown of quasi-periodic solutions in Symplectic maps and 1-D Statistical Mechanics models. Depending on the physical interpretation of the model, the analyticity breakdown may correspond to the onset of mobility of dislocations, or of spin waves (in the 1-D models) and to the onset of global transport in symplectic twist maps. The criterion we propose here is based on the blow-up of Sobolev norms of the hull functions. The justification of the criterion suggests fast numerical algorithms that we have implemented using Fourier methods in several examples.

#### Speaker: Stephen Gustafson (University of British Columbia)

#### Title: Global symmetric Schrödinger maps

Abstract: I will describe some results on singularity (non-)formation and stability, in the energy-critical 2D setting, for a nonlinear Schroedinger equation of geometric and physical (ferromagnetism) origin – the Schroedinger map. In particular, radial solutions are global. This is joint work with Eva Koo.

#### Speaker: Philippe Guyenne (University of Delaware)

#### Title: A Hamiltonian higher-order NLS equation for surface gravity waves

Abstract: We present a systematic and consistent Hamiltonian approach to nonlinear modulation of surface water waves on arbitrary depth, both in two and three dimensions. It is based on the reduction of the problem to a lower-dimensional system involving surface variables alone. This is accomplished by introducing the Dirichlet–Neumann operator which gives the normal fluid velocity at the free surface, and expressing it as a Taylor series in terms of the surface elevation. In this framework, we derive new Hamiltonian envelope models describing the weakly nonlinear modulation of quasi-monochromatic surface gravity waves both on

finite and infinite depth. In particular, we derive Hamiltonian versions of Dysthe's equation which is valid at one order higher than the cubic NLS equation. In the deep-water case, we analyze the stability properties of our Hamiltonian Dysthe equation regarding the Benjamin–Feir instability of a Stokes wave, and compare them with existing non-Hamiltonian results. We also perform numerical simulations using a symplectic time integrator, to test these stability results as well as to check the conservation of the Hamiltonian.

This is joint work with W. Craig (McMaster University) and C. Sulem (University of Toronto).

#### Speaker: Ernst Hairer (University of Geneva)

#### Title: Modulated Fourier expansions

Abstract: The theory of modulated Fourier expansions has its origin in the study of the long-time behaviour of numerical integrators when standard backward error analysis cannot directly be applied due to the presence of high oscillations. The main idea is to separate fast oscillatory motion from slow dynamics in the solution. It is successfully applied to yield information over long times for the analytic solution of the differential equation as well as for the numerical solution obtained by suitable discretizations.

New insight is gained for the numerical energy conservation in Hamiltonian systems that are perturbations of highly oscillatory harmonic oscillators. In the case of several high frequencies, resonance plays an important role. Closely connected is the near conservation of oscillatory energies.

Modulated Fourier expansions also allow to explain long-time regularity of solutions for non-linearly perturbed wave equations. The techniques carry over to numerical discretizations, which results in an understanding of the long-time near-conservation of energy, momentum, and harmonic actions. The ideas can also be applied to get insight into the distribution of mode energies over long times, when the initial data are small and concentrated in one Fourier mode.

Yet another application of the technique of modulated Fourier expansions is for the Fermi-Pasta-Ulam (FPU) problem. Insight into the long-time dynamics is obtained for small initial data, where only a few low frequency modes are excited. Suitable numerical discretizations retain the correct qualitative behaviour.

This is a joint-work with Christian Lubich. Parts of it are in collaboration with David Cohen, Ludwig Gauckler, and Daniel Weiss.

#### Speaker: Thomas Kappeler (University of Zürich)

#### Title: NLS & KAM

Abstract: In this talk I will survey recent results on the normal form of the defocusing and focusing NLS and its applications.

#### Speaker: Mohammed Lemou (CNRS & University of Rennes 1)

#### Title: Orbital Stability of Spherical Galactic Models.

Abstract: We consider the three dimensional gravitational Vlasov Poisson system which is a canonical model in astrophysics to describe the dynamics of galactic clusters. A well known conjecture is the stability of spherical models which are nonincreasing radially symmetric steady states solutions. This conjecture was proved at the linear level by several authors in the continuation of the breakthrough work by Antonov in 1961. In a previous work, we derived the stability of anisotropic models under spherically symmetric perturbations using fundamental monotonicity properties of the Hamiltonian under suitable generalized symmetric rearrangements first observed in the physics literature. In this work, we show how this approach combined with a new generalized Antonov type coercivity property implies the orbital stability of spherical models under general perturbations.

#### Speaker: Melvin Leok (University of California - San Diego)

#### Title: General Techniques for Constructing Variational Integrators

Abstract: The numerical analysis of variational integrators relies on variational error analysis, which relates the order of accuracy of a variational integrator with the order of approximation of the exact discrete Lagrangian by a computable discrete Lagrangian. The exact discrete Lagrangian can either be characterized variationally, or in terms of Jacobi's solution of the Hamilton–Jacobi equation. These two characterizations lead to the Galerkin and shooting-based constructions for discrete Lagrangians, which depend on a choice of a numerical quadrature formula, together with either a finite-dimensional function space or a one-step method. We prove that the properties of the quadrature formula, finite-dimensional function space, and underlying one-step method determine the order of accuracy and momentum-conservation properties of the associated variational integrators. We also illustrate these systematic methods for constructing variational integrators with numerical examples.

#### Speaker: Rafael de la Llave (University of Texas)

#### Title: An a-posteriori KAM theorem for whiskered tori for some ill-posed Hamiltonian PDE.

Abstract: We develop a framework to study whiskered tori in some Hamiltonian PDE. We formulate an equation that is satisfied by the parameterization of the solution and its whiskers and show that if there is aan approximate solution, that satisfy some non-degeneracy conditions, then there is a true solution close by. The abstract theory applies to several ill-posed equations that were proposed as models for water waves by Boussinesq. This is joint work in progress with Yannick Sire.

#### Speaker: Fleur McDonald (Massey University)

#### Title: Travelling Wave Solutions for Multisymplectic Discretisations of Wave Equations.

Abstract: Symplectic integrators for Hamiltonian ODEs have been well studied over the years and a lot is known about these integrators. They preserve the symplecticity of the system which automatically preserves other geometric properties of the system, such as a nearby Hamiltonian and periodic and quasiperiodic orbits. It is then natural to ask how this generalises to Hamiltonian PDEs, which leads us to the concept of multisymplectic integration. We ask how well do multisymplectic integrators capture the long time dynamics of multi-Hamiltonian PDEs? As multi-Hamiltonian PDEs possess travelling wave solutions, we wish to see how well multisymplectic integrators preserve these types of solutions. This will give us an idea of how well the multisymplectic integrator is replicating the dynamics of the PDE.

#### Speaker: Florian Méhats (University of Rennes 1)

#### Title: Stroboscopic averaging for highly oscillating nonlinear Schrodinger equations

Abstract: We present a numerical method that enables to integrate highly oscillating nonlinear Schrodinger equations without resolving the fast oscillations in time. This method is based on the so-called stroboscopic averaging, which constructs an averaged dynamics that possesses the following properties : this differential system is still Hamiltonian and its solution coincides with the solution of the initial problem at the stroboscopic points. The stroboscopic averaging method (SAM) integrates numerically the averaged system without using its analytical expression. This is a joint work with F. Castella, P. Chartier and A. Murua

#### Speaker: Alexander Ostermann (University of Innsbruck)

#### Title: Meshfree integration of evolution equations

Abstract: For the numerical solution of time-dependent partial differential equations, a class of meshfree exponential integrators is proposed. These methods are of particular interest in situations where the solution of the differential equation concentrates on a small part of the computational domain which may vary in time. For the space discretization, radial basis functions with compact support are suggested. The reason for this choice are stability and robustness of the resulting interpolation procedure. The time integration is performed with an exponential Rosenbrock method or an exponential splitting method. The required matrix functions are computed by Newton interpolation based on Leja points. The proposed integrators are fully adaptive in space and time. Numerical examples that illustrate the robustness and the good stability properties of the method are given. This is joint work with Marco Caliari, Verona and Stefan Rainer, Innsbruck.

#### Speaker: Chus Sanz-Serna (University of Valladolid)

#### Title: Numerical mathematics and the method of averaging

Abstract: We shall explain ho to perform averaging analytically throught the combinatorial techniques now used to study the properties of numerical integrators. The novel approach systmatizes the derivation of high-order averaged systems. This is a joint work with Ph Chartier and A Murua.

#### Speaker: Zaijiu Shang (Chinese Academy of Sciences, Beijing)

Title: Numerical Stability of Hamiltonian Systems by Symplectic Integration

Abstract: Symplectic numerical integration theory for Hamiltonian systems has been developed rapidly in recent twenty five years. The recent monographs [1] and [2] summarize the main developments and important

results of this theory. Qualitative behavior of symplectic integrators applied to Hamiltonian systems has been investigated by many authors. Some stability results either in the spirits of the KAM theory or based on the backward analysis have been well established. The typical stable dynamics of Hamiltonian systems, e.g., quasi-periodic motions and their limit sets — minimal invariant tori, can be topologically preserved and quantitatively approximated by symplectic integrators. In this talk I give a brief review about old results and some new studies. The main emphasis is on the understanding of stability of Hamiltonian systems by symplectic numerical integration in the framework of KAM theory and backward analysis theory.

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#### Speaker: Carles Simó (University of Barcelona)

#### Title: Jet transport and applications

Abstract: Many problems in dynamics require the knowledge of the local dependence of some orbits on the changes of initial conditions and/or parameters. As an example we can mention bifurcations, integrability conditions, checking KAM conditions, etc. This can require some symbolic manipulation to obtain, e.g., a suitable normal form and it is relatively easy when dealing with the behavior around a given point.

However, when this is desired around some orbit which is known only numerically, like a periodic orbit not known analytically, one has to obtain information from variational equations and, possibly, higher order variational equations. This can be systematically carried out by transporting a jet at the desired order along the orbit. The method can be based on any numerical integrator, but it is specially convenient to use high order Taylor methods.

Some applications will be done to checking integrability conditions, to the applicability of KAM theorem and to the next passage of asteroid Apophis. Part of this work has been done with R. Martínez [3,4] and T. Kapela [2] and other coworkers [1]. The computations can be converted into rigorous proof by using standard CAP (Computer Aided Proofs) techniques.

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#### Speaker: Yannick Sire (University of Marseille)

Title: KAM theory for whiskered tori on lattices

Abstract: I will report on some joint work with E. Fontich and R. de la Llave about the construction of quasiperiodic and almost-periodic solutions on lattices. I will develop an a posteriori KAM theory, which does not require the reduction to action-angle variables and does not need transformation theory.

Speaker: **Laurent Thomann** (University of Nantes) Title: *Resonant dynamics for the quintic non linear Schrödinger equation*  Abstract: We consider the quintic nonlinear Schrödinger equation on the circle. We prove that the solution corresponding to an initial datum built on four Fourier modes which form a resonant set have a non trivial dynamic that involves periodic energy exchanges between the modes initially excited. It is notable that this nonlinear phenomena does not depend on the choice of the resonant set. The dynamical result is obtained by calculating a resonant normal form up to order 10 of the Hamiltonian of the quintic NLS and then by isolating an effective term of order 6. Notice that this phenomena can not occur in the cubic NLS case for which the amplitudes of the Fourier modes are almost actions, i.e. they are almost constant.

# **List of Participants**

Bambusi, Dario (University of Milano) Bao, Weizhu (National University of Singapore) Calleja, Renato (McGill University) Cohen, David (University of Basel) Craig, Walter (McMaster University) de la Llave, Rafael (University of Texas at Austin) Dujardin, Guillaume (INRIA Lille Nord-Europe) Faou, Erwan (Ecole Normale Superieure de Cachan Bretagne) Figueras, Jordi-Lluis (Universitat de Barcelona) Grebert, Benoit (Universite de Nantes, France) Gustafson, Stephen (University of British Columbia) Guyenne, Philippe (University of Delaware - Department of Mathematical Sciences) Hairer, Ernst (University of Geneva) Imekraz, Rafik (University Paris Dauphine) Kappeler, Thomas (University of Zurich) Lemou, Mohammed (CNRS and University of Rennes) Leok, Melvin (University of California, San Diego) McDonald, Fleur (Massey University Manawatu) Mehats, Florian (Universite Rennes) Ostermann, Alexander (University of Innsbruck) **Paturel, Eric** (University of Nantes) Penati, Tiziano (University of Milan) Sanz-Serna, J M (Universidad de Valladolid Spain) Shang, Zaijiu (Chinese Academy of Sciences) Simo, Carles (Universitat de Barcelona) Sire, Yannick (Universite Paul Cezanne) Thomann, Laurent (University of Nantes) Vilmart, Gilles (Ecole Polytechnique Féérale de Lausanne)

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# Chapter 20

# **Triangulated categories and applications** (11w5009)

# Jun 12 - Jun 17, 2011

**Organizer(s):** Paul Balmer (University of California Los Angeles (UCLA)) Dan Christensen (University of Western Ontario (UWO)) Amnon Neeman (Australian National University)

# **Overview of the Field**

The best way to think of triangulated categories is as a powerful technical tool which has had amazing applications over the last 30 years. Homological algebra was first introduced quite early in the 20th century, and by the 1950s the subject was viewed as fully developed: so much so that the authoritative book, by Cartan and Eilenberg, dates from this decade, and until recently no one bothered to write an update. Around 1960 Grothendieck and Verdier introduced a new twist (triangulated categories), a refinement no one expected. It took about 20 years before people started realizing the power of the method, and in the last 30 years the applications have reached corners of mathematics no one would have foreseen. In organizing the conference we tried to bring in people from diverse fields, who use triangulated categories in their work, to give them a chance to interact. Many of the participants told us it was the best conference they had been to in a long lime.

# **Recent Developments and Open Problems**

It's hard to know where to begin, there has been so much recent progress and it's been all over the place. Some of the progress has been on foundational questions, such as Brown representability [27, 11, 26, 5] and understanding the Balmer spectrum [1, 2, 4] of a tensor triangulated category. There has been considerable progress in understanding *t*-structures on various derived categories, for example the theory of Bridgeland stability conditions [8, 9, 10]. There are several theorems about obstructions to finding model structures for triangulated categories, examples of categories without model structures [25], and theorems telling us about the existence and uniqueness of model structures for large classes of triangulated categories [28, 23]. There has been major progress in computing the Balmer spectrum [3], as well as generalizations to categories with coproducts and applications in the specific cases [6, 7]. There has also been progress on applying triangulated categories to mathematical physics [12, 20, 21, 22] and to the study of  $C^*$ -algebras [24].

Every bit of progress opens up a myriad new questions, the very fact that we are making so much progress is evidence of how little we know.

## **Presentation Highlights**

We began the conference with three very introductory presentations: we decided that, for such a diverse audience, there was a need to have experts present an overview of how their field finds triangulated categories relevant. Somewhat arbitrarily we decided to split up the applications into three broad areas: Mark Hovey talked about topology, Yujiro Kawamata introduced algebraic geometry, and Henning Krause spoke about representation theory. Of course this leaves out many of the fields to which triangulated categories are applied, but we couldn't very well have a conference that was just a string of introductory talks.

In choosing the speakers we kept diversity in mind; we tried to have as many fields as possible represented, and specifically asked each speaker to bear in mind that he or she will be addressing an audience most of whom know nothing about their specialty. As already mentioned, the participants were enthusiastic about the outcome.

Ralf Meyer and Ivo Dell'Ambrogio gave talks with a  $C^*$ -algebra perspective, Gonçalo Tabuada introduced us to how to reframe a whole bunch of conjectures in terms of suitable model liftings of triangulated categories and their localizations. Neil Strickland talked about the right axiomatization of tensor products in triangulated categories. Greg Stevenson and Srikanth Iyengar both gave talks about two (quite different) generalizations of the Balmer spectrum to infinite triangulated categories, that is to ones with coproducts, and each gave examples of applications. Jon Carlson and Julia Pevtsova both talked about applications to representation theory and group cohomology. Sabin Cautis and Tony Licata talked about categorified representation theory and the triangulated categories that arise there. John Greenlees told us about cohomological descriptions of complete intersection, with a derived category tilt. Brooke Shipley presented results on the equivariant version, where the group G is a compact Lie group; this improves on work by Greenlees in the special cases where G is either a finite group or the group  $S^1$ . Don Stanley gave a talk about the progress made in the attempts to classify t-structures in certain interesting cases. Fernando Muro told us about the current confused status of our understanding of Brown representability, including the (published) theorem of Rosický that unfortunately happens to be false and counterexamples to it. Wendy Lowen and Amnon Yekutieli each gave a talk about (totally different) results of interest in non-commutative algebraic geometry. And finally Daniel Murfet explained to us the problem of constructing finite dimensional models of the pushforward of a matrix factorization: it's easy to show, by theoretical arguments, that such a model exists, but an effective procedure for constructing one is very new.

It goes without saying that there were many topics we could not cover, and the fact that some topics were left out was because speakers chosen to cover them cancelled their participation at the last minute.

# Scientific Outcomes of the Meeting

The meeting aimed to bring together a very diverse group of mathematicians who employ the methods of triangulated categories in totally different fields. They certainly were interested in listening to each other, and we hope that the interactions and exchange of ideas will continue. Over time we will be able to form a more accurate picture of what the scientific benefits will be.

### Abstracts

#### **Mark Hovey**

To open this conference on triangulated categories and applications, we first describe how triangulated categories arose in algebraic topology. Thus we explain the process that leads from topological spaces to specta to the stable homotopy category. The stable homotopy category is a compactly generated tensor triangulated category. The most basic feature of any such category is the graded commutative ring of self-maps of the unit, which in this case consists of the stable homotopy groups of the sphere. We describe what is known about this ring, but it is so complex that there are no prospects for ever computing it entirely. So we need new approaches. We describe two such approaches, both worked out by Mike Hopkins and Jeff Smith. We first describe all the field objects of the category; these turn out to be the Morava K-theories. We then describe the thick subcategories of compact objects and the associated prime ideal spectrum, in the sense of Paul Balmer. Finally, we describe how the stable homotopy category gives rise to all of the commonly studied triangulated categories, including ones seemingly far away from algebraic topology. Building on work of Stefan Schwede and Brooke Shipley, Andreas Heider has recently shown that every well-generated triangulated category with a model is a localization of the triangulated category of modules over a symmetric ringoid spectrum.

#### Yujiro Kawamata

This was a survey talk on the structure of the bounded derived categories of coherent sheaves on algebraic varieties  $D^b(X) = D^b(Coh(X))$ , viewed as new kind of spaces. I started with results on explicit structures given by exceptional collections of objects such as

$$D^b(\mathbf{P}^n) \cong \langle \mathcal{O}(-n), \dots, \mathcal{O}(-1), \mathcal{O} \rangle$$

by Beilinson, and by semi-orthogonal decompositions such as

$$D^b(X) \cong \langle U^+, \mathcal{O}_X, D^b(C) \rangle$$

for a Fano 3-fold X of degree 12 and a curve C of genus 8 by Kuznetsov.

Then I went on to more complicated derived categories when the canonical divisor is trivial. I explained an equivalence called the Fourier-Mukai transform

$$\Phi_P: D^b(A) \to D^b(\hat{A})$$

for an abelian variety A and its dual abelian variety  $\hat{A}$  defined as an integral functor whose kernel is the Poincaré line bundle. I also explained a more complicated case of K3 surfaces and the derived Torelli theorem.

I explained the representability theorem by Bondal and Van den Bergh, which says that the category  $D^b(X)$  is saturated. I also explained the representability theorem by Orlov, which says that equivalences of derived categories are expressed as integral functors. I also talked about the Fourier-Mukai partners.

I talked about invariants of the categories. I explained Hochshild (co)homology, and the Hochshild-Kostant-Rosenberg isomorphism. I explained the moduli spaces of stability conditions defined by Bridgeland, and his structure theorem on the autoequivalence group of the derived category of a K3 surface.

Finally I explained the relationship between the semiorthogonal decompositions and the minimal model program. Especially I explained so-called K to D conjecture. I explained a problem of replacing the categories when the varieties have singularities.

#### **Henning Krause**

When one studies the representations of a finite dimensional algebra A (over some field k), there are two triangulated categories which naturally arise: the bounded derived category  $D^b(\text{mod } A)$  of the category mod A of finite dimensional representations, and the stable category stmod A where one takes the quotient modulo all morphisms factoring through a projective module. For the second construction, one needs to assume that the algebra is self-injective; a typical example would be the group algebra kG of a finite group G. An important example for the first construction arises from the path algebra kQ of a finite quiver Q without oriented cycles.

Historically, the first interesting results are those of Beilinson and Bernstein–Gelfand–Gelfand (both published in 1978). They provide a beautiful connection between algebraic geometry and representation theory and contain already a number of important ideas, which led in the following years to further exciting results. Beilinson describes for the projective space  $\mathbb{P}_k^n$  an equivalence of the form  $R \operatorname{Hom}(T, -)$  between  $D^b(\operatorname{coh} \mathbb{P}^n)$  and  $D^b(\operatorname{mod} \operatorname{End}(T))$  via a tilting object T, while the BGG-correspondence gives an equivalence between  $D^b(\operatorname{coh} \mathbb{P}^n)$  and the stable category of graded modules over the exterior algebra of an n + 1dimensional vector space.

Then I gave the basic results from tilting theory, in particular Rickard's theorem characterising the fact that two algebras have equivalent derived categories. Also the stable category was explained in further detail, based on work of Buchweitz for Gorenstein algebras.

Next I moved to hereditary categories such that its derived category admits a tilting object. Happel's theorem tells us that there are just two types: the representations of path algebras and the coherent sheaves on weighted projective lines in the sense of Geigle–Lenzing.

Auslander-Reiten theory for triangulated categories and Serre duality form another interesting aspect. A theorem of Happel says that  $D^b \pmod{A}$  has AR-triangles if and fonly if A has finite global dimension.

One of the great success stories in representation theory is based on the notion of cohomological support for modular group representations. A theorem of Benson, Carlson, and Rickard gives a complete classification of all thick subcategories of stmod kG, using the support defined in terms of the group cohomology  $H^*(G, k)$ .

Finally, I moved to the theory of exceptional sequences which is well developed for quiver representations. A recent result of Ingalls and Thomas implies a classification of all admissable thick subcategories of  $D^b \pmod{kQ}$  in terms of non-crossing partitions associated to the underlying diagram of the quiver Q. Taking as an example the Kronecker quiver (two vertices and two parallel arrows), this classification complements the classification of the thick tensor ideals which one gets from the equivalence with  $D^b (\operatorname{coh} \mathbb{P}^1_k)$ .

#### **Ralf Meyer**

Noncommutative topology views C\*-algebras as a generalization of pointed compact topological spaces. The basis of this is that the category of commutative C\*-algebras is anti-equivalent to the category of pointed compact spaces by Gelfand's Theorem.

An important source of C\*-algebras are stacks, which may be described by groupoids and corresponding C\*-algebras. The C\*-algebra associated to a groupoid is, however, only well-defined up to an appropriate C\*-algebraic notion of Morita equivalence. Thus we add a Morita invariance condition to the axioms for homology theories in the C\*-algebraic context.

This has rather drastic effects: it turns out that any Morita invariant and split-exact functor on C\*-algebras behaves essentially like K-theory. In particular, the universal such functor deserves to be called bivariant K-theory. This is the analogue of the stable homotopy category in noncommutative topology. It is a triangulated category as well.

Several results in homotopy theory can be extended to noncommutative topology by first generalizing them to triangulated categries and then specializing to bivariant K-theory. In many cases, this requires some further work because C\*-algebras do not admit uncountable coproducts or internal Hom functors. Hence standard notions from homotopy theory do not apply directly. It seems also quite difficult to relate bivariant K-theory to model categories.

One of the most powerful techniques in this context is homological algebra in triangulated categories. It provides an abelian approximation to a triangulated category, starting with a stable homological ideal. This is a powerful substitute for t-structures. The latter do not apply to bivariant K-theory because of Bott periodicity.

Approximating bivariant K-theory and its variants by Abelian categories also leads to some interesting phenomena in ring theory. The search for universal coefficient theorems for equivariant versions of bivariant K-theory has led to several examples of hereditary exact categories that deserve further study by algebraists.

#### **Goncalo** Tabuada

I will start by introducing the category Mot of *noncommutative motives*, as invisioned by Drinfeld and Kontsevich in their noncommutative algebraic geometry program. This category is the natural setting for the study of several classical invariants such as cyclic homology (and its variants), algebraic K-theory, topological Hochschild homology, etc. Among other results, I will show that algebraic K-theory becomes corepresentable in Mot by the tensor unit object. Then, I will present joint work with Ivo Dell'Ambrogio on the tensor triangular geometry of noncommutative motives. Making use of Hochschild homology, periodic cyclic homology, and algebraic K-theory, I will describe some explicit points in the Balmer spectrum of Mot. This will illustrate the complexity of the Balmer spectrum of Mot. Finally, I will present joint work with Paul Balmer on the assembly isomorphism conjectures. Our main result asserts that the *fundamental assembly isomorphism conjecture* (which implies all the conjectures on the market) is simply a coefficients variant of the classical Farrell-Jones conjecture in K-theory. This will illustrate the central role played by the classical Farrell-Jones conjecture among all isomorphic conjectures.

#### **Neil Strickland**

Many important examples of triangulated categories come equipped with a symmetric monoidal tensor product. There are some basic features of the interaction between these structures that are well-known. However, Peter May has pointed out that there are more subtle interactions present in the usual examples, which are important for certain applications. Here we report on a project to make May's results more complete and symmetrical. For simplicity, we restrict attention to the homotopy category  $\mathcal{D}$  of ungraded differential modules over a fixed commutative  $\mathbb{Z}/2$ -algebra. This has a canonical triangulation for which the suspension functor is the identity. We believe that, with more bookkeeping, our constructions can be generalised to cover all the usual algebraic examples of tensor triangulated categories.

Suppose we have two distinguished triangles in  $\mathcal{D}$ , say  $A_0 \to A_1 \to A_2 \to A_0$  and  $B_0 \to B_1 \to B_2 \to B_0$ . By tensoring these together, we obtain a functor  $F: \mathcal{U} \to \mathcal{D}$ , where  $\mathcal{U}$  is an evident additive category with object set  $(\mathbb{Z}/3)^2$ . Our elaboration of May's results shows that this has a canonical extension over a larger category  $\mathcal{V} \supset \mathcal{U}$ . More specifically, the category  $\mathcal{V}$  has objects  $u_{ij}$  (for  $i, j \in \mathbb{Z}/3$ ) and  $v_k$ . There are morphisms

$$v_{i+j+1} \xrightarrow{\mu_{ij}} u_{ij} \xrightarrow{\lambda_{ij}} v_{i+j-1}$$

and the full category is generated freely by these, subject only to the relations  $\mu_{i+1,j+1}\lambda_{i-1,j-1} = 0$  and  $\sum_{i+j=k} \lambda_{ij}\mu_{ij} = 0$ . The category  $\mathcal{V}$  has only finitely many morphisms, which can be listed explicitly. It also has a rich group of automorphisms. For each morphism in the image of the extended functor  $F: \mathcal{V} \to \mathcal{D}$ , the cofibre can be described as an object in the image of F, or a direct sum of two or three such objects.

#### **Greg Stevenson**

We will discuss a framework for proving classification theorems for localizing subcategories of compactly generated triangulated categories using actions of tensor triangulated categories. As both motivation and an application we will discuss the classification of localizing subcategories of the stable derived category of a complete intersection over a field.

An action of a tensor triangulated category T on a triangulated category K is a functor  $T \times K \to K$ which is exact and coproduct preserving in each variable and is compatible with the tensor structure on T. In the case that T is rigidly-compactly generated and K is compactly generated this gives rise to a theory of supports which extends the theory of Balmer and Favi and categorifies work of Benson, Iyengar, and Krause.

We will indicate briefly how one constructs the associated support theory and its relationship to the classification problem. This leads to the one of the central abstract results: the local-to-global principle for actions. This theorem allows one to reduce the classification problem to (hopefully) more tractable problems.

As a demonstration of the utility of this machinery we explain recent progress on understanding the lattice of localizing subcategories of the stable derived category of a noetherian separated scheme. In particular, the classification for hypersurfaces in terms of the singular locus will be discussed.

#### Ivo Dell'Ambrogio

As an illustration of the general methods of relative homological algebra in triangulated categories developed by Christensen, Beligiannis and Meyer-Nest, we explain the following equivariant generalization of two classical, and very useful, results of Rosenberg and Schochet, namely, their universal coefficient and Künneth theorems for complex C\*-algebras.

Let G be a finite group. For any G-C\*-algebra A, the collection of all H-equivariant topological K-theory groups of A, with H running through all subgroups of G, assemble to form a  $\mathbb{Z}/2$ -graded Mackey functor  $k_*(A)$ . The assignment of  $k_*(A)$  to A lifts to a stable homological functor defined on the G-equivariant Kasparov category,  $KK^G$ . We obtain from this construction, and from the general machinery, the existence of previously unobserved universal coefficient and Künneth spectral sequences abutting to  $KK^G(A, B)$  and  $K^G(A \otimes B)$ , respectively. As input for these spectral sequences we find Ext and Tor groups, respectively, that can be computed in the abelian category of Mackey modules over the complex character ring of G. Convergence – conditional and strong, respectively – is obtained if A is "cellular", in the sense that it belongs to the localizing subcategory of  $KK^G$  generated by the algebras C(G/H). Such algebras form a rather large class, containing all commutative G-C\*-algebras and closed under the classical "bootstrap" operations.

#### Jon Carlson

This lecture is a survey of results on endotrival modules over finite groups and group schemes. Assume that k is a field of characteristic p and G is a finite group or group scheme. A kG-module is endotrivial provided  $\operatorname{Hom}_k(M, M) \cong M^* \otimes M \cong k \oplus P$  where P is a projective kG-modules. Thus, M is an endotrivial module if its k-endomorphism rings is a trivial module in the stable category  $\operatorname{stmod}(kG)$  of kG-modules modulo projectives. Dade and Puig showed that the endotrivial modules play a substantial role in the block theory of modular group representations. In addition, tensoring with an endotrivial module is a self-equivalence on the

stable category. Consequently the group of endotrivial module, which has elements the isomorphism classes of endotrival modules in the stable category and operation given by the tensor product, is an important part of the Picard group of self-equivalences of stmod(kG). It is group of self-equivalences of Morita type.

Everett Dade introduced the group of endotrivial modules more than thirty years ago. He classified them in the case that G is an abelian p-group. A complete classification of endotrivial modules for all p-groups was achieved a few years ago by Jon Carlson and Jacques Thévenaz building on the work of many others, notably Dade and Jon Alperin. Classifications of the endotrivial modules over other types of groups are included in works by various combinations of Jon Carlson, Dave Hemmer, Nadia Mazza, Dan Nakano, Gabriel Navarro, Geoff Robinson and Thévenaz. Some progress has also been made by Carlson and Nakano on the structure of endotrivial modules for infinitesimal finite group schemes. We review this work in the lecture and also demonstrate a construction of exotic endotrivial modules. The construction relys on the theory of support varieties for kG-modules and connects the work of Paul Balmer and Giordano Favi on gluings in triangulated categories.

#### Julia Pevtsova

The study of representations of a finite group (scheme) over a field of characteristic p via their restrictions to the subalgebras of the form  $k[t]/t^p$ , known as cyclic shifted subgroups or  $\pi$ -points, goes back to the work of J. Carlson in the 80's and has an extensive literature base. In this talk, I'll report on the ongoing project joint with J. Carlson and E. Friedlander in which we initiate the study of representations of an elementary abelian p-group E via their restrictions to "rank r shifted subgroups", that is, subalgebras of kE of the form  $k[t_1, \ldots, t_r]/(t_1^p, \ldots, t_r^p)$ .

In this framework, we introduce various geometric invariants that generalize familiar concepts in the special and well studied case of r = 1. In particular, we investigate a somewhat surprising behavior of "r-support varieties" and "nonmaximal r-support varieties" for r > 1. Inspired by the concept of a module of constant Jordan type that lead to new constructions of vector bundles on projective spaces, we introduce modules of constant *r*-socle and *r*-radical type and show how such a generalization leads to constructing algebraic vector bundles on Grassmannians. The talk will be spiced up with numerous examples of modules with prescribed properties and of corresponding algebraic bundles on Grassmannians.

#### Srikanth Iyengar

The goal of my talk was to give an introduction to on-going work with Dave Benson and Henning Krause concerning, what we have called, stratification of triangulated categories. The main achievement of our collaboration so far, and the principal driving force behind it, has been a classification of the localizing subcategories of the stable module category of a finite group, in the spirit of Neeman's result for the derived category of a commutative noetherian ring. To this end it has been necessary to develop a theory of local cohomology and derived completion, from commutative algebra, in the context of fairly general triangulated categories. Beyond clarifying what it takes to classify localizing, and also colocalizing, subcategories, these techniques have allowed us to deduce many results that are consequences, but by no means obvious ones, of such classifications. In my talk, I tried to illustrate these by explaining various answers we could obtain for the question: When is there a non-zero morphism between objects in a triangulated category? The talk was based on the following papers, all co-authored with Benson and Krause and available on the math arXiv:

- Colocalizing subcategories and cosupport, J. Reine. Angew. Math., to appear.
- Stratifying triangulated categories, J. Topology, to appear.
- Stratifying modular representations of finite groups, Ann. of Math. 175 (2012); to appear.
- Local cohomology and support for triangulated categories, Ann. Sci. École Norm. Sup. (4) **41** (2008), 575–621.

#### John Greenlees (Joint work with Benson, Hess and Shamir).

The talk described three different characterizations of complete intersections for Noetherian local rings R. The sci condition (regular ring mod regular sequence), the mci condition (eventually multiperiodic resolutions for finitely generate modules), and the gci condition (polynomial growth of Ext algebra). The aim of the talk

was to give a homotopy invariant definition, and in particular to give versions of these definitions which apply to  $R = C^*(X; k)$  (cochains on a space X).

Before one gets to complete intersections, one needs to deal with the regular case. There are corresponding definitions (s-regular, m-regular and g-regular) for regular local rings. One can make good sense of g-regular (Ext algebra finite dimensional) and then use the putative m-regular condition (finitely generated implies small) to give a *definition* of finite generation. The substitute for the Noetherian condition on a ring R is that there is a map  $Q \rightarrow R$  from a regular ring, making R a small Q-module. An R-module M is then said to be finitely generated if it is small as a Q-module.

Now, a space is sci if it is obtained as an iterated spherical fibration from a regular space. A space is gci if  $H_*(\Omega X)$  has polynomial growth. To make sense of the mci condition, the eventual multiperiodicity states that a Koszul complex is small, but to get equivalence one needs to require that this natural in a suitable sense. So we reach the eci condition which says that iterated cofibrations in the category of bimodules reach a non-trivial small object. The sci condition is stronger than the others, but in the rational and mod p contexts, the gci and eci conditions are equivalent.

The talk also provided some illustrative examples with X the classifying space of a finite group.

#### **Brooke Shipley**

For a compact Lie group G of rank r, Greenlees has conjectured that there is an abelian category A(G) of injective dimension r such that the homotopy category of rational G-equivariant cohomology theories is modeled by the derived category of A(G). This conjecture holds for finite groups since rational G-equivariant cohomology theories are just graded rational Mackey functors (which are all injective). This conjecture also holds for SO(2), O(2) and SO(3) by work of Greenlees [13, 14, 15]. In this talk we discussed joint work with Greenlees on this conjecture for G a torus. Specifically we outlined this new, simplified, proof for SO(2) and indicated the changes needed for higher rank tori.

Theorem [19] For any torus,  $T^n$ , there is an abelian category  $\mathcal{A}(T^n)$  of sheaves over the space of closed subgroups of  $T^n$  and a Quillen equivalence of model categories:

Rational  $T^n$ -spectra  $\simeq_Q$  Rational  $dg\mathcal{A}(T^n)$ 

*Furthermore,*  $\mathcal{A}(T^n)$  *has injective dimension* n *(the rank.)* 

In the case of T = SO(2) this Quillen equivalence appears in [29] based on the work in [14]. In [16], Greenlees uses this work to construct SO(2)-equivariant elliptic cohomology. Our generalization to higher dimensional tori leads to the possibility of constructions of  $T^g$ -equivariant cohomology theories associated to complex curves of genus q; see also [17].

One can also specialize to families versions of the above Theorem for rational G-spectra with fixed points concentrated in a given family,  $\mathcal{F}$ . For example, free  $T^n$ -spectra are modeled by differential graded torsion modules over  $H^*BT^n$ ; this gives a new proof for tori of the results in [18].

#### Don Stanley Joint work with Adam-Christiaan van Roosmalen

Let R be an abelian category, and D(R) the derived category of R. An aisle  $U \subset D(R)$  is a full subcategory closed under extensions and suspensions, such that the inclusion has a right adjoint. Keller and Vossieck observed that aisles and t-structures are equivalent data. Given an aisle, consider the function

$$\phi(\mathcal{U}): \mathbb{Z} \to \{\text{specialization closed subsets of } Spec(R)\}$$

$$n \mapsto \bigcup_{M \in \mathcal{U}} Supp H_n(M),$$

where Spec(R) is the ideal spectrum, and Supp is the support. It turns out that this function determines the *t*-structure if we restrict to *t*-structures in  $D_{fg}^b(R)$ , the bounded derived category with finitely generated homologies. If *R* also has dualizing complex, then it is understood which functions can occur, and hence there is a classification of the *t*-structures.

On the other hand even for slightly more general abelian categories A, such as the coherent sheaves on  $P^1$ , the support data of  $\phi$  does not give enough information to determine t-structures. In this talk we introduce other data that replaces the sequences of support that worked in the commutative ring case. This data is a function

$$\phi'(\mathcal{U}) \colon \mathbb{Z} \to (W(n), T(n))$$

where W(n) is a wide subcategory of A and T(n) is a tilting torsion theory in the orthogonal of W(n-1) inside W(n). If A is a category of modules over a finite hereditary algebra, then this data classifies t-structures in  $D_{fg}^b(A)$ .

#### Fernando Muro The talk is based on joint work with Oriol Raventós (Barcelona).

There are two representability theorems that a compactly generated triangulated category  $\mathcal{T}$  may satisfy: Brown's theorem says that any product-preserving functor  $\mathcal{T}^{op} \to Ab$  which takes exact triangles to exact sequences of abelian groups is representable. Adam's theorem says that if  $\mathcal{T}^c$  is the category of compact objects in  $\mathcal{T}$ , any additive functor  $(\mathcal{T}^c)^{op} \to Ab$  which takes exact triangles to exact sequences is the restriction of a representable functor  $\mathcal{T}^{op} \to Ab$ , and any natural transformation  $\mathcal{T}(-, X)_{|\mathcal{T}^c} \to \mathcal{T}(-, Y)_{|\mathcal{T}^c}$  is represented by a morphism  $X \to Y$ . These theorems were first proved for the stable homotopy category and later generalized by Neeman, Krause, Franke... to triangulated categories under suitable assumptions.

The classical Adams representability theorem is seldom satisfied. For instance, the derived category of a finite-dimensional hereditary algebra over an uncountable algebraically closed field satisfies Adam's theorem if and only if it is of finite representation type. A failed theorem of Rosický claimed that any well generated triangulated category with a model would asymptotically satisfy a transfinite version of Adams' theorem: for big enough regular cardinals  $\alpha$ , if  $\mathcal{T}^{\alpha}$  is the category of  $\alpha$ -compact objects in  $\mathcal{T}$ , any functor  $(\mathcal{T}^{\alpha})^{op} \to Ab$  which preserves products of less than  $\alpha$  objects and takes exact triangles to exact sequences is the restriction of a representable functor  $\mathcal{T}^{op} \to Ab$ , and any natural transformation  $\mathcal{T}(-, X)_{|\mathcal{T}^{\alpha}} \to$  $\mathcal{T}(-, Y)_{|\mathcal{T}^{\alpha}}$  is represented by a morphism  $X \to Y$ . Such a result for a given triangulated category would still have amazing consequences, therefore this problem deserves to be studied in specific cases.

In my talk I presented an approach to this problem from the classical point of view of obstruction theory, leading to counterexamples to Rosický's theorem based on recent results by Braun–Göbel and Bazzoni– Štovíček. These counterexamples are about the representability of natural transformations for  $\mathcal{T}$  the derived category of  $\mathbb{Z}$  or  $\mathbb{C}[x, y]$ . I also showed that there would be counterexamples to the representability of functors  $(\mathcal{T}^{\alpha})^{op} \rightarrow Ab$  if there were a hereditary ring R with  $\alpha$ -pure global dimension > 2 for  $\alpha$  big enough. The existence of such rings is an open problem.

#### **Amnon Yekutieli**

Let A be a noetherian commutative ring, and  $\dashv$  an ideal in it. In this lecture I will talk about several properties of the derived  $\dashv$ -adic completion functor and the derived  $\dashv$ -torsion functor.

In the first half of the talk I will discuss GM Duality (first proved by Greenlees and May, then treated by Alonso, Jeremias and Lipman), and the closely related MGM Equivalence. The latter is an equivalence between the category of cohomologically  $\dashv$ -adically complete complexes and the category of cohomologically  $\dashv$ -torsion complexes. These are triangulated subcategories of the derived category D(Mod A).

I will explain how the derived completion functor can be studied using the concept of  $\dashv$ -adically projective modules.

In the second half of the talk I will discuss new results: (1) A characterization of the category of cohomologically  $\dashv$ -adically complete complexes as the right perpendicular to the derived localization of A at  $\dashv$ . This shows that our definition of cohomologically  $\dashv$ -adically complete complexes coincides with the original definition of Kashiwara and Schapira. (2) The Cohomologically Complete Nakayama Theorem. (3) A characterization of cohomologically cofinite complexes. This is related to t-dualizing complexes, in the sense of Alonso, Jeremias and Lipman. (4) A theorem on completion by derived double centralizer. This last result extends earlier work of Dwyer-Greenlees and Efimov.

This is joint work with Marco Porta and Liran Shaul.

For full details see the lecture notes

www.math.bgu.ac.il/~amyekut/lectures/cohom-complete/notes.pdf or the paper arxiv:1010.4386.

#### **Anthony Licata**

A categorical  $sl_2$  action consists of a sequence of k-linear additive categories  $D(-N), \ldots, D(N)$  together with functors, for  $\ell \in \mathbb{Z}$ ,

$$E(\ell) : D(\ell - 1) \rightarrow D(\ell + 1)$$
 and  $F(\ell) : D(\ell + 1) \rightarrow D(\ell - 1)$ 

satisfying the relations

$$E(\ell-1) \circ F(\ell-1) \cong id_{D(\ell)}^{\oplus \ell} \oplus F(\ell+1) \circ E(\ell+1) \text{ if } \ell \ge 0.$$
(20.1)

$$F(\ell+1) \circ E(\ell+1) \cong id_{D(\ell)}^{\oplus -\ell} \oplus E(\ell-1) \circ F(\ell-1) \text{ if } \ell \le 0$$
(20.2)

On the complexified (split) Grothendieck groups  $V(\ell) := K(D(\ell)) \otimes_{\mathbb{Z}} \mathbb{C}$ , the functors  $E(\ell)$  and  $F(\ell)$  induce maps of vector spaces  $e(\ell) := [E(\ell)]$  and  $f(\ell) := [F(\ell)]$ . By the above relations,  $V = \oplus V(\ell)$  is a locally finite representation of  $sl_2(\mathbb{C})$ , where  $e = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$  acts by  $\bigoplus_{\ell} e(\ell)$  and  $f = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$  acts by  $\bigoplus_{\ell} f(\ell)$ .

Any such  $sl_2$  action on  $\oplus_{\ell} V(\ell)$  integrates to an  $SL_2$  action. Hence the reflection element

$$t = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

induces an isomorphism of vector spaces  $V(\ell) \xrightarrow{\sim} V(-\ell)$ . An interesting question is whether this isomorphism can be lifted to an equivalence of categories  $T : D(\ell) \to D(-\ell)$  coming from a lift of the reflection element.

In their seminal work, Chuang and Rouquier constructed such an equivalence under the assumption that the underlying weight space categories are abelian, and the categorical  $sl_2$  action is by exact functors. More precisely, they constructed an equivalence between the corresponding derived categories.

In our motivating geometric examples, however, the natural functors are not exact, and as a result the weight space categories  $D(\ell)$  are triangulated instead of abelian. Nevertheless, it is still natural to ask for an equivalence between  $D(\ell)$  and  $D(-\ell)$ .

The setup we use in order to modify the Chuang-Rouquier construction is that of *strong categorical*  $sl_2$  *actions*. In particular, this means that categories  $D(\ell)$  are graded and the Es and Fs satisfy a graded version of relations (20.1) and (20.2). The grading implies that on the level of the Grothendieck group there is an action of the quantum group  $U_q(sl_2)$ .

As an additional data, we demand functors

$$\mathbf{E}^{(r)}(\ell): \mathbf{D}(\ell-r) \to \mathbf{E}^{(r)}(\ell+r) \text{ and } \mathbf{F}^{(r)}(\ell): \mathbf{D}(\ell+r) \to \mathbf{D}(\ell-r)$$

which categorify the elements  $e^{(r)} = \frac{e^r}{r!}$  and  $f^{(r)} = \frac{f^r}{r!}$  along with natural transformations X, T which are used to rigidify the isomorphisms (20.1) and (20.2).

Here is a sketch of the construction. If we restrict  $t \in SL_2$  to the weight space  $V(\ell)$  with  $\ell \ge 0$ , then one can write t as

$$t = f^{(\ell)} - f^{(\ell+1)}e + f^{(\ell+2)}e^{(2)} \pm \dots$$

where the sum is finite since  $V(\ell) = 0$  for  $\ell \gg 0$ . We can lift  $f^{(\ell+s)}e^{(s)}$  to the composition of functors  $F^{(\ell+s)} \circ E^{(s)}$ . We then form a complex of functors  $\Theta_*$  whose terms are

$$\Theta_s := \mathbf{F}^{(\ell+s)}(s) \circ \mathbf{E}^{(s)}(\ell+s) \langle -s \rangle.$$

(the  $\langle \cdot \rangle$  represents a shift in the grading). The connecting maps of the complex are defined via various adjunction morphisms.

The main result of the talk states that if our categories  $D(\ell)$  are triangulated then the convolution of this complex is an equivalence  $T : D(\ell) \xrightarrow{\sim} D(-\ell)$ .

#### **Sabin Cautis**

In 2004 Chuang and Rouquier proved a version of Broué's abelian defect group conjecture for the symmetric group by introducing the notion of a strong categorical sl(2) action. Their key idea was to show that the Weyl involution of sl(2) can be lifted to give an equivalence of categories.

More recently, in joint work with Joel Kamnitzer and Anthony Licata, we constructed similar categorical sl(2) actions on (derived) categories of coherent sheaves on cotangent bundles to Grassmannians  $DCoh(T^*G(k, N))$ . Furthermore we showed that such actions also induce equivalences and thus were able to construct a natural equivalence  $DCoh(T^*G(k, N)) \simeq DCoh(T^*G(N-k, N))$  generalizing earlier work of Namikawa and Kawamata on derived equivalences in algebraic geometry. More recently, in joint work with Joel Kamnitzer, we extend this notion to define categorical sl(n) actions. We show that such an action induces an action of the braid group on n strands (this should be thought of as a cover of the symmetric group which is the Weyl group of sl(n)). By constructing such an sl(n) action on (derived) categories of coherent sheaves on n-step partial flag varieties we obtain a braid group action on them.

In this talk I will explain what is a categorical sl(n) action and how it can be used to construct braid group actions. This definition will be motivated by braid group actions constructed via Seidel-Thomas spherical twists. I will illustrate all of this by defining an sl(3) action on the resolution of  $\mathbb{C}^2/\mathbb{Z}_3$ , thus obtaining the well known braid group action on (the derived category of) this space.

This method of constructing braid group actions has applications to geometry (as described above), knot theory (e.g. algebro-geometric constructions of Khovanov homology) and representation theory of finite group (e.g. the work of Chuang and Rouquier). It is also natural to ask if there are similar constructions for other groups, for instance, mapping class groups.

#### Wendy Lowen

Compact generation of triangulated categories was introduced by Neeman. One of the motivating situations is given by "nice" schemes (i.e. quasi-compact separated schemes, later extended to quasi-compact quasiseparated schemes by Bondal and Van den Bergh). The ideas of the proofs later crystallized in Rouquier's (co)covering theorem which describes a certain covering-by-Bousfield-localizations situation in which compact generation (later extended to  $\alpha$ -compact generation by Murfet) of a number of "smaller pieces" entails compact generation of the whole triangulated category. The notions needed in the (co)covering concept can be interpreted as categorical versions of standard scheme constructions like unions and intersections of open subsets, and in the setup of Grothendieck categories rather than triangulated categories they have been important in non-commutative algebraic geometry. In this talk we present a (co)covering theorem for Grothendieck categories based upon these notions, which can be used to prove compact generation of the derived category of certain Grothendieck categories. As such, the result follows from the triangulated (co)covering theorem, and it implies Neeman's original result for schemes by application to the Grothendieck category of quasicoherent sheaves. Our interest in such an intermediate result comes from its applicability to Grothendieck categories that originate as "non-commutative deformations" of schemes, more precisely abelian deformations of categories of quasi-coherent sheaves in the sense of Lowen and Van den Bergh. In general, there remain obstructions to the lifting of compact generators of some of the relevant categories under deformation. On the other hand, in some situations (eg. for quasi-projective surfaces) we can use the (co)cover theorem in combination with techniques of Keller and Lowen to obtain compact generation of all deformations.

#### **Daniel Murfet**

Functors between triangulated categories are often described in terms of integration against a kernel. In the categorical setting this integration takes the form of a pushforward. I will describe a new approach to constructing finite models of pushforwards for matrix factorisations and some applications including, if time permits, computations of homological link invariants.

## **List of Participants**

Balmer, Paul (University of California Los Angeles (UCLA))
Benson, David (University of Aberdeen)
Carlson, Jon (University of Georgia)
Casacuberta, Carles (Universitat de Barcelona)
Cautis, Sabin (Columbia University)
Christensen, Dan (University of Western Ontario (UWO))
Dell'Ambrogio, Ivo (Universität Bielefeld)
Dugger, Dan (University of Oregon)
Friedlander, Eric (University of Southern California)
Greenlees, John (University of Sheffield)
Hovey, Mark (Wesleyan University)

Iyengar, Srikanth (University of Nebraska, Lincoln) Kawamata, Yujiro (The University of Tokyo) Klein, Sebastian (Utrecht University) Krause, Henning (University of Bielefeld) Licata, Anthony (Institute for Advanced Study and the Australian National University) Lowen, Wendy (Universiteit Antwerpen) Lowrey, Parker (UWO) Meyer, Ralf (Universitat Gottingen) Murfet, Daniel (University of California Los Angeles) Muro, Fernando (Universidad de Sevilla) Neeman, Amnon (Australian National University) Pauwels, Bregje (UCLA) Pevtsova, Julia (University of Washington) Rickard, Jeremy (University of Bristol) Sanders, Beren (University of California Los Angeles (UCLA)) **Shipley, Brooke** (University of Illinois, Chicago) Smith, Paul (University of Washington) **Smith, Jeffrey** (University of British Columbia) Stanley, Don (University of Regina) Stevenson, Gregory (ANU) **Stovicek, Jan** (Charles University in Prague) Strickland, Neil (University of Sheffield) Tabuada, Goncalo (Universidade Nova de Lisboa) Takahashi, Ryo (Shinshu University) Wang, Gaohong (UWO) Wolcott, Luke (University of Washington) Wu, Enxin (UWO) Yekutieli, Amnon (Ben Gurion University) **Zhang, James** (University of Washington)

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# Chapter 21

# Groups, graphs and stochastic processes (11w5141)

Jun 19 - Jun 24, 2011

**Organizer(s):** Miklos Abert (Renyi Institute of Mathematics) Balint Virag (University of Toronto)

## Goals and an Overview of the Field

This workshop aimed to bring together experts and young researchers in the following fields: asymptotic group theory, ergodic theory,  $L^2$ -cohomology, geometric group theory, percolation, random walks, 3-manifold theory, analytic graph theory, free probability and logic. A common object of interest was unimodular random networks (in the language of probability), measure preserving actions of a countable group (in the language of group theory) or graphings (in the language of graph theory). Each field investigates this object from a different angle, and although there has already been considerable interaction, the organizers felt that learning each other's math in more depth would be productive.

The main topics of the workshops were:

- Graph convergence, both Benjamini-Schramm and local-global
- Stochastic processes on Cayley graphs
- Finite approximation of infinite graphs and processes
- $L^2$  cohomology, Rank gradient and cost of measure preserving actions
- Random walks on groups and compression

**Limits of finite graphs.** Benjamini and Schramm introduced a natural topology on bounded-degree finite graphs which has since become a central object of study in many areas of mathematics. Two graphs are close if they agree with high probability in a neighborhood of a randomly chosen vertex, called the root. This space has a natural compactification and a limit of convergent graph sequences is always a unimodular random network, that is, a probability distribution on rooted graphs that stays the same if we move the root (see work of Aldous and Lyons).

Groups come into the game at this point; for instance, if the limit is concentrated on one graph, then it must be vertex transitive. If the limit is not one point, then one gets something close to a measure-preserving group action. This connection allows one to use ergodic theory to understand finite graphs and has been succesfully used by Szegedy, Elek, Schramm and others. Energy also moves in the other direction, as some of the known phenomena on finite graphs translate to unimodular random networks and even to general ergodic theory. An example for the last is the recent theorem of Abert and Weiss that for a countable group, every free measure preserving action weakly contains its Bernoulli actions. The analogous theorem is trivial for finite graphs. Much more is expected in both ways.

Another very recent, largely unexplored area is local-global convergence, that has been defined by Hatami, Lovasz and Szegedy. Groups again come into the picture, as cowering towers of graphs, in particular, graph sequences coming from chains of subgroups of finite index are local-globally convergent. On the other hand, the corresponding notion has been recently introduced in ergodic theory by Kechris as weak containment by measure preserving actions.

**Stochastic processes on Cayley graphs.** One can also get unimodular random networks starting directly from groups. A finitely generated group with a generating set gives rise to a so-called Cayley graph. This graph carries a lot of information on the group and one can use geometric methods to exploit this. This area of investigation started with the work of Gromov, who characterized groups with Cayley graphs of polynomial growth.

Probabilists are interested in Cayley graphs because they are a rich source of natural homogeneous (vertex transitive) test spaces. Now one can look at natural random subgraphs of the Cayley graph. An example is edge percolation, another is a random spanning forest. In both cases, the resulting distribution will be invariant under the group action, so one gets a unimodular random network. Again, there is an interesting interplay between group invariants and the behaviour of natural stochastic processes on the Cayley graph and energy flows both ways on these connections. For instance, by the work of Lyons, the most natural definition of the first  $L^2$  Betti number of a group is through free spanning forests. One can also study other invariant subgraphs of Cayley graph, for instance, Lyons and Nazarov recently proved that every nonamenable bipartite Cayley graph admits a factor of i.i.d. perfect matching.

**Finite approximation.** A group is residually finite, if the intersection of its subgroups of finite index is trivial. Many of the most interesting groups, including lattices in linear Lie groups, fall into this category. There is no strong general infinite group theory, as one can construct weird examples that defy any reasonable conjecture. However, residual finiteness is a restriction that allows one to build such a theory. For instance, by work of Zelmanov, finitely generated residually finite groups of finite exponent are finite. Another class of groups with a well-built theory are amenable groups.

It is easy to see, that for both residually finite and amenable groups, their Cayley graphs can be obtained as the Benjamini-Schramm limit of finite graphs, that is, they are sofic. It is an exciting question whether every Cayley graph (or even every unimodular random network) is sofic. A positive answer would have a farreaching consequence on group theory, as some of the machinery invented for residually finite or amenable groups can be used for sofic groups as well. Note that the famous Connes embedding problem asks the same question, just instead of finite permutations, we want to approximate the group by finite dimensional matrices, using the trace norm.

Similarly, one can try to approximate invariant processes on infinite Cayley graphs using processes on sequences of finite graphs converging to the Cayley graph in the Benjamini-Schramm sense.

**Rank,**  $L^2$  cohomology and cost. Another invariant under intense investigation is the so-called cost, introduced by Levitt and analyzed in depth by Gaboriau. The cost is a rank-type invariant for countable measure preserving actions. It comes up naturally in probability on Cayley graphs, as it derives from the expected degree of invariant connected random subgraphs and in asymptotic group theory, as, by work of Abert and Nikolov the cost of a profinite action can be expressed in terms of the growth of rank on the corresponding subgroup chain. The main question in this direction is whether the cost depends on the action, or is a group invariant (fixed price problem). This question has natural translations in both group theory, percolation theory and finite graph theory. For finite graphs, the task would be to understand how many edges one can erase from a large graph to stay bi-Lipshitz to it in the graph metric. Logicians, including Kechris or Hjorth are also interested in the cost, as it is a natural orbit equivalence invariant on measure preserving equivalence relations.

While the cost is not understood satisfactorily,  $L^2$  theory is in much better shape. Lück approximation implies that the first  $L^2$  Betti number equals the growth of homology on a normal chain with trivial intersection, at least for finitely presented groups. Gaboriau has recently introduced  $L^2$  Betti numbers of measure preserving equivalence relations and showed that they are actually group invariants. That is, fixed price does hold homologically and one can hope that this will help attacking the general problem.

**Random walks and compression.** The structure of graphs and unimodular random networks can also be understood by studying the properties of random walks on them. An example is Kesten's theorem – a Cayley graph is amenable if and only if the return probabilities of random walks decay exponentially. A similar characterization via percolation is still open: it is widely believed that a graph is amenable if there is a parameter for which Bernoulli percolation has infinitely many infinite clusters.

Similarly, a Cayley graph supports bounded harmonic functions if and only if the random walk has positive speed – whether this property depends on the graph or only the group is a central open question. The more general connection between the asymptotic rate of escape and group-theoretic properties is also an object of recent scrutiny. Peres recently gave a simple elegant proof that random walks on groups are at least  $n^{1/2}$  away after *n* steps. Rate of escape of walks has also been connected to Hilbert compression and other geometric properties of graphs and groups by work of Naor and Peres.

## **Recent Developments and Open Problems**

We list some recent examples where ideas from one subject were applied in a ground-breaking way in another:

- Gaboriau's work on distinguishing ergodic equivalence relations by developing a measure-theoretic analogue of L<sup>2</sup> Betti numbers;
- Lackenby's seminal work on asymptotic invariants of finitely presented groups;
- Lück Approximation and its follow-ups;
- Abert and Nikolov's work on profinite actions connected the fixed price problem to the 'rank vs. Heegaard genus problem' in 3-manifold theory;
- Gaboriau and Lyons solved the measurable version of von Neumann's problem using percolation on transitive graphs;
- Osin constructed a finitely generated non-amenable torsion group, using cost;
- Kechris re-proved fixed price for free groups (originally a theorem of Gaboriau that used treeings) using that the cost is monotonic to weak containment and the Abert-Weiss result;
- Abert and Weiss showed that for a countable group, every free measure preserving action weakly contains its Bernoulli actions
- Monod and Epstein have used minimal spanning forests to partially solve the Diximier problem that asks whether non-amenable groups are necessarily non-unitarizable;
- Bowen has introduced a new entropy notion for actions of non-amenable groups, using sofic approximations.

Major open problems in the area include:

- Is every group sofic? That is, is every Cayley graph the limit of finite graphs?
- Does every non-hyperfinite measure preserving equivalence relation admit a free action of a free group?
- Is it true, that every invariant process on the 3-regular tree that is approximable on every sequence of finite graphs Benjamini-Schramm converging to the infinite tree, lies in the weak closure of factor of i.i.d. processes?
- Does the rank gradient depend on the chain, assuming it approximates the ambient group?

- Is the cost of a free action an invariant of the group?
- Is it true that the speed of random walk being positive does not depend on the generating set?
- What is the essential girth of finite Ramanujan graphs?
- Does every nonamenable Cayley graph admit a factor of i.i.d. perfect matching?

# People at the workshop

The following people participated in the workshop. We put a \* next to people who gave a presentation. The schedule and list of talks can be found at www.birs.ca/workshops/2011/11w5141/Schedule11w5141.pdf.

- 1. Abert, Miklos, Renyi Institute of Mathematics
- 2. \* Amir, Gidi, Bar-Ilan University
- 3. \* Babai, Laszlo, University of Chicago
- 4. \* Bowen, Lewis, Texas A&M
- 5. \* Brieussel, Jeremie, Neuchatel University
- 6. Candellero, Elisabetta, Graz University of Technology
- 7. Csoka, Endre, Eötvös Loránd University
- 8. \* Elek, Gabor, Renyi Institute
- 9. \* Friedman, Joel, University of British Columbia
- 10. \* Gilch, Lorenz, Graz Technical University
- 11. \* Glasner, Yair, Ben Gurion University of the Negev
- 12. \* Grabowski, Łukasz, Goettingen University
- 13. Gurel-Gurevich, Ori, UBC
- 14. \* Harangi, Viktor, Renyi Institute
- 15. Hegedus, Pal, Central European University
- 16. \* Kaimanovich, Vadim, University of Ottawa
- 17. \* Karlsson, Anders, University of Geneva
- 18. Kassabov, Martin, Cornell University
- 19. \* Lee, James, University of Washington
- 20. Li, Xiang (Janet Lisha), University of Toronto
- 21. \* Lippner, Gabor, Harvard
- 22. \* Lyons, Russell, Indiana University
- 23. Matter, Michel, University of Geneva
- 24. \* Mineyev, Igor, University of Illinois at Urbana-Champaign
- 25. \* Nachmias, Asaf, MIT
- 26. Navas, Andres, Universidad de Santiago de Chile

- 27. \* Peres, Yuval, Microsoft Research
- 28. Pete, Gabor, University of Toronto
- 29. \* Saloff-Coste, Laurent, Cornell University
- 30. \* Smirnova-Nagnibeda, Tatiana, University of Geneva
- 31. Stewart, Andrew, University of Toronto
- 32. \* Szegedy, Balazs, University of Toronto
- 33. Thompson, Russ, Cornell University
- 34. \* Timar, Adam, Hausdorff Center for Mathematics, Bonn University
- 35. Virag, Balint, University of Toronto
- 36. Weinberger, Shmuel, University of Chicago
- 37. \* Woess, Wolfgang, Technische Universität Graz
- 38. \* Young, Robert, University of Toronto at Scarborough

### **Presentation Highlights**

The following is the list of presentations given at the workshop.

Speaker: Gideon Amir (Bar Ilan University)

Title: Liouville property of automaton groups

**Abstract:** Many classical fractals, such as the Sierpinski gasket, and Julia sets of polynomials can be described through groups generated by finite automata. Automaton groups also provide a rich source of examples (such as Grigorchuk group of intermediate growth) and play an important role in geometric group theory. In this talk we will show a phase transition in the Liouville property of automaton groups, and deduce that all automaton groups with activity growth of degree up to 1 are amenable. A key ingredient is the analysis of random walks on the Schreier graphs of these groups: We will discuss how further understanding of the structure of these Schreier graphs, and in particular estimation the resistances between vertices may be used to further our knowledge of automaton groups.

This talk is based on joint works (some in progress) with O. Angel and B. Virag.

Speaker: Laszlo Babai (University of Chicago)

**Title:** Asymptotic characterization of finite vartex-transitive graphs with bounded Hadwiger number via rooted limits

#### Abstract:

Speaker: Lewis Bowen (Texas A&M)

Title: Entropy for sofic group actions

**Abstract:** In 1958, Kolmogorov defined the entropy of a probability measure preserving transformation. Entropy has since been central to the classification theory of measurable dynamics. In the 70s and 80s researchers extended entropy theory to measure preserving actions of amenable groups (Kieffer, Ornstein-Weiss). My recent work generalizes the entropy concept to actions of sofic groups; a class of groups that contains for example, all subgroups of GL(n,C). Applications include the classification of Bernoulli shifts over a free group, answering a question of Ornstein and Weiss.

Speaker: Gabor Elek (Renyi Institute, Budapest)

Title: Groups and graph limits

**Abstract:** Convergence of finite graphs was introduced by Benjamini and Schramm. Finer notion of convergence was studied by Bollobas and Riordan. We survey these basic notions of convergence and the respective limit constructions; measurable graphings and unimodular networks.

Speaker: Joel Friedman (UBC)

Title: Fancy Linear Algebra and the Hanna Neumann Conjecture

**Abstract:** In this talk we describe a proof of the Hanna Neumann Conjecture of the 1950's based on linear algebra, and an invariant of a collection of linear maps that we call the "maximum excess." The maximum excess has a number of remarkable properties, and can be viewed as an analogue of the  $L^2$  Betti numbers defined by Atiyah. Our linear algebra can be intuitively understood in terms of a very simple type of sheaf cohomology theory on graphs; however, as we shall show, our proof can be given without cohomology theory or any heavy-handed techniques from sheaf theory.

Speaker: Yair Glasner (Ben Gurion University)

Title: A probabilistic Kesten theorem and counting closed circles in graphs

**Abstract:** We give explicit estimates between the spectral radius and the densities of short cycles for finite *d*-regular graphs. This allows us to show that the essential girth of a finite *d*-regular Ramanujan graph G is at least  $c \log \log |G|$ .

We prove that infinite *d*-regular Ramanujan unimodular random graphs are trees. Using Benjamini-Schramm convergence this leads to a rigidity result saying that if most eigenvalues of a *d*-regular finite graph G fall in the Alon-Boppana region, then the eigenvalue distribution of G is close to the spectral measure of the *d*-regular tree.

We also show that for a nonamenable invariant random subgroup H, the limiting exponent of the probability of return to H is greater than the exponent of the probability of return to 1. This generalizes a theorem of Kesten who proved this for normal subgroups.

Speaker: Lukasz Grabowski

Title: Turing machines, graphings and the Atiyah problem

**Abstract:** It is shown that all non-negative real numbers are  $l^2$ -Betti numbers. The main new idea is embedding Turing machines into integral group rings. The main tool developed generalizes known techniques of spectral computations for certain random walk operators to arbitrary operators in groupoid rings of discrete measured groupoids.

Speaker: Lorenz Gilch (Graz)

Title: Branching Random Walks on Free Products of Groups

**Abstract:** In this talk we will consider discrete-time branching random walks on free products of groups, which can be described in the following way. An initial particle starts at some vertex of the free product. At each instant of time, each particle produces in a first stage some offspring according to an offspring distribution

and in a second stage each of the offspring particles moves independently to a neighbour element in the free product. That is, each particle performs its own independent single random walk from its place of birth. We investigate the phase of branching random walks, where the branching process survives and where the process vacates each finite subset almost surely after finite time. The purpose of this talk is to describe the boundary to which the particle cloud moves. We give an explicit phase transition criterion in order to describe the set of ends of the Cayley graph of the free product, where the branching random walk accumulates. Furthermore, we give an explicit formula for the box-counting dimension and the Hausdorff dimension of the boundary set (in comparision to the dimensions of the boundary of the whole free product), which is reached by the branching random walk.

Speaker: Viktor Harangi (Renyi Institute, Budapest)

Title: Low moments are sofic

**Abstract:** We explicitly describe the possible pairs of triangle and square densities for regular ifnite simple graphs. We also prove that every r-regular unimodular random graph can be approximated by r-regular infinite graphs with respect to these densities. As a corollary one gets an explicit description of the possible pairs of the third and fourth moments of the spectral measure of r-regular unimodular random graphs.

Speaker: Vadim Kaimanovich (Ottawa)

Title: Finite approximations of invariant measures

**Abstract:** Although the notion of an invariant measure is usually formulated for a single transformation or in the presence of a (semi)group action, the theory of foliations provided a first example where it was done without these assumptions (holonomy invariant measures, Plante 1975). Soon afterwards Feldman and Moore (1977) defined the notion of invariance with respect to a discrete equivalence relation. As it was noticed by the author (1998), the space of rooted locally finite graphs has a natural "root moving" equivalence relation, so that one can talk about invariant measures on this space as well.

A similar notion of invariance for measures on graphs ("unimodular measures") was later developed by probabilists (these two notions coincide for graphs with trivial group of isomorphisms). For any finite graph the uniform distribution on the set of its vertices is unimodular. Benjamini and Schramm (2001) showed that any weak limit of a sequence of such measures is also unimodular, which naturally leads to the question about the measures which can be obtained in this way (Aldous and Lyons, 2007). In particular, for Cayley graphs existence of such an approximation is equivalent to the group being sofic. Elek (2010) by using an earlier idea of Bowen (2003) proved that any unimodular measure on the space of rooted trees with uniformly bounded vertices is finitely approximable.

In this talk we show that if an invariant measure on the space of rooted graphs is such that the "root moving" equivalence relation is amenable with respect to this measure, then the measure is finitely approximable. The proof is based on ergodic considerations. Namely, amenability (i.e., hyperfiniteness) of the equivalence relation allows one to apply the martingale convergence theorem to obtain the approximation in question.

Speaker: Anders Karlsson (Royal Institute of Technology, Sweden)

Title: Spanning forests, heat kernels, and Epstein zeta values

**Abstract:** I will describe rather detailed asymptotics of the number of spanning trees, and rooted spanning forests for discrete tori,  $Z^d/AZ^d$  as the integral matrix A tends to infinity. In dimension d = 2 this was known from the statistical physics literature. In these asymptotics several interesting constants appear, often special values of Epstein zeta functions associated to a limiting torus. In particular, the determinant of the Laplacian of the limiting torus appears in the spanning tree case. The methods involve heat kernel analysis on the graph tori and the manifold tori. Joint work with G. Chinta and J. Jorgenson.

Speaker: James Lee (University of Washington)

Title: Rate of escape and harmonic functions

**Abstract:** We prove that on any infinite, connected, transitive graph, the random walk escapes at rate at least  $t^{1/2}$  after t steps. Following Erschler, we use non-constant equivariant harmonic mappings to reduce the problem to a study of  $L^2$ -valued martingales. For the case of discrete, amenable groups, we present a new construction of such harmonic mappings based on the heat flow from a Folner set.

Speaker: Gabor Lippner (Harvard University)

Title: Nodal domains on graphs

**Abstract:** We show how to discretize Cheng's result on bounding the multiplicity of Laplacian eigenvalues by the genus. The proof is based on a discrete version of the Courant Nodal Domain theorem. Though certain versions of this theorem have been around, they are insufficient for our application of bounding multiplicities. Extending ideas of Davies et al, we prove two new forms of the Nodal Domain Theorem, one for bounded degree graphs and another for 3-connected graphs with bounded genus.

Speaker: Russell Lyons (Indiana)

Title: From probability to measured group theory

**Abstract:** We explain the differing viewpoints of probability theory on the one hand and measured group theory on the other. This involves passing from random processes on, say, Cayley graphs to random rooted graphs to graphings of measured equivalence relations. We illustrate with an outline of joint work with Gaboriau of the proof that every non-amenable group contains a "measurable free subgroup" of rank 2.

Speaker: Igor Mineyev (University of Illinois Urbana-Champaigne)

Title: Groups, graphs and the Hanna Neumann Conjecture

**Abstract:** The Hanna Neumann Conjecture asserts a specific upper bound on the rank of the intersection of two finitely generated subgroups in a free group. Walter Neumann proposed a strengthened version of the Hanna Neumann Conjecture (SHNC). We will present a proof of SHNC in terms of groups and graphs. We will also discuss trees, flowers, forests, gardens, and leafages. There is an analytic version of this proof using Hilbert modules which allows for generalizations of SHNC to complexes.

Speaker: Asaf Nachmias

Title: Is the critical percolation probability local?

**Abstract:** We show that the critical probability for percolation on a d-regular non-amenable graph of large girth is close to the critical probability for percolation on an infinite d-regular tree. This is a special case of a conjecture due to O. Schramm on the locality of  $p_c$ . We also prove a finite analogue of the conjecture for expander graphs

Speaker: Yuval Peres (Microsoft Research)

Title: Embedding groups in Hilbert space and rate of escape of random walks.

**Abstract:** A metric space X has Markov type 2 if for any stationary reversible finite hidden Markov chain taking values in X, the second moment of the distance from the starting point grows at most linearly in the number of steps. Since Hilbert space  $L_2$  has Markov type 2 (K. Ball 1992) this can be used to bound from below the distortion of any embedding into  $L_2$  of a space where Markov chains can escape faster, e.g. the hypercube. We derive from this a general inequality that bounds the compression exponent for embeddings

of infinite amenable groups via the escape exponent for random walks. The inequality is sharp in lamplighter type groups (Talk based on joint work with Assaf Naor).

Speaker: Laurent Saloff-Coste (Cornell University)

Title: Random walks driven by low moment measures

**Abstract:** On finitely generated groups, we consider symmetric probability measures satisfying some natural moment conditions and prove lower bounds for the probability of return to the starting point after n steps. For instance, on a polycyclic group of exponential volume growth and for a symmetric measure with finite first moment, we prove that the probability of return after n step is bounded below by  $\exp(-cn^{1/2})$ . The proofs involve the notion of trace, comparison of Dirichlet forms and other tools from functional analysis.

Speaker: Tatiana Smirnova-Nagnibeda (Geneva)

Title: Abelian sandpile model, unimodular rooted random networks and self-similar groups

**Abstract:** We propose to consider the Abelian sandpile model on unimodular random rooted networks and address in this context the problem on criticality of the model. This viewpoint allows us to exhibit a multitude of examples of infinite graphs where we prove rigorously criticality of the ASM.

Speaker: Balazs Szegedy

Title: Higher-order Fourier Analysis

**Abstract:** In a famous paper Timothy Gowers introduced a sequence of norms U(k) defined for functions on abelian groups. He used these norms to give quantitative bounds for Szemeredi's theorem on arithmetic progressions. The behavior of the U(2) norm is closely tied to Fourier analysis. In this talk we present a generalization of Fourier analysis (called k-th order Fourier analysis) that is related in a similar way to the U(k+1) norm. Ordinary Fourier analysis deals with homomorphisms of abelian groups into the circle group. We view k-th order Fourier analysis as a theory which deals with morphisms of abelian groups into algebraic structures that we call "k-step nilspaces". These structeres are variants of structures introduced by Host and Kra (called parallelepiped structures) and they are close relatives of nil-manifolds. Our approach has two components. One is an uderlying algebraic theory of nilspaces and the other is a variant of ergodic theory on ultra product groups. Using this theory, we obtain inverse theorems for the U(k) norms on arbitrary abelian groups that generalize results by Green, Tao and Ziegler. As a byproduct we also obtain an interesting limit theory for functions on abelian groups in the spirit of the recently developed graph limit theory.

Speaker: Adam Timar (Vienna)

Title: Approximating Cayley graph versus Cayley diagrams

**Abstract:** We construct a sequence of finite graphs that weakly converge to a Cayley graph, but there is no labelling of the edges that would converge to the corresponding Cayley diagram. This is related to the question whether soficity of a group depends only on the Cayley graph and not on its orientation and labelling by the generators.

Speaker: Robert Young (University of Toronto)

Title: Pants decompositions for random surfaces

**Abstract:** Every hyperbolic surface has a decomposition into a union of three-holed spheres glued along their boundaries, which is called a pants decomposition. The length of a pants decomposition gives one way to describe the geometric complexity of a surface: it describes how difficult it is to break the surface into simple pieces. Bers proved that every hyperbolic surface of genus g has a pants decomposition which has

length bounded by a constant that depends only on g, and one natural question is how this constant depends on g. In this talk, we will give a brief introduction to some techniques from the geometry of hyperbolic surface, describe some results on pants decompositions of surfaces, and present some recent work showing that random surfaces are difficult to decompose into pairs of pants. This talk is joint work with Larry Guth and Hugo Parlier.

Speaker: Wolfgang Woess (Technical University, Graz)

Title: On the spectrum of lamplighter random walks and percolation clusters

Abstract: Let G be a finitely generated group and X its Cayley graph with respect to a finite, symmetric generating set S. Furthermore, let H be a finite group. We consider the lamplighter group over G with group of "lamps" H. This is the wreath product of G with H. We show that the spectral measure (Plancherel measure) of the "switch-walk-switch" random walk on the lamplighter group coincides with the expected spectral measure (integrated density of states) of the random walk with absorbing boundary on the cluster of the group identity for Bernoulli site percolation on X with parameter p = 1/|H|. The return probabilities of the lamplighter random walk coincide with the expected (annealed) return probabilities on the percolation cluster. In particular, if the clusters of percolation with parameter p are almost surely finite then the spectrum of the lamplighter group is pure point. This generalizes results of Grigorchuk and Zuk, resp. Dicks and Schick regarding the case when G is infinite cyclic.

(Joint work with F. Lehner and M. Neuhauser, published in Mathematische Annalen 342 (2008) 69-89.)

# **Scientific Progress Made**

The greatest progress of the meeting was to make the attending researchers of various areas meet and talk to each other. Participants learned each other's angles on the topic of the workshop. Some new questions and directions also emerged from the talks.

# **List of Participants**

Abert, Miklos (Renyi Institute of Mathematics) Amir, Gidi (Bar-Ilan University) Babai, Laszlo (University of Chicago) Bowen, Lewis (Texas A&M) Brieussel, Jeremie (Neuchatel University) Candellero, Elisabetta (Graz University of Technology) Csoka, Endre (Eötvös Loránd University) Elek, Gabor (Renyi Institute) Friedman, Joel (University of British Columbia) Gilch, Lorenz (Graz Technical University) **Glasner, Yair** (Ben Gurion University of the Negev) Grabowski, ?ukasz (Goettingen University) Gurel-Gurevich, Ori (UBC) Harangi, Viktor (Renyi Institute) Hegedus, Pal (Central European University) Kaimanovich, Vadim (University of Ottawa) Karlsson, Anders (University of Geneva) Kassabov, Martin (Cornell University) Lee, James (University of Washington) Li, Xiang (Janet Lisha) (University of Toronto) Lippner, Gabor (Harvard) Lyons, Russell (Indiana University)

Groups, graphs and stochastic processes

Matter, Michel (University of Geneva) Mineyev, Igor (University of Illinois at Urbana-Champaign) Nachmias, Asaf (MIT) Navas, Andres (Universidad de Santiago de Chile) **Peres, Yuval** (Microsoft Research) Pete, Gabor (University of Toronto) Saloff-Coste, Laurent (Cornell University) Smirnova-Nagnibeda, Tatiana (University of Geneva) Stewart, Andrew (University of Toronto) Szegedy, Balazs (University of Toronto) Thompson, Russ (Cornell University) Timar, Adam (Hausdorff Center for Mathematics, Bonn University) Virag, Balint (University of Toronto) Weinberger, Shmuel (University of Chicago) Woess, Wolfgang (Technische UniversitŁt Graz) Young, Robert (University of Toronto at Scarborough)

# Chapter 22

# **Emerging Challenges at the Interface of Mathematics, Environmental Science and Spatial Eco (11w5106)**

# Jul 03 - Jul 08, 2011

**Organizer(s):** Steve Cantrell (University of Miami) Robert Holt (University of Florida) Mark Lewis (Alberta)

## **Overview and Recent Developments**

Traditional mathematical models in ecology, epidemiology, evolution, and related areas typically assume that the environment is uniform in time and space and that the transport of organisms, chemicals, genes, and pathogens through the environment is random. In reality, many environments are heterogeneous in time and/or space and many physical processes and behavioral responses involve nonrandom transport.

Incorporating heterogeneity and nonrandom transport into models for biological processes and then analyzing such models leads to significant new mathematical challenges. There are three unifying features that many of those challenges have in common: (i) The first is that quantities of interest that can be computed readily for random transport in homogeneous environments are, at present, difficult or even impossible to compute or analyze for parameter dependence when there is heterogeneity and/or biased movement; (ii) The second, which often gives rise to the first, is that the mathematical methods and physical or biological insights that allow us to understand simple models cannot be used in the presence of heterogeneity, anisotropy, or nonrandom transport; for example, it is easy to obtain an explicit formulae for the principal eigenvalues of the relevant Laplace operators in simple geometries and uniform space, and these immediately lead to a simple formulation for the minimal size required for a region to sustain a diffusing population with given growth and diffusion rates. On the other hand, there are no such formulae for the principal eigenvalue of a periodic parabolic operator with advective terms and variable coefficients, and there are few results on how the eigenvalues of such operators depend on parameters. Thus, it is much harder to determine the minimal habitat size needed for persistence in environments with semi-realistic patterns of spatial variation. A significant reason for this limitation in our current understanding is that orthodox analytic methods (such as the variational formulation of eigenvalues) can no longer be used, so progress requires the development of new methods; (iii) The third feature concerns the nonlocal nature of many transport processes which can include long-distance displacement or jumps. When transport is nonlocal, local partial differential equation models must be extended to include nonlocal interactions, resulting in integrodifferential or related integrodifference equations. Here, standard mathematical tools for classical spatial models based on partial differential equations, such as regularity theory, maximum principles or the existence of principal eigenvalues, do not necessarily apply.

There is considerable empirical evidence that nonlocal dispersal occurs in some populations, but its significance has rarely been addressed outside of the context of invasion theory. New mathematics will be needed for the analysis of nonlocal dispersal models in other contexts. We envisage that the workshop help define and develop the new mathematics needed for such analysis.

Properly addressing these important issues will not only require new mathematical ideas but also close and on-going interaction between researchers who analyze models (mainly mathematicians) and those who pose questions and formulate models and attempt to link model to data (mainly biologists). Our workshop brought both groups together to identify important analytic challenges associated with models for environmental heterogeneity and nonrandom transport and to develop new mathematical approaches to addressing them. New mathematical challenges have come to the fore in various ways; to illustrate the nature of these challenges and to frame the problems more concretely, we the following describes a number of specific examples.

The rate of spread of a diffusing population into a uniform environment can, typically, be determined by a direct calculation based on a linear analysis, and such an analysis can often be extended to interacting populations. There are some abstract mathematical extensions of these notions to variable and stochastic environments, and there has been some empirical work on the topic, but analytic computations or estimates of spread rates are available only in a few special cases. Similarly, the basic reproduction number for epidemiological models,  $R_0$ , can be computed explicitly by matrix theoretic methods, assuming a nonspatial context and a temporally constant environment. Recently, there have been extensions of R0 theory to include infinite-dimensional models and temporally periodic environments. However, in practice, it remains a challenge as how to calculate the quantity in variable or spatially complex environments. Quantities such as R0 and spread rates that play a critical role in our understanding of models can sometimes be characterized in terms of eigenvalues for certain operators or matrices or as Floquet coefficients, but determining those analytically in terms of model parameters in the context of spatio-temporal heterogeneity presents many difficulties that will require new mathematical ideas to resolve. By mixing top mathematicians and quantitatively skilled environmental scientist together in the workshop, we not only addressed the above challenges mathematically but to also provided insight back to the questions of environmental concern that originally inspired the mathematical models.

Additional new mathematical challenges have recently arisen from issues of pressing environmental concern with anisotropic and directional movement. Examples include streams and rivers, where diffusion is augmented by downstream advection plus anthropogenic water flow manipulation, and terrestrial environments where structures such as roads can lead to movement anisotropy. Advection has been treated in connection with various purely physical processes, and anisotropic diffusion has been studied in the context of image processing, but neither of those areas of research addresses how spatial effects interact with nonlinear population or community dynamics. In the case of models with advection, standard methods based on variational principles do not apply directly, so alternative methods must be developed. These were the subject of discussion and development at the workshop.

Finally, we also considered the impacts of environmental change on populations from the context of optimal dispersal strategies. How should individuals within a population adjust their movement behavior in response to increasing environmental heterogeneity (both spatial fragmentation and temporal fluctuations in environmental conditions)? The issue of the evolution of dispersal strategies under changing environmental conditions is a question of very substantial interest in theoretical biology. It is also of urgent applied interest given the growing evidence for rapid evolutionary shifts in dispersal rates in organisms subsequent to land use changes and alterations in climatic range limits. There has been work on this problem from a number of diverse mathematical viewpoints, ranging from game theory, adaptive dynamics, to optimization to mathematical quantitative genetics, but each of those approaches emphasizes certain aspects of the phenomenon and ignores others. A major mathematical challenge in this area is the development of a synthesis of the different modeling approaches that has the capacity to address topics ranging from mechanistic descriptions of movement under environmental heterogeneity, to the evolutionarily and convergent stability of dispersal strategies, all within a unified framework.

# **Presentation Highlights**

Dr. Chris Cosner presented an overview of research on models for the evolution of conditional dispersal in spatially heterogeneous environments. Here partial differential equation models were coupled to methods from game theory to determine evolution of dispersal. Ideas such as evolutionarily stable strategies, convergent stable strategies and neighborhood invaders were developed in the context of infinite dimensional dynamical systems. Methods based on variational approaches for eigenvalues were developed. A repeating theme in the research was that, under temporally constant environmental conditions, evolution would select diminished dispersal or ideal free dispersal. A challenge for the future is how to incorporate temporal environmental variation into our understanding of evolution of dispersal. This was the subject of much discussion.

Dr. Wenxian Shen addressed the challenge of analyzing spatially heterogeneous dynamical systems with nonlocal dispersal. Much of the analysis investigated the principal eigenvalues of nonlocal dispersal operators in spatially heterogeneous domains. Here, spectral results rely upon constraints regarding the nonlocal operator and the explicitly spatial environmental variation encountered. Conditions for population persistence and methods for analysis of spreading speeds and travelling waves were discussed.

Dr. Wei-Ming Ni reviewed some recent progress in spatially inhomogeneous Lotka-Volterra competitiondiffusion systems. A two species reaction-diffusion system for Lotka-Volterra type competition was investigated for an environment with heterogeneous carrying-capacity. New results concerning which combinations of diffusion coefficients and interspecific competition coefficients result in either a globally attracting coexistence equilibrium or extinction for one of the species. It was shown that if two ecologically equivalent species compete there is a lower limit for diffusivity beyond which slower diffusion can be detrimental. This was compared to the homogeneous case where the slower diffuser always wins. Two open questions were presented regarding the single species equilibrium of a logistic-diffusion equation with heterogeneous carrying-capacity:

- 1. Is the L-1 norm of the difference between the population equilibrium and the carrying-capacity monotone increasing in relation to the diffusion coefficient; and,
- 2. For a fixed total carrying capacity, can the local carrying capacity be distributed in such a way that can yield an arbitrarily large total population at equilibrium?

Dr. Vlastimil Krivan used the ideal free distribution (IFD) and game theory models to study the dispersal of multiple species of omniscient animals in a multi-patch environment. Population dynamics were included into the model by assuming that the animals' adaptive dispersal behavior happened on a faster time-scale than the population dynamics. Predator-prey and Lotka-Volterra competition modules were considered. A variety of dynamics were exhibited including ESS coexistence states, and multiple alternative coexistence states at higher competition levels. It was shown that in some cases adding IFD dispersal can destabilize population equilibriums in multi-species models.

Dr. Robert Holt addressed the role of predation and evolutionary dynamics in determining species range limits. Most species have genetic variation, which allows them to adapt to spatially varying environmental conditions. Models of adaptation and population dynamics in continuous or discrete space show that the interplay of demography, selection, and dispersal (including gene flow) can influence the habitat use and geographical range of a species. A predator-prey model illustrates how the ecological factor of predation can alter the balance of these forces, and thus alter the evolutionary trajectory of a prey species. Sometimes, predation can shift the equilibrial distribution of a prey species and expand its range of habitats, but in other circumstances, predation can constrain prey invasion and hence range limits. Open questions include accounting for the fact that dispersal itself can provide a source of genetic variation; that dispersal is often not simply diffusive; and that predators themselves have genetic variation and can thus evolve. The specific topic of the talk centered around spatially heterogeneous population dynamics, which is exactly the topic of this workshop.

Dr. Henri Berestycki presented new developments regarding reaction-diffusion equations in heterogeneous media. His talk introduced definitions of a General Transition Wave (Front) and its global mean speed for a type of reaction-advection-diffusion equations with temporally and spatially varying diffusion, advection and growth functions in an unbounded domain. For reaction-diffusion equations of KPP and bistable types with spatially varying growth function but constant diffusion rate, the existence or nonexistence of the general transition wave have been given in  $\mathbb{R}^n$  space and in more general unbounded domains with a star-shaped or compact obstacle. However, the existence of the general transition wave in the most general heterogeneous habitats still needs to be investigated and the computation approaches for estimating the mean speed also remain open. The general transition wave in non-local cases is also an interesting problem. The results greatly enrich the study of propagation patterns of population in general heterogeneous habitats.

Heterogeneity enters dynamical models in different ways, one of which is that individuals can switch between phases that may be connected to differential properties of the habitat. Dr. K. Hadeler analyzed diffusively coupled dynamical systems, which are constructed from two dynamical systems in continuous time by switching between the two dynamics. If one of the vector fields is zero, it is called a quiescent phase. His research shows that introducing quiescent phases damps oscillations or even causes them to disappear. In their most recent work, exponentially distributed sojourn times is replaced by general distributions that lead to novel types of delay differential (diffuse) equations. One of the question pointed out in the talk is that the quiescent phase is somehow similar to a refuge which has infinite capacity. In the classic non-spatial competing species models introduced by Lotka and Volterra, the competitive exclusion principle (CEP) plays a significant role. However, in the recent work, Dr. J. Lopez-Gomez proved that even in the simplest cases when the species disperse through random transport, the spatial heterogeneities can lead to a modification of the CEP that might explain the earth biodiversity through the existence of refuge patches for some of the competing species, where they can segregate when the intensity of the aggression from the antagonists increases. An interesting question arouse from the talk is that since the coexistence of species requires that the refuse size for each species should be large enough, the number of different species will be limited if refuses for difference species do not overlap between each other, which is permitted in their model. Then the question is what the maximum number of different species is if they are able to coexist in the same habitat.

Hantavirus is a recent emerging zoonotic disease that is carried by wild rodents. Based upon ODEs, continuous-time Markov chains and branching processes, Dr. Linda Allen presented patch models with three regions reflecting reservoir habitat, spillover habitat and the boundary between them. The key result is that interaction of the species in the boundary region spreads the disease, i.e. there is an amplification rather than a dilution effect due to increased contacts (aggressiveness). It is therefore possible for the spillover species to contribute to the maintenance of the disease in the wild. This is facilitated by the workshop theme of spatial structure. Furthermore, cross-species transmission may lead to host shifts when a new viral strain is able to reproduce in a new host. It was suggested that the model could be used as a starting point to identify in general necessary ingredients for diseases to spill over and back, as well as to suggest key processes to measure in the wild (Mark Lewis). With 16 ODEs, the model is rather complicated, and suggestions have been made how to simplify the model (time scale arguments / Bob Holt; focussing on states of new infection to reduce the NGM / Odo Diekmann). Connections were drawn to reaction-diffusion models with overlapping habitats and competitive interactions (Chris Cosner).

Bacteriophages are viruses that parasitize bacteria and the most numerous life form on the planet. Their spread can be observed on agar plates, where they wipe out bacteria after bursting. The speed of the spreading plaques can be seen as a surrogate for fitness and is therefore of biological interest. Existing models significantly overestimate the wave speed. Dr. Hal Smith presented a model in which the exponential distribution of the latent period is replaced by a fixed delay. The key result is the effect of this delay on the existence and speed of travelling waves. This has been accomplished by applying asymptotic spreading speed theory to a related scalar equation. It appears that this scalar equation can be connected to quiescence (Karl Hadeler). Alan Hastings suggested similarities to certain nematodes and Odo Diekmann to use the fundamental solution of the Laplacian. The rate of plaque advance could be further slowed down by fixing the life time of free virus (Bob Holt). Chris Cosner pointed out that there may be hidden Allee effects breaking down the linear determinacy. Lyme disease is a vector-borne disease and transmitted to humans by the bite of infected ticks. Dr. Xiao-Qiang Zhao based his presentation on a reaction-diffusion model that takes into account the vector's stage structure (Caraco et al., Am. Nat. 2002). Using monotone semiflows in bounded and unbounded spatial domains, the key finding is that host movement spreads the disease spatially. The model could be applied to spatially heterogeneous environments by making some parameters space-dependent. Tying in with spatial control management, the model could be modified to include control to make uniform disease persistence impossible. As an example, Mark Lewis referred to the culling of white-tailed deer in Alberta with the aim to control chronic wasting disease. Jim Powell pointed out that deer move very differently within and between habitats (also, prions are very persistent and should therefore be an interesting spread problem). Furthermore, it was suggested that the basic model might be modified to include frequency-dependent transmission (vector-borne disease) and passive movement of the vector proportional to the host movement.

Dr. Sergei Petrovskii tackled a major question of dispersal when realistic individual movement is taken into account. Specifically, given a point source release of N individuals at time t=0, with population density r(x,t), the main question is "what is the rate of decay for large |x| as t evolves?" It is known that realistic movement often involves (at least for some ranges) a statistical distribution with fat tails, so the initial question can be rephrased in terms of: (1) What is the process behind fat tails? (2) Do fat-tails mean non-Brownian motion? (3) Is diffusion irrelevant? The answer to all questions is "diffusion prevails", and the method to reach this conclusion is via a diffusivity distribution function. The theoretical framework was put to test with real-world data, and results are encouraging; the next step is to widen the validation of this framework with more species.

The main question of the talk of Dr. William F. Fagan was how complex population-level patterns arise as a result of (1) population-level movement, (2) individual-level movement, and (3) dynamic resources. Resources vary according to amount, spatial variability, temporal variability, and resource predictability. The movement mechanisms are either non-oriented (diffusion), oriented (perception-based), and spatial memory (own history, communication, genetic inheritance, path integration, cognitive maps). It was noted that consumers evolved to use different mechanisms in different situations, leading to patterns of residency, migration, nomadism in which there is no pattern, and nomadism in which there is no repetition of terrain. The talk addressed the problem of how landscapes influence movement, and identifies, for several ungulate species, mechanisms of response to dynamic resources, and infotaxis, i.e. when information directs movement due to spatial memory, and communication. The main question opened is how to incorporate these phenomena into an analytical framework capable of explaining phenomena whose qualitative properties are well understood.

Dr. Roger Nisbet linked mathematics to a conservation problem in environmental sciences. Specifically, he used the Pacific salmon as a study case to illustrate that for species which encounter strongly varying spatial scales at different life stages, it is important to consider entire life cycle. Dynamic Energy Budget Theory (DEB) offers a good vehicle in which to take behavior, physiology and space into account simulataneously. A standard DEB model can represent the complete life cycle in a parameter-sparse way and provide a generic model. Comparison of salmon data with model predictions shows agreement on both inter-species level and intra-species level. The biological importance of considering varying spatial scales across different life stages wass highlighted throughout the presentation.

Dr. Thomas Hillen discussed how transport equations can be employed in spatial ecology to model movement in habitats with directional features that provide faster travel routes. Scaling methods for these transport equations that were previously considered separately (moment closure, hyperbolic scaling and parabolic scaling), are shown to lead to the same drift-diffusion limit, where the drift and diffusion are determined by the expected orientation of the habitat and its variance, respectively. Depending on the scaling, drift- or diffusiondominated limits can be obtained. The parabolic scaling is only applicable if the expected habitat orientation is zero. Application to wolf movement shows that they prefer to move along seismic lineswhich enables them to spread out faster from a point compared to uniform movement. The talk brings together different mathematical tools for the modeling of an ecological phenomenon, and mathematics is linked with ecological data.

Dr. Otso Ovaskainen discussed animal movement and evolution of dispersal in heterogeneous space using the Glanville fritillary butterfly as an example. He proposed a simple model incorporating random walk and habitat selection for butterfly movement. Linear landscape elements such as corridors and barriers are explicitly considered in the model. He used diffusion-advection-reaction models to fit mark-recapture data. The model can be applied to predict the probability that a butterfly visits a specific meadow and to examine effects of a movement corridor. In the second part, he discussed two ways of modeling dispersal evolution: ESS and ESFD, and simulated the movement of an individual with short-ranged dispersal kernel and an individual with long-ranged dispersal kernel. The models are analyzed by moment closures or perturbation expansions. Furthermore, he discussed how life-history and land structure influence the evolution of dispersal. As for the connection to the theme of the workshop, this talk provides a good study example for animal movement and its evolution. More empirical evidence needs to be accumulated for validating and calibrating the evolutionary dispersal models.

Dr. Alan Hastings presented a talk on the stochastic aspects of dispersal and on the control of invasive

species. He employed the stochastic Ricker model with various stochasticities: demographic stochasticity, environment stochasticity, demographic heterogeneity, and sex ratio stochasticity, to discuss species extinction. His group performed a series of experiments on red flour beetles to validate the model. His study suggested that typical deterministic models can be misleading. For instance, many species could be at much higher risk than we think. In the second part of his talk, he computed stochastic spread speed using a stochastic modeling framework. In the last part, he discussed the management of invasive species (cost versus risk) and showed that an Allee effect slows invasion considerably. As for the relationship to the theme of the workshop, this talk was the only one discussing stochastic aspect of dispersal and the control of invasive species .

Dr. Donald DeAngelis discussed several ecological issues of significance a specific locale, namely the Florida Everglades: (1) the ecotone dynamics of halophytic and freshwater vegetation types under rising sea levels, changing ground water salinity, and storm surges; (2) dynamics of fish under a hydrology with strong temporal dependence; (3) dynamics of highly mobile hydrology dependent species with small populations, such as the snail kite. The approach outlined is that of supplementing rigorous mathematical models (ODE, PDE, matrix) with less rigorous but flexible individual or agent based models.

Dr. Mark Lewis discussed issues related to the analysis of spatiotemporal models for steam and river populations. Such ecosystems consitute instances where biology meets physics, in that population dynamics are coupled to stream flow. In this regard, Dr. Lewis examined the role of spatial heterogeneity and flow rate in mediating predictions of persistence for both a single pelagic population in the drift and for a population with drift and benthic states. Following was a discussion of biogeographic issues related to the "drift paradox", in particular the interplay between upstream spread rate and the stream length needed to sustain a population. He then showed how the notion of net reproductive rate from epidemiology can be formulated in the current ecological context for a single pelagic species based on the concept of a next generation operator, and how this formulation can then recover mathematical results pertaining to biogeographical aspects of the drift paradox.

## **Scientific Progress Made**

This meeting has highlighted important issues at the interface mathematics, environmental science and ecology. We had particular foci for each morning/afternoon of each day of the meeting, in discussing important, fundamental mathematical and ecological issues, around which the talks were built: dispersal, impact of spatial heterogeneity, invasion and spread, scale, determinism and stochasticity and real-world applications. The talks keyed-in markedly on each of these themes, much to the credit of speaker who made concerted effort to connect closely with the workshop themes.

Perhaps unsurprisingly, many of the connections that were made were unanticipated. In particular, the discussions generated new ways to connect seemingly disparate areas. For example, dynamic energy budgets were connected to optimal spatial movement modelling; analysis of detailed animal migration patterns was connected to transport equation models and their scaling limits; spatial competition models and analysis was connected to issues of biodiversity, spatial segregation, niche theory and promotion of spatial coexistence; the ideal free distribution and game theory was connected to predator-prey dynamics and evolution of species ranges. The list goes on.

Mathematically the structure of the meeting rested upon new developments in nonlinear infinite-dimensional spatial operators arising from reaction-diffusion-advection models, integrodifference and integrodifferential systems, games theory, stochastic processes and stochastic differential equations. These developments including methods of analyzing spectra and eigenvalues, comparison methods, construction of super- and sub-solutions, energy methods, dynamical systems theory, and functional analysis. Here the new mathematical models, arising from ecological, environmental and evolutionary questions, challenged mathematical theory to investigate fundamental model properties, such as well-posedness, spreading speeds, persistence, anisotropy, invasibility, and optimality. In several cases, classical ecological theory was turned on its head. For example we learned how evolutionary pressures actually allow predators to enhance prey growth and spread (R. Holt), quiescent stages in life history can actually destabilize systems , promoting temporal oscillations (K. Hadeler), and variation between individuals can have dramatic population-level effects, such as greatly magnified spreading speeds (S. Petrovskii).

In other areas no ecological theory existed, and the talks outlined new ways to use mathematics to develop this theory. For example the concepts of spatial learning and memory in animal movement are in their infancy. However, new mathematical models can explain how different spatial movement strategies result in characteristic movement patterns such as nomadism, range residency and migration (W. Fagan). We are just beginning to study optimal dispersal in nonautonomous nonlocal systems and there will be considerable mathematical challenges going forward.

Spatial and temporal scales have been a recurring element, arising time and again in different areas. The key element is being able to formulate mathematically tractable models where movement, demographic processes, and population structure are included at the level needed for scientific insight.

### **Outcome of the Meeting**

The meeting brought together mathematicians and biologists in new ways. We held extensive break-out sessions and discussion that lead to a deepening of our understanding of the mechanistic construction and analysis of mathematical models. Indeed several entirely new areas of mathematical model development were suggested at the meeting. These include physiologically-based movement modelling etc.

Moving towards a more profound mechanistic basis for ecological and environmental models is a key element in the maturation of the field of mathematical ecology. This meeting has taken us on the first steps.

There are several ideas for follow-up meetings, including potentially, future meetings at BIRS.

## Abstracts of Talks

#### Linda J. S. Allen, Texas Tech University, Spread of Disease from Reservoir to Spillover Populations

Interspecies pathogen transmission is a primary route for emergence of new infectious diseases. Spatial overlap of habitats leads to greater numbers of interspecies encounters which in turn may lead to pathogen transmission in a nave host or adaptation of the pathogen to create a new reservoir. Deterministic and stochastic patch models for spread of disease among reservoir and spillover populations are used to investigate the dynamics of interspecies pathogen transmission when habitats overlap.

#### Henri Berestycki EHESS-Paris and University of Chicago Reaction-Diffusion Equations in Heterogeneous Media

I will review several recent developments regarding the mathematical theory of reaction-diffusion equations in general non-homogeneous framework. Issues such as non-uniform stationary states, generalized transition waves and what determines the speed of propagation will be discussed. These topics are relevant for ecology modeling in heterogeneous environment.

#### Chris Cosner University of Miami Models for the Evolution of Conditional Dispersal in Spatially Heterogeneous Environments

Mathematical models predict that in environments that are heterogeneous in space but constant in time, there will be selection for slower rates of unconditional dispersal, including specifically random dispersal by diffusion. However, some types of unconditional dispersal may be unavoidable for some organisms, and some organisms may disperse in ways that depend on environmental conditions. In some cases, models predict that certain types of conditional dispersal strategies may be evolutionarily stable within a given class of strategies. For environments that vary in space but not in time those strategies are often the ones that lead to an ideal free distribution of the population using them, provided that such strategies are available within the class of feasible strategies.Problems in the evolution of dispersal have been addressed from two complementary mathematical viewpoints, namely game theory and mathematical population dynamics. This talk will describe some results and open problems from the viewpoint of spatially explicit models in population dynamics, including reaction-diffusion-advection models and models for nonlocal dispersal. Some of the results and problems are related to the evolutionary stability of dispersal strategies leading to an ideal free distribution and the mechanisms that might allow organisms to realize such strategies.

#### Donald L. DeAngelis U. S. Geological Survey and University of Miami Plant Herbivore Defense: Modeling Optimal Defense Allocation as a Function of Light and Nutrient Availabilities and Intensity of Herbivory

Woody plants allocate their acquired resources, energy (or carbon) and nutrients, to meet their several essential functions. In order to grow and reproduce, plants allocate resources to acquire solar radiation (grow leaf biomass) and to acquire nutrients (grow fine root biomass). Investment instem wood, beyond what is needed structurally by the foliage and roots, is provided to obtain a competitive advantage through height for capturing light. In addition to the allocation of resources to these essential functions, resources are usually allocated to chemical antiherbivore defense, or other types of defense, such as spines or thickening of leaf surfaces, because herbivory can significantly reduce growth and increase mortality, thereby reducing plant fitness. Optimization of physiological trade-offs between growth and defense has been termed a central dilemma of plants. However, despite extensive research on chemically mediated plant herbivore interactions over the past three decades, an improved synthesis of plant defenses as a part of plant resource allocation strategies is lacking. Although such a synthesis will ultimately depend upon on empirical examination of patterns of chemical defense over a broad variety of environments, the efficiency of this empirical research can be greatly increased by appropriate use of modeling. The purpose of this study is to interpret theory using a quantitative framework for determining optimization of trade-offs between growth and chemical (or other) defense in terms of phenotypic responses of a plant as a function of spatial and temporal variation, external conditions, including available solar radiation (influenced by the degree of shadiness), external nutrient input, and intensity of herbivory. The model treats plant components and the herbivore compartment as variables. The herbivory is currently assumed to be purely folivory. Three alternative functional responses are used for herbivory, two of which are variations on donor dependent herbivory and one of which is a Lotka-Volterra type interaction. All three are modified to include the negative effects of chemical defenses on the herbivore. In preliminary results, optimal strategies of carbon allocation are found and shown to vary with most changes in environmental conditions. Increased intensity of herbivory led to an increase in the optimal allocation of carbon with increasing intensity of herbivory. Decreases in available limiting nutrient generally led to increasing importance of defense. Increases in shading also led, in one of the models, to increases in defense allocation, though not in the other two. Because the plant defense was only in the foliage, increases in allocation to plant defense were usually accompanied by shifts in carbon allocation from foliage to fine roots, because the effects of herbivory on foliage decreased.

#### William F. Fagan and Thomas Mueller University of Maryland Migration, Nomadism, and Range-Residency: How Landscape Dynamics Link Individual Movements to Population-Level Patterns

To help synthesize existing research, I will outline a unifying conceptual framework that uses spatio-temporal resource dynamics to bridge the gap between individual-level behaviors and population-level spatial distributions. This framework distinguishes among (1) non-oriented movements based on diffusion and kinesis in response to proximate stimuli, (2) oriented movements utilizing perceptual cues, and (3) memory mechanisms that assume prior knowledge of movement targets. Species use of these mechanisms depends on life-history traits and resource dynamics, which together shape population-level patterns. Static and well-dispersed resources should facilitate sedentary ranges, whereas resources with predictable spatial distributions but seasonal variation should generate migratory patterns. A third pattern, 'nomadism', should emerge when resource distributions are unpredictable in both space and time. Extensive empirical datasets detailing animal movements, remote sensing imagery time series, and a variety of mathematical models will all be used to demonstrate the connections among individual movements, landscape dynamics, and population-level patterns.

#### K.P. Hadeler University of Tuebingen and Arizona State University Coupled Dynamics, Quiescent Phases, and Distributed Sojourn Times

Heterogeneity enters dynamical models in different ways. For example, consider a population distributed in space that evolves in time. The whole population can be subject to temporal (e.g. seasonal) changes of the habitat, individuals can move in a heterogeneous habitat, or individuals can switch between phases that may be connected to differential properties of the habitat. These different views of what happens to individuals lead to models that may appear similar but which may greatly differ with respect to stability of stationary states, properties of periodic orbits, and traveling waves. Phases of quiescence (resting phases) or reduced activity provide illuminating examples. In our most recent research (with Frithjof Lutscher) we replace exponentially distributed sojourn times (the usual Poisson assumption) by general distributions that lead to novel types of delay differential (diffusion) equations.

#### Alan Hastings University of California, Davis Spatial Population Dynamics and Control of Spatial Populations

I will discuss two related issues in spatial ecology. I will consider the dynamics of spatial spread when all appropriate sources of stochasticity are included. This work shows that calculations from typical deterministic models can be very misleading. A key issue is that in natural systems have only a single realization of a stochastic process. I will then consider how to optimally control the spread of invasive species, using the case of Spartina alterniflora as an example. This work shows the difficulties of drawing on rules of thumb to determine control strategies.

#### Thomas Hillen and Kevin J. Painter University of Alberta Kinetic Models for Movement in Oriented Habitats and Scaling Limits

Kinetic models for movement in oriented habitats are a useful tool if the environment shows some distinct directional features, such as roads, rivers, seismic lines, or row-plantations. Historically, kinetic models were considered for diluted gases (Boltzmann equations), and various scaling limits were developed. In my talk I plan to review the three most common scaling methods (i) parabolic scaling, (ii) hyperbolic scaling, and (iii) moment closure, in the ecological context. I will show how these scalings are related and I will discuss in which case which scaling is more appropriate. I will illustrate the theory on examples of movement in habitats with linear features, on attraction to a food source, and on life in a stream.

#### Robert D. Holt University of Florida Predation and the Evolutionary Dynamics of Species Ranges

Gene flow that hampers local adaptation can constrain species distributions and slow down invasions. Predation as an ecological factor mainly limits prey species ranges, but a richer array of possibilities arise once one accounts for how predation alters the interplay of gene flow and selection. In this talk, I will extend previous single species theory on the interplay of demography, gene flow, and selection, by investigating how predation modifies the coupled demographic-evolutionary dynamics of the range and habitat use of a prey species. I first consider a model for two discrete and heterogeneous patches, coupled by movement, and then a complementary model for species distributed along continuous environmental gradients. The latter involves an extension of familiar reaction-diffusion models, stemming back to Skellam. I show that predation can strongly influence the evolutionary stability of prey habitat specialization and range limits. Predators can permit prey to expand in habitat use or geographical ranges, or conversely cause range collapses. Transient increases in predator tightens or loosens evolutionary constraints on the invasion speed and ultimate size of the range of its prey depends on the predator effectiveness, its mobility relative to its prey, and the preys intraspecific density dependence, as well as the magnitude of environmental heterogeneity. These results potentially provide a novel explanation for lags and reversals in species invasions.

#### Vlastimil Krivan Czech Academy of Sciences The Ideal Free Distribution

The IFD is a game theoretical model that describes a theoretical distribution of a population in a patchy environment consisting of habitat or foraging patches. Under the IFD, payoff in all occupied patches is the same and individuals cannot increase their fitness by changing their strategy. Thus, the IFD is a Nash equilibrium of the underlying habitat selection game. Originally, this concept was defined for a single population that does not undergo population dynamics. In my talk I will discuss some extensions of his concept to situations with more interacting populations (e.g., two competing species), and with populations that undergo population dynamics. I will show that distributional models based on the IFD when combined with population dynamics. Some of these simple models that combine population dynamics with distributional dynamics can be analyzed provided we assume time scale separation. In my talk I will focus on the situation where behavioral (distributional) dynamics operate on fast time scale when compared with population dynamics. The resulting models lead to piece-wise continuous differential equations that, in the case of two or three interacting species, are often analyzable.

#### Mark Lewis University of Alberta Analysis of Spatiotemporal Models for Stream Populations

Water resources worldwide require management to meet industrial, agricultural, and urban consumption needs. Management actions change the natural flow regime, which impacts the river ecosystem. Water managers are tasked with meeting water needs while mitigating ecosystem impacts. We develop process-oriented advection-diffusion-reaction equations that couple hydraulic flow to population growth, and analyze them to assess the effect of water flow on population dynamics. We present a mathematical framework, based on the net reproductive rate  $R_0$  for advection-diffusion-reaction equations and on related measures. We apply the measures to populations in rivers under various flow regimes. This work lays the groundwork for connecting  $R_0$  to more complex models of spatially structured and interacting populations, as well as more detailed habitat and hydrological data. This is achieved through explicit numerical simulation of two dimensional depth-averaged models for river population dynamics. This talk is is based on recent collaborative work with Frank Hilker, Jon Jacobsen, Yu Jin, Hannah McKenzie, and Peter Steffler as well as earlier collaborative work with Frithjof Lutscher, Ed McCauley, and Roger Nisbet.

#### Julian Lopez-Gomez Complutense University of Madrid Biodiversity through High Intensity Competition

Classical non-spatial competing species models, as introduced by A. J. Lotka and V. Volterra, predict extinction of some of the species when the level of the aggressions between antagonists is sufficiently large. As a byproduct, in non-spatial models the principle of competitive exclusion plays a significant role in describing the dynamics. Rather strikingly, even in the simplest cases when the species disperse through random transport, the spatial heterogeneities might explain the Earth biodiversity through the existence of refuge patches for some of the competing species, where they can segregate when the intensity of the aggression from the antagonists increases. If the refuge patches can support each of the species in the absence of competitors, some further adaptation mechanisms to the inherent territorial specificities might explain the extraordinary biodiversity of Gaia; possibly enhanced by some additional, eventually hidden, facilitative mechanisms between the species which might increment, even dramatically, the productivity and stability of the ecosystem, as it seemingly occurs in the tropical habitats. The importance of mathematical models in designing stable and productive ecosystems will become apparent when scientists can predict, by simply analyzing a prototype model, some hidden unexpected relevant phenomenology, like it was the prediction of the curvature of the light in Physics, by A. Einstein, one century ago. Here relies the great power of mathematics in dealing with real world problems. Besides estimating the relevant parameters of the models, mathematics provides with very simple toys to think about and order the available information in a rather systematic way.

#### Wei-Ming Ni University of Minnesota and East China Normal University Some Recent Progress in Spatially Inhomogeneous Lotka-Volterra Competition-Diffusion Systems

In recent years, lots of extremely interesting research in understanding the interaction among diffusion, directed movements and spatial heterogeneity have been done. In this talk I wish to report some of the recent progress in this direction.

#### Roger M Nisbet University of California Santa Barbara A Salmon's Perspective on Spatial Ecology

The dynamics of a population are determined by the interactions of individual organisms with their environment. However, different spatial characteristics of the environment are important at each life stage. I shall illustrate this by considering the full life cycle (egg/embryo, juvenile adult) of Pacific salmon. Eggs mature in gravel in upland streams, young fish grow in stream and river habitat before migrating to the ocean, and returning fish migrate upstream and spawn. Key physiological rates in all life stages can be described by a Dynamic Energy Budget (DEB) model that relates growth, development and reproduction to the fishs environment. The models qualitative predictions have been tested for five species: pink, chum, sockeye, coho and chinook. Practical application of the model to any particular salmon population requires considering processes at many spatial scales. Embryonic development and survival is influenced by spatial heterogeneity at the scale of 10-2m. Growth of young fish is influenced by the flow mediated dispersal of benthic macroinvertebrates that comprise their major food; food supply in upland streams will vary over 1-10m. Migrating juveniles face challenges of high temperatures and low water quality on a scale of 1-100km. Returning adults do not feed but face energetic challenges in upstream migration with large spatial heterogeneity in currents. I shall review how each is treated when working with the DEB model, and end with some general remarks on integrating multi-scale spatial and physiological heterogeneity into population models.

#### Otso Ovaskainen University of Helsinki Environmental Heterogeneity in Continuous-Space Continuous-Time Models

I discuss models of animal movement, population dynamics and evolutionary dynamics, focusing on the interplay between environmental heterogeneity and a biological process. I consider both theoretical approaches examining the link between the underlying assumptions and the emerging patterns, and statistical approaches aimed at interpreting data. I first discuss how mark-recapture data (e.g. on butterfly movements) can be fitted to diffusion-advection-reaction models. Here environmental heterogeneity is modeled either through a discrete set of habitat types (with habitat selection at boundaries) or through continuously varying habitat quality. Inclusion of linear elements (such as movement corridors or barriers) leads to a mixture of twoand one-dimensional diffusions. I then discuss how diverse ecological and evolutionary phenomena can be modeled by spatio-temporal point processes. In this framework environmental heterogeneity is modeled e.g. through a smoothed point field, allowing one to control parameters such as patch size, patch quality, and patch turnover rate. The spatial and stochastic individual-based models can be analyzed mathematically by constructing a perturbation expansion around the mean-field obtained at the limit of global interactions. As an example I discuss how the evolution of dispersal distance depends on landscape structure, life-history parameters and the approach taken to model evolutionary dynamics (adaptive dynamics vs. mutation-selection-drift balance).

#### Sergei Petrovskii University of Leicester A Tale of Two Tails: The Impact of Statistical Structure

The rate of decay in the population density at large distances from the species main range has been an issue of controversy, a subject of heated debate and a focus of intensive research for at least two decades. The traditional random walk/diffusion-based theoretical framework that predicts a thin Gaussian tail was eventually opposed by superdiffusion theories resulting in a fat tail with either exponential or even a slower power law rate of decay. Indeed, field data often show a decay rate slower than Gaussian. This issue is apparently very important for understanding invasion rates as a fatter tail normally results in a faster spread of the invading species. Here we show that the thin tail is, in fact, an artifact of an over-simplified description of the dispersing population and not an immanent property of the random walk diffusion. Specifically, we show that a fat-tailed dispersal curve arises naturally in a population of non-identical individuals, i.e. in a population with some inherent statistical structure. Therefore, contrary to a widely spread opinion, a thick dispersal tail is not necessarily a fingerprint of Levy flights or superdiffusion. A good understanding of population dispersal and biological invasions is hardly possible without knowing what happens on the microscale of the individual movement. Correspondingly, we then proceed to the analysis of animal's individual paths. Movement paths are characterized by the duration of bouts of continuous movements. Studies on different species have revealed that the distribution of bout durations often has a fat tail well described by a power law. The relation between this pattern and the underlying processes remains poorly understood though. Basing on the concept of statistically structured population introduced in the first part of the talk, here we formulate an approach that allows us to describe data on bout duration within a unified framework and show that a truncated fat-tail in the bout distribution of animal movement is an immediate consequence of the inherent statistical variation of individual traits.

#### Wenxian Shen Auburn University Nonlocal Dispersal in Spatially Periodic Media

The current talk is concerned with two separate, but related dynamical aspects associated to nonlocal dispersals in spatially periodic media, that is, the principal eigenvalue of spatially periodic nonlocal dispersal operators and the spatial spread and front propagation dynamics of monostable equations with nonlocal dispersal in spatially periodic habitats. First, a principal eigenvalue theory for nonlocal dispersal operators with space periodic dependence is developed, which plays an important role in the study of spatial spread and front propagation of spatially periodic nonlocal monostable equations and is also of independent interest. It is seen that a nonlocal dispersal operator with space periodic dependence has a principal eigenvalue for following cases: the nonlocal dispersal is nearly local; the periodic dependence is nearly globally homogeneous or it is nearly homogeneous in a region where it is most conducive to the growth of the solutions of the associated evolution equation. It is also seen that in general, a nonlocal dispersal operator may not have a principal eigenvalue, which reveals some essential difference between nonlocal and random dispersal operators. Second, by applying the principal eigenvalue theory mentioned above, it establishes some general theory about spatial spreading speeds and traveling wave solutions of spatiallyperiodic nonlocal monostable equations, including the existence of spatial spreading speeds and the existence, uniqueness, and stability of traveling wave solutions in any given direction with speed greater than the spreading speed in that direction. It is seen that the spatial spreading speeds is independent of the existence of principal eigenvalue of the linearized nonlocal dispersal operator at the trivial solution. It is also seen that the spatial variation of the underline medium speeds up the spatial spread. The talk will also present some ongoing research on nonlocal monostable equations in locally spatially inhomogeneous habitats.

#### Hal Smith, Don Jones, Horst Thieme, Gergely Rost Arizona State University Spread of Viruses in a Growing Plaque

A reaction diffusion system with time delay is proposed for virus spread on bacteria immobilized on agarcoated plate. The delay explicitly accounts for a virus latent period of fixed duration. The focus is on the speed of spread of the plaque and on the existence of traveling wave solutions of the model equations, which represent a spreading plaque. We give a rigorous proof of upper and lower spreading speeds associated with the system and provide a proof of the existence of traveling wave solutions. Our spreading speeds give better quantitative agreement with experimental results than earlier, non-rigorous, results.

#### Xiaoqiang Zhao Memorial University Global Dynamics of a Reaction and Diffusion Model for Lyme Disease

In this talk, I will report our recent research on a reaction and diffusion model for Lyme disease. In the case of a bounded spatial habitat, we obtain the global stability of either disease-free or endemic steady state in terms of the basic reproduction number  $R_0$ . In the case of a unbounded spatial habitat, we establish the existence of the spreading speed of the disease and its coincidence with the minimal wave speed for traveling fronts. Our analytic results show that  $R_0$  is a threshold value for the global dynamics and that the spreading speed is linearly determinate.

## **List of Participants**

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## Chapter 23

# Mathematical Biology of the Cell: Cytoskeleton and Motility (11w5050)

## Jul 31 - Aug 05, 2011

**Organizer(s):** Anders Carlsson (Washington University) Adriana Dawes (University of Alberta) Leah Edelstein-Keshet (University of British Columbia) David Sept (University of Michigan)

## **Overview of the Field**

#### **Introduction and Rationale**

Cell biology and mathematics have traditionally been distinct areas of science, each with its own culture, techniques, and approaches. Until recent times, the only points of contact were a few key biophysical concepts, with relevant mathematical formulations, that were applied in a cell biology context. However, this situation has drastically changed. First, cell biology has become increasingly quantitative and new experimental techniques allow researchers to collect extremely detailed information for both *in vitro* as well as *in vivo* systems. Concomitant with this, there has been explosive growth of computational biology with essential aspects of mathematics, physics, and computational methods at its core. These new techniques and areas of focus have been used to gain a deeper understanding of eukaryotic cells, how these cells orient and move, and what roles are played by the underlying biopolymers and regulators.

Cell biology, and the cytoskeleton in particular, constitute a particularly promising area of contact between mathematics and the life sciences due to the abundance and complexity of the available data. This means that biologists are more inclined to actively seek collaboration with mathematicians, physicists, and computer scientists, and there is an obvious need for mathematical analysis of complex pathways to decipher data sets that cannot be understood by traditional methods. This workshop was in essence a follow-up to a BIRS meeting held in the summer of 2005 (Mathematical Modeling of the Cell: Cytoskeleton and Motility 05w5004). That first meeting planted many ideas that have now come to fruition, and many participants from the 2005 meeting were able to return and participate in this workshop.

#### The Cytoskeleton and the Cell

In order to put the developments and presentations from the workshop in the proper context, it is useful to first present some basic background on the relevant biology. All eukaryotic cells, or cells with a nucleus, contain an array of polymers collectively referred to as the cytoskeleton. There are three primary filament types: actin filaments, microtubules and intermediate filaments. The cytoskeleton is involved in a wide range

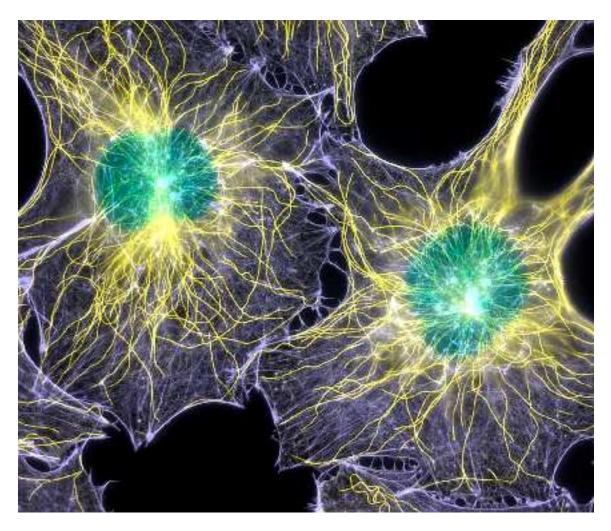


Figure 23.1: Fluorescent micrograph of a cell highlighting the microtubules (yellow), actin filaments (blue) and cell nucleus (green). Image courtesy of Torsten Wittmann (UCSF).

of cellular functions including cell division and cell migration. Further, the cytoskeleton provides a structural framework within the cell, allowing it to both exert and respond to extracellular stimuli.

As shown in Figure 1, actin filaments and microtubules often assume semi-regular arrays within cells. Microtubules are the most rigid structures in the cell, typically emanating from the microtubule organizing center (MTOC) next to the nucleus. Actin filaments can assume a variety of different conformations including bundles, where the filaments are arranged in a parallel or antiparallel fashion, or branched networks. These branched networks typically found at the edge of migrating cells, form a broad thin structure called a lamellipod. The cytoskeleton is involved in determining cell shape and movement.

It should not be surprising that actin filaments and microtubules do not act alone. Rather, their function is regulated by a multitude of associated proteins. Some of these associated proteins help to polymerize or depolymerize the filaments, crosslink filaments into networks or bundles. Motor proteins exert forces between filaments, organelles, cell membrane and extracellular matrix. Biochemistry and cell biology have given us a wealth of data about the components and parts of this system, but many details are still missing. More than that, how the system is organized to work coherently in space and time is still an elusive question. Given the inherent complexity of this system, mathematical and physical models are playing an increasingly important role in elucidating the underlying behaviour of the cytoskeleton and its role in many cellular functions.

## **Recent Developments and Open Problems**

#### **Experimental Advances**

Cell biology has been significantly impacted by the introduction of many new experimental techniques that allow more accurate and quantitative measurements to be made. There are several burgeoning areas of technology development, such as super-resolution microscopy, that hold promise to further revolutionize the field, but in this section we highlight a few recent advances that have had major impact on our understanding of cell motility and the cytoskeleton.

In 2008, the Nobel Prize in Chemistry was awarded to Shimomura, Chalfie and Tsien for their discovery and development of green fluorescent protein (GFP). The ability to express GFP tagged proteins in cells and observe their localization, movement and interaction has led to a completely new understanding of the cell. This technology was further exploited with Total Internal Reflection Fluorescence (TIRF) microscopy. This technology uses the evanescent wave resulting from total internal reflection to illuminate only a narrow portion of the viewing field, eliminating the background that would result in standard fluorescent microscopy. This technology allows researchers to view processes at or near the cell membrane, in the case of live cells, but is also very useful in purely *in vitro* systems where the dynamics and interactions of actin filaments or microtubules can be observed in detail. These advances in protein labelling and microscopy now allow researchers to make detailed measurements on cell processes to the point of determining the order of events and assigning kinetic rate constants to individual interactions. One of the workshop participants, Tom Pollard (Yale), has long advocated that to truly understand a process knowledge of rate constants is essential. This viewpoint meshes well with mathematical modellers, whose description of these cellular phenomena using coupled differential equations relies on estimates for such rate constants.

One clever extension of fluorescent labeling is known as fluorescent speckle microscopy. In this scenario the concentration of the fluorescent proteins is low enough that individual proteins appear as dots or speckles. For example, polymers appear as a series of puncta that move and flow as filaments polymerize or are translocated by motor proteins. Multiple particles can be simultaneously followed using different fluorescent labels. Gaudenz Danuser (Harvard Medical School) has developed elaborate methods to track these particles and quantify their movements. These methods have been widely adopted, giving new insight into many complex processes including cell migration, dynamics within lamellipodia, and cell division.

One final advance that must be mentioned is the development of new (biological) model systems and cell environments. For many years, researchers studying cell motility and migration used two-dimensional systems of cell(s) crawling on glass. This has been ideal for microscopy and, in some cases, for determining biochemical details underlying motility. However it has become apparent that some essential details are missing. First, the mechanics of the substrate strongly affect the cell, and many researchers, including work-shop participant Paul Janmey (University of Pennsylvania), have now shown that hard surfaces, like glass, affect cells differently than softer, more biologically appropriate substrates such as collagen or fibrin. Second, although it is easier to study cells in a 2D environment, cells within the body interact in a 3-dimensional network of cells and matrix. Denis Wirtz (Johns Hopkins), has shown how motility in 3D differs in many aspects from previous 2D studies. This factor will undoubtedly become more fully explored in future research.

#### **Theory and Modeling Advances**

Recent years have seen an increasingly close two-way interaction between theory and experiment, in which theory is beginning to guide experimentalists to particular systems and parameter ranges for performing experiments that discriminate between competing hypotheses. This trend has been manifested in several methodologies and approaches to the theory of complex systems which have expanded over the past decade.

Multiscale modeling, which originated in materials science but is now increasingly practiced in biology, involves grafting approaches which treat a complex system at differing length scales. For example, it could constitute a "wedding" of an atomistically based approach with one based on continuum elasticity. Such modeling has the advantage that it can, in principle, combine the accuracy of atomistic methods with the ability of more coarse-grained methods to treat spatial scales of micrometers and time scales of minutes. One could never treat all of the molecules in a cell in a single computer simulation, but with the use of continuum models based on molecular-level calculations one can incorporate molecular-level information

into a treatment of a whole cell. Examples of such work at the meeting included simulations of whole-cell behavior from the lab of Alex Mogilner (UC Davis), and work by David Sept (University of Michigan) and Fred MacKintosh (Vrije Universiteit) developing elastic models of microtubules based on information from intensive molecular-level simulations of small microtubule fragments.

Stochastic simulation has increasingly become a standard component of a theorist's portfolio. This is important for cell biology because a number of phenomena, such as transcription regulation by small-copynumber proteins or the growth of a microtubule, involve a small number of constituents so that fluctuations are important. This arm of theory is further driven by the ability to watch the growth of biopolymers such as microtubules at sufficiently high resolution to see the stochastic nature of the growth. Stochastic simulation, in its simplest form, involves assigning a random number to each possible event which could occur during a time interval, and in more complex realizations uses algorithms in which the time step is variable, and determined by the rates. Provided that distinct events are not too strongly correlated, such methods describe the fluctuations accurately. Applications of stochastic-simulation methods at the workshop included simulations by Pollard and Dimitrios Vavylonis (Lehigh University) of the self-assembly of the contractile ring in yeast, simulations by Anders Carlsson (Washington University) of F-actin waves moving on the substrate-attached surface of cells, simulations by the labs of Holly Goodson (University of Notre Dame) and Melissa Gardner (University of Minnesota) of the growth of microtubules, and simulations of chemotaxis and sensing from Herbert Levine (UC San Diego).

An increasing influx of nonlinear-dynamics methods into the mathematical biology of cells has been a recent trend. Simple mathematical models based on reaction-diffusion equations and related nonlinear interaction models provide key concepts for understanding complex cell phenomena, such as bifurcations leading to spontaneous symmetry breaking or limit cycles, or even to chaos. Such nonlinear-dynamics models are being applied in an increasingly quantitative way to cells, based on our growing understanding of the underlying protein-protein interactions. Such quantitative applications were seen in work from the group of Leah Edelstein-Keshet (University of British Columbia) treating cell polarization and migration using a model based on several modules, including membrane lipids, Rho GTPAses, and actin. Basic nonlineardynamics concepts were also utilized in work presented by the Levine lab on cell chemotaxis and sensing, work from the lab of Adriana Dawes (Ohio State University) treating Par protein segregation, work from the Mogilner, Vavylonis, and Carlsson labs of F-actin waves, and very recent work from the Vavylonis lab on Cdc42 oscillations.

## **Presentation Highlights**

#### **Cell Migration**

The meeting included several outstanding talks about recent progress in tracking and modeling cell migration. Alex Mogilner (UC Davis) talked about a recent models under development joint with experimentalists (Kinneret Keren (Technion, Israel), Julie Theriot and others) for the migration of cells derived from fish scales (keratocytes). The models are based on the idea that actomyosin behaves like a viscoelastic material, graded from front to back in these cells, and that membrane tension forms an important dynamically changing regulator of the motion. His talk was followed by Kinneret Keren's beautiful lecture on the experimental results probing the role of membrane tension in assembly, contraction of actomyosin, and formation of adhesions. Keren's lab is able to experimentally manipulate each of these variables, and measure the response of the others using innovative experiments. For example, she fuses giant vesicles to motile cells to rapidly change their membrane area. Surprisingly, the cells keep moving with little change. She summed up the results by the statement "tension is generated by growing actin filaments at the leading edge pushing against the inextensible membrane, and is relieved due to centripetal actin flow generated by myosin-powered contraction and mediated by the adhesion strength".

Alexander (Sasha) Verkhovsky (EPFL Lausanne) described similar keratocyte experiments. He used osmotic manipulations to investigate the role of tension, and concluded that cell speed increases with membrane tension. In his hands, inhibiting myosin resulted in irregular cell shapes, lower tension, and slower speed. Some of the differences in results between the Verkhovsky experiments and those of Keren are not fully resolved. Several talks focused on the importance of understanding multiscale processes in cell motility for both basic science and clinical applications. John Condeelis (Albert Einstein College of Medicine) presented an overview of his research on the motility and invasive properties of mammary carcinoma cells and their response to a growth factor (EGF). Using bioinformatic analysis of the invasive tumor cells, he has deciphered the changes in their actin-related regulatory networks that are a "signature" of invasion/metastasis. Among these factors is a well-know protein, cofilin, that breaks actin filaments. Work in recent years identifies cofilin as an actin-nucleating agent (creating new filament ends that can grow and lead to membrane protrusion). Condeelis described the spatial distribution of cofilin and its regulators (Rho, LIM kinase) in structures called invadopodia and lamellipodia, and pointed to recent modeling work (with UBC postdoc Nessy Tania) that has helped to decipher the dynamics of the intermediates.

Inke Näthke (University of Dundee) gave a visually stunning lecture about how changes in tissue structure (crypts) are linked to colorectal cancer. Hers was a second talk about tissue organization. Jennifer Zallen (Sloan-Kettering Institute) showed the polarity reorganization in fly embryos that results in elongation along the head-tail axis. By labeling proteins responsible for adhesion and contraction, Zallen showed that they become asymmetrically distributed and generate cell polarization. She returned to the dominant theme of tension, noting that myosin generates tension and tension then leads to recruitment of more myosin to the cortex of the cells.

A number of lectures specifically addressed the issue of single-cell polarization, both in the context of chemotaxis and in other cases. Adriana Dawes described her joint experiment-modeling work on the polarity of (PAR) proteins in the worm embryo, *C. elegans*. Herb Levine summarized recent work with experimental and theoretical colleagues on the chemotaxis of the social amoeba (*Dictyostelium discoideum*). He described a 2D motility simulation that can account for the unique motion of this kind of cell by successive random formation of extensions (pseudopods). The model is based on a reaction-diffusion system operating around the cell periphery, and giving rise to hot spots that become protrusions. Good comparison with experimental observation was evident.

Orion Weiner (UC San Francisco) gave an intriguing lecture about probing the polarity of white blood cells (neutrophils). Returning to the theme of tension, his group showed that manipulating membrane tension in these cells (e.g. by micropipette aspiration) can lead to dramatic changes in cell polarization from the level of signaling proteins (such as Rac) up to the level of actin and protrusive activity. He also described unusual experiments with cells that form two parts, connected by long thin membranous "tubes". So long as the tube remains intact, only one of the parts acts as "cell front". Once the tube is severed, the second part also develops a "front". Such experiments were used to infer that tension plays a role in polarity signaling, and that diffusible inhibitors cannot be the only mechanism for preventing multiple fronts.

Talks in this workshop had a spectrum of levels of detail. Les Loew (University of Connecticut) presented an argument in favor of including details in models of actin regulation and turnover. Herb Levine noted that, as few details are known, models with known dynamic properties are useful. Edelstein-Keshet's talk motivated a range of approaches, including detailed as well as simplified (analytically tractable) "toy models". She pointed out that some details (e.g. differences in diffusion of proteins on the membrane versus in the fluid interior) are important. Other details (such as how feedback is wired, enhancing rates of activation or damping rates of inactivation) may be less important for the dynamic behavior of a given signaling circuits.

#### **Cell Mechanics**

The role of cell mechanics in cell migration and morphology, and potential mutual regulation of mechanical and biochemical processes, was a common thread through many presentations at the workshop. About the role of forces and tension, Michael (Misha) Kozlov (Tel Aviv University) summarized the status in his introduction to a lecture on focal adhesions. He said that ".. in past years, membrane tension was hardly mentioned as an exotic factor. Now, everyone talks about membrane tension, and we who know how to model it physically have become very popular.".

Sean Sun (Johns Hopkins University) addressed the topic of mechanosensation in migrating cells. Cells form stress fibers, bundles of polymerized actin filaments, to adhere to a substrate or neighboring cells. The formation of these stress fibers can be induced by applying an external force, indicating that cells can modulate internal structures in response to external forces. His results suggest that in this case, mechanics may be the origin of the biochemical response.

During migration, some cell types exhibit bipedal motion where the front extends at a constant speed, but there is an alternating body contraction that moves the sides of the cell forward in a rhythmic pattern that is reminiscent of walking. Using a highly abstracted mechanical model of a migrating cell consisting of cross-linked springs, Jay Tang (Brown University) was able to reproduce the bipedal motion. He was able to demonstrate configurations that give the same qualitative agreement with experimental observations and suggestions for experiments to distinguish between the potential configurations.

One talk focused on understanding mechanical properties of actin networks with a novel use of atomic force microscopy (AFM). Actin polymers can organize into many different types of structures that are branched or bundled and can extend over long or short space scales. Dan Fletcher (UC Berkeley) demonstrated that imposing stiffness on an actin network can alter its behavior. Using a broad flat tip during AFM, he applied either a constant force or constant height to a sample of actin polymers and measured the equilibration time. The results varied depending on the imposed conditions suggesting that actin networks dynamically remodel in response to mechanical regulation.

A series of talks looked at the assembly, stability and regulation of contractile actomyosin networks. Karen Oegema (Ludwig Institute for Cancer Research) uses the nematode worm *C. elegans* to explore mechanisms of cell division and regulation of the contractile ring. Her experiments have shown that during constriction the contractile ring maintains a constant concentration and thickness, although the constriction rate decreases, potentially by contacting the spindle midzone. One of the highlights of the conference was an outstanding lecture by Ewa Paluch (MPI for Molecular Cell Biology and Genetics), who specializes in the phenomenon of cell blebbing. Paluch studies blebbing both in the context of motility and cell-division. Large cytoplasmic oscillations during cytokinesis lead to failure of division, while small cytoplasmic oscillations accompanied by bleb formation at the pole allow the cell to divide successfully. She proposes that the blebs are essential to release membrane tension at the poles and allow cytokinesis to proceed. Tatyana Svitkina (University of Pennsylvania) discussed assembly of sarcomere-like structures of actin and myosin in non muscle cells. The exquisite and compelling images showed a striated organization before and after recovery from blebbistatin treatment, and demonstrated that unpolymerized non-muscle myosin II may play a role in forming focal adhesions.

#### **Microtubule and Actin Dynamics**

There was a provocative series of talks relating to microtubule dynamics and mechanics. Jennifer Ross (University of Massachusetts Amherst) started the session by discussing microtubule length regulation and severing and two newly identified microtubule severing proteins, katanin and fidgetin. Using TIRF microscopy, she has been able to characterize and localize the function of these proteins in vitro. Melissa Gardner also spoke on microtubule length regulation, but via different mechanisms. Microtubules exhibit an interesting property called *dynamic instability* where they undergo stochastic periods of growth and shrinkage. Gardner showed how the distribution of catastrophes, the transition from growth to shrinkage, follows a gamma distribution with k = 3, suggesting there is a series of 3 transitions that precede a catastrophe. She next demonstrated how microtubule associated proteins can alter this behavior by either affecting the rate of these individual steps or by changing the number of steps. David Odde (University of Minnesota) spoke on microtubule assembly kinetics and showed how our understanding of this seemingly simple process is incorrect. Polymerization processes have typically been modeled using mass action chemical kinetics where the growth rate is a second-order process that depends on the free monomer concentration and the off rate is simply a first order rate constant. New data from high-resolution experiments that can track polymerization at the nanoscale have shown that this model is too simplistic since the structure of the microtubule tip changes as the growth rate increases. This gives rise to a very different kinetic model that fundamentally changes the way we understand microtubule polymerization.

Holly Goodson spoke on computational modeling of microtubule dynamics and how observed dynamics can be related to the biochemistry, mechanics, and structure of the microtubule. As with Odde's talk, her results suggest that we may need to fundamentally rethink the details of microtubule polymerization. Finally, David Sept spoke on efforts to connect all-atom molecular dynamics simulations of microtubules with more coarse-grained simulations and ultimately continuum mechanics. In his talk he showed how a bootstrap approach allows one to connect atomically detailed descriptions to polymer level models and thereby explain the effects of drugs or protein mutations on the mechanics that are observed.

New results for actin dynamics focused on spontaneous patterning and wave formation. In cell types including neutrophils and the slime mold Dictyostelium, polymerized actin often forms spontaneous patterns including clumps of actomyosin crucial for cytokinesis, traveling waves moving around the edge of the cell pushing the membrane out, waves traveling along the substrate-attached surface of the cell, or patches which can either remain stationary or move. Work out of the Pollard and Vavylonis laboratories demonstrated that actomyosin clumping and subsequent ring formation results from a "search, capture, pull, and release" mechanism in which actin filaments growing from preexisting foci find other foci, pull on them, and then release due to the action of actin-binding proteins which disassemble actin filaments. They showed that such a mechanism explains contractile ring formation for parameters consistent with experiment. Furthermore, they showed that under other conditions, the clumps remain isolated - without forming rings; this prediction is consistent with experiments.

Complementary to this work, calculations out of the MacKintosh laboratory showed that the active motion of myosin in actin networks can give rise to diffusive-like behavior of the networks. Several talks and posters, out of the laboratories of Vavylonis, Mogilner, and Carlsson, treated these waves using a combination of positive and negative feedback acting between two chemical constituents. Such feedback effects, when coupled to diffusion of at least one of the constituents, are known from the mathematics of nonlinear dynamics to have the ability to produce spontaneous traveling waves and patches. The models generally focused on the combination of F-actin and the nucleation-promoting factors which act upstream of it, with either of the constituents assumed to feed back on itself positively. The negative feedback terms were based on a mechanism in which F-actin "bites the hand that feeds it" - by inactivating the nucleation-promoting factors. Arpita Upadhyaya (University of Maryland) found experimental evidence for actin based traveling waves in spreading kinetics of T cells. Work out of Martin Falcke's laboratory (Max Delbrück Center Berlin) focused on the dynamics of filament attachment and detachment from the membrane. This work showed that the velocity response of a cell to a sudden applied force is often has a delayed component coming from dynamic rearrangements of the actin network.

John Cooper (Washington University) investigated actin assembly during cytokinesis in yeast cells. In particular, he focussed on the mechanism of Arp2/3 action and regulation. His lab has found that N-WASP associates with Arp2/3 at the membrane where it nucleates an actin filament branch point, but N-WASP is replaced by cortactin as Arp2/3 is pushed away from the membrane by actin polymerization. Mutants of Arp2/3 regulators exhibit longer actin filaments and fewer branches, consistent with reduced Arp2/3 activity. Margaret Gardel (University of Chicago) gave a comprehensive overview of recent understanding of the lamellar actin cytoskeleton, while Cécile Sykes (Institut Curie) discussed biomimicking systems of cell shape changes. When actin gels form around rigid beads, the ability of the bead to break symmetry and initiate movement depends on the ratio of Arp2/3 to capping protein: too much Arp2/3 and the actin gel is overly branched while too much capping protein produces an actin shell that is too small. To further clarify the role of the actin cortex, she presented recent work with liposomes (oil droplets with no actin) and membrane blebs (with an intact actin cytoskeleton). She demonstrated that the actin cytoskeleton slows spreading compared to liposomes, but when force is applied using a tube pulling assay, force exerted by the liposomes depends on the tube length. Taken together, this suggests that differences in liposomes and cells d not lie entirely in the cytoskeleton, but also in the membrane proteins, and the membrane bilayer in cells can help regulate mechanical properties in the cell.

### **Scientific Progress Made**

The cytoskeleton and motility community has a diverse constituency, made up of cell biologists, biophysicists, mathematicians and engineers. There are few opportunities and/or venues that brings this group together. This alone makes the BIRS workshop unique. Although these researchers continually read and follow each other's work, there is often not an efficient transfer of information since a biologist can face challenges in reading an article in a *SIAM* journal, and likewise an engineer may not glean all the details and nuances from a *Nature Cell Biology* paper.

The small size of the workshop, the ample time for discussion, and the informal interactions during meals and other social times, gave valuable opportunities for in-depth and informative scientific exchange. Experimentalists were exposed to new theoretical ideas and modeling platforms. Likewise, theorists and

modelers saw novel experimental measurements and data that provides contact with reality and motivation for new approaches. This type of interaction goes far beyond what is possible at a typical mathematics (or cell biology) meeting. The workshop created many new opportunities that will bear fruit in the coming months and years.

## **Outcome of the Meeting**

Experimental biology has come a long way in allowing precise measurements of forces between cells, cells and their environment, and even between individual molecules. Similarly, our visualization techniques have dramatically improved, with fluorescent labeling techniques and ever improving microscopy. Consequently, we have more data at every level, and a greater need for synthesis and understanding of that data. Modeling is playing a prominent role in this process and has become an integral part of quantitative cell biology, helping to focus experimental directions and distinguish between competing hypotheses.

Although this report is being written in the weeks immediately following our workshop, we can already document at least 11 new collaborations that have been established, 3 grant proposals that are being written or planned, and 2 manuscripts that will acknowledge the contribution of BIRS. The previous workshop held in 2005 had far-reaching effects that impacted all sectors of this interdisciplinary field. We anticipate nothing less to arise from this latest workshop and look forward to the next opportunity to bring together such an interdisciplinary group at BIRS.

## **Remaining Open Questions**

When comparing the 2005 meeting to the one in 2011, there has been a significant move from modeling at the level of individual proteins and polymers to large systems of proteins, cells and even tissues. This trend will undoubtedly continue in the future, but significant challenges remain. Experimental complexity greatly increases when dealing with full-scale signaling cascades in cells, cell-cell interactions, and communication between cells in a tissue, let alone a whole organism. Modeling methods and techniques for the analysis of models, as well as simulation methods are still emerging to treat large-scale dynamics that depend on both time and space.

Although we have a plethora of data, some very basic questions remain, such as "Where is force produced in the cell?", "What is the relative contribution of polymerization forces and motor proteins?", "What are the key feedback elements leading to cell polarization?", and "What are the specific roles of the various actin nucleators and their activators?". At this point, each of these questions has been addressed by a substantial body of theory and experiment, and investigations are crystallizing around a few competing hypotheses. Over the next five years, we would expect several of these questions be definitively answered. But we are only beginning to understand the larger question of the logic of the complex mechano-chemical protein networks that control cell behavior. Systems biology efforts are well-poised to begin addressing these issues and we hope that at least rudimentary answers will be given over the next few years.

## **List of Participants**

Carlsson, Anders (Washington University) Condeelis, John (Albert Einstein College of Medicine) Cooper, John (Washington University School of Medicine) Danuser, Gaudenz (Harvard Medical School) Dawes, Adriana (University of Alberta) Edelstein-Keshet, Leah (University of British Columbia) Falcke, Martin (Max Delbrck Center Berlin) Fletcher, Dan (University of California Berkeley) Gardel, Margaret (University of Chicago) Gardner, Melissa (University of Minnesota) Goodson, Holly (University of Notre Dame)

Holmes, Bill (University of British Columbia) Janmey, Paul (University of Pennsylvania) Kasza, Karen (Sloan-Kettering Institute) **Keren, Kinneret** (Technion University) Kozlov, Michael (Tel Aviv University) Levine, Herbert (University of California San Diego) Loew, Leslie (University of Connecticut) MacKintosh, Fred (Vrije Universiteit) Mogilner, Alex (University of California, Davis) Nathke, Inke (University of Dundee) Odde, David (University of Minnesota) Oegema, Karen (Ludwig Institute for Cancer Research) Paluch, Ewa (Max Planck Institute of Molecular Cell Biology and Genetics) Pollard, Thomas D. (Yale University) Rodewald, Richard (National Science Foundation) Ross, Jennifer (University of Massachusetts Amherst) Sept, David (University of Michigan) Sun, Sean (John Hopkins) Svitkina, Tatyana (University of Pennsylvania) Sykes, Cécile (Institut Curie) Tang, Jay (Brown University) Tania, Nessy (University of British Columbia) Upadhyaya, Arpita (University of Maryland) Vavylonis, Dimitrios (Lehigh University) Verkhovsky, Alexander (EPFL Lausanne) Weiner, Orion (University of California San Francisco) White, Diana (University of Alberta) Wirtz, Denis (Johns Hopkins University) Zallen, Jennifer (Sloan-Kettering Institute)

# Chapter 24

# **Twenty-five years of representation theory of quantum groups (11w5096)**

## Aug 07 - Aug 12, 2011

**Organizer(s):** Pavel Etingof (Massachusetts Institute of Technology) Victor Ginzburg (University of Chicago) Nicolas Guay (University of Alberta) David Hernandez (Université Paris 7) Alistair Savage (University of Ottawa)

## **Overview of the Field**

Quantum groups first appeared under different disguises in the first half of the 1980's, in particular in the work of physicists and mathematicians interested in the quantum inverse scattering method in statistical mechanics. For instance, one of the simplest examples, the quantized enveloping algebra of  $\mathfrak{sl}_2$ , first surfaced in a paper of P. Kulish and N. Reshetikhin in 1981 about integrable systems. Quantized enveloping algebras of Kac-Moody algebras, the most studied examples of quantum groups, are non-commutative and non-cocommutative Hopf algebras discovered around 1985 independently by V. Drinfeld and M. Jimbo. The address of V. Drinfeld at the International Congress of Mathematicians in 1986 brought quantum groups to the attention of mathematicians worldwide and laid the foundations of this theory. In one fell swoop, Drinfeld gave birth to a new branch of algebra which started growing at tremendous speed and has remained a very active area of research to this day.

Quantum groups have found applications in other branches of mathematics, topology being one notable example present at the workshop. Quantum groups have even made their appearance in subjects more distant from algebra, for instance in probability theory, harmonic analysis and number theory (the last one being the subject of the BIRS workshop "Whittaker functions, crystal bases and quantum groups" held in June 2010). Some ideas that have been fruitful in the study of quantum groups have gained in popularity and have started spreading across mathematics, for instance the philosophy of categorification.

Several different approaches to the study of representations of quantum groups have been successful. An algebro-combinatorial approach has led to the discovery of crystal bases and of more general crystal structures, which have had a profound influence in Lie theory. Geometric realizations of representations have been obtained via equivariant K-theory of appropriate varieties, e.g. Steinberg varieties and quiver varieties. Of course, Lie theorists have been very much interested in highest weight modules for quantum groups, their characters and also in some specific families of finite dimensional modules, e.g. Weyl modules and Kirillov-Reshetikhin modules. The representation theory of quantum groups is a lively area of research and it is reasonable to expect it to remain this way for the foreseeable future.

### **Recent developments and open problems**

One of the most exciting recent developments surrounding quantum groups is the categorification of quantized Kac-Moody enveloping algebras by M. Khovanov and A. Lauda and, independently, by R. Rouquier. Their work has led to the introduction of a very interesting new family of algebras, the Khovanov-Lauda-Rouquier algebras or quiver Hecke algebras, which have a rich representation theory. These have had applications to the study of other algebras of interest in Lie theory: for instance, they have been used by J. Brundan and A. Kleschev to create new gradings on blocks of Hecke algebras. Of course, all this leads to the open problem of categorifying many other interesting algebraic structures in representation theory (e.g. highest weight modules, Heisenberg algebras, etc.). Moreover, these ideas have also lead to applications in topology (e.g. categorification of knot invariants) and open problems in this direction were mentioned in the talks of C. Stroppel and B. Webster.

One of the first celebrated theorems about quantum groups is the Khono-Drinfeld theorem which states that the monodromy representation of the braid group  $B_{\mathfrak{g}}$  coming from the Knizhnik-Zamolodchikov connection is isomorphic to a representation constructed from the *R*-matrix of  $U_q\mathfrak{g}$ . Recent work of V. Toledano Laredo on the trigonometric Casimir connection is in the same vein and leads naturally to an analogous conjecture about the monodromy of this connection whose proof in the  $\mathfrak{sl}_2$ -case was announced at the workshop.

Cluster algebras have been one of the hottest topics in algebra in the last ten years, rapidly developing in connection with various subjects. Rather recent work of D. Hernandez, B. Leclerc, H. Nakajima and others has investigated connections between these and finite-dimensional representations of quantum affine algebras. Starting from the observation that the cluster exchange relations are of the same form as the T-system equations satisfied by Kirillov-Reshetikhin modules, D. Hernandez and B. Leclerc [17] have conjectured that the Grothendieck ring of a certain tensor category of finite dimensional modules is isomorphic to a cluster algebra (this is another example of categorification, called monoidal categorication). Their work and subsequent work of Nakajima [25], imply their conjecture at "level 1" (and imply as a byproduct the positivity conjecture for finite type cluster algebras). Furthermore, it has been shown recently that certain quantized coordinate rings have the structure of a quantum cluster algebra. Cluster algebras were the subject of the BIRS workshop "Cluster algebras, representation theory, and Poisson geometry" in September 2011. Several participants of our workshop participated in the September workshop and talked about the connection with quantum groups.

There has been a lot of progress made recently on other aspects of quantum group theory, for instance on generalization of Kirillov-Reshetikhin modules, on quantization of structures analogous to Lie bialgebras, on crystals, on quantum toroidal algebras and on ring theoretical properties of quantized coordinate rings. The meeting featured talks on all these subjects and many of these ended with important conjectures. Moreover, the presentation of IFrenkel paved the way for a completely new direction of research for years to come. We have outlined in the previous paragraphs three exciting avenues for future advances in quantum group theory. More information about recent developments and open problems is contained in the following section.

### **Content of the talks**

The speakers all gave talks about their recent research projects, sometimes on topics that have now become "classical" in the representation theory of quantum groups (e.g. crystals), and sometimes on topics that are somewhat more remote but inspired by work originally done on quantum groups (for instance, categorification of various mathematical structures). Four of the speakers were postdocs (Sachin Gautam, David Jordan, Peter Tingley, Charles Young). There was also one poster presented by another postdoc, Stewart Wilcox, based on his Ph.D. thesis about rational Cherednik algebras: these are related to the representation theory of quantum groups in various ways – for instance, the Knizhnik-Zamolodchikov connection plays a very important role for quantum groups and for rational Cherednik algebras and the Ph.D. thesis of Stewart Wilcox provides a detailed study of that connection in a very important special case.

#### Monday, August 8

The workshop started with a presentation by Professor Evegeny Mukhin (Indiana University - Purdue University Indianapolis) entitled *Representations of Toroidal Quantum*  $\mathfrak{gl}[1]$  about his joint work with B. Fei-

gin, E. Feigin, M. Jimbo and T. Miwa [12, 13]. Toroidal quantum algebras (double affine quantum groups) have been investigated for about twenty years and connections with theoretical physics (e.g. Fock space constructions) have been established. They are very interesting mathematical objects, but also very mysterious since they are hard to investigate. Until this recent work, quantum toroidal algebras were defined only for finite dimension simple Lie algebras and for the Lie algebra  $\mathfrak{gl}[n]$  with  $n \geq 2$ . It turns out that Fock spaces depending on a continuous complex parameter also appear in the representation theory of the toroidal quantum gl[1] and can be shown to be tame, irreducible highest weight modules. Furthermore, E. Mukhin presented constructions of various tame, irreducible representations with natural bases parameterized by certain plane partitions (e.g. Macmahon modules) with, possibly, various boundary conditions. They can be identified with subspaces of certain tensor products of Fock modules. He also gave character formulas after various specializations of parameters. As a byproduct, he explained how to obtain Gelfand-Zetlin like bases in a family of lowest weight irreducible  $\mathfrak{gl}_{\infty}$ -modules. A connection with double affine Hecke algebras for the symmetric group was also mentioned: the spherical subalgebra of type A is a quotient of the quantum toroidal algebra of  $\mathfrak{gl}[1]$ . Double affine Hecke algebras are another fascinating topic in representation theory which has garnered a lot of attention in the last fifteen years and were the subject of another talk (by E. Vasserot). It was mentioned at the end of his talk that all the results he presented should be extendible to the quantum toroidal algebra for  $\mathfrak{gl}[n]$  for any  $n \geq 1$ .

The second talk, Quantum foldings by Professor Jacob Greenstein (University of California at Riverside), was the first of a few on the subject of crystals. The discovery of crystal bases by M. Kashiwara in the 1990's is one of the most important in the representation theory of quantum groups and has found a lot of applications in representation theory and in combinatorics. He presented the results of his joint work [2] with A. Berenstein on the following natural question. A classical result in Lie theory stipulates that a simple finite dimensional Lie algebra that is not simply laced can be constructed as the subalgebra  $g^{\sigma}$  of a Lie algebra g of type A,D or E fixed by a diagram automorphism  $\sigma$  of the latter. This construction is called "folding" and extends to Kac-Moody Lie algebras when  $\sigma$  is admissible. It is well-known that foldings do not admit direct quantum analogues, so it is natural to ask if there is a less direct way to relate the representation theory of  $U_q(\mathfrak{g})$  and of  $U_q(\mathfrak{g}^{\sigma})$ . The answer is yes if  $\mathfrak{g}^{\sigma}$  is replaced by  $(\mathfrak{g}^{\vee})^{\sigma}$  where  $\mathfrak{g}^{\vee}$  is the Langlands dual Lie algebra: it can be shown that there exists an embedding of crystals (or of Lusztig's canonical bases) for g and  $\mathfrak{g}^{\sigma}$ . The aim of their work is to introduce algebraic analogues and generalizations of foldings in the quantum setting which yield new flat quantum deformations of non-semisimple Lie algebras and of Poisson algebras. Perhaps the most spectacular example is an algebra that can be regarded as a new algebra of quantum nby n matrices. Their work has led them to introduce new interesting examples of so-called überalgebras (which appear to have interesting ring theoretical properties as mentioned in the talk of M. Yakimov): he explained a general setting where such algebras can be useful (namely as a substitute when a linear map between algebras does not extend to an algebra homomorphism) and he provided an explicit construction of an überalgebra in the case of the dual pair of type  $(D_{n+1}, C_n)$  via a flat deformation of the enveloping algebra of  $\mathfrak{sl}_n \ltimes (\mathbb{C}^n \otimes \mathbb{C}^n)$ . A link with Hall algebras and with cluster algebras (a very hot topic over the past twelve years) was briefly mentioned at the end of his talk.

Dr. Anthony Licata (Stanford University) was the first to speak on the subject of categorification. The title of his talk on joint work with Sabin Cautis was *Heisenberg Categorification and Hilbert Schemes*. Given a finite subgroup G of SU(2), he defined a monoidal category whose Grothendieck group is isomorphic to the homogeneous Heisenberg algebra corresponding to G. A very interesting property of this category is that it acts on the direct sum of the derived categories of Hilbert schemes of points on the resolution of the corresponding simple singularity; from this, one can recover a known representation of the Heisenberg algebra on the direct sum of the Grothendieck groups of these resolutions. Their work sheds some light on the connection between two realizations of Fock space representation theory has grown tremendously since the seminal works of Khovanov-Lauda and Rouquier a few years ago on the categorification of quantum groups. The work of A. Licata and S. Cautis uses ideas derived from the discoveries of M. Khovanov and A. Laura and can be viewed as an indirect application to a problem in classical representation theory of ideas stemming from quantum groups.

The following talk by Professor Weiqiang Wang (University of Virginia), *Spin fake and generic degrees for the symmetric group*, was not only about the symmetric group itself, but also about associated Hecke algebras, in particular the Hecke-Clifford algebras and the spin Hecke algebras. Quantum groups have been

known to be related to Hecke algebras since the paper [18] of M. Jimbo, one of the first on the subject of quantized enveloping algebras. The fake degrees are graded multiplicities of an irreducible module of a Weyl group in its coinvariant algebra. The generic degrees arise from Hecke algebras, and their evaluation at a prime power are degrees of irreducible characters of finite Chevalley groups. In his talk, based on joint work with Jinkui Wan, W. Wang formulated and computed the spin analogues of fake and generic degrees for the symmetric group and related Hecke algebras. Of importance in this work is the Morita equivalence between the spin Hecke algebras and the Hecke-Clifford algebras introduced by S. Sergeev and G. Olshanski over twenty years ago in their work on (quantum) supergroups of type Q. He gave explicit formulas for the fake degrees (in terms of a Schur function) and stated that it was equal to the generic degree in this super context. He also presented results about trace forms on spin Hecke and Hecke-Clifford algebras.

Professor Milen Yakimov (Louisiana State University) gave the last talk of the first day about *Ring theory of quantum solvable algebras*. It was the only one on this topic, although a large body of literature has been produced about the subject. The area of quantum groups has supplied a very large number of examples where general methods for studying noncommutative rings can be tested and developed, using representation theoretic methods. A. Joseph, T. Hodges, T. Levasseur, and Y. Soibelman obtained a great deal of information about the spectra of quantized coordinate rings of simple Lie groups, and K. Goodearl and G. Letzter developed a general stratification theory putting the area in the framework of quantum affine toric varieties. The De Concini-Kac-Procesi quantum nilpotent algebras were another large class of algebras which were heavily investigated.

This talk was a great overview of known results on spectra of quantum solvable algebras, normal separation, the extension of Gabber's catenarity theorem to these classes, and the classification of their automorphism groups along the Andruskiewitsch-Dumas conjecture. It was partly an historical review about important theorems from the 1990's, and partly one about the recent work of the speaker. For instance, he stated his very recent theorem to the effect that the center of A. Joseph's localization of a quantized coordinate ring is a Laurent polynomial algebra; another of his theorems provides a homeomorphism between the space of maximal ideal of a quantized function algebra and a Laurent polynomial ring, which answers a question of Goodearl and Zhang to the effect that maximal ideals in such a ring all have finite codimension. He finished with an overview of open problems in the ring theoretic side of quantum groups: for example, he stated a conjecture to the effect that a Cauchon-Goodearl-Letzter extension (which a type of iterated skew polynomial algebra) is catenary.

#### **Tuesday, August 9**

The second day started with a talk of Dr. Charles Young from the University of York about his joint work with Evgeny Mukhin on Extended T-systems. Kirillov-Reshetikhin modules form a family of representations of quantum affine algebras with a lot of interesting properties and which have been studied rather extensively. One of their most important properties is that they satisfy certain systems of recurrence relations called Tsystems (this is the Kirillov-Reshetikhin conjecture, proved by H. Nakajima and D. Hernandez). The goal of their work is to replace Kirillov-Reshetikhin modules by a wider class of modules from which it is possible to build generalized T-systems. Such a wider class of modules includes all minimal affinizations (Kirillov-Reshetikhin modules are special types of minimal affinizations) and so-called snake modules. Their work is restricted to categories of finite-dimensional representations of quantum affine algebras of types A and B, but he commented on what can be expected in other types (based on some "experimental" preliminary results). He outlined the proofs of their results using the theory of q-characters and also briefly explained how to compute the q-character of a snake module by computing a certain sum over non-overlapping tuples of paths, so that snake modules are in fact thin and special. Their main theorem is the existence of a short exact sequence for snake modules, modulo the direction of the arrows. He concluded with a couple of open problems, one of which was about hypothetical relations between the generalized T-systems and the cluster algebra conjecture of D. Hernandez and B. Leclerc.

C. Young was followed by Professor Anne Schilling (University of California at Davis) with a talk entitled *Crystal energies via the charge in types A and C*. Hers was the first of a few talks about the combinatorial approach to representation theory. The discovery of crystal bases by M. Kashiwara in the early 1990's [19] is one of the most important in the history of quantum groups and has had applications to more classical (i.e. non-quantum) problems in representation theory. The axiomatic notion of crystal can be extolled from his

result on crystal bases and the rich combinatorial structure of crystals has been studied quite a lot for more than fifteen years.

The energy function of affine crystals is an important grading used in one-dimensional configuration sums of statistical mechanical models and generalized Kostka polynomials. It is defined by the action of the affine Kashiwara crystal operators through a local combinatorial rule and the R-matrix. Nakayashiki and Yamada have related the energy function in type A to the charge statistic of Lascoux and Schuetzenberger. Computationally, it is much more efficient to compute charge than energy since its definition involves a recursive definition of local energy and the combinatorial R-matrix, for which not in all cases efficient algorithms exist. In her talk, she related energy to a new charge statistic in type C which comes from the Ram-Yip formula for Macdonald polynomials. This involves in particular the generalization of parts of the Kyoto path model for perfect crystals to the nonperfect setting, which yields an isomorphism between affine highest weight crystals and tensor products of Kirillov-Reshetikhin crystals. This is joint work with Cristian Lenart [23].

The first speaker of the afternoon was Professor Maxim Nazarov from the University of York who spoke about his joint work with S.Khoroshkin and E.Vinberg on a *Generalized Harish-Chandra isomorphism* [22]. The classical Harish-Chandra isomorphism is one of the most important results in the representation theory of semisimple Lie algebras. The motivation for seeking to generalize it was to obtain explicit realizations of all simple finite-dimensional modules of Yangians and of their twisted analogues. Yangians are one important family of quantum groups of affine types and the classification of their irreducible representations has been known for almost twenty-five years; it has also been known for a long time that, for the Yangians of  $\mathfrak{sl}_2(\mathbb{C})$ , those are isomorphic to tensor products of evaluation representations. However, finding explicit, concrete realization of irreducible representations of the other Yangians (twisted and non-twisted) has been a very challenging problem which has been solved in impressive recent work of M. Nazarov and S. Khoroshkin [21].

For any complex reductive Lie algebra  $\mathfrak{g}$  and any locally finite  $\mathfrak{g}$ -module V, M. Nazarov and his collaborators extended to the tensor product A of  $U(\mathfrak{g})$  with V the Harish-Chandra description of  $\mathfrak{g}$ -invariants in the universal enveloping algebra  $U(\mathfrak{g})$ . Their description of the algebra of invariants  $A^{\mathfrak{g}}$  is in terms of the invariants of the action of Zhelobenko operators on the zero weight space of a certain quotient of A and their proof uses the Mickelsson algebras. The case relevant for Yangians is when V is a the Grassmann algebra of  $\mathbb{C}^{mn}$  since, in this case, the (twisted) Yangian of  $\mathfrak{g}$  admits a non-trivial homomorphism to  $A^{\mathfrak{g}}$ . He explained the role played by Howe duality in their work, and also how to construct a functor  $\mathcal{F}$  from the category of finite dimensional modules over a certain finite dimensional reductive Lie algebra  $\mathfrak{k}$  to the category of finite dimensional modules for a (twisted) Yangian  $Y(\mathfrak{f})$  when  $\mathfrak{k}$  and  $\mathfrak{f}$  form an Howe dual pair. He finished by stating his main theorem which says that any irreducible representation of  $Y(\mathfrak{f})$  can be obtained as the image of an intertwining operator between two modules over  $Y(\mathfrak{f})$  obtained via the functor  $\mathcal{F}$  applied to Verma modules over  $\mathfrak{k}$ .

The last two talks were more of a combinatorial nature. Professor Masato Okado of Osaka University delivered a presentation about Open problems related to Kirillov-Reshetikhin crystals. It is widely known that Kirillov-Reshetikhin modules of quantum affine algebras admit extremely rich structures, such as Tsystems, fermionic character formulas, existence of crystal bases (Kirillov-Reshetikhin crystals), Kyoto path realization of affine highest weight crystals, existence of the corresponding geometric crystals, and positive birational Yang-Baxter maps (also called tropical R maps). There are many conjectures related to Kirillov-Reshetikhin crystals. Although some of these have been settled recently, many are still open. M. Okado reviewed recent progress and surveyed important open problems on this subject. The first conjecture he presented was divided into two parts: the first one about the existence of crystal bases for Kirillov-Reshetikhin modules (he recalled all the cases which have been proved so far), and a second part which says that, if a finite dimensional module over a quantum affine algebra has a crystal basis, then it must be a tensor product of Kirillov-Reshetikhin modules. His second conjecture gave a criterion for the perfectness of Kirillov-Reshetikhin crystals. The third one was about a connection, already established in type A and many other non-exceptional types, between perfect crystals and ground state paths; he illustrated it using an example in type  $G_2^{(1)}$ . Finally, he presented a conjectural fermionic character formula which has been resolved in some cases through the work of H. Nakajima, D. Hernandez, P. Di Francesco, R. Kedem, A. Schilling, M. Shimozono and himself. He explained some of the steps and ideas (Q-systems, rigged configurations) in the proof of those cases which have been established so far.

The day ended with a talk of a combinatorial and geometric nature by Professor Joel Kamnitzer (Uni-

versity of Toronto) about *Components of quiver varieties and affine Mirkovic-Vilonen polytopes*. G. Lusztig introduced quiver varieties whose components index the semicanonical basis for symmetric Kac-Moody Lie algebras. The speaker explained a method for understanding these components in finite and affine types us-

describe crystals of affine Lie algebras, generalizing ideas of Beck-Chari-Pressley, Dunlap, and others. He started by recalling Lusztig's bijection defined using the crystal structure on Lusztig's canonical basis for  $U^+\mathfrak{g}$  (with  $\mathfrak{g}$  finite) and stated a theorem of Lusztig and Berenstein-Zelevinsky which provides the connection between canonical bases and certain GGMS polytopes in  $\mathfrak{h}^*_{\mathbb{R}}$  called Mirkovic-Vilonen (MV) polytopes. These are characterized by the fact that a GGMS polytope is an MV polytope if and only if all of its 2-faces are, and MV polytopes of rank 2 are known by an explicit rule. One of the goal of his research was to generalize them to the case when  $\mathfrak{g}$  is an affine Kac-Moody algebra  $\mathfrak{g}$ . An important role is played by certain polytopes Pol(M) associated to modules M over a preprojective algebra of the Dynkin quiver Q of  $\mathfrak{g}$ . His main theorem in the affine case consisted of two results, the first one being the existence of a bijection (constructed using these Pol(M)) between the canonical basis and affine MV polytopes and the second one stating that a decorated GGMS polytope is an affine MV polytope if and only if all of its 2-faces are. This is joint work with Pierre Baumann and Peter Tingley, who had more to say about this on Friday.

ing the combinatorics of Mirkovic-Vilonen polytopes. In the affine type, this gives a new combinatorics to

#### Wednesday, August 10

The first presentation of the day was delivered by Professor Benjamin Enriquez (Université de Strasbourg) and pertained to *Solutions of some problems in the quantization of Lie bialgebras*. A famous conjecture of V. Drinfeld going back twenty years ago [4] states that any Lie bialgebra could be quantized. It was proved in the 1990's in a series of papers by P. Etingof and D. Kazhdan using the theory of associators, see for instance [9, 10]. B. Enriquez started by giving an overview of the quantization problem which consists of constructing a functor from a classical object (e.g. a Lie bialgebra) to a quantum object (e.g. a bialgebra) such that the classical object can be recovered by taking the semi-classical limit of the quantum one. The other two families of classical objects that he considered are the Lie quasibialgebras and the coboundary Lie bialgebras, the corresponding quantum objects being quasibialgebras and coboundary bialgebras.

The existence of quantization for coboundary Lie bialgebras and quasi Lie bialgebras was solved by himself and G. Halbout in the impressive papers [6, 7]. After his introduction to the progress made on those quantization problems, he presented the formalism of PROPS which are symmetric tensor categories equipped with a functor from the Schur category which is the identity on objects and introduces a certain PROP which is relevant for the quantization problem of Lie bialgebra. (PROPS playing an analogous role exist also for the other classes of objects mentioned above.) The rest of this talks was devoted to explaining the main ideas in the proofs of their very important results using the formalism of PROPS and translating the quantization problem into this language.

Afterwards, Professor Valerio Toledano Laredo of Northeastern University gave a talk entitled Yangians, quantum loop algebras and trigonometric connections. Let G be a semisimple complex algebraic group (or  $GL_n(\mathbb{C})$ ) with maximal torus H. He started with a general result about flat connections on  $H_{reg}$  and explained how the trigonometric Casimir connection, which is flat and W-equivariant, is constructed using Yangians [27]. In the case of  $GL_n(\mathbb{C})$  and when the fiber of the vector bundle affording this connection is a tensor product of evaluation modules, the connections thus obtained is essentially the dynamical differential equation of V. Tarasov and A. Varchenko. He stated a conjecture to the effect that the action of the affine braid group on a representation V of the Yangian  $Y_{\hbar}(\mathfrak{g})$  which comes from the Casimir connection is equivalent to its action via quantum Weyl group operators on a representation  $\mathcal{V}$  of the quantum loop algebra  $U_{\hbar}(L\mathfrak{g})$ . This is reminiscent of a famous fundamental theorem of V. Drinfeld and Kohno [5] about the Knizhnik-Zamolodchikov connections and can be viewed as an affine extension of it. Matching those two classes of representations involves in particular the construction of a functor relating finite-dimensional modules of those two quantum groups. He devoted a good amount of time explaining a theorem of his which provides an isomorphism between a completion of the Yangian of g and a completion of the corresponding quantum loop algebra (see [16]). This is a Lie algebra analog of Lusztig's isomorphism between an affine Hecke algebra and a completion of its associated degenerate version. That isomorphism induces an equivalence of categories between graded representations of the Yangian and filtered representations of the quantum loop algebra and it also induces Drinfeld's degeneration map between the Yangian and the associated graded ring of the quantum loop algebra with respect to the evaluation ideal. All these results are of the utmost importance in the representation theory of quantum groups of affine type: it had been believed for a long time that such an isomorphism existed after completion and that the categories of finite dimensional representations of Yangians and of quantum loop algebras were almost "the same" since the simple objects in both cases are parametrized by the so-called Drinfeld polynomials, but this had never been giving a rigorous treatment. He finished by presenting explicitly that isomorphism in the  $\mathfrak{sl}_2$ -case.

This is based on joint work with Sachin Gautam of Columbia University who was the next speaker and talked about *Monodromy of the trigonometric Casimir connection for*  $\mathfrak{sl}(2)$ , which is another joint project. He explained the proof of their theorem to the effect that the monodromy of the trigonometric Casimir connection for a tensor product of evaluation modules of the Yangian of  $\mathfrak{sl}(2)$  is described by the quantum Weyl group operators of the quantum loop algebra. One of the main ideas of the proof is to use commuting action of  $\mathfrak{gl}_n$  and  $\mathfrak{gl}_k$  in a polynomial ring with kn variables to relate the Casimir connection for  $\mathfrak{sl}_n$  with the KZ-connection on n points and the Drinfeld-Khono theorem. He also explained how to extend the proof to the case of  $\mathfrak{gl}_2$ . In the course of the proof, he obtained an explicit expression for the lattice part of the affine braid group action.

#### Thursday, August 11

Professor Catharina Stroppel (Universität Bonn) was the first speaker of the day and she talked about *Fractional Euler characteristics and categorified colored Jones polynomials*. Some of the most fascinating applications of quantum groups can be found in topology, especially in the construction of manifold invariants. In Khovanov's categorification of the Jones polynomial, a polynomial invariant of links is upgraded to an invariant with values in complexes of graded vector spaces such that taking the graded Euler characteristic gives back the original polynomial. One would like to extend this construction to other invariants like colored Jones or Turaev-Viro 3-manifold invariants. The problem hereby is that the polynomial invariant (or at least its construction) is not defined integrally anymore, but it is defined instead over the rational numbers, hence one would like to interpret rational numbers as Euler characteristics and linear maps with not necessarily integral matrix entries as maps induced by functors on the Grothendieck group. These questions and their relevance in existing categorifications were addressed in her talk.

She started by recalling basic ideas about categorification and sketched a categorification of the  $U_q\mathfrak{sl}_2$ module  $\mathbb{Q}(q)^{\otimes 2}$  using derived categories built from various blocks of the category  $\mathcal{O}$  for  $\mathfrak{gl}_n$ . She then raised the question of categorifying the whole of  $\operatorname{Rep}(U_q\mathfrak{sl}_2)$  with a view towards 3-manifolds invariants. She explained some ideas about how to make sense of fractional Euler characteristics by working with completed Grothendieck groups [1] and certain intermediate subcategories of bounded derived categories. This is certainly going to be very useful for further work on categorification. Afterwards, she stated two major theorems of hers, obtained alongside I. Frenkel and J. Sussan [15]: the first one states how to categorify the Jones-Wenzl projector using certain Serre quotients of blocks of the category  $\mathcal{O}$  for  $\mathfrak{gl}_n$ , and the second one gives a construction of a categorification of the colored Jones polynomial using tensor products of  $U_q\mathfrak{sl}_2$ -modules.

The last part of her talk dealt with applications of these results, in particular to categorification of 3j-symbols,  $\Theta$ -networks (interpreted as the Euler characteristic of  $\text{Ext}^*(L, L)$  for some simple Harish-Chandra bimodule L) and tetrahedron networks. Her work in this direction has applications in representation theory: for instance, 3j symbols can be viewed as generalizations of the Kazhdan-Lusztig polynomials.

She was followed by Professor Wolfgang Soergel from the University of Freiburg who spoke on *Koszul duality in positive characteristic*, mainly in the context of the category  $\mathcal{O}$  of a reductive algebraic group. The main new point was a formality result for the derived category of sheaves on the complex analytic flag variety with coefficients in a finite field, constructible along the Bruhat stratification: the extension algebra of parity sheaves as a dg-ring with trivial differential already describes this triangulated category. The method to prove this is splitting by the action of the Frobenius, which can be done under very mild and explicit restrictions on the characteristic.

In the afternoon, Professor Igor Frenkel from Yale University gave an intriguing presentation on *Quantum* groups associated to the split real Lie groups, their representations and future perspectives. He outlined the beginning of a new ambitious program to study the representation theory of certain quantum groups when the norm of q is 1, extending to the case |q| = 1 many results already known when |q| < 1. Slightly

more precisely, one of the main goals of his program is to construct *q*-deformations of minimal (spherical) principal series representations for split real Lie groups with properties similar to those in the compact case. This involves notions from functional analysis, namely the theory of positive self-adjoint operators. His program is expected to be connected to canonical bases, topological invariants and some notion of continuous categorification. He gave a very brief overview of work from the past twenty-five years which should be relevant for his program (e.g. Drinfeld double, equivalence of categories between quantum groups and affine Lie algebra).

Most of his talk focused on the case of  $\mathfrak{sl}_2$  (both on  $U_q\mathfrak{sl}_2$  and on  $F_q^+(GL_2(\mathbb{R}))$ ), starting with an observation of Faddeev to the effect that a pair of quantum torus algebras (or modular double of quantum plane algebra) can be derived from the simplest Heisenberg algebra. This suggests to consider a similar modular double for  $U_q\mathfrak{sl}_2$  and a family of representations realized via operators on  $L^2(\mathbb{R})$  belonging to the quantum plane algebra and satisfying a certain transcendental relation. He presented concrete, explicit formulas involving properties of the quantum dilogarithm (a quotient of two q-deformations of gamma functions) which are relevant for the  $\mathfrak{sl}_2$ -picture. One surprising aspect is that only continuous series representations appear in the decomposition of the tensor product of two continuous series representations.

The last part of his talk was about the modular double of  $F_q^+(GL_2(\mathbb{R}))$ . He finished by stating a Peter-Weyl type theorem which provides a decomposition of  $L^2(F_q(GL_2^+(\mathbb{R})))$  as a representation of the quantum group  $U_{q\tilde{q}}\mathfrak{sl}_2(\mathbb{R})$ . (This is partly based on work of Ivan Ip.)

Professor Alexander Molev (University of Sydney) followed with a talk about the Feigin-Frenkel center for classical types. For each simple Lie algebra  $\mathfrak{g}$ , consider the corresponding affine vertex algebra  $V(\mathfrak{g})$  at the critical level. The center  $\mathfrak{z}(\hat{\mathfrak{g}})$  of this vertex algebra is a commutative associative algebra whose structure was described about two decades ago by a remarkable theorem of B. Feigin and E. Frenkel [11] which is fundamental in the study of affine Lie algebras and has applications in the celebrated Langlands program [14]. That theorem states that the center is generated by rank(g) Segal-Sugawara vectors and the translation operator given by the derivative. However, only recently simple formulas for the generators of the center were found for the Lie algebras of type A following Talalaev's discovery of explicit higher Gaudin Hamiltonians. AMolev was able to obtain explicit formulas for generators (Sugawara operators) of the centers of the affine vertex algebras  $V(\mathfrak{g})$  associated with the simple Lie algebras  $\mathfrak{g}$  of types B, C and D and he presented those formulas at the workshop. (For  $\mathfrak{gl}_N$ , such formulas were obtained earlier by T. Talalaev using the Bethe subalgebra of the Yangian of  $\mathfrak{gl}_N$ .) The construction relies on the Schur-Weyl duality involving the Brauer algebra, and the generators are expressed as weighted traces over tensor spaces and, equivalently, as traces over the spaces of singular vectors for the action of the Lie algebra  $\mathfrak{sl}(2)$  in the context of the Howe duality. He presented concrete examples to show what his formulas looked like. His explicit formulas could also be used to give a simpler proof of the theorem of B. Feigin and E. Frenkel. Applying the state-field correspondence map to a complete set of Segal-Sugawara operators in  $\mathfrak{z}(\hat{\mathfrak{g}})$  yield generators for the center of the completed enveloping algebra of  $\hat{\mathfrak{g}}$ . It also leads to an explicit construction of a commutative subalgebra of the universal enveloping algebra  $U(\mathfrak{g}[t])$  and to higher order Hamiltonians in the Gaudin model associated with each Lie algebra g. It would be possible to introduce analogues of the Bethe subalgebras of the Yangians Y(g) and show that their graded images coincide with the respective commutative subalgebras of  $U(\mathfrak{g}[t])$ .

The day ended with a presentation by Professor Eric Vasserot (Université de Paris 7) on Cyclotomic rational double affine Hecke algebras and categorification. It was proved by P. Shan that, from the category  $\mathcal{O}$  of a cyclotomic rational double affine Hecke algebra H, one can obtain a categorification of the quantum Fock space. It is conjectured in [28] that this category is equivalent to a certain subcategory of a parabolic category  $\mathcal{O}$  at negative level of an affine Kac-Moody algebra. This subcategory can be seen as a higher analogue of the q-Schur algebra because the category of modules over the latter is known to be equivalent to a highest weight subcategory of the affine category  $\mathcal{O}$  of  $GL_N$  at a negative level. This is a consequence of the famous work of D. Kazhdan and G. Lusztig [20] which provides an equivalence between the category of finite dimensional representation of  $U_q \mathfrak{gl}_N$  and a certain affine category  $\mathcal{O}$  for  $\mathfrak{gl}_N$ .

He started by recalling general results about rational Cherednik algebras, in particular a theorem of his and P. Shan [26] which describes the support of modules obtained via the induction and the restriction functors. He then gave a present statement of a conjecture of P. Etingof [8] to the effect that the number of irreducible modules in the category  $\mathcal{O}$  for H with a given support is equal to the dimension of a certain vector space obtained from weight spaces of a representation of an affine Lie algebra. The rest of his talk was devoted to his proof [26] of this conjecture for cyclotomic H using a categorification of the Heisenberg algebra action on

the Fock space and a reinterpretation of the support of modules in  $\mathcal{O}$  in terms of actions of affine Lie algebras on the Fock space. This is a major result in the representation theory of Cherednik algebras since, from the conjecture of P. Etingof, one obtains a formula for the number of irreducible finite dimensional modules over H.

#### Friday, August 12

The first two talks on Friday morning were delivered by postdoctoral researchers. Dr. David Jordan of the University of Texas at Austin spoke on *Quantized multiplicative quiver varieties*. He started by recalling a "diamond" of degenerations relating the quantized enveloping algebra  $U_q\mathfrak{g}$  with  $\mathfrak{U}\mathfrak{g}$ ,  $\mathbb{C}[G]$  and  $\mathrm{Sym}(\mathfrak{g})$  for  $\mathfrak{g}$  a semisimple Lie algebra. His goal was to obtain a similar diamond for quiver varieties,  $\mathfrak{U}\mathfrak{g}$ ,  $\mathbb{C}[G]$  and  $\mathrm{Sym}(\mathfrak{g})$  being replaced by, respectively, the quantized quiver varieties of Gan-Ginzburg, the multiplicative quiver varieties of Crawley-Boevey-Shaw and Lusztig's quiver varieties. The role of  $U_q\mathfrak{g}$  is played by new algebras  $D_q(Mat_d(Q))$  associated to a quiver Q and dimension vector d which can be defined explicitly in terms of generators and relations. An important theorem about these is that they yield a flat (PBW) q-deformation of the algebra of differential operators on the space of matrices associated to Q and that, furthermore, a certain localization of  $D_q(Mat_d(Q))$  quantizes a quasi-Poisson structure on an open subset of the cotangent bundle of that space of matrices.  $D_q(Mat_d(Q))$  admits a q-deformed moment map from the quantum group  $U_q(\mathfrak{gl}_d)$ , acting by base change at each vertex. The quantum Hamiltonian reduction,  $A_d^{\xi}(Q)$ , of  $D_q$  by  $\mu_q$  at the character  $\xi$  is simultaneously a quantization of the multiplicative quiver variety, and a q-deformation of the quantized quiver variety associated to Q.

Specific examples of the data  $(Q, d, \xi)$  yield q-deformations of important algebras in representation theory: for example, the spherical double affine Hecke algebra of type  $A_n$  may be obtained in this way when Q is the Calogero-Moser quiver. (This is a deformation of a construction of the spherical rational Cherednik algebra by Gan and Ginzburg.) Given the ubiquity of quiver varieties in geometric representation theory, it is natural to anticipate further connections. He ended his talk by presenting briefly the construction of a functor from the category of modules over  $D_q(Mat_d(Q))$  to the category of representations of the elliptic Weyl group.

Afterwards, Dr. Peter Tingley of the Massachusetts Institute of Technology delivered a presentation on *Combinatorics of affine*  $\mathfrak{sl}(2)$  *MV polytopes* based on his joint work with Pierre Baumann, Thomas Dunlap and Joel Kamnitzer. MV polytopes give a useful realization of finite type crystals, which are combinatorial objects related to representations of complex simple Lie algebras and their quantized enveloping algebras. Recent work of Baumann and Kamnitzer constructs MV polytopes from Lusztig's quiver varieties, which are well defined outside of finite type. This work has now been extended to give a definition of MV polytopes in all symmetric affine cases, and to show that understanding the resulting combinatorics reduces to understanding the  $\mathfrak{sl}(3)$  and affine  $\mathfrak{sl}(2)$  cases. (This was explained on Tuesday by J. Kamnitzer.) In his talk, P. Tingley gave a simple characterization of the polytopes and a description of the crystal operators in the affine  $\mathfrak{sl}(2)$  case, thereby completing the picture in all symmetric affine cases. He also explained what the combinatorics meant in terms of quiver varieties.

The meeting concluded with a talk by Professor Ben Webster of Northeastern University about *Categorification, Lie algebras and topology*. It is a long established principle that an interesting way to think about numbers is as the sizes of sets or dimensions of vector spaces, or better yet, as the Euler characteristic of complexes. You cannot have a map between numbers, but you can have one between sets or vector spaces. For example, Euler characteristic of topological spaces is not functorial, but homology is functorial. One can try to extend this idea by taking a vector space and trying to make a category by defining morphisms between its vectors. This approach (interpreted suitably) has been a remarkable success within the representation theory of semi-simple Lie algebras and their associated quantum groups. This speaker gave an introduction to this area, with a view toward applications in topology, in particular to replacing polynomial invariants of knots that come from representation theory with vector space valued invariants that reduce to knot polynomials under Euler characteristic.

Let  $\mathfrak{g}$  be a semisimple Lie algebra and  $U_q\mathfrak{g}$  be Lusztig's quantized enveloping algebra obtained by adding extra idempotents. The speaker started with an overview of the Chang-Rouquier-Khovanov-Lauda diagrammatic categorification of the universal enveloping algebra  $\mathfrak{U}\mathfrak{g}$  and of  $U_q\mathfrak{g}$ , insisting on the wonderful observation that the grading on their category  $\mathcal{U}$  (whose Grothendieck group is  $\mathfrak{U}\mathfrak{g}$ ) easily yields a graded version  $\mathcal{U}$  whose Grothendieck group is  $U_q \mathfrak{g}$ . He then explained briefly how to categorify, using again diagrams, the irreducible finite dimensional representations of  $\mathfrak{g}$  with a given highest weight. He recalled how some of these categorifications where already known from previous work on the symmetric groups and Hecke algebras.

By analogy with how one obtains polynomial knot invariants from ribbon tensor categories of representations of  $U_q \mathfrak{g}$ , he proposed to construct quantum knot homologies from a categorification of tensor product of simples modules of  $\dot{U}_q \mathfrak{g}$ . This is envisioned as one step in a bigger schema to construct quantum knot homologies via conjectural ribbon 2-categories of representations of  $\mathcal{U}$ . For  $\mathfrak{g} = \mathfrak{sl}_n$  and  $\mathfrak{g} = \widehat{\mathfrak{sl}}_n$ , some of these categorifications can be obtained from familiar categories in classical representation theory (e.g. blocks of a parabolic category  $\mathcal{O}$ ).

He finished by stating an amazing theorem, related to the conjecture of P. Etingof whose proof was explained on the previous day by E. Vasserot, which says that the category of finite dimensional representations of a symplectic reflection algebra for the wreath product of the symmetric group  $S_n$  with a finite subgroup  $\Gamma$  of  $SL_2(\mathbb{C})$  is derived equivalent to a certain weight space of a categorification of a simple  $\mathfrak{g}$ -module.

## Outcome of the meeting

The workshop was an occasion for researchers to get an overview of some important recent progress in the representation theory of quantum groups. Many positive comments have been received by the organizers to that effect. For instance, Professor Evegeny Mukhin (Indiana University - Purdue University Indianapolis) commented that "The conference was great. Everything was right – the organization, the participants, the timing, etc. It was my fourth time at BIRS and I would come again anytime. I have surely learned many things and even started a couple of new projects. It is too early to say how they will go, but it is certainly a very interesting twist." Some participants also took the opportunity to exchange ideas relevant to their research, work on projects with their collaborators or start new ones, as exemplified by the following testimonials.

"I had some fruitful discussions with my collaborator Catharina Stroppel, in which we made some progress towards the categorification of matrices using Harish-Chandra bimodules. I also had some useful conversations with Weiqiang Wang, through which I learnt of some exciting new progress that he has made in the representation theory of Lie superalgebras." Professor Jonathan Brundan, University of Oregon.

"It was a great workshop and very productive for me. Peter Tingley and I worked on our papers on affine MV polytopes, which should be completed soon. Ben Webster and I worked on our project involving quantization of slices in the affine Grassmannian using Yangians. During a hike, I talked to Evgeny Mukhin about monodromy of Bethe vectors. This conversation continued with Valerio Toledano Laredo the next day, and I hope that it will lead to a future project.

On the bus to the airport, I had a very good discussion with Jon Brundan, which gave me a much better understanding of how the category  $\mathcal{O}$  work on categorification (see papers of Brundan, Kleshchev, Stroppel, Frenkel, Sussan, etc.) fits in with the affine Grassmannian and I hope this will lead to some future projects." Professor Joel Kamnitzer, University of Toronto.

"The workshop has been a wonderful experience for me. It brought together leaders in several areas of representation theory; their talks provided a comprehensive and inspiring picture of the cutting edge research in the field. I received a valuable feedback for my own talk from several participants, including David Jordan, Valerio Toledano Laredo, Maxim Nazarov, Weiqiang Wang and Milen Yakimov. Through conversations with these people I discovered new approaches to develop a promising direction of research which will involve quantum versions of centers of vertex algebras." Professor Alexander Molev, University of Sydney.

"I was able to meet with my collaborator Anne Schilling and we could discuss our ongoing research about the conjecture on the equality of one-dimensional sums and generating functions of rigged configurations. The presentations delivered by Toledano Laredo, Gautam and Frenkel were completely new to me and they will inspire my future research. The presentation delivered by Kamnitzer will become useful for my research about the combinatorial structure of Kirillov-Reshetikhin crystals." Professor Masato Okado, Osaka University.

"Igor Frenkel made some useful remarks regarding my talk afterwards. Also, Peter Tingley had interesting comments regarding my talk on how to possibly generalize work to the nonperfect setting. We are still in discussion about this via e-mail. It was very useful for me to discuss some aspects of the crystal commutator with Joel Kamnitzer." Professor Anne Schilling, University of California at Davis.

"The conference had many interesting talks, and was productive for me in several ways. Most particularly, I was able to meet with Joel Kamnitzer, and we made significant progress on our joint project on affine MV polytopes. Also, Anne Schilling's presentation gave me some new ideas which may be useful in understanding a relationship between Demazure characters and Macdonald polynomials in type C." Dr. Peter Tingley, Massachusetts Institute of Technology.

"From Eric Vasserot's talk I learned about results which will be very relevant to classifying the possible support sets of modules over the cyclotomic rational Cherednik algebra. I was also inspired by the talks in general to try to use more abstract machinery." Dr. Stewart Wilcox, University of Alberta.

## **List of Participants**

Benkart, Georgia (University of Wisconsin - Madison) Brundan, Jonathan (University of Oregon) **Cliff, Gerald** (University of Alberta) Enriquez, Benjamin (Universit de Strasbourg) Frenkel, Igor (Yale University) Gautam, Sachin (Northeastern University) Ginzburg, Victor (University of Chicago) Greenstein, Jacob (University of California Riverside) Guay, Nicolas (University of Alberta) Hernandez, David (Université Paris 7) Jordan, David (Massachusetts Institute of Technology) Kamnitzer, Joel (University of Toronto) Kim, Jeong-Ah (University of Seoul) Licata, Anthony (Institute for Advanced Study and the Australian National University) Moley, Alexander (University of Sydney) Moura, Adriano (Universidade Estadual de Campinas) Mukhin, Evgeny (University-Purdue University Indianapolis) Nakanishi, Tomoki (Nagoya University) Nazarov, Maxim (University of York) Okado, Masato (Osaka University) Savage, Alistair (University of Ottawa) Schilling, Anne (University of California Davis, Department of Mathematics) Shin, Dong-Uy (Hanyang University) Soergel, Wolfgang (University of Freiburg) Stroppel, Catharina (Universitat Bonn) **Tingley. Peter** (Massachusetts Institute of Technology) Toledano Laredo, Valerio (Northeastern University) Varagnolo, Michela (Universite de Cergy-Pontoise) Vasserot, Eric (University Paris 7) Wang, Weiqiang (University of Virginia) Webster, Ben (University of Oregon) Wilcox, Stewart (University of Alberta) Yakimov, Milen (Louisiana State University) Young, Charles (University of York)

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## Chapter 25

# Algebraic Structure in Network Information Theory (11w5074)

## Aug 14 - Aug 19, 2011

**Organizer(s):** Michael Gastpar (University of California, Berkeley) Frank Kschischang (University of Toronto)

Mathematics has always played an important role in the design and optimization of communication systems, particularly following Shannon's groundbreaking work in 1948 that gave theorems establishing fundamental limits on the rates of reliable communication over point-to-point channels (i.e., those involving a single transmitter-receiver pair). In order to develop fundamental bounds, concepts from probability and statistics and arguments involving averages taken over random code ensembles have been of key importance in most of the communications problems studied to date. Endowing these code ensembles with particular algebraic structure (e.g., the structure of a vector space) was not necessary to establish fundamental limits, and entered the stage only to allow for compact code descriptions and computationally-efficient encoding and decoding algorithms.

In *networks* (i.e., communication systems involving multiple transmitters or receivers or relay nodes) the situation becomes much more complicated, and a general framework that establishes fundamental limits is lacking. The current grand challenge in information theory is to devise communication strategies and architectures that optimally exploit communication networks. An emerging key insight—and the motivation for this workshop—is that in certain network information theory problems, endowing code ensembles with algebraic structure is a key necessity, not only for engineering convenience, but for the derivation of fundamental limits. The goal of the workshop was to bring together experts from information theory, coding theory, and algebra to shed light on this observation, with the goal of beginning to understand the type and extent of algebraic structure needed to extend Shannon's insights about point-to-point channels to the more general case of networks.

## **Overview of the Field**

In his groundbreaking paper [23], Shannon determined the fundamental limits of reliable communication across a noisy channel and set forth the bit as the underlying unit of information. The mathematical frame-work used to prove these results involved statistical averages taken over ensembles of codebooks chosen at random, and thus forged a deep connection between information theory, probability, and statistics. Following Shannon, information theorists proving capacity theorems often resort to probabilistic arguments to prove the existence of good codes. As no particular algebraic structure is imposed, the resulting codebooks are generally regarded as being unstructured. In fact, Shannon's original random coding arguments do indeed determine optimal performance for all single-user noisy channels as well as for several multi-user networks.

In this classical context, algebraic structure is not a necessity, but it is a practical convenience, as such structure often allows for efficient encoding and decoding. The simplest examples are linear block codes, where the codewords form a finite-dimensional vector space over a finite field, allowing an exponentiallylarge number of codewords to be described as linear combinations of only a small number of basis codewords, and where decoding algorithms can exploit this algebraic structure for efficiency. In this classical context, it seems that there may be a price to pay for this algebraic convenience: a folk theorem holds that, in general, codes with algebraic structure perform worse than the best unstructured codes. (This is in fact true for the case of a single noisy channel, where it is known that group codes are suboptimal except in the case of additive noise [1].)

More recently, it has become clear that this folk theorem may give the wrong insight in the network setting. That is, when several users communicate over noisy channels and interfere with each other (as occurs, for example, in wireless communications), requiring algebraic structure can be advantageous, even in the context of proving a capacity theorem. More precisely, proving the existence of a good algebraically-structured code becomes possible, even when arguments involving unstructured code ensembles fail. A first inkling of this appeared in the paper by Körner and Marton [12], which considers a very simple, non-standard distributed coding problem where the goal is to recover, not the original bits, but only their modulo-2 sum. For this problem, it was shown that linearly-structured codes attain optimal performance, while standard arguments involving ensembles without algebraic structure are not able to show that good codes exist.

Recent work by several groups has shown that arguments involving algebraically-structured codes for communicating bits across a network can result in proofs for the existence of codes having significant gains relative to what can be proved about codes drawn from unstructured ensembles, and specific examples (with references) will be given in the sequel. These gains appear to stem from the fact that algebraic structure enables users to perform distributed processing as if it were centralized.

Beyond these examples, algebraic structure is emerging as a key argument in several of the most important and challenging problems in network information theory, including the following:

**Interference alignment:** One of the long-standing open problems in information theory is the determination of the capacity of the so-called interference channel, wherein several transmitter-receiver pairs share the same communication channel. For many years, it was assumed that the maximum bit rate per user is inversely proportional to the number of active users. Surprisingly, each user can achieve half its interference-free bit rate, regardless of the number of interferencs. The key is to carefully assign subspaces for transmission such that all signals (except the desired one) end up in a single subspace at each receiver [4]. Codes with algebraic structure have a crucial role, as recent work has shown [3, 21]. Algebraic structure also enters as an argument determining the maximum amount of interference alignment possible. An early account of this can be found in [8].

**Distributed interference cancellation:** Consider a power-limited transmitter and receiver that communicate over a noisy channel subject to interference. One of the celebrated results of information theory is that the effects of the interference can be completely removed as soon as the transmitter has prior knowledge of the interfering signal, regardless of its strength [6]. What if multiple users communicate to a single receiver over interfering links? When each transmitter has partial knowledge of the interference, cancellation of an additional interference is possible, but only if algebraically structured codes are used. For an additive white Gaussian noise model, this involves lattice codes and has been studied in [22].

**Computation over noisy channels:** The traditional view of interference is that it is an obstacle to reliable communication. This is true if the objective of each receiver is to recover the message sent by a particular transmitter. However, if the receiver is only interested in a function of the messages, then interference can be harnessed to compute the function more efficiently, provided the transmitters use a structured code that is appropriately matched to the function of interest (e.g., see [20]).

**Wireless "Network Coding":** Even in simple networks, it is not sufficient to just route packets; instead, intermediate nodes may have to forward linear combinations of their incoming packets. This insight was found in [2] and has since sparked a great deal of research under the name of "network coding." If we

consider said intermediate node, all it really needs to know is a particular linear combination of its incoming packets. Using codes with algebraic structure, we can enable just this, as advocated in [19], and further developed in recent work such as [18, 17]. Beyond this local perspective, codes with algebraic structure are also crucial at the end-to-end level, as recent work has shown [13].

**Distributed quantization:** It is increasingly the case that data is collected at several locations and then compressed for transmission across a network. The receiver may only be interested in a function of the sampled data and, in this case, it has been shown that gains are possible through the use of group and lattice codes [14, 15].

**Secrecy:** Algebraic structure enables several users to collude against adversaries and eavesdroppers directly over a wireless link, without any prior coordination (e.g., see [11]).

The emerging theme is that algebraically-structured codes can enable powerful new schemes, especially for wireless channel models, that have the potential to dramatically increase end-to-end bit rates. To date, most of the above research has used existing algebraic code constructions in a "plug-and-play" fashion. For discrete channels, these are mostly codes over finite fields, and for continuous-input channels, lattice codes [5]. Much work has focused on showing that lattice codes can approach the capacity of a single-user additive white Gaussian noise channel, beginning with [7] and culminating in several successful constructions [16, 24, 9], see [10] for a commentary. While these codes already give interesting results in networks, they are optimal only in certain limited special cases. One of the most interesting avenues for future research will be to develop new approaches to the construction of algebraically structured codes that are particularly well-suited for a given network communication scenario.

The research described above is the beginning of a new algebraic methodology for existence proofs in network information theory. To complement these methods, new tools for proving impossibility results will be needed as well. As it stands, impossibility results focus on which statistical dependencies can be established between different transmitters and receivers. Quite recently, new bounds have emerged for the interference channel that make use of results in additive combinatorics [8]. Much work is needed to bring algebraic structure to the forefront in impossibility results.

# **Recent Developments and Presentation Highlights**

The presentation of recent developments was organized into five sessions, not necessarily mutually exclusive.

 Mathematical Foundations. This session started with a tutorial lecture by Ram Zamir (Tel Aviv University) on the fundamentals of random lattices and how they relate to network information theory. Starting from the Minkowski-Hlawka ensemble, he gave an extensive coverage of the basic tools and ended with a series of intriguing starting points for discussion, which came under the heading of "antistructure problems," namely, problems where algebraic arguments are not of key importance.

Uri Erez (Tel Aviv University) presented a refined analysis of algebraic codes in network information theory, including a new result on error exponents on the Gaussian multiple-access channel.

Sandeep Pradhan (University of Michigan, Ann Arbor) continued the exposition of the basic foundations with the discussion of nested linear constructions, going beyond the classical construction of nesting a "fine" linear code inside a "coarse" one.

Nigel Boston (University of Wisconsin, Madison) presented on the mathematical foundations of convolutional codes.

The session was completed by two short talks by graduate students about very recent work, namely Katie Morrison (University of Nebraska, Lincoln) on rank-metric codes, and Anna-Lena Trautmann (University of Zurich, Switzerland) on cyclic orbit codes.

2. Algebraic Structure in Relay Networks. This session started with a longer lecture of a certain tutorial character by Shlomo Shamai (Technion, Israel), diligently summarizing the state of the art of algebraic

arguments as they appear in the recent literature, with a particular connection to the important emerging topic of interference management.

This was followed by a sequence of shorter, more focused talks.

Bobak Nazer (Boston University) started with a discussion of the "compute-and-forward" paradigm and then gave a thought-provoking presentation about the main missing ingredients and open problems in the use of lattice coding in Gaussian networks. To underline the importance of his open problems as well as his Canadian heritage, he carefully chose names for each of the open problems, including the "icewine" problem, referring to the prizes offered for the solution of these problems.

Urs Niesen (Bell Labs, New Jersey) presented an improved "compute-and-forward" construction for Gaussian networks that performs significantly better in the limit as the noise process disappears (but requires a significant amount of channel state information at the coding devices in turn).

Krishna Narayanan (Texas A&M University) talked about practical code constructions for lattice codes, showing ways of explicitly going beyond binary codes.

In the second part of this session, the talks focused on questioning the ultimate need for algebraic structure.

Sae-Young Chung (Korea Advanced Institute of Science and Technology) started this part in a classical devil's advocate fashion. He considered one of the flagship results that are widely used to underline the need for algebraic structure, namely, the Gaussian two-way relay channel. For this channel, he showed that in the limit as the noise process disappears, almost the same performance can be attained by a code without any algebraic structure.

Gerhard Kramer (Technical University of Munich) presented a well-structured review of the emerging "noisy network coding" approach, again an approach that chooses not to deal with algebraic structure, as well as some intriguing extensions of this approach, in particular pertaining to what he referred to as "short messages."

Slawomir Stanczak (Technical University of Berlin) presented a complementary set of ideas about practical approaches to compute-and-forward (as well as an intriguing connection to Hilbert's 15th problem).

The final three talks considered in detail specific network problems for which it does not seem that algebraic structure is needed.

Natasha Devroye (University of Illinois, Chicago) considered the classical relay channel and showed that codes with algebraic structure can attain all results of codes without algebraic structure.

Liang Xie (University of Waterloo) presented list decoding ideas for the classical relay channel.

Ashish Khisti (University of Toronto) talked about delay-efficient coding for streaming applications.

This session was completed by several graduate student talks, covering recent developments. Chen Feng (University of Toronto) presented an algebraic approach to compute-and-forward. Matthew Nokleby (Rice University) presented ideas on "cooperative" compute-and-forward. Yiwei Song (University of Illinois at Chicago) presented further results on lattices in Gaussian relay networks (involving list decoding). Jiening Zhan (University of California, Berkeley) presented on algebraic structure and receiver architectures in networks.

3. Algebraic Structure and Interference Alignment. Algebraic structure of a slightly different kind is of key importance to another promising emerging direction in network information theory, namely, interference alignment. The third session of the workshop was devoted to this.

Alex Dimakis (University of Southern California) started off from the real-world problem of distributed database repair, and showed how codes with algebraic structure play a key role in this problem.

Viveck Cadambe (University of California, Irvine) posed the interference alignment problem as a problem of finding common invariant subspaces for a collection of (linear) operators. He elegantly expressed the problem as a canonical (though unsolved) question about tensors.

Sriram Vishwanath (University of Texas, Austin) considered lattice codes for interference scenarios.

Aylin Yener (Pennsylvania State University) expanded the horizon by considering the problem of communication under secrecy constraints, and showed how algebraic structure again plays a key role.

This session was completed by a graduate student talk on very recent developments. Guy Bresler (University of California, Berkeley) presented new results on interference alignment for vector channels.

 Algebraic Structure and Network Coding. This session covered the important topic of network coding and its many connections to algebraic structure.

Joachim Rosenthal (University of Zurich) started the session with an introduction to Schubert calculus and its connection to rank-metric codes.

Frederique Oggier (Nanyang Technological University, Singapore) discussed wiretap code design.

Emanuele Viterbo (Monash University, Australia) presented results about network coding over finite rings, giving explicit constructions.

Babak Hassibi (California Institute of Technology) discussed the important connections between network coding and matroid theory.

Danilo Silva (Federal University of Santa Catarina, Brazil) presented the key ideas behind using algebraic codes to obtain error control for noncoherent network coding.

Tracey Ho (California Institute of Technology) used an intriguing "zigzag" network example to illustrate fundamental algebraic questions in network coding.

Alex Vardy (University of California, San Diego) then talked about a third class of codes of fundamental importance to the workshop, namely, subspace codes. He presented novel list decoding algorithms for these codes.

 Algebraic Structure and Source Coding. The final session concerned the role of algebraic structure in distributed source coding.

Aaron Wagner (Cornell University) presented fundamental results delineating those distributed source coding problem for which structure is important.

Prakash Ishwar (Boston University) talked about interactive source coding.

Mohammad Maddah-Ali (Bell Labs) presented new algebraic approaches to distributed source coding, giving crisp examples that showed the need for algebraic structure.

### **Open Problems**

The workshop also allowed ample time for the discussion of open problems. For one, short breaks were scheduled between all talks to enable addressing detailed open problems arising in a narrower context. On top of this, dedicated open problems sessions were held in the evenings. These sessions happened both in the lecture halls as well as in the BIRS lounge and were very well attended.

One of the most heavily debated open question concerned the information expressions for the Gaussian networks. In particular, typical information-theoretic capacity results for Gaussian channels involve expressions of the type  $\log(1 + \text{SNR})$ . When using lattices for the "compute-and-forward" problem, in the two-terminal setting, it is possible to show a formula of the type  $\log(\frac{1}{2} + \text{SNR})$ . This might appear to be a small difference, but it has important ramifications when it comes to layering and multi-level codes. Therefore, the question is whether this difference is fundamental to the problem, and if it is not, what kinds of constructions might permit to improve performance. A fair amount of discussion was devoted to understanding this.

Another open problem, raised by Uri Erez, concerns the so-called "dirty paper" problem, where the received signal is of the form  $Y^n = X^n + hS^n$ , where h is a constant known only to the receiver and  $S^n$  is a sequence known only to the transmitter (in a non-causal fashion, at the beginning of time). Several approaches were developed during the session, but it remains to be determined whether they will work.

Bobak Nazer posed several questions pertaining to the possibility of doing "compute-and-forward" in a fast-fading environment, and Krishna Narayanan considered a simple two-way relay channel to understand the trade-offs between compute-and-forward and decode-and-forward, for which it seemed highly tempting that a final capacity result should be within reach.

Many other open problems, beyond this short sampling, were discussed, and we hope to see solutions in the literature shortly.

# **Concluding Remarks**

The workshop achieved its main goal of providing a focused environment for in-depth discussion of this emerging research direction. None of the existing forums could provide a similarly dedicated setting. Deep technical discussions were enabled by the many high-quality research talks providing a steady stream of input, but perhaps even more importantly by several sessions dedicated to open problems. The BIRS setup provides a uniquely stimulating environment for this, including lecture halls of various sizes with ample blackboard space. While algebraic arguments provide network information-theoretic results that are out of reach of the classical random coding arguments, they can at present rarely be proved to be strictly optimal. This nagging fact provided ample open problems and many intriguing discussions. Another factor that contributed to the highly interactive environment was the fact that room and board were provided by BIRS, free of charge to participants. Therefore, many interesting discussions took place over breakfast, lunch and dinner and well into the night over coffee and other drinks in the well-equipped lounge at the BIRS facility. Holding a workshop at BIRS was a truly enjoyable experience for all involved.

# **List of Participants**

Boston, Nigel (University of Wisconsin) **Bresler, Guy** (University of California at Berkeley) Cadambe, Viveck (University of California at Irvine) Chung, Sae-Young (Korea Advanced Institute of Science and Technology) Devroye, Natasha (University of Illinois at Chicago) Dimakis, Alex (University of Southern California) Erez, Uri (Tel Aviv University) Feng, Chen (University of Toronto) Gastpar, Michael (University of California, Berkeley) Hassibi, Babak (California Institute of Technology) Ho, Tracey (California Institute of Technology) Ishwar, Prakash (Boston University) Khisti, Ashish (University of Toronto) Kramer, Gerhard (Technical University Munich) Kschischang, Frank (University of Toronto) Maddah-Ali, Mohammad Ali (Alcatel-Lucent Bell Laboratories) Morrison, Katie (University of Nebraska - Lincoln) Narayanan, Krishna (Texas A&M University) Nazer, Bobak (Boston University) Niesen, Urs (Alcatel-Lucent Bell Laboratories) Nokleby, Matthew (Rice University) **Oggier, Frederique** (Nanyang Technological University) Pradhan, Sandeep (University of Michigan at Ann Arbor) Rosenthal, Joachim (University of Zurich) Shamai, Shlomo (Technion Israel Institute of Technology) Silva, Danilo (Federal University of Santa Catarina) Song, Yiwei (University of Illinois at Chicago) Stanczak, Slawomir (Fraunhofer Heinrich-Hertz-Insiut and Technical University of Berlin) Trautmann, Anna-Lena (University of Zurich) Vardy, Alexander (University of California San Diego) Vishwanath, Sriram (University of Texas at Austin) Viterbo, Emanuele (Monash University Melbourne) Wagner, Aaron (Cornell University)

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# Chapter 26

# **Crossing Numbers Turn Useful** (11w5144)

# Aug 21 - Aug 26, 2011

**Organizer(s):** Dan Archdeacon (University of Vermont) Gelasio Salazar (Universidad Autonoma de San Luis Potosi) Laszlo Szekely (University of South Carolina)

### An Overview of Crossing Numbers

A graph G represents a relation between pairs of items. The items are commonly called *vertices* and the set of vertices is denoted V(G). A relation is a pair of vertices  $\{v_1, v_2\}$ . Each relation is called an *edge*, and the set of all edges is denoted E(G). For example,  $G = K_5$  is the graph with 5 vertices, every pair of which are together in an edge. This is called the *complete graph* of order 5.

Graphs are important models in many contexts because of their generality. For example, the vertices may represent people and the edges represent when a pair of people are friends. Analysis of this abstracted graph can reveal an underlying structure of the social relationship. Or the vertices may represent processors in a computer network and the edges represent communication networks. The analysis of this graph can reveal the connectivity of the underlying network.

An important class of graphs are those that can be drawn on a plane so that edges do not cross. Continuing the application where the graph represents a computer network, such a graph can be laid out on a circuit board so that communication channels do not cross, so no insulation is needed to avoid electrical shorts. Graphs so drawn without edge crossings are called *planar graphs*.

Not every graph is planar; for example, the graph  $K_5$  described above is not planar. In this case the next best thing would be to draw the graph G in the plane with as few crossings as possible. This minimum taken over all drawings is called the *crossing number of G*, denoted cr(G).

The problem of minimizing crossings when drawing a graph was first raised by Paul Turán. He tells [27] of how he posed the problem while in a forced labor camp in World War II. Here there were a set of n kilns making bricks and m railroad terminals to ship the bricks. Each kiln was connected to each terminal by a rail line. When two lines crossed cars carrying bricks could derail, creating extra work. Turán's idea was to lay out the camp so as to minimize the number of crossing tracks. Here the graph is denoted  $K_{n,m}$  (there are n kilns related to each of m terminals, called a *complete bipartite graph*), so in modern terms he was asking for  $cr(K_{n,m})$ .

Despite the simple nature of the problem not much is known about this parameter. For example, neither the crossing number of the complete graph  $cr(K_n)$  or the crossing number of the complete bipartite graph  $cr(K_{n,m})$  is known exactly, or even their asymptotic trend.

Applications of the crossing number include VLSI circuit layouts as described above. In 1983 Leighton [17] proved the that the area needed to represent a layout of an electric circuit is closely related to the crossing

number of the underlying graph. Another application of crossing number is in the visualization of graphs. Minimizing the number of edge crossings is desirable, albeit competing with other properties such as symmetry and the shape of the edges. Purchase [20] says "... reducing the number of edge crossings is by far the most important aesthetic, while minimizing the number of bends and maximizing symmetry have a lesser effect."

# A Closer Look at Crossing Numbers

We turn to a more specific description of problems involving crossing numbers.

### Three classes of graphs

Our first question is about the crossing number of the complete graph.

**Conjecture 26.0.1**  $cr(K_n) = \frac{1}{4} \lfloor \frac{n}{2} \rfloor \lfloor \frac{n-1}{2} \rfloor \lfloor \frac{n-2}{2} \rfloor \lfloor \frac{n-3}{2} \rfloor.$ 

The formula comes from the optimal known drawings with few crossings. Conjecture 26.0.1 is true for  $n \leq 12$  and is known to be an upper bound for general n. Proving that the formula is a lower bound is much harder. An important partial result would be to establish the asymptotic behavior of the crossing number:

#### Question 26.0.2 Determine

$$\lim_{n \to \infty} \frac{cr(K_n)}{n^4}$$

We turn next to the crossing number of complete bipartite graphs.

**Conjecture 26.0.3**  $cr(K_{n,m}) = \lfloor \frac{n}{2} \rfloor \lfloor \frac{n-1}{2} \rfloor \lfloor \frac{m}{2} \rfloor \lfloor \frac{m-1}{2} \rfloor$ .

Equality was thought to be established by Zarankiewicz [46], but a flaw in his proof was detailed by Guy [29]. Again, the formula is known to be an upper bound as given by constructions.

The third class of interesting graphs is the *Cartesian product of two cycles*  $C_n \times C_m$ . The vertex set of this graph is the product of two cyclic groups  $Z_n \times Z_m$  with edges joining pairs where one coordinate is the same and the other coordinate differs by one.

**Conjecture 26.0.4**  $cr(C_n \times C_m) = n(m-2)$  where  $n \ge m$ .

These graphs embed on the torus. They were originally examined by Harary, Kainen, and Schwenk [16] who showed these crossing numbers grow with  $\min\{n, m\}$ . In particular, this showed that the crossing numbers of toroidal graphs can be arbitrarily large when drawn in the plane. Again, drawings illustrate that n(m-2) is an upper bound on the crossing number. Once more, demonstrating the lower bound is harder.

These are of course three specific classes of graphs. They are important as they give rise to other natural questions. For example, the crossing number of the complete graph leads to the crossing number of a graph and its minors [22, 11], the crossing number of the complete bipartite graph is important in the theorem of set systems [46], and the crossing number of the product of cycles leads to the number of intersections in meshes of curves [21]. The common theme is that a question about a specific class of graphs can evolve into questions about the general structure of graphs.

### The Geometric Crossing Number

Heretofore we have been examining arbitrary drawings in the plane. A common restriction is to require that edges be line segments. A *geometric drawing* represents vertices by points in the plane with edges being straight-line segments between their ends. By convention, no edge is allowed to pass through another vertex. The *geometric crossing number*  $\bar{cr}(G)$  is the minimum number of crossings over all geometric drawings. Note that the geometric crossing number is at least the crossing number, since we are taking the minimum over a smaller collection of drawings.

Perhaps surprisingly, the geometric crossing number can be strictly greater than the crossing number. In particular  $\bar{cr}(K_8) = 19 > 18 = cr(K_8)$ . This is the smallest complete graph for which the difference is strict. Lovász et al. invoked [8] to show that  $cr(K_n)$  and  $\bar{cr}(K_n)$  differ by  $\Omega(n^4)$ . In contrast:

**Conjecture 26.0.5**  $c\bar{r}(K_{n,m}) = cr(K_{n,m}).$ 

We would like to present a conjecture for the exact value of  $\bar{cr}(K_n)$ , but its value is unclear. Upper bounds are demonstrated by examples, and there is a long history of these that give sequentially smaller number of crossings. Attention has focused on the following (see [3]):

Conjecture 26.0.6 Find

$$\lim_{n \to \infty} \frac{\bar{c}r(K_n)}{\binom{n}{4}}.$$

This limit is called  $q_*$  for reasons discussed in the next section. It is known to exist and that

$$379972 < \frac{277}{729} \le q_* \le \frac{83247328}{218791125} < .380488.$$

Observe that the difference between the upper and lower bounds is quite small (or, from another view, quite large).

### **Sylvester's Four-Point Problem**

An important motivation of the geometric crossing number is *Sylvester's Four-Point Problem* from geometric probability (see [9], with [10] for a more rigorous statement). Let R be an open set in the plane with finite area. What is the probability q(R) that four points chosen randomly from R form a convex quadrilateral? It is known [5] that if R is convex, then q(R) is minimized when R is a disk and maximized when R is a triangle. Let  $q_*$  denote the infimum of q(R) over all R. Scheinerman and Wilf [62] showed this was closely related to the geometric crossing number  $\bar{cr}(K_n)$ , specifically, that

$$q_* = \lim_{n \to \infty} \frac{\bar{cr}(K_n)}{\binom{n}{4}}$$

### Lower Bounds on the Crossing Number

The literature abounds with examples of upper bounds for the crossing numbers of classes of graphs. These are given by drawings which realize specific classes of graphs. However, establishing lower bounds is much more difficult. There are two main techniques.

**Theorem 26.0.7** Let G be a simple graph with n vertices and m edges. Then

- 1. (Euler Bound):  $cr(G) \ge m 3n + 6$ ; and
- 2. (Crossing Lemma Bound): If m > 4n, then  $cr(G) \ge \frac{m^3}{64n^2}$ .

The first bound comes from the observation that the largest number of edges in a simple planar graph is 3n - 6. Hence each edge beyond this must be involved in at least one crossing. The second bound is harder to prove (see [5, 17, 19]), but is much stronger for dense graphs.

### k-Edges

Consider a set P of n points in general planar position, that is, no three are collinear. We consider these as the vertices of a geometric drawing of  $K_n$ . A *k*-edge is a line through two of the points with exactly k points on one side. Choosing the smaller side we assume that  $k \leq \lfloor n/2 \rfloor - 2$ . A  $(\leq k)$ -edge is a *j*-edge with  $j \leq k$ . Denote the number of  $(\leq k)$ -edges by  $E_{\leq k}$ . A remarkable theorem by Lovász, Vesztergombi, Wagner and Welzl [18] and independently by Ábrego and Fernández-Merchant [2] shows

$$\bar{cr}(P) = \sum_{k=0}^{\lfloor n/2 \rfloor - 2} (n - 2k - 3) E_{\leq k}(P),$$

so that a lower bound on  $E_{\leq k}(P)$  determines a lower bound on the crossing number of that point set. References [2, 18] also show that  $E_{\leq k}(P) \geq 3\binom{k+2}{2}$  for any point set k. These two inequalities combine to prove that

$$\bar{cr}(K_n) \ge \frac{3}{8} \binom{n}{4} + \Theta(n^3).$$

Hence the constant  $q_*$  of Sylvester's Four-Point Problem is at least 3/8. A more subtle analysis can improve the bound on  $E_{\leq k}(P)$ , resulting on an improved estimate for  $q_*$ , as well as on the exact calculation of  $\bar{cr}(K_n)$ for  $n \leq 27$  [1] (see also [1]).

## **Workshop Presentation Highlights**

The workshop was characterized by three factors:

- 1. The emphasis on short, interactive presentations;
- 2. a flexible schedule; and
- 3. the willingness of the participants to interact.

To emphasize the first point the entire first day was devoted to short individual presentations. These were originally intended to be 5-minutes presenting an interesting problem or a report on recent research. These quickly turned into more interactive events with the audience asking for further information, mentioning relations with other problems, and offering generalizations. This back-and-forth exchange was greatly appreciated. The format was especially helpful since it introduced each participant to the others and let everyone know who was interested in what sort of problems.

The flexible schedule was also very helpful. As the success of the individual presentations became apparent we quickly expanded the time for them from Monday morning only through the afternoon session as well. The extra time was well spent. We also had our first problem session Tuesday morning. We worried about it being redundant given the extensive discussions on the first day, but were proved wrong. A night's reflection led to some expansions on the first day's talks and the led participants to think of other ideas.

The first major presentation was by Pedro Ramos. This was rescheduled from later in the week because it provided some important background on issues raised in the introductory discussions. Dr. Ramos began with a review of the current state of the rectilinear crossing number, focusing on its relation with Sylvester's 4-point constant and with ( $\leq k$ )-edges. Specific details about this topic were given in Section 26.

The next two major presentations were by Dan Cranston and Peter Hlinéný. Dr. Cranston spoke on "Crossings, colorings and cliques", in which he addressed results related to Albertson's conjecture described in Section 26. Dr. Hlinéný took crossing numbers off of the plane, introducing a new embedding-density parameter *stretch* for a graph embedded on an arbitrary surface. This can be used for lower bounds on the planar crossing number.

The final two presentations were given by Eva Czabarka and Markus Chimani. Dr. Czabarka spoke on lower bounds for crossing numbers. She raised the question of finding the optimal Crossing Lemma type bound. For more information on this the reader is referred to Section 26. Dr. Chimani spoke on approximation algorithms calculating the crossing number. In particular he discussed vertex- and edge-insertation algorithms and gave several clever examples. For details see Section 26.

The format provided several times for group discussions. Tuesday we as a group decided on several topics on which to focus (for details see Section 26). We then broke into smaller groups to brainstorm on specific projects. One "requirement" set by the organizers was that groups had to meet in Max Bell so that individuals were available for quick questions between groups. This requirement was agreed to, adhered to, and worked perfectly to ensuring the hoped-for frequent collaboration.

Late Thursday we met in full session to report on our group discussions and offer some further problems. Among the other open problems discussed were:

1. Is computing the crossing number was APX-hard? That is, does there exist a polynomial-time algorithm to approximate the crossing number within a factor of  $1 + \epsilon$ ?

- 2. A 2-page drawing is a drawing with all vertices on a line, and with no edges crossing that line. The 2-page crossing number of a graph is the minimum number of crossings in a 2-page drawing of the graph. Conjecture 26.0.1 can be achieved by a 2-page drawing of  $K_n$  as well. Is the 2-page crossing number of  $K_n$  equal to its crossing number?
- 3. Is the sequence  $\{cr(K_n)\}_{n=1}^{\infty}$  convex?
- 4. Does every optimal drawing of  $K_n$  contain an edge that is in no crossing? (This is false for general graphs.)
- 5. How does the crossing number change upon the deletion of a random subset of edges?

# **Workshop Research Highlights**

We next give some specifics of problems discussed and discoveries made during the meeting.

### **The 3-Cut Problem**

Suppose that a graph G has a cut-set of 3 edges whose deletion leaves graphs  $G_1, G_2$ . Let  $\bar{G}_1, \bar{G}_2$  denote the graphs resulting by contracting the other subgraph to a single point. How is cr(G) related to  $cr(\bar{G}_1)+cr(\bar{G}_2)$ ? During this workshop Jesús Leaños, Markus Chimani, and Drago Bokal proved the following:

**Theorem 26.0.8**  $cr(G) = cr(\bar{G}_1) + cr(\bar{G}_2).$ 

The proof, while too technical to include here, has already been written up [8]. Bruce Richter praised the effort as an example of the best type of collaboration, saying "There are three independent important new ideas in the proof, one created by each of the three authors."

### **Crossing Numbers of Periodic Graphs**

Consider a graph T with two disjoint distinguished sets of vertices  $\ell_1, \ldots, \ell_k$  and  $r_1, \ldots, r_k$ . Build a graph  $T^n$  from n disjoint copies  $T_j$  of T by adding edges between each  $r_i$  in the  $j^{th}$  copy to  $\ell_i$  in the  $j + 1^{st}$  copy for  $j = 1, \ldots, n-1$ . The graph can be visualized by drawing  $T_j$  in a rectangle, or *tile*, with the vertices  $\ell_i$  on the left boundary and  $r_i$  on the right boundary, placing the tiles next to each other left-to-right along a line, and adding in the connecting edges between adjacent tiles. The drawing suggests that the crossing number of  $T^n$  might be linear in n. Confirming this intuition is more difficult. In fact, the first goal is to show that determining  $\lim_{n\to\infty} cr(T^n)/n$  is computable.

This problem was proposed by Bruce Richter. A large group of people, led by Zdenek Dvorak and Bojan Mohar worked on the problem. Eventually, the group hammered out a proof that the limit was indeed computable, with the details still to be filled in.

### **Optimizing Density Lower Bounds**

Drago Bokal, Mojča Bračič, Éva Czabarka and László Székely have been working recently on optimizing the density bounds for the crossing number of graphs, as density bounds can be better for a subgraph than for the whole graph. Density bounds come in two shapes. The first is a linear lower bound from the Euler formula, which has variations for genus and girth conditions. The second is a Crossing Lemma type bound, which is nonlinear, and in most of the cases comes by a bootstrapping from the linear bound. (There are exceptions, however, which came from the bisection width or other methods.) To be more specific, a Crossing Lemma type lower bound is like  $m^3/n^2$ , where n = n(H) denotes the number of vertices and m = m(H) is the number of edges in an induced subgraph H of G. The group conjectures that if  $d_1 \ge d_2 \ge \cdots \ge d_{n(G)}$  is the degree sequence of the graph G, realized by vertices  $v_1, v_2, ..., v_n$ , and  $H_i = G|_{\{v_1,...,v_i\}}$ , then

$$m^{3}(G)/n^{2}(G) \ge \max_{1 \le i \le n} m^{3}(H_{i})/n^{2}(H_{i}) = \Omega\left(\frac{m^{3}(G)/n^{2}(G)}{n^{2/3}}\right)$$

as a construction suggests the correctness of this suboptimal algorithm.

The optimization of an Euler-type lower bound of the form  $\alpha m(H) - \beta n(H)$  for the crossing number of a graph is equivalent to finding the optimal solution in the Dual Program, which is equivalent in finding the orientation  $\vec{G}$  of G where we minimize the following quantity:

$$\sum_{\substack{v \in V(G) \\ d_{\vec{G}}^+(v) \ge 3}} (d_{\vec{G}}^+(v) - 3) = m(G) - 3n(G) + \sum_{\substack{v \in V(G) \\ d_{\vec{G}}^+(v) \ge 3}} (3 - d_{\vec{G}}^+(v)).$$
(26.1)

In a particular case, de Fraysseix and Ossona de Mendez [13] showed that

**Corollary 26.0.9** If G is a graph such that for each subgraph  $H \frac{m(H)}{n(H)} \leq 3$ , then G has an orientation where the indegree of any vertex is at most 3. In particular, planar graphs have such orientation.

The authors solved (26.1) and then realized that an early work of Frank and Gyárfás [12] essentially solves the minimization problem in (26.1) and implies Corollary 26.0.9, except for the crossing number application.

#### Albertson's Conjecture and Convexity

Albertson's Conjecture states that the crossing number of a graph with chromatic number r is at least that of  $cr(K_r)$ . Barát and Tóth [9] showed that the conjecture is true for  $r \le 16$  and is also true up to a multiplicative constant. A group including Dan Cranston, Jozsef Balogh, Drago Bokal, Eva Czabarka, and László Székely worked on this conjecture, hoping to expand the work of Albertson, Cranston and Fox [6].

This group made positive progress in that they showed several approaches would not work. Their work led to a new conjecture that the sequence is *convex*: that is,  $cr(K_{n+1}) + cr(K_{n-1}) \ge 2cr(K_n)$ . The conjecture *should* be true, but is expected to be difficult as even the asymptotic behavior of  $cr(K_n)$  is only known up to a multiplicative constant.

### The Crossing Number of Twisted Planar Tiles

The following problem was posed by Bojan Mohar. Let T be a graph embedded (without crossings) in a tile. Let  $\ell_1, \ldots, \ell_n$  be the vertices top-to-down order on the left edge of the tile and  $r_1, \ldots, r_m$  be those in order on the right. The goal is to *twist the tile*, that is, to draw (possibly with crossings) the graph in the tile so that  $\ell_1, \ldots, \ell_n$  appear on the left in top-to-down order but  $r_1, \ldots, r_m$  appear on the right in down-to-top order. How can we calculate the crossing number of this twisted tile  $\tilde{T}$ ?

If there exist k disjoint paths from the left to right edge of T, then the crossing number to  $\hat{T}$  must be at least  $\binom{k}{2}$ . However, this bound need not be tight. A group of participants examined this problem made some interesting progress on this problem, refining the bound mentioned above, but the exact answer remains elusive.

### k-Edges in Drawings

Consider a planar geometric (straight-line) drawing of a complete graph. Recall from Section 26 that the number of  $(\leq k) - edges$  is related to the crossing number of the drawing. However, the concept has not been applied to classic crossing number problems when the drawings are not geometric.

During the workshop a group around Gelasio Salazar, Silvia Fernandez, Pedro Ramos, and Oswin Aichholzer generalized the underlying concepts to topological graphs. Several promising properties of this new concept have already been obtained. Together with Bernardo Ábrego they are currently investigating the crossing number of the complete graph.

### **Approximating Crossing Numbers**

A very interesting problem is to approximate the crossing number for *sparse* graphs; those with relatively few edges compared to vertices. The general idea is to find a large planar subgraph, then extend a planar drawing of this subgraph by adding in the few remaining edges without creating too many crossings. There is a

polynomial-time algorithm to determine how to insert an edge to minimize the number of resulting crossings [14], and it is known [10] that this algorithm provides a constant approximation factor for almost all graphs with  $\Delta(G-2)/2$ . Similar work [11] gives similar results for vertex insertion.

At the workshop a group investigated if the results above can be generalized for inserting a fixed number of edges. Some interesting and promising process was made.

# **Closing Comments from the Organizers**

The meeting was very successful. We put together a diverse group by all acounts. We had 20 participants: 7 from the US, 3 from Canada, 2 from Germany, 2 from Mexico, 2 from the Czech Republic, 2 from Slovenia, 1 from Austria, and 1 from Spain. Of those 20 participants, 3 were female researchers, and 3 were junior researchers (who obtained their Ph.D.'s in 2007 or later).

The combination of a location where we were free to concentrate on research all day, the flexibility of the schedule, the size of the group, and choice of topics all contributed to its success. To this end we thank the staff and directorship at the BIRS facility for all of their help. Equally if not more importantly, the organizers thank the participants for their willingness to participate and to contribute to this collaboration.

# **List of Participants**

Aichholzer, Oswin (TU Graz) Archdeacon, Dan (University of Vermont) **Balogh, Jozsef** (University of Illinois at Urbana) Bokal, Drago (University of Maribor) Cabello, Sergio (University of Ljubljana) Chimani, Markus (Friedrich-Schiller-University Jena) Cranston, Dan (Virginia Commonwealth University) Czabarka, Eva (University of South Carolina) Duncan, Christian (Louisiana Tech University) **Dvorak, Zdenek** (Charles University, Prague) Fernandez-Merchant, Silvia (California State University, Northridge) Hlineny, Petr (Masaryk University) Leanos, Jesus (Universidad Autonoma de Zacatecas) Mohar, Bojan (Simon Fraser University) Mutzel, Petra (Technische UniversitLt Dortmund) Ramos, Pedro (Universidad de Alcala) Richter, Bruce (University of Waterloo) Salazar, Gelasio (Universidad Autonoma de San Luis Potosi) Szekely, Laszlo (University of South Carolina) Toth, Csaba (University of Calgary)

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# Chapter 27

# Self Adjoint Extensions and Singularity Resolution in String Theory and Quantum Gravity (11w5080)

# Aug 21 - Aug 26, 2011

**Organizer(s):** Robert Brandenberger (McGill University) Walter Craig (McMaster University) Thomas Thiemann (Albert Einstein Institute, Golm) Neil Turok (Perimeter Institute) Mark Van Raamsdonk (University of British Columbia)

Fundamental cosmological theories describing the origin of structure in the early universe include the standard big bang model (SBB), and the inflationary cosmology which is the current paradigm; the latter was introduced to avoid problems of causality which would otherwise occur given the uniformity of the cosmic microwave background (CMB). However despite its successes, current models of inflation suffer from several drawbacks, which has led to the effort to find alternatives. The most serious problem is the fact that these cosmological models all contain an initial space-like singularity. In the present state of theoretical cosmology, there are a number of competing approaches to resolve this cosmological singularity. Some of the competing theories that have the most currency include on one hand holographic cosmologies making use of the anti-deSitter/conformal field theory (AdS/CFT) correspondence (which emerges from string theory) [1-4], and on the other loop quantum gravity [5,6]. Similar mathematical challenges appear in both approaches, e.g. the need to extend the dynamics via self-adjoint extensions. In addition to the demands of making sense mathematically, such theories are held to the high standard of corresponding to observational data, of which there is now an increasingly large quantity. It is a requirement of each of these theories to resolve the singularities of general relativity, either at the big bang, at a bounce, or at the formation of a black hole. Furthermore, some of the current theories have specific problems associated with boundary conditions, for example the ekpyrotic scenario envisions that one must impose boundary conditions at a time-like singularity, while the AdS/CFT scenario involves a five dimensional space-time, with boundary conditions on a four dimensional boundary which possesses its own Lorentzian metric.

The objective of our workshop was to bring together physicists and mathematicians who are interested in problems of physical importance in quantum mechanics, quantum field theories, and general relativity. In particular we sought out experts in the problem of self-adjoint extensions in operator theory, in order to promote discussions between physicists and mathematicians related to the goal of resolving cosmological singularities, and ideally to stimulate new collaborations that would be of benefit to both disciplines. The physicists that we invited to the workshop included string theorists, experts in loop quantum gravity, and cosmologists who are involved in the AdS/CFT approach to resolving cosmological singularities. While our first goal was to stimulate interactions between mathematicians and physicists, a secondary goal of this workshop was to encourage more discussions and collaborations between the relevant research communities in theoretical physics itself.

**Participants.** There were 16 participants, who can be roughly classified into the following groups or topics:

Loop quantum gravity. Martin Bojowald (Pennsylvania State University) Bianca Dittrich (Albert Einstein Institute/Perimeter Institute) Wojciech Kaminski (Albert Einstein Institute - Max Planck) Tomasz Pawlowski (University of New Brunswick) String theory. David Lowe (Brown University) Vaidya Sachindeo (Indian Institute of Science) Sumit Das (University of Kentucky) Misha Smolkin (Perimeter Institute) Omid Saremi (University of California - Berkeley) Cosmology. Robert Brandenberger (McGill University) Yi Wang (McGill University) Elisa Ferreira (University of Sao Paolo/McGill University) Mathematics. Walter Craig (McMaster University) Niky Kamran (McGill University) Jared Wunsch (Northwestern University) Jakob Yngvason (Universität Wien)

**Details of the workshop.** The structure of the workshop was atraditional, in that several key participants were assigned by the organizers to give tutorials rather than more traditional research presentations, not all participants spoke (in the Oberwolfach style of meeting), and furthermore the lectures and their order of presentation, other than those on the first day, were decided by public acclaim in a discussion at the end of the first afternoon session. In particular the mathematics talks were essentially all pre-assigned tutorials, and they were distributed through the workshop as punctuation to the physics lectures.

The workshop opened with an summary lecture by Robert Brandenberger, who set the tone and stated the challenges of current theoretical cosmology. Essentially the goal of cosmology is to understand the history and the dynamics of the early universe, drawing information from theoretical physics, and to make connections with the wealth of data on the large-scale structure of the universe. At present there is a lot of data, both on the homogeneous character of the universe as well as on its inhomogeneities. Key information comes from the cosmic microwave background (CMB) - specifically from the size and structure of its anisotropies, but this is not the sole source. Standard cosmologies are based on classical physics, with space-time evolving according to Einstein's general relativity and matter assumed to be an ensemble of ideal gasses. There is a well known Lagrangian, an action principle, and equations of motion, and their homogeneous solutions which admit a singularity (the big bang), the standard from which the typical physicist works, are the Friedmann - Robertson - Walker space-times. Already this basis presents problems, as for one there is no information in a completely homogeneous singlarity. Furthermore, the degree of homogeneity of the CMB violates the principle of causality in the standard big bang model. The current paradigm by which one escapes this latter difficulty is to posit a period of exponential inflation. This is a theory that has been a phenomenological success, whose predictions have been verified with great accuracy. Nonetheless, inflation has its own difficulties. It is still based on an initial space-time singularity which is governed by standard cosmology, and it is not clear that classical physics is valid at length scales less than the Planck length which arise in inflationary cosmology since current data which we are measuring eminates from sub-(or trans-) Planck scales which have grown to cosmological scales through the inflation process. Hence the first question before the workshop has to do with resolution of such a space-time singularity. One such possibility is a 'bounce', a cosmology which begins in a contracting phase and makes a smooth transition to an expanding period at a nonzero local minimum of the scale factor which is sufficiently large to avoid trans-Planckian length scales. Cosmological bounces occur in several recent early universe scenarios based either on string theory or on loop quantum gravity. Other scenarios are also possible, in particular an "emergent" scenario in which the universe begins in a quasi-static phase, and which can be realized in the context of "string gas cosmology", and which leads to measurable, and thus verifiable consequences (slight red shifts vs slight blue shifts in the gravitational wave spectrum). It remains to understand the content of the new physics that would go into such proposals.

The main body of the physics lectures of the workshop were essentially on the theme of proposals for the new physics with which to understand either the non-classical physics on sub-Planck scales, or a theory of quantum mechanics and gravitation that will give rise to one of the alternate scenarios to a singularity. Omid Saremi gave a tutorial on the core material of the AdS/CFT scenario, which works with a five dimensional space-time (the bulk manifold) with a high degree of gauge symmetries, which has a four dimensional boundary with its own Lorentzian metric. Classical fields in the bulk manifold give rise to quantum fields and their observables on the boundary manifold. This is a beautiful picture geometrically, and the correspondence between bulk fields and boundary fields is through the self-adjoint boundary conditions of the title of the workshop. However the quantum theory of this sceario suffers on the rigorous mathematical level from the physical assumption that the Euclidian version of the theory (that is, one in which the metric signature is switched to being Riemannian) gives the same answers as the original Lorentzian metric. Martin Bojowald gave a series of talks, essentially a tutorial, on the foundations of loop quantum gravity. This theory also starts out very geometrically, describing the receipe for quantizing classical fields, the standard approach (as yet unsuccessful) to quantize the classical theory of gravity, and then the ideas behind a quantization of a theory based on closed curves (loops) and their dual objects. We understood from his lectures that the structures behind the quantum algebras that are constructed in this field are very complicated, and that the necessary algebraic manipulations are nontrivial. To a mathematician, this program gave the impression that, although the basic objects of the theory are simple and geometrically beautiful, the direction taken in developing this field is a receipe that is strongly guided by a close analogy with classical quantization. David Lowe gave the principal presentation from the string theory point of view, starting with a classical description of space-time in conformally compact coordinates, onto which he introduced a potential and the string theory landscape. He gave the he estimate that there are roughly  $10^4$  six-dimensional Calabi-Yau manifolds, which after around 100 cycles of a bouncing universe, gives rise to the possibility of  $10^{500}$  possible vacuua, definitely a problem of non-uniqueness. He then went on to outline some selection principles, old and new, which if successful would partial resolve this problem.

There were four mathematics tutorial talks for the workshop. Walter Craig gave a talk on the classical result of Weyl's limit point/limit circle theory, which is principle for selection of self-adjoint boundary conditions for ordinary differential operators. Jakob Yngvason completed this discussion of self-adjoint boundary conditions with the theory of deficiency indices, and their extension to partial differential operators in the form of a Fredholm condition. Niky Kamran spoke on the theory of stability of space-times, including the wel developed theory (by now) of the nonlinear stability of Minkowski space-time, and the newly developing theory of the stability of Schwarzschild space-times. This made a good impression on many of our physicist colleagues, and will we believe have an impact on their future point of view with regard to the topic of classical general relativity. Finally, Jared Wunsch spoke on the method of energy estimates, from which, when microlocalized, one may derive theorems of energy transport for both linear and nonlinear hyperbolic systems. He also mentioned versions of this form of energy transport for quantum mechanical systems, as well as commutator estimates in general and Morawetz estimates in particular.

Several of the participants formed a working group to study an extension of an approach to AdS/CFT cosmology proposed by Sumit Das and his collaborators [4]. The goal of the participants of the working group is to extend the analysis to the case of inhomogeneous universes (with small amplitude inhomogeneities which correspond to the observed cosmological fluctuations). The members of the working group met at informal evening discussion sessions. Key members of the working group were Brandenberger, Das, Ferreira, Kamran and Wang. The work of this group has continued after the workshop. It is being explored whether the new mathematics results related to the initial and boundary value problems in AdS space-time which Kamran and collaborators have recently developed can be applied to construct a model in which the inhomogeneities corresponding to cosmological fluctuations can be carried forwards from the initial contracting phase of a bouncing cosmology to the expanding phase.

Definition of success. In the back of our mind was the possibility that this mix of cosmologists on the

forefront of their research discipline, and mathematical analysts would hit upon a solution to a major problem in the discipline, or at least make a significant step in the direction of a solution of a major problem, to which subsequent collaboration would progress (as was achieved in a different context in [7][8]). Our BIRS program has indeed led to new collaborations being formed with the goal of solving the challenge from cosmology which motivated the workshop. More generally, it was agreed by all participants that the week at BIRS was very intensive, with well prepared short courses both on the mathematical side and on the physics content, that were very well received. It seems as though the several disciplines of theoretical cosmology that were represented were able to benefit from the opportunity to present their work to each other, something which, we learned, seems to be unfortunately rarer than it should be. We came away from the workshop with a better appreciation of the rigor of an analytical argument and the scope of some of the theorems of general relativity that have been proved over the last decade or so. We also came away with a deeper appreciation of the demands that observations make on cosmologists, that is, one must not only construct a conceptially rigorous theory, but it is also demanded to be quantitative and predictive. That is, it must make specific predictions that have the possibility to be verified or falsified within a forseeable future.

# **List of Participants**

Bojowald, Martin (The Pennsylvania State University) Brandenberger, Robert (McGill University) Craig, Walter (McMaster University) Das, Sumit (Univ. of Kentucky) Dittrich, Bianca (Albert Einstein Institute) Ferreira, Elisa (Univ. of Sao Paulo - McGill University) Kaminski, Wojciech (Albert Einstein Institute in Golm, Max Planck) Kamran, Niky (McGill University) Lowe, David (Brown University) Pawlowski, Tomasz H (University of New Brunswick) Saremi, Omid (University of California Berkeley) Smolkin, Misha (Perimeter Institute) Vaidya, Sachindeo (Indian Institute of Science and McGill University) Wang, Yi (McGill University) Wunsch, Jared (Northwestern University) Yngvason, Jakob (Universität Wien)

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# **Chapter 28**

# **Stochasticity in Biochemical Reaction Networks (11w5140)**

Sep 11 - Sep 16, 2011

**Organizer(s):** Sotiria Lampoudi (University of California Santa Barbara) Brian Munsky (Los Alamos National Laboratory) David Thorsley (Biotechnology HPC Software Applications Institute) Aleksandra Walczak (Ecole Normale Superieure)

#### Abstract

Cellular functions in biological organisms are comprised of the complex interactions of many molecular species: proteins, DNA and mRNA molecules, hormones, etc. Recent experimental developments in molecular biology have enabled researchers to characterize many of the biochemical pathways involved in these functions, and enormous amounts of data are currently available. However, despite this wealth of data, we still lack a sufficient understanding as to how cellular mechanisms combine to form the observable properties of cellular behavior. Key obstacles that restrict this understanding are the inherently complex and stochastic properties of cellular systems. Not only must we overcome the complex many-body nature of the interactions between the cellular components, but we are also we are faced with an additional difficulty, stemming from the stochastic, nonequilibrium nature of chemical reactions. The  $3^{rd}$  Workshop on Stochasticity in Biochemical Reaction Networks was held to discuss recent progress on the role of intrinsic stochasticity in many-body biochemical networks.

# **Overview of the Field**

Cells in biological organisms are subject to vast amounts of random variation, which can cause isogenic cells to respond differently. There are many factors that may contribute to this phenotypical diversity. The simplest of these include fluctuations in environmental conditions such as nutrients, heat, radiation, etc. But even in homogenous environments, diversity can arise from the rare and discrete nature of chemical interactions within a cell. In general, molecules that are present in smaller numbers are prone to a greater extent of variable response, as single molecule events take on greater relative importance. In particular, since cells contain only one or two copies of many important genes, these cells can express vastly different behaviors when these genes become active (on) or inactive (off). Switching times from on to off and back are controlled by an uncountable number of random or chaotic events as the many cellular constituents move and interact within the cell. Effectively, genes can be (de)activated simply due to chance reactions with gene regulatory molecules. In turn, these regulatory molecules undergo their own complicated set of events, including degradation, dimerization, folding, etc. Any of these events may assist or impede a chemical's reaction with a corresponding regulatory site of a given gene.

As alluded to above, gene regulation is particularly prone to stochastic fluctuations due their extremely small population numbers. The variability in gene regulation subsequently affects the downstream regulation of other processes [30, 10, 55, 22, 41, 11, 25]. This variability is often deleterious to the organism's survival, and biology has developed many mechanisms to suppress this variability, such as negative feedback or auto-regulation [2, 9, 38], which can reduce fluctuations for a given mean expression level. As an alternative, dynamics in one regulatory sub-network can introduce low- or band-pass filters that help diminish fluctuation frequencies coming from other sources [3, 54].

In different systems, stochastic fluctuations may be be used to the cell's advantage. When combined with nonlinear effects, stochastic behaviors can be used to amplify [43] or damp external fluctuations and tune a system's sensitivity to its environment. Fluctuations may also be used to excite and/or improve the robustness of resonant behaviors [29]. Stochastic fluctuations may also allow for the phenomena of stochastic switching, and allow organisms to express two or more very different phenotypes [1, 59, 31, 57]. For certain organisms that exist in especially hostile environments, such as parasites, this ability to switch unpredictably from one state to another ability provides an important evolutionary advantage. If the host cannot predict the response of a parasite, then it has a much harder task to devise a strategy to combat that parasite. Even in the absence of direct competition, random switching can still provide a vital role in survival within an uncertain environment [6].

Measurement of the phenotypic and/or molecular variability of single cells is a field of great progress over the recent years [45]. These techniques enable today's experimentalists to prepare cells such that the dynamics of their gene expression, protein localization, or other traits can be observed through the presence or activation of fluorescent markers. Antibodies can be attached to fluorescent dyes and then made to bind specific cellular proteins or phosphoproteins. DNA and RNA molecules can be measured with fluorescence *in situ* hybridization (FISH) techniques [42, 24, 44]. With these techniques, researchers can simultaneously measure multiple different molecule types, and even explore the spatial dynamics and colocalization of biological molecules with fluorescence (Förster) resonance energy transfer (FRET) techniques or with split fluorescent proteins [16, 4, 5]. Once tagged with fluorescent reporters, there are many techniques with which one can then measure the highlighted cellular properties. These include fluorescence microscopy, confocal microscopy, time lapse microscopy, and flow cytometry.

Once measured, biochemical reaction networks could be modeled at many different scales. At the finest level of detail, molecular dynamics simulations are used to explore how protein movement, folding and interactions with surrounding molecules. At the other end of the scale, continuous-valued concentrations and ordinary differential equations describe large-volume chemical processes. Measurements of single-cell and single-molecule data require an approach at the *mesoscopic* scale. At this scale, each chemical species is described by an integer population, which is assumed to evolve according to Markovian dynamics. The majority of analyses at the mesoscopic scale have been conducted using kinetic Monte Carlo (MC) algorithms, such as Gillespie's Stochastic Simulation Algorithm (SSA) [17], or one of many improvements upon that approach [7, 53, 21, 51, 19, 56, 8, 46, 18]. Other analyses have been developed to approximate the solution of the chemical Master Equation, which describes the evolution of the probability densities for the Markov Process. These techniques include Finite state Projection approaches, [32, 33] and the spectral method [70, 71, 72, 73].

The participants of our workshop have also been involved in constructing and using algorithms for inferring molecular models of gene regulation [79, 78] and moment matching optimization algorithms.

### A Need for Multi-Disciplinary Investigations

As discussed above, cell-to-cell variability has been studied in many different contexts and within many different disciplines, including molecular and cellular biology, physics, chemistry, computer science, optics, applied mathematics, mechanical and electrical engineering, statistics and others. The simple fact that so many different disciplines are actively researching within a relatively new topic introduces a unique set of research challenges and opportunities. One key challenge is that a strong language barrier exists that divides one discipline from another. When even physicists and engineers use unrelated sets of terminology to describe the same simple phenomena, there is little hope that mathematicians and molecular biologists could freely discuss more subtle behaviors. Faced with this concern, very few traditional journals, workshops or conferences exist to bring these myriad fields together, and established researchers have little incentive to learn the foreign terminology of another seemingly unrelated discipline. In many cases, this lack of communication leads to the duplication of efforts. On the other hand, the fact that so many different groups are focusing on similar problems has led to vast improvements in specific areas of research.

The workshop was committed to unite a broad array of young, international researchers who work on different aspects of the problem of understanding the role of stochasticity in biochemical systems. Experts in developing mathematical methods to describe cellular behavior, experimentally analyzing biochemical processes, performing advanced computations of stochastic behavior, and designing novel biological devices worked together to share the latest results in this exciting area of research, and defined new research directions for future study.

Together, the participants of this workshop formed an intellectually diverse group of researchers united by their interest in the subject of stochasticity in biochemical reaction networks and complex biological matter; they represented the fields of biology, biophysics, engineering, chemistry, mathematics, and computer science. Each has contributed to the field of biochemical networks in either the theoretical or experimental sphere and many have contributed in both areas.

### New Tools and Approaches to Study Stochastic Biochemical Reactions

Recent experimental techniques make it possible to measure the variation in gene expression, protein abundance, and cellular behavior. Combined with computational modeling, these techniques enable us to uncover the causes and effects of stochastic cellular dynamics. Depending on cellular function, biochemical processes may act to minimize stochastic variations or exploit them to the cell's advantage; in both cases, cellular processes have evolved to be remarkably robust to both intrinsic and extrinsic noise. By exploring this robustness in naturally occurring biological systems, we hope not only to improve our understanding of cellular biology, but also to formulate the "design principles" necessary to build similarly robust biochemical circuits and nanoscale devices.

This workshop brought together several multidisciplinary experts, who introduced the audience to many different aspects of this exciting research topic. First, we heard from experimental molecular biologists, who are continually developing and perfecting new quantitative techniques to observe single cell and single molecule dynamics. Tools such as flow cytometry and fluorescence activated cell sorting (FACS) were used by many presenters (including Lingchong You, Robert Egbert, Narendra Maheshri, Attila Becksei, and Ophelia Venturelli) measure the protein levels for millions of individual living cells in the time span of a single minute–thus conducting millions of simultaneous experiments. Time-lapse fluorescence microscopy and microfluidics studies were described by other researchers (including Rob Egbert, Nacho Molina, Gurol Suel, Gabor Balazsi) which made it possible for these researchers to measure, track and/or manipulate the behavior of single cells in carefully controlled micro-environments. Fluorescence *in situ* hybridization (FISH) techniques were presented by Gregor Neuert and Allistair Boettiger which were used to explore the spatial distributions of specific, individual RNA molecules within a cell or developing embryo. Jim Werner presented a new technique of three-dimensional single molecule tracking that could examine cellular dynamics at an even greater time and spatial resolution [85].

Next, the theorists and mathematicians among us presented new quantitative methods to analyze and explain the vast amounts of statistical data gathered from such experiments. It is known that stochasticity in cells is caused in part by intrinsic noise – the variability caused by the statistical dynamics of a chemical reaction with a small number of reactants – and in part by extrinsic noise – the variability caused by random fluctuations in a cell's environment. The participants in this workshop have already developed many methods to understand and differentiate between these types of noise in experimental data. For example, Peter Swain and Andreas Hilfinger presented new theoretical approaches to discriminate between various possible sources of stochastic variation in cellular fluctuation, while Gregor Neuert, Nacho Molina [79, 78] and Gabrielle Laillacci discussed integrated experimental and computational approaches to use cell-to-cell variability to learn more about the underlying mechanisms. In addition, as experimental techniques such as FISH provide more and more information on the spatial dynamics of intracellular processes, it becomes more useful to extend these techniques to spatially heterogenous reaction dynamics, such as those discussed by Eldon Emberly and Pablo Meyer-Rojas.

Finally, these theorists and experimentalists have successfully integrated their various analyses to understand how, why and when different cellular mechanisms transmit noise in different ways, i.e. some suppress it while others amplify or exploit it. For example, control theory can help us understand feedback and feedforward regulatory motifs in cellular architectures, while an information theoretic perspective can help us to understand how cells in a developing multicellular organism can determine their exact spatial location. These analyses suggest new methods and appropriate models for mathematically demonstrating how certain motifs are useful for dealing with noise and uncertainty. Such analyses are then directly applicable to the work of more applied researchers, who can use these theories to better constructing synthetic biological circuits and devices at the nanoscale level, including biomolecular motors and DNA molecular machines. For example, Yannick Rondelez and Elisa Franco both discussed new results in the field of synthetic biology where they have designed and experimentally validated biomolecular computational devices [47, 48, 49, 12, 13]

In the following subsections, we briefly discuss a few presentations that introduced most important advances in various fields of the experimental, theoretical, and computational investigation of stochasticity in biochemical reaction, followed by a section on how these tools have successfully been combined to gain new insight into biological behaviors.

### **Presentation Highlights**

We assembled a list of presentation highlights based on the top ranked speakers from an anonymous participant survey. The vast majority of the workshop participants presented unpublished work for the first time. The interactive environment allowed them to both get feedback on their research and presentation, but also to drastically adapt the presentation of their work to suit the audience. In what follows we discuss some of the workshop's highlights. Where applicable, we have included citations to relevant past work.

### **Recent Discoveries of Biological Stochasticity**

There is a clear shift in the experimental and theoretical parts of the field to go beyond simply characterizing noise, towards attempting to understand the possible functions of noise. This was clear in most of the experimental talks:

- Gurol Suel [6, 26, 50] talked about the role of noise in the competence circuit. He specifically contrasted the large noise present in the native circuit versus the synthetic circuits, which are less noisy. He also pointed out the importance of the correct sequential timing of events in how the cell makes its decision to sporulate or not [27, 28].
- Alistair Boettiger [65, 67, 66, 68] pointed out that the apparently redundant repetition of regulatory elements can be important in the spatial macroscopic precision of expression patterns in fly development.
- Careful characterization by means of combining dynamical theoretical models with experiments by Nacho Molina resulted in surprising gene-specific bursting characteristics in mammalian cells, that have never been observed in prokaryotes [78, 79].

- Tom Shimizu talked about linking the biochemical network that controls chemotaxis with its function in the presence of signal fluctuations [77, 60, 61, 62].
- Narendra Maheshri [58, 39, 34] and Gregor Neuert talked about linking dynamical encoding of function in gene switches.
- Gabor Balazsi [38] discussed the interplay of noise and evolution in circuits in yeast.

### **Cellular environment**

Several speakers with a biological background pointed to the need for a more holistic view of the cell.

- One of the highlights was a thought provoking lecture by biochemist Diego Ferreiro [80, 81, 82, 83, 84] about the need for a dynamical view of regulation in the cell.
- Pablo Meyer Rojas [35, 36] discussed the importance of localization of reactions in the cell.

### Synthetic Circuits

Another series of experimental talks presented ideas about how our increased knowledge of molecular biology, chemistry and noise can be used in the field of synthetic biology to build more precisely designed switches and networks:

- Rob Egbert described how design of regulatory sequences can lead to precise tuning of observed gene regulatory circuit dynamcs.
- Yannick Rondelez [47, 48, 49] described a toolbox for building predictable switches using DNA elements.
- Elisa Franco [12, 13] directed our attention to interactions between well-functioning modules and biochemical switches.

### **Theoretical Techniques**

On the theoretical side, there was a strong emphasis on understanding the environment in which biochemical networks function: the temporally changing signals and resources. Similarly to experimental and computational approaches the theoretically-focused speakers discussed the time varying response of gene expression.

- Pointing to the fact that gene expression occurs in a cellular environment, Rosalind Allen talked about the effects of mRNAs competing for ribosomes [20].
- The precision of temporal signaling in the context receptors was discussed by Thierry Mora.
- Peter Swain [40] and Andreas Hilfinger [23] both talked about novel frameworks for distinguishing between intrinsic and extrinsic fluctuations in dynamical systems.
- Paul Francois discussed the evolution of function in the context of morphogenic gradients [14, 15].
- Eldon Emberly presented a computational model based on simple physical ideas of spatial patterning of proteins in bacteria [52].

### **Computational Techniques**

Important computational advances were discussed in the context of both analyzing experimental data and developing novel methods for model selection. Once again the topic of understanding the dynamics of gene regulation was prominent.

- Gregor Neuert and Nacho Molina [78, 79] discussed computational approaches that allow for the efficient analysis of gene expression data.
- Gabrielle Lillacci talked about how to increase the reliability of model selection algorithms while reducing computational costs.

## **Scientific Progress Made**

A few new topics emerged as a result of the workshop. Many of the discussions aimed to point out that biochemical networks function in a specific context: they are part of the cellular environment, they rely on nutrients, they evolve, they interpret signals, they fulfill a function. Biochemical networks involve proteins, which are dynamical entities. As a result, a dynamical picture of both gene regulation and signaling is needed, to understand the functioning of cells. The importance of the dynamics of molecular interactions was addressed both theoretically (e.g. Peter Swain, Nils Becker) and experimentally (Atilla Becksei, Tom Shimizu). However, it clearly emerged as an important future direction.

On a similar note, it became clear that more attention must be directed to understanding the ability of biochemical circuits to react in a wide range of environments and conditions.

Discussions also pointed towards the abundance and spatial availability of proteins, enzymes and molecular machinery in the cell. This direction emerged as a worthwhile direction to study both theoretically and experimentally.

As noted before, many of the discussion centered around function and evolution of biological circuits. These topics were present in the talks (see section 28), but also in private discussions.

During the specially allocated discussion time, groups of varying size met to brainstorm about new ideas. One fruitful interdisciplinary interaction concerned protein and DNA interactions, and involved discussions between molecular biologists, physicists, chemists and control theorists. Specifically the group considered the analogies and differences between the chemical circuits used in bio-engineering ("molecular devices") and the existing biochemical networks in cells. The workgroup led to experimental ideas that the participants will try to verify.

An exchange between participants interested in creating DNA switches in cells and theorists working on describing real noisy biochemical networks resulted in a discussion about how feedback can be encoded in molecular circuits. The portraying of this seemingly simple questions in the light of DNA switches led the participants to re-visit some basic assumptions made in molecular modeling. As a result, the experimentalist had new ideas that could be tested. This exchange also resulted in sharing existing literature among the theorists.

In the field of DNA switches, it became clear that many of the initial technical problems have now been solved. However to obtain well functioning molecular devices, it is now necessary to consider many different ways of implementing feedback. The interactions between participants working on DNA switches from a chemical and control interaction background led them to establish international collaborations.

Similarly the workshop put in touch people interested in the relevance of spatial positioning of biochemical networks in pathways.

In the anonymous survey, the participants clearly claimed that the workshop led them to start new collaborations, discover new fields and point their research in novel directions. Since the survey was anonymous, we do not know the names of these participants, but we are excited to learn about these projects in a future meeting.

## **Outcome of the Meeting**

The workshop emphasized recent improvements in the theoretical, computational, and experimental investigation of stochasticity at the cellular and nanoscale levels. Each of the participants at the meeting contributed to this progress in at least one, and in many cases two or three, of these advances. The workshop promoted cross-disciplinary communication and collaboration between researchers in mathematical fields such as stochastic processes, Markov models, stochastic simulation and information theory, engineering fields such as control theory, computer science, and circuit design, and scientific fields such as computational biology, nucleic acid research, biophysics, biochemistry, and nanotechnology. The event was highly successful in encouraging the development of a research community uniquely qualified to investigate the phenomenon of stochasticity in biochemical reaction networks.

In addition to presenting significant progress on the topics of stochasticity in biochemical reactions, the workshop also highlighted the persisting need for continued improvements in the analysis of such reactions.

For example, combining new techniques for measuring spatial variability in cellular components with spatially non-homogenous analyses may yield new insights into cell regulatory behaviors. Similarly, the expanding usage of experimental techniques such as flow cytometry, time lapse fluorescence microscopy, and other techniques involving the use of fluorescent proteins leads to a demand of a much more quantitative characterization of these important proteins. Finally, with researchers from many diverse disciplines exploring stochasticity in the fields of synthetic and computational biology, a real need is arising for an improved and standardized toolkit for researchers to describe and computationally analyze cellular variability. These and other discussion topics that arose during the meeting will be revisited in the next workshop on stochasticity in biochemical reaction networks.

### **Open and Emerging Questions**

Recent advances in experimental molecular biology have revolutionized the way people conduct biological research. Techniques such as flow cytometry, fluorescence activated cell sorting, time-lapse fluorescence microscopy, and microfluidics have made it possible for researchers to measure and manipulate the behavior of single cells and even single molecules within them. These experiments have shown that cellular dynamics are intrinsically noisy and that individual cells may both regulate and exploit this noise. To further understand the mechanisms of organism development, evolution, cancer, disease and drug efficacy, we must improve our understanding of the effects of noise on the corresponding biochemical reaction processes. Such explanations require the close integration of new mathematical models, techniques and theories with these emerging experimental techniques. An improved understanding of these systems will help explain newly observed phenomena and may suggest methods by which new behaviors can be engineered.

The main goal of the workshop was to suggest new research directions and new synergies between researchers in complementary fields within the main field of systems biology. As becomes clear from participant testimonies, the workshop fulfilled this goal. Many new directions that emerged from discussions have been summarized in sections 28 and 28. Here we present them from the point of view of the questions we asked before the workshop. The workshop was organized around a sequence of questions that begins and ends with experimental evidence:

- What new experiments are possible and what can they tell us? In the last few years, many of our participants have devised new experimental techniques to measure intracellular dynamics. Even in their infancy, the tools previously presented at BIRS in September 2009 have already improved our understanding of intrinsic and extrinsic noise biochemical reaction networks. During this workshop it became clear that there has been a shift from studying prokaryotic cells to developing tools to study eukaryotic cells, including mammalian cells. The experimental talks on biological cells can be divided into those that talked about techniques to describe noise in eukaryotic cells (e.g. Neuert, Molina) and those that looked at the level of the whole organism (e.g. Boettiger, Shimizu, Meyer-Rojas). We note that many of the experimental results were presented with advanced statistical or theoretical analysis (e. g. Molina, Neuert, Shimizu), marking a significant shift in the field. The experimental advances presented at the workshop, including new, unpublished techniques offered the starting point of the workshop.
- What are the available computational tools? How good do they need to be? What new mathematical approaches may be developed to meet these requirements? The addition of stochasticity to gene regulatory network models severely complicates numerical analyses. Several of the workshop participants have pioneered new techniques for the analysis, reduction, and solution of stochastic processes in the context of gene regulatory networks and many are extending these results to treat spatially heterogeneous systems. Many efficient computational methods were presented in the context of the analysis of experimental data (e. g. Molina, Neuert). Others (Becker, Lilacci) pioneered new techniques to target spatially and temporally fluctuating environments.
- How does noise affect cellular mechanisms? How do cellular mechanisms affect noise? The signaling network in the cell is vast and only approximately known. Many of our participants have developed new ways to examine control, stability, robustness, adaptability, computation and information transfer under this highly uncertain setting. As noted above a key shift has been to try and link

the observed stochasticity to function (e.g. Suel, Balazsi) or understand the dynamics of the response in fluctuating environments (e.g. Maheshri). Once again it is worth emphasizing that our participants discussed the role of precision of expression at the multicellular level, by means of both theoretical (Francois) and experimental (Boettiger) techniques. An interesting novel topic was considering the fluctuations in resources (Allen) and the spatial precision of events (Meyer-Rojas).

- What sorts of synthetic biochemical processes can be designed and constructed? As our computational and theoretical understanding of cell regulation improves, we can obtain more detailed quantitative characterizations of biochemical building blocks. Many of our workshop participants in synthetic biology used these "design principles" to build new organic constructs to perform specific biological and micro-mechanical tasks, both in gene regulatory (Egbert) and DNA-switch circuits (Franco, Rondelez).
- What new experiments should we do? Measurements at the single cell level are difficult, expensive and sometimes even disappointingly uninformative. One of the main objectives of this workshop was to suggest new approaches and collaborations to integrate stochastic modeling and experimental studies. This goal has been realized in a much wider range of interactions than we anticipated. Not only did experimentalists and computational researchers interact to build better data analysis software, but experimentalists and theorists discussed the prospect of tackling the newly emerging questions, such as the dynamics and spatial organization in cells.

### **Comments on the Workshop Organization and Logistics**

Although other meetings had previously been organized to explore stochasticity in biochemical reaction networks, this workshop was unlike any other in the field. Upon conclusion of the workshop, it seems beneficial to discuss the particular items that made this a success. The key ingredients that set this workshop apart were (i) a multi-disciplinary and international organizing committee and participant list, (ii) an emphasis on young researchers and new ideas rather than tenured professors and established techniques, (iii) a flexible schedule with ample discussion time, and (iv) a specific focus on the integration of experimental and theoretical/computational investigations. Even though we adopted our title and location from two previous Workshops on Stochasticity in Biochemical Reaction Networks, these ingredients represented a significant and very successful shift in focus and organization. The original workshop was organized and attended almost exclusively by researchers connected to the control engineering community in the USA, whereas this workshop brought together a multi-disciplinary group of international researchers-including not only control engineers, but also physicists, chemists, mathematicians and biologists (including new organizers). Whereas the original workshops considered mostly theoretical and computational studies of small networks, this workshop emphasized the systematic integration of computational, theoretical and experimental techniques to investigate the interactions of cellular components at myriad length and time scales. Moreover, the five-day length of the workshop allowed much more time for discussion and collaboration than the breakneck pace of the previous two-day workshops.

As discussed above, one of the main goals of this workshop was to encourage collaboration between researchers from diverse fields, who often might not be aware of each others' research. The diverse participant list helped us to achieve this goal. The workshop participants included representatives of diverse fields: chemists, engineers, control theorists, molecular biologists, physicists, mathematicians and computer scientists. These researchers also represented a diverse set of locations including US (19), Canada (4), Europe (12), Asia (1) and South America (1). Most of the participants were young: 14 are pre-tenure faculty members; 7 will have just started their faculty positions this year; and 6 are currently post-doctoral researchers. 7 women attended the workshop: five invited attendees and two organizers, all of them junior faculty (4), post-docs (1) or graduate students (2). This is a high ratio for research disciplines which include such male dominated fields as physics, computer science, engineering and theoretical chemistry.

We note that the ability to bring together such a young internationally diverse group of people was made possible by the award we received from International Complex Adaptive Matter Institute (ICAM). This award allowed us to subsidize the rather high travel costs of young faculty and post-docs, allowing many of them to attend. The Director of ICAM, Professor Daniel Cox, attended our workshop as a participant and acknowledged our success in achieving the goals of the institute to foster the exchange of scientific ideas.

#### **Meeting Researchers From Diverse Communities**

One of the major positive outcomes of the workshop was successfully bringing together people from extremely different backgrounds. Although many workshops invite people from different communities and create the potential for the exchange of ideas, our workshop was truly unique compared to other meetings we have attended. Unlike in other events, the participants exchanged ideas and points of view and engaged in discussion both during the sessions and during the plentifully designated discussion time. Due to the variety of backgrounds, not a lot of "basal" knowledge was shared by participants. We strongly encouraged our participants to ask questions, and *every single talk at the workshop elicited several questions and discussions*. This suggestion on one hand resulted in incredibly lively discussions. On the other hand it allowed for a bridging of the gap between the different backgrounds of participants. These prolonged introductions often led to the emergence of interesting questions (see section 28 for details). Frankly, the level of interactions, exchange of ideas and mixing of fields greatly surpassed the expectations of the organizers.

We believe that the unusually successful and creative atmosphere during our workshop is a combination of a number of factors:

- The wonderfully intimate facilities at BIRS, that forced people who did not know each other to interact (for example: eat together and engage in discussions).;
- The schedule of the meeting that left plenty of time for discussions and collaborations. For this reason people were not tempted to skip sessions to work, they paid attention during the sessions and could continue discussions privately after the sessions;
- Most of our participants were young faculty members experienced researchers who are very open minded and curious about other fields.
- The strong emphasis and encouragement to ask questions.

To second the fact that this is not only our subjective impression, we quote samples of post-workshop surveys that specifically say this was the best conference people have ever attended.

To emphasize one of the main successes of the workshop we will cite the comment of one participant who met and started to collaborate with another participant - Rosalind Allen. After the week, this participant decided to spend his or her sabbatical visiting the newly found collaborator whom they previously did not know existed:

"Because of the workshop, I realized Rosalind Allen's research interests overlap with my own. Consequently, I am arranging to spend a sabbatical in Edinburgh next summer. That connection certainly would not have been made if not for the fortuitous arrangement of speakers."

Some additional quotes from participants:

"Through the workshop I've developed one potential collaboration with someone whose research I was unaware of before coming to Banff. ..."

"... I was able to establish collaborations with two different scientists during this event, which would have been extremely hard to achieve without such an intimate environment."

"The amply allocated discussion time allowed for deep communition with people whom I'm unlikely to have interacted with otherwise, and has led to three (or possibly more) concrete leads for future collaborations. This would not have occurred in a typical conference setting ..."

"I really enjoyed the feeling that we were on the cutting edge of defining the future course of this very new field of study."

"This workshop allowed work on a collaboration that includes two people from different European countries and one from the US."

"Time is the most valuable thing for people, and this workshop did a good job in allowing people to have just the right amount of time to meet and talk with each other, by organizing properly informal discussions slot (including meals)."

"This was the BEST workshop I ever attended. I learned deeply from topic that i believed to be out of my specific field but turned out to be very close. I feel this will mark a before/after point in my career."

"Very much like the emphasis on promoting the field in a collaborative way - this is exemplary!"

### The Continued Demand for Such a Meeting

The views cited above (and the ones we did not have room to quote) clearly show that the most important outcome of the workshop was for people to meet, exchange ideas and start new collaborations, often with people whose research they were previously unfamiliar with. A large number of participants noted the importance of fostering a collaborative environment, the time and space to exchange ideas, and meeting other young researchers. Practically all participants emphasized the non-standard nature of this meeting (the large allocation of time to questions and discussions) as opposed to the many talks + posters format present elsewhere.

To illustrate the demand for such a workshop in the community, we can recall the large number of participants who were eager to apply to organize the subsequent meeting from this series. Finally four participants were chosen, from four different communities (molecular biology, physics, control theory and bioengineering), and we fully expect that future meetings will retain the kind of scientific diversity and energy that made this meeting a strong success.

### Summary

We organized a workshop that aimed to bring together researchers studying different aspects of the emergent behavior of cellular networks. Despite extreme progress over the last decade, our understanding of how many cellular components, which interact in an intrinsically stochastic manner, come together and result in reliable outcomes of cell behavior is still in its infancy. The organization of our workshop allowed for free discussion between scientists who have been studying similar problems with very different tools. Although the large scale goal of understanding the complexity of cells (the space of possible output states, their relation to biological phenotypes and genotypes, the stability of these states, and their connectivity) is clear, the intermediate problems the community needs to solve are, in general, not obvious. This workshop made precise some missing links in our understanding of how cells function. By studying eukaryotic cells, we saw that many ideas the community considered to be resolved in prokaryotes are not at all simple in eukaryotic cells and at the multi-cellular level. The resulting main idea of the workshop is to call for a more holistic view of cells. At this stage of the development of the field it is essential to keep bringing together diverse young scientist to attempt to propose novel approaches to these problems. Our goal was to provide such a venue, introduce scientists from different fields to each other, and encourage informal discussions and strong, long-lasting collaborations. We feel we have been very successful in providing this platform for the exchange of ideas.

# **List of Participants**

Allen, Rosalind (University of Edinburgh) Balazsi, Gabor (The University of Texas MD Anderson Cancer Center) Becker, Nils (AMOLF) Becskei, Attila (University of Zurich) **Boettiger, Alistair** (University of California at Berkeley) Burger, Anat (University of California at San Diego) Cox, Daniel (University of California at Davis) Daigle, Bernie (University of California at Santa Barbara) Dunlop, Mary (University of Vermont) Egbert, Robert (University of Washington) **Emberly, Eldon** (Simon Fraser University) Estevez-Torres, Andre (Centre national de la recherche scientifique) Ferreiro, Diego (Universidad de Buenos Aires) Franco, Elisa (University of California at Riverside) Francois, Paul (McGill University) Hellander, Andreas (University of California at Santa Barbara) Hilfinger, Andreas (Harvard Medical School) Joo, Jaewook (University of Tennessee- Knoxville)

Lampoudi, Sotiria (University of California Santa Barbara) Lillacci, Gabriele (University of California at Santa Barbara) Maheshri, Narendra (Massachusetts Institute of Technology) Meyer-Rojas, Pablo (IBM research) Molina, Nacho (Ecole Polytechnique Federale de Lausanne) Mora, Thierry (Ecole normale superieure) Mulger, Andrew (Fundamental Research on Matter Institute, Amsterdam) Munsky, Brian (Los Alamos National Laboratory) Nemenman, Ilya (Emory University) Neuert, Gregor (Massachusetts Institute of Technology) Payne, Stephen (Duke University) Rondelez, Yannick (The University of Tokyo) Scott, Matthew (University of Waterloo) Shimizu, Tom (AMOLF) Singh, Abhyudai (University of Delaware) Suel, Gurol (University of Texas Southwestern Medical Center) Swain, Peter S. (Centre for Systems Biology at Edinburgh, University of Edinburgh) Thorsley, David (Biotechnology HPC Software Applications Institute) Venturelli, Ophelia (Caltech) Walczak, Aleksandra (Ecole Normale Superieure) Werner, James (Los Alamos National Laboratory) You, Lingchong (Duke University) Zilman, Anton (University of Toronto)

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# **Chapter 29**

# Foundations of Stochastic Analysis (11w5077)

Sep 18 - Sep 23, 2011

**Organizer(s):** Zhen-Qing Chen (University of Washington) Takashi Kumagai (RIMS Kyoto)

### Scientific agenda of the conference

Over the years, the foundations of stochastic analysis included various specific topics, such as the general theory of Markov processes, the general theory of stochastic integration, the theory of martingales, Malliavin calculus, the martingale-problem approach to Markov processes, and the Dirichlet form approach to Markov processes. To create some focus for the very broad topic of the conference, we chose a few areas of concentration, including

- Dirichlet forms
- Analysis on fractals and percolation clusters
- Jump type processes
- Stochastic partial differential equations and measure-valued processes

Dirichlet form theory provides a powerful tool that connects the probabilistic potential theory and analytic potential theory. Recently Dirichlet forms found its use in effective study of fine properties of Markov processes on spaces with minimal smoothness, such as reflecting Brownian motion on non-smooth domains, Brownian motion and jump type processes on Euclidean spaces and fractals, and Markov processes on trees and graphs. It has been shown that Dirichlet form theory is an important tool in study of various invariance principles, such as the invariance principle for reflected Brownian motion on domains with non necessarily smooth boundaries and the invariance principle for Metropolis algorithm. Dirichlet form theory can also be used to study a certain type of SPDEs.

Fractals are used as an approximation of disordered media. The analysis on fractals is motivated by the desire to understand properties of natural phenomena such as polymers, and growth of molds and crystals. By definition, fractals are mathematical objects that are very rough and lack smoothness, so one can not use the standard analytic methods that were developed for Euclidean spaces and for manifolds. It turns out that Dirichlet form theory is well suited for studying fractals—significant progress has been made in this area in the last fifteen years. Detailed study of heat kernel estimates and parabolic Harnack principle on fractals require techniques both from probability and analysis. Stability of such estimates under perturbations of operators and spaces can be proved by translating the problem into some analytic and geometric conditions. Such equivalent conditions are often obtained in the framework of graphs and general metric measure spaces, and Dirichlet forms are one of the key tools for the analysis. As an example, we mention that this approach

turned out to be very useful in the analysis of random walks on random media such as percolation clusters. We believe that Dirichlet forms can play a more important role in studying scaling limits of nearest neighbor random walk and long range random walk on percolation clusters—this is an example of a concrete research project that was discussed at the conference.

In recent years there was an explosion of activity in the area of jump type processes. There are diverse reasons for this increased interest in the area. One is that many physical and economic systems are best modeled by discontinuous Markov processes. On the theoretical side, jump type processes provide a hard but elegant challenge for mathematical methods, because the infinitesimal generators of jump type Markov processes are non-local operators. Research on Markov processes generated many new results for non-local operators and for pseudo-differential operators as well, such as heat kernel estimates, parabolic Harnack principle and a priori Hölder estimates of parabolic functions. These new directions in the development of the de Giorgi-Moser-Nash theory for non-local operators made it possible to give general criteria for convergence of Markov chains with jumps, and they also provided a new approach to long-range random walk in random media.

A stochastic partial differential equation (SPDE) is a partial differential equation containing a random (noise) term. The study of SPDEs is an exciting topic which brings together techniques from probability theory in general and stochastic analysis in particular, functional analysis, and the theory of partial differential equations. SPDEs have many diverse applications: study of random evolution of systems with a spatial extension (random interface growth, random evolution of surfaces, fluids subject to random forcing), study of stochastic models where the state variable is infinite dimensional (for example, a curve or surface). The solution to a stochastic partial differential equation may be viewed in several manners. One can view the solution as a random field (set of random variables indexed by a multidimensional parameter). In the case when the SPDE is an evolution equation, the infinite dimensional point of view is to consider the solution at a given time as a random element in a function space and thus the SPDE is represented as a stochastic evolution for (almost) every realization of the noise and then view the solution as a random variable on the set of (infinite dimensional) paths thus defined. SPDEs are closely related to measure-valued processes, which are a class of strong Markov processes that model the spatial and temporal evolution of a population with reproductive mechanism.

The goal of the conference was to encourage the invited participants to bring their own perspectives on the foundations of stochastic analysis and help trigger activity in various exciting areas.

# **Presentation Highlights**

The opening two lectures were related to the rough path theory. Y. Le Jan opened the conference and discussed his recent work showing that the signature of Brownian motion completely determines Brownian motion in the sense that the completions of the  $\sigma$ -fields of the two processes coincide. M. Hairer discussed SDEs driven by fractional Brownian motions. He discussed the existence of smooth densities of the solution of SDE under Hörmander's condition and uniqueness of the invariant measure.

The talks were diverse but included several well defined clusters centered on specific topics. The first cluster of talks was on jump-type processes, especially their potential theoretical aspects. M. Kassmann presented his recent works on a new formulation of the Harnack inequalities that implies regularity estimates for solutions of heat equations. P. Kim, R. Song and Z. Vondracek talked about subordinate Brownian motions; oscillation of harmonic functions and its application to Fatou's theorem, (boundary) Harnack inequalities and two-sided estimates of the Green functions for subordinate Brownian motions with and without Gaussian components. T. Kulczycki discussed the trace of reflected Brownian motion in D on a flat part of the boundary  $F \subset \partial D$ ; the connection of the process with the Dirichlet to Neumann map and with the mixed Steklov problem, and some geometric conditions on D and F so that the hot spot conjecture is true. M. Kwasnicki discussed boundary Harnack inequalities for pure-jump processes under mild assumptions on metric measure spaces. R. Schilling discussed sample path properties of Feller processes such as estimates for maximal values of the process, transience/recurrence using the symbol of the semigroup. M. Takeda discussed Feynman-Kac penalisations for multi-dimensional symmetric  $\alpha$ -stable processes. R. Banuelos summarized recent applications of the sharp martingale inequalities of Burkholder to various Fourier multipliers including

some that arise from transformations of Lévy processes via the Lévy-Khintchine formula. A talk by S. Evans was also related to jump processes. He discussed Lipschitz minorants of Lévy processes and showed that if a Lévy process indexed by the real line has a *K*-Lipschitz minorant, then the set of times where the process is in contact with its minorant is a stationary regenerative set and hence it is the closed range of a subordinator "made stationary". He also characterized this subordinator in many cases and determined properties such as whether or not its range is countable or has zero Lebesgue measure. T. Uemura presented some sufficient condition for a non-symmetric bilinear form to be a lower bounded semi-Dirichlet form so that there is a jump-diffusion associated with it.

Some of the talks on processes with jumps described above used tools from the Dirichlet form theory. Dirichlet forms played a significant role in a number of other presentations. P.J. Fitzsimmons discussed two problems related to quadratic variation and diffusions. One is a decomposition of CAF to a CAF determined by a quasi-continuous function and a local MAF. The other is that the infinite-dimensional Brownian motion constructed by Gross fails to satisfy the axiom of polarity, namely there exists a semipolar set that is not polar. M. Fukushima presented his recent results on how to apply Brownian motion with darning to conformal mappings of multiply connected planar domains and to the associated Komatu-Loewner differential equation. A. Winter constructed a continuum-tree-valued diffusion via a quasi-regular Dirichlet form. She showed that Aldous' Markov chain on N-cladogram (which is a semi-labeled, unrooted and binary tree with N leaves) suitably rescaled and started in the uniform cladogram converges in the weak Gromov topology to this diffusion. S. Feng discussed some progresses on the construction of a reversible diffusion process with the two-parameter Dirichlet process (which is a random measure generalizing Ferguson's Dirichlet process) as the reversible measure. In some cases, such a reversible diffusions can be constructed by using Dirichlet form method.

Another cluster of talks reported recent progress on SPDEs, measure-valued processes and SDEs. R. Bass considered the heat equation on an interval with random mechanism given by A(u)(x) (with current temperature u) times space-time white noise, where A is Hölder continuous. He showed the uniqueness in law holds for the SPDE under some reasonable conditions on A. E. Perkins discussed non-uniqueness (in law and pathwise) of similar type SPDE where A(u)(x) part is  $|u(t,x)|^{\gamma}$ . He showed that the SPDE with zero initial conditions has a non-zero solution for  $0 < \gamma < 3/4$  (hence solutions are not unique in law or pathwise) whereas it is pathwise unique when  $\gamma > 3/4$ . D. Khoshnevisan described sensitiveness of randomly-forced heat equations on the choice of the initial function. A family of parabolic Anderson models is one such example, and he described some connection of the Anderson models to the so called KPZ relation. M. Röckner talked about recent extinction results for SPDE (with multiplicative noise) of porous media type and applications to self-organized criticality (SOC). He discussed recent results, where for the SOC-case asymptotic extinction was proved for all spatial dimensions and shown to be locally exponentially fast. K. Xian presented his recent results on a Schilder-type sample large deviation for super-Brownian motions with an explicit good rate function. J. Xiong discussed well-posedness of the martingale problem for superprocesses with interactions. Y. Ren discussed a supercritical Galton-Watson branching processes with immigration. She discussed the recent results on the small valued probabilities of the random variable arising as a non-degenerate limit for the normalized population size under some mild condition. X. Li discussed the construction of a stochastic process (called the derivative process) associated to the SDE whose coefficients are not differentiable. She presented a probabilistic representation for the derivative of the corresponding semi-group and the convergence of approximating SDEs.

The third cluster of talks was focused on stochastic processes on fractals and related topics. M. Barlow summarized the equivalent conditions for sub-Gaussian heat kernel estimates and discuss the role and application of the so-called cut-off Sobolev inequalities. D. Croydon introduced a notion of spectral Gromov-Hausdorff convergence and used it to prove the convergence of mixing times for a sequence of finite graphs. B. Hambly summarized recent results on quenched and annealed asymptotic order of eigenvalue counting functions for the generator on random fractals. J. Kigami discussed non-local Dirichlet forms on *p*-adic numbers and its heat kernels. Some heat kernel estimates were also derived. N. Kajino presented his recent results on Weyl's Laplacian eigenvalue asymptotics for the harmonic Sierpinski gasket.

Mass transport was also an important topic in the workshop. E.P. Hsu presented generalizations of Talagrand's transportation cost inequality to the heat kernel measure on a Riemannian manifold and the Wiener measure on the path space over a Riemannian manifold. S. Pal considered rank-based models which are certain interacting diffusion processes. Using transportation cost inequalities, he derived uniform Gaussian tail bounds for the empirical least-square estimate of the index over large intervals of time. K.-T. Sturm considered couplings of the Lebesgue measure and the Poisson point process. He showed that the minimal mean  $L^p$ -transportation cost of the coupling is finite for all p provided  $d \ge 3$ , and when  $d \le 2$  it is finite if and only if p < d/2. When p = 2, the relation of the optimal coupling and a random tiling of  $\mathbb{R}^d$  by convex polytopes of volume 1 was also discussed.

Some talks given during the week covered stochastic analysis themes harder to classify. Roughly speaking, they were related to heat kernel estimates and Gaussian processes. K. Bogdan presented recent results on Schrödinger perturbations of integral kernels. Under some integrability condition of the kernels, existence of the transition density for the perturbed operator and its upper bound were derived. J-D. Deuschel discussed Markov chain approximations to non-symmetric uniform elliptic divergence forms. He showed Gaussian heat kernel estimates for the centered random walks (a class of non-symmetric Markov chains), and as an application he proved the approximation by such random walks. M. Gordina talked about recent results on functional inequalities on infinite-dimensional curved spaces and applications. For instance, integrated Harnack inequalities for the heat kernel measures were discussed with an application to prove quasi-invariance of heat kernel measures on certain infinite-dimensional groups.

N. Eisenbaum discussed some properties of Gaussian processes. Given a Gaussian process  $\{\eta_x\}_{x\in E}$  with continuous covariance, the equivalence of infinite divisibility of  $\eta^2$  with other conditions such as  $\eta^2$  satisfying FKG condition, the law of  $\eta^2$  being Radon measure etc., were presented. J. Swanson discussed recent results on an explicit expression for the weak Stratonovich integral for a fractional Brownian motion with Hurst parameter 1/6. Using this expression, an Itô-type formula for this integral was derived.

# **Participants**

The participants spanned a wide spectrum by any measure. There were many participants from Canada and the US, but also a large number of probabilists from various European and Asian countries. There was a healthy mix of senior mathematicians and junior researchers. Although women were a minority at the conference, their number was significant and their contributions were among the most interesting.

# Abstracts

#### Speaker: Rodrigo Banuelos (Purdue University)

#### Title: Martingales and Fourier multipliers, sharp estimates

Abstract: We shall discuss some recent applications of the sharp martingale inequalities of Burkholder to various Fourier multipliers including some that arise from transformations of Lévy processes via the Lévy–Khintchine formula. While these results are of interest on their own right, they are motivated by some well known open problems in analysis and PDE's.

#### Speaker: Martin Barlow (University of British Columbia)

#### Title: Energy of cutoff functions and applications

Abstract: A well known theorem of Grigoryan and Saloff Coste states that Gaussian heat kernels bounds are equivalent to volume doubling (D) plus Poincare inequalities(PI). In the sub-Gaussian case, which arises on various regular fractals, Rich Bass and I showed that these are equivalent to (D), (PI) and an additional condition, denoted CS(b). The condition CS(b) gives the existence of low energy cutoff functions. In this talk I will give some additional applications of CS(b), which hold without (PI). This is joint work with Sebastian Andres.

#### Speaker: Richard F. Bass (University of Connecticut)

#### Title: Uniqueness in law for parabolic SPDEs and infinite dimensional SDEs

Abstract: We consider the heat equation on an interval with heat being introduced according to a random mechanism. When the random mechanism is space-time white noise, this equation has been much studied. We look at the case where the white noise is modified by a function A(u)(x) of the current temperatures u and where A is Hölder continuous as a function of u. Unlike other work along these lines, A(u)(x) can

depend on the temperatures throughout the interval. Our method involves looking at the Fourier coefficients, which leads to an infinite dimensional system of stochastic differential equations. This is joint work with Ed Perkins.

#### Speaker: Krzysztof Bogdan (Wrocław University of Technology, Poland)

#### Title: Schrödinger perturbations

Abstract: I will report joint work in progress with Wolfhard Hansen, Tomasz Jakubowski and Sebastian Sydor on Schrödinger perturbations of integral kernels; ones which produce comparable integral kernels.

- [1] W. Hansen. Global comparison of perturbed Green functions. Math. Ann. 334 (2006), no. 3, 643-678.
- [2] K. Bogdan, W. Hansen, T. Jakubowski. Time-dependent Schrödinger perturbations of transition densities. Studia Math. 189 (2008), no. 3, 235–254.
- [3] T. Jakubowski. On combinatorics of Schrödinger perturbations. Potential Anal. 31 (2009), no. 1, 45–55.
- [4] T. Jakubowski, K. Szczypkowski. Time-dependent gradient perturbations of fractional Laplacian. J. Evol. Equ. 10 (2010), no. 2, 319–339.

#### Speaker: David Croydon (University of Warwick, UK)

Title: Mixing time convergence for sequences of random walks on graphs

Abstract: The main conclusion of this work, which is a joint project with Ben Hambly (University of Oxford) and Takashi Kumagai (Kyoto University), is that the mixing times of the simple random walks on a sequence of graphs converge to the mixing time of a limiting diffusion whenever the corresponding state spaces, invariant measures and heat kernels converge in a suitable Gromov-Hausdorff sense. In addition to presenting this result, I will describe how it can be applied to a number of interesting examples, including some simple lattice models, self-similar fractal graphs with random weights, critical Galton-Watson trees, the Erdos-Renyi random graph at criticality and the range of a random walk in high dimensions.

#### Speaker: Jean-Dominique Deusche (Berlin Technical University, Germany)

Title: Markov chain approximations to non-symmetric diffusions with bounded coefficients

Abstract: We consider a certain class of non-symmetric Markov chains and obtain heat kernel bounds and parabolic Harnack inequalities. Using the heat kernel estimates, we establish a sufficient condition for the family of Markov chains to converge to non-symmetric diffusions. As an application, we approximate non-symmetric divergence forms with bounded coefficients by non-symmetric Markov chains. This extends the results by Stroock-Zheng ([SZ]) to the non-symmetric divergence forms. Joint work with Takashi Kumagai.

[SZ] D.W. Stroock and W. Zheng. Markov chain approximations to symmetric diffusions. Ann. Inst. Henri. Poincaré-Probab. Statist. 33 (1997), 619-649.

#### Speaker: Nathalie Eisenbaum (Université Paris VI, France)

Title: Some properties of Gaussian processes

Abstract: We will describe and characterize some properties of Gaussian processes.

#### Speaker: Steve Evans (University of California at Berkeley)

#### Title: Uplift under Lévystan: Lipschitz minorants of Lévy processes

Abstract: Motivated by problems in statistical density estimation, Groeneboom 1983 established a number of remarkable properties of the greatest convex function dominated by the path of a one-dimensional Brownian motion. Pitman, Bass, Cinlar, Bertoin and others extended these results and showed how they could be derived more easily using techniques such as excursion theory and last exit decompositions. There has been a resurgence of interest in this area with a flurry of recent work on convex minorants of Lévy processes and random walks by various combinations of Abramson, Pitman, Ross and Uribe Bravo. Researchers in non-linear optimization, particularly optimal transport, have developed the notion of c-convexity that greatly generalizes the familiar definition of convex function while keeping many of its important features such as Legendre-Fenchel duality. Within this theory, the set of functions from the reals to the reals with a given upper bound K on their Lipschitz constant share many of the features of the convex functions. I will show

that if a Lévy process indexed by the real line has a *K*-Lipschitz minorant, then the set of times where the process is in contact with its minorant is a stationary regenerative set and hence it is the closed range of a subordinator "made stationary". It is possible to characterize this subordinator in many cases and determine properties such as whether or not its range is countable or has zero Lebesgue measure. If the Lévy process is a Brownian motion with drift, then there are explicit distributions for a number of random variables related to the minorant. This work is joint with Josh Abramson.

#### Speaker: Shui Feng (McMaster University)

#### Title: An Open Problem Associated with the Two-parameter Dirichlet Process

Abstract: The two-parameter Dirichlet process is a random measure generalizing Ferguson's Dirichlet process. This talk will discuss progresses and difficulties in constructing a reversible diffusion process with the two-parameter Dirichlet process as the reversible measure.

#### Speaker: Patrick J. Fitzsimmons (University of California at San Diego)

#### Title: Zero-Energy Functions of a Symmetric Diffusion

Abstract: Consider a continuous function f on the state space of a symmetric diffusion  $X = (X_t : t \ge 0)$ such that  $t \mapsto f(X_t)$  is locally of zero energy. Using time-reversal arguments, I will show that f must be constant along the paths of X. The space-time version of this result will also be discussed. Time permitting, I will examine a representation of general continuous additive functionals of X, extending a result of Tanaka for one-dimensional Brownian motion.

#### Speaker: Masatoshi Fukushima (Osaka University, Japan)

Title: On Brownian motion with darning and Komatu-Loewner equation for multiply connected planar domains

Abstract: Brownian motion with darning (BMD in abbreviation) is applied to the study of conformal mappings of multiply connected planar domains and the associated Komatu-Loewner differential equations. The notion of BMD and its basic properties are presented in Chapter 7 of a forthcoming book [CF] in a more general context. It is a diffusion process obtained from the absorbing Brownian motion on a multiply connected planar domain by rendering each hole of the domain into one point. Especially the zero period property of a general BMD-harmonic function and the conformal invariance of BMD will be used to derive the continuity of some fundamental quantities for the Komatu-Loewner equation. We are motivated by the works [BF1],[BF2],K and [L]. This talk is based on an ongoing joint work with Z.-Q. Chen and S. Rohde.

- [BF1] R.O. Bauer and R.M. Friedrich, On radial stochastic Loewner evolution in multiply connected domains. J. Funct. Anal. 237 (2006), 565-588.
- [BF2] R.O. Bauer and R.M. Friedrich, On chordal and bilateral SLE in multiply connected domains. *Math.* Z. 258 (2008), 241-265.
- [CF] Z.-Q. Chen and M. Fukushima, *Symmetric Markov Processes, Time Change, and Boundary Theory*. Princeton University Press, to appear.
- [K] Y. Komatu, On conformal slit mapping of multiply-connected domains. Proc. Japan Acad. 26 (1950), 26-31.
- [L] G. F. Lawler, The Laplacian-b random walk and the Schramm-Loewner evolution. *Illinois J. Math.* **50** (2006), 701-746.

#### Speaker: Maria Gordina (University of Connecticut)

#### Title: Functional inequalities in infinite dimensions

Abstract: we will talk about recent results on functional inequalities on infinite-dimensional curved spaces and applications of such inequalities. One type of such results concerns integrated Harnack inequalities for the heat kernel measures, and how these inequalities can be used to prove quasi-invariance of heat kernel measures on certain infinite-dimensional groups. These results use geometric data such as lower Ricci bounds. Therefore these techniques is not applicable to sub-elliptic Laplacians. Most of finite-dimensional methods for such heat kernels are dimension-dependent. Nevertheless, recently we were able to prove several types of functional inequalities for a sub-elliptic Laplacian on an infinite-dimensional Heisenberg group. The results of this talk are based on joint work with F. Baudoin, B. Driver, T. Melcher.

#### Speaker: Martin Hairer (University of Warwick, UK)

#### Title: Hypoelliptic SDEs driven by rough paths

Abstract: We present a number of recent results extending Hörmander's theorem to a larger class of SDEs driven by Gaussian stochastic processes. In particular, we focus on the case when the driving process is rougher than Brownian motion, using the theory of rough paths to give meaning to the equations. Our main ingredient in the implementation of Malliavin's programme is a deterministic version of Norris's lemma. This relies on a quantitative property of the driving process (a "modulus of Hölder roughness") ensuring that it is sufficiently non-degenerate. One application of the theory is to demonstrate ergodicity of such equations under conditions that are qualitatively similar to those in the classical ergodic theory for SDEs.

#### Speaker: Ben Hambly (University of Oxford)

#### Title: Spectral asymptotics for random fractals

Abstract: I will discuss some results concerning the high frequency asymptotics of the eigenvalue counting function for a variety of random fractals. The focus will mainly be on the continuum random tree where we can show the size of the second order term in the asymptotic expansion. We will also discuss other random recursive fractals where a variety of behaviors is possible.

#### Speaker: Elton Hsu (Northwestern University)

#### Title: Brownian Motion and Transpotation Inequality on Path Spaces

Abstract: We will show how to use synchronizing Riemannian Brownian motion to prove generalizations of Talagrand's transportation cost inequality to the heat kernel measure on a Riemannian manifold and the Wiener measure on the path space over a Riemannian manifold.

#### Speaker: Naotaka Kajino (University of Bielefeld)

# Title: Weyl's Laplacian eigenvalue asymptotics for the measurable Riemannian structure on the Sierpinski gasket

Abstract: On the Sierpinski gasket K, Kigami [Math. Ann. 340 (2008), 781–804] has introduced the notion of the measurable Riemannian structure, with which the gradient vector fields of functions, the Riemannian volume measure  $\mu$  and the geodesic metric  $\rho$  are naturally associated. Kigami has also proved in the same paper the two-sided Gaussian bound for the corresponding heat kernel, and I have further shown several detailed heat kernel asymptotics, such as Varadhan's asymptotic relation, in [Potential Anal., in press, doi: 10.1007/s11118-011-9221-5].

In the talk I will talk about the Weyl's Laplacian eigenvalue asymptotics for this case. The correct scaling order for the asymptotics of the eigenvalues is given by the Hausdorff dimension d of the metric space  $(K, \rho)$ , and in the limit of the eigenvalue asymptotics we obtain a constant multiple of the d-dimensional Hausdorff measure  $H^d$ . Moreover, we will also see that this Hausdorff measure  $H^d$  is Ahlfors d-regular with respect to  $\rho$  but that it is singular to the Riemannian volume measure  $\mu$ .

#### Speaker: Moritz Kassmann (University of Bielefeld, Germany)

#### Title: Harnack's inequality: a new formulation and applications

Abstract: We present a formulation of Harnack's inequality which is applicable to local and nonlocal operators at the same time. We show that this version of Harnack's inequality implies regularity estimates for solutions to several integrodifferential operators. We apply the method to some nonlocal symmetric Dirichlet forms and to generators of jump processes. We discuss how this approach extends known results. The talk is based on three works: [K. 2010], [K.-Mimica 2011] and [Dyda-K. 2011]

#### Speaker: Davar Khoshnevisan (University of Utah)

#### Title: On the chaotic character of some parabolic SPDEs

Abstract: I will describe how a family of randomly-forced heat equations depends sensitively on the choice of the initial function. Time permitting, we will see a surprising connection, and derivation, of the so called KPZ relation between the spatial and temporal fluctuation exponents of the solution to a family of parabolic Anderson models. This talk is based on joint works with D. Conus, M. Foondun, M. Joseph, and S. Shiu.

Speaker: Jun Kigami (Kyoto University, Japan)

Title: Dirichlet forms on a noncompact Cantor set and random walks on its defining tree

Abstract: First we will construct a class of Dirichlet forms on a noncompact Cantor set, which is a generalization of *p*-adic numbers, from prescribed sets of eigenvalues and measures. At the same time, we have concrete expressions of the jump kernel and the transition density. Assuming the volume doubling condition, we construct an intrinsic metric under which estimates of transition density and jump kernel are obtained. Secondly transient random walks on the defining tree of the noncompact Cantor set are shown to induce a subclass of Dirichlet forms discussed in the first part on the noncompact Cantor set as traces.

#### Speaker: Panki Kim (Seoul National University)

Title: Oscillation of unbounded harmonic functions for subordinate Brownian motion and its applications Abstract: In this talk we discuss the oscillation of unbounded harmonic functions for pure-jump subordinate Brownian motion. As an application, we give a probabilistic proof of relative Fatou's theorem for harmonic functions for such subordinate Brownian motion. This is a joint work with Yunju Lee.

Speaker: **Tadeusz Kulczycki** (Polish Academy of Sciences and Wrocław University of Technology, Poland) Title: *On jump processes which are traces of reflected Brownian motion* 

Abstract: Let  $B_t$  be a reflected Brownian motion in a bounded domain  $D \subset R^d$ . Assume that there exists a part F of a boundary of D which is flat (for example D can be a cylinder and F one of its bases or D can be a triangle and F one of its sides). Let us consider the process  $X_t$  which trajectories are traces of the process  $B_t$  on F. More formally  $X_t = B_{\eta_t}$ , where  $\eta_t$  is the inverse of a local time of  $B_t$  on F.

We will show the connection of the process  $X_t$  with the Dirichlet to Neumann map and with the mixed Steklov problem. Such Steklov problem appears very naturally in some problems of hydrodynamics.

It occurs that the jump process  $X_t$  on F shares many properties of a reflected Brownian motion on F. In particular we will show that under some geometric assumptions on D and F the hot spots property holds for the process  $X_t$ . That is, the first non-constant eigenfunction corresponding to the semigroup of the process  $X_t$  attains its maximum and minimum on the boundary of F. We will also study some properties of the process  $X_t$  under continuous deformation of the domain D. Some open questions will be also discussed.

#### Speaker: Mateusz Kwasnicki (Wrocław University of Technology, Poland)

#### Title: Boundary Harnack inequality for jump-type processes

Abstract: I will present the results of my recent work with Krzysztof Bogdan and Takashi Kumagai. We consider a Hunt process  $X_t$  in a metric measure space. Under relatively mild assumptions, we prove a boundary Harnack inequality for nonnegative functions harmonic with respect to  $X_t$  in an arbitrary open set. We require:

- (1) existence of the dual process  $X_t^*$ ,
- (2) existence of bump functions in the domains of the Feller generators of  $X_t$  and  $X_t^*$ ,
- (3) boundedness (away from the diagonal) of the jumping kernel and the potential kernel.

Under these assumptions, we prove boundedness near the boundary point  $z \in \partial D$  of the ratio f(x)/g(x) of any two nonnegative harmonic functions f, g in an open set D, given that f and g vanish off D in some neighbourhood of z. More precisely, we prove that in this case, if d(x, z) < r and d(y, z) < r, then

$$\frac{1}{C}\frac{f(x)}{g(x)} \le \frac{f(y)}{g(y)} \le C\frac{f(x)}{g(x)},$$

where C does not depend on D, x, y, f and g, given that f(x) = g(x) = 0 whenever  $x \notin D$  and d(x, z) < 2r.

When  $X_t$  is a symmetric (i.e. self-dual) process which admits local stable-like bounds for the transition density (i.e. heat kernel), then (1) and (3) are satisfied automatically. The only restrictive assumption is in this case (2). In Euclidean setting, (2) holds true if the jumping kernel is sufficiently regular. In general metric measure spaces, (2) can often be proved when there is a sub-Gaussian diffusion process. Under these assumptions, our boundary Harnack inequality is scale-invariant and, in some sense, stable under small perturbations.

The proof involves a new, probabilistic method for proving a priori supremum bounds for nonnegative harmonic functions, which may be of independent interest.

#### Speaker: Yves Le Jan (Université Paris-Sud, France)

Title: The signature of Brownian paths

Abstract: We show that in dimension larger than two, Brownian paths indexed by [0,T], are determined by their iterated integrals taken up to T.

#### Speaker: Xue-Mei Li (University of Warwick, UK)

#### Title: The derivative process for SDEs with non-smooth coefficients

Abstract: For an SDE with smooth coefficients, the solution depends continuously on the initial data. The latter is a basic assumption for numerical schemes. In this talk we discuss the construction of a stochastic process, which we call the derivative process, associated to the SDE in the case of the coefficients not differentiable. This is used to give a probabilistic representation for the derivative of the corresponding semi-group. For this construction we also studied the convergence of approximating SDEs and make sense of of an SDE with random coefficients. As a by product we have an existence theorem for the smooth solution flow.

#### Speaker: Soumik Pal (University of Washington)

#### Title: Transportation Cost Inequalities for rank-based models

Abstract: Transportation Cost inequalities are functional inequalities that compare the Wasserstein distance between two probability measures with their relative entropy. Via an argument by Marton these inequalities are powerful methods to show concentration of measure properties. We focus on applications to certain interacting diffusion processes called rank-based models. This is a multidimensional diffusion model where each particle (coordinate index) gets an instantaneous drift and diffusion coefficient depending on its rank among all the particles. It is known that if we exponentiate the coordinates and rescale to have a total sum of one, the ordered values exhibit power law decay in equilibrium. Using Transportation Cost Inequalities we derive uniform Gaussian tail bounds for the empirical least-square estimate of the index of this power law over large intervals of time. Part of this talk is based on joint work with Misha Shkolnikov.

#### Speaker: Edwin Perkins (University of British Columbia)

Title: Nonuniqueness for a parabolic SPDE with  $\frac{3}{4} - \epsilon$ -Hölder diffusion coefficients

Abstract: We prove an analogue of the Girsanov examples for SDE's for the parabolic stochastic partial differential equation (SPDE)

$$\frac{\partial u}{\partial t} = \frac{\Delta}{2} u(t, x) + |u(t, x)|^{\gamma} \dot{W}(t, x),$$

with zero initial conditions. Here  $\dot{W}$  is a space-time white noise on  $R_+ \times R$ . More precisely, we show the above stochastic pde has a non-zero solution for  $0 < \gamma < 3/4$ , and hence solutions are not unique in law or pathwise unique. The case  $\gamma = 1/2$  arises as a scaling limit point of a system of branching annihilating random walks. An analogue of Yamada-Watanabe's theorem for SDE's was recently shown by Mytnik and Perkins for SPDE's by establishing pathwise uniqueness of solutions to

$$\frac{\partial u}{\partial t} = \frac{\Delta}{2}u(t,x) + \sigma(u(t,x))\dot{W}(t,x),$$

where  $\sigma$  is Holder continuous of index  $\gamma > 3/4$ . The situation for the above class of parabolic SPDE's is therefore similar to their finite dimensional counterparts, but with the index 3/4 in place of 1/2. This is joint work with Carl Mueller and Leonid Mytnik.

#### Speaker: Yanxia Ren (Peking University)

#### Title: Small value probabilities for supercritical branching processes with immigration

Abstract: We consider a supercritical Galton-Watson branching process with immigration. It is well known that under suitable conditions on the offspring and immigration distributions, there is a finite, strictly positive and non-degenerate limit for the normalized population size, denoted as W. The main purpose of this paper is to investigate the small value probabilities of W, that is to estimate  $P(W \le \varepsilon)$  for  $\varepsilon > 0$  small. In comparison with the well-studied results for supercritical Galton-Watson branching process without immigration, precise effects of the balance between offspring and immigration distributions on small value probability of W, are obtained. Several illustrative examples are analyzed carefully. They demonstrate the sharpness of our results

and the significant effect of the immigration which can cause the near-constancy phenomena even when there is no oscillation in the setting without immigration.

#### Speaker: Michael Röckner (University of Bielefeld, Germany)

Title: Recent extinction results for stochastic porous media equations and applications to self-organized criticality

Abstract: The first part of the talk will recall extinction results for stochastic partial differential equations (with multiplicative noise) of porous media type. These include stochastic fast diffusion equations and more singular cases, where e.g. the nonlinearity is given by a Heaviside or sign function, so is multivalued. The latter describe certain continuum models for the phenomenon of self-organized criticality (SOC). These extinction results have been obtained in the past two years. In the SOC-case, however, extinction was only shown if the underlying spatial domain is one-dimensional and only with positive (though high) probability. The second part of the talk is devoted to very recent results, where for the SOC-case asymptotic extinction was proved for all spatial dimensions and shown to be locally exponentially fast. One main technique in the proofs is to transform the stochastic PDE into a deterministic PDE with a random parameter. The resulting deterministic PDE is of an entirely new type and new methods had to be invented for its analysis.

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- [5] V. Barbu, M. Röckner On a random scaled porous media equation, BiBoS–Preprint, publication in preparation, 22 pp., 2010.
- [6] V. Barbu, M. Röckner Stochastic porous media equations and self-organized criticality: convergence to the critical state in all dimensions, BiBoS–Preprint, publication in preparation, 21 pp., 2011.

#### Speaker: Rene Schilling (Technical University at Dresden, Germany)

#### Title: Sample Path Properties of Feller Processes

Abstract: We present sufficient conditions for the transience and the existence of local times of a Feller process, and the ultracontractivity of the associated Feller semigroup. These conditions are sharp for Lévy processes, and they are based on the local symmetrization technique and a uniform upper bound for the characteristic function of a Feller process. As a byproduct, we obtain for stable-like processes (in the sense of R. Bass) on  $\mathbb{R}^d$  with smooth variable index  $\alpha(x) \in (0, 2)$  a transience criterion in terms of the exponent  $\alpha(x)$ ; if d = 1 and  $\inf_{x \in \mathbb{R}} \alpha(x) \in (1, 2)$ , then the stable-like process admits local times.

This work is joint with Jian Wang (Fujian Normal University and TU Dresden)

#### Speaker: Renming Song (University of Illinois)

#### Title: Potential theory of subordinate Brownian motions

Abstract: A subordinate Brownian motion is a Levy process which can be by replacing the time parameter of Brownian motion by an independent subordinator. The subordinator can thought of as "intrinsic" time or "operational" time. Subordinate Brownian motions form a large subclass of Levy processes and they are widely used in applications.

Recently, a lot of progress has been made in the study of the potential theory of subordinate Brownian motions. In this talk, I will give a survey of some recent results on the potential theory of subordinate Brownian motions without Gaussian components. In particular, I will present a boundary Harnack principle and two-sided estimates on the Green functions of these processes in bounded smooth open sets.

This talk is based on joint works with Panki Kim and Zoran Vondracek.

Speaker: **Karl-Theodor Sturm** (University of Bonn, Germany) Title: *Optimal Transport from Lebesgue to Poisson*  Abstract: We study couplings  $q^{\bullet}$  of the Lebesgue measure and the Poisson point process  $\mu^{\bullet}$ , i.e. measurevalued random variables  $\omega \mapsto q^{\omega}$  s.t. for a.e.  $\omega$  the measure  $q^{\omega}$  on  $\mathbb{R}^d \times \mathbb{R}^d$  is a coupling of  $\mathfrak{L}^d$  and  $\mu^{\omega}$ . For any given  $p \in (0, \infty)$  we ask for a minimizer of the mean  $L^p$ -transportation cost

$$\mathfrak{C}(q^{\bullet}) = \sup_{B \subset \mathbb{R}^d} \frac{1}{\mathfrak{L}^d(B)} \mathbb{E}\left[ \int_{\mathbb{R}^d \times B} |x - y|^p \, dq^{\bullet}(x, y) \right].$$

The minimal mean  $L^p$ -transportation cost turns out to be finite for all p provided  $d \ge 3$ . If  $d \le 2$  then it is finite if and only if p < d/2.

Moreover, in any of these cases we prove that there exist a unique translation invariant coupling which minimizes the mean  $L^p$ -transportation cost. In the case p = 2, this 'optimal coupling' induces a random tiling of  $\mathbb{R}^d$  by convex polytopes of volume 1.

#### Speaker: Jason Swanson (Central Florida University)

#### Title: The calculus of differentials for the weak Stratonovich integral

Abstract: The weak Stratonovich integral is defined as the limit, in law, of Stratonovich-type symmetric Riemann sums. We derive an explicit expression for the weak Stratonovich integral of f(B) with respect to g(B), where B is a fractional Brownian motion with Hurst parameter 1/6, and f and g are smooth functions. We use this expression to derive an Itô-type formula for this integral. As in the case where g is the identity, the Itô-type formula has a correction term which is a classical Itô integral, and which is related to the so-called signed cubic variation of g(B). Finally, we derive a surprising formula for calculating with differentials. We show that if dM = X dN, then Z dM can be written as ZX dN minus a stochastic correction term which is again related to the signed cubic variation.

#### Speaker: Masayoshi Takeda (Tohuku University)

#### Title: Feynman-Kac Penalisations of Symmetric Stable Processes

Abstract: B. Roynette, P. Vallois and M. Yor have studied limit theorems for Wiener processes normalized by some weight processes. K. Yano, Y. Yano and M. Yor studied the limit theorems for the one-dimensional symmetric stable process normalized by non-negative functions of the local times or by negative (killing) Feynman-Kac functionals. Our aim is to extend their results on Feynman-Kac penalisations to positive Feynman-Kac functionals of multi-dimensional symmetric  $\alpha$ -stable processes.

#### Speaker: Toshihiro Uemura (Kansai University)

#### Title: On multidimentional diffusion processes with jumps

Abstract: Let  $a_{ij}$  and  $b_i$  be coefficients of a second order partial differenctial operator defined on an open set D of  $R^d$  and k a Levy-type kernel over D. We define a non-symmetric billinear form on  $L^2(D; dx)$  having the dates above

Under some conditions on the datas, we will show the form becomes a lower bounded semi-Dirichlet form and there exists a diffusion process with jumps associated with the form.

#### Speaker: Zoran Vondracek (University of Zagreb)

#### Title: Potential theory of subordinate Brownian motions with Gaussian components

Abstract: In this talk I will look at a subordinate Brownian motion with a Gaussian component and a rather general discontinuous part. The assumption on the subordinator is that its Laplace exponent is a complete Bernstein function with a Lévy density satisfying a certain growth condition near zero. The main result that I will present is a boundary Harnack principle with explicit boundary decay rate for non-negative harmonic functions of the process in  $C^{1,1}$  open sets. I will also discuss an example showing that the boundary Harnack principle fails for processes with finite range jumps. As a consequence of the boundary Harnack principle, one can establish sharp two-sided estimates on the Green function of the subordinate Brownian motion in any bounded  $C^{1,1}$  open set D and identify the Martin boundary of D with respect to the subordinate Brownian motion with the Euclidean boundary.

Joint work with Panki Kim and Renming Song

Speaker: **Anita Winter** (Friedrich-Alexander-Universität Erlangen-Nürnberg ) Title: *Aldous move on cladograms in the diffusion limit*  Abstract: A N-cladogram is a semi-labeled, unrooted and binary tree with N leaves labeled  $\{1, 2, ..., N\}$  and with unit edge lengths. Aldous constructed a Markov chain on cladograms and gave bounds on its mixing time.

In this talk we use Dirichlet form methods to construct a continuous tree-valued diffusion and show that Aldous move on cladograms suitably rescaled converges in the weak Gromov topology to this diffusion provided that started in the uniform cladogram.

#### Speaker: Kai-Nan Xian (Nankai University, China)

#### Title: An Explicit Schilder-type Theorem for Super-Brownian Motions

Abstract: Like ordinary Brownian motion, super-Brownian motion, a central object in the theory of superprocesses, is a universal object arising in a variety of settings. Schilder-type theorems and Cramér-type theorems are two of the major topics for large-deviation theory. A Schilder-type (which is also a Cramér-type) sample large deviation for super-Brownian motions with a good rate function represented by a variation formula was established in 1993 and 1994 (see [1]-[3]). There have been very valuable contributions for giving an affirmative answer to the question of whether this sample large deviation holds with an explicit good rate function since then. In [4], thanks to previous results on this issue and the Le Gall's Brownian snake, we established such a large deviation for nonzero finite initial measures. Then in [5], we proved the mentioned large deviation holds for infinite initial measures. Those concluded the attacking on the long-standing conjecture proposed in [1].

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#### Speaker: Jie Xiong (University of Tennessee)

Title: Uniqueness problems for some measure-valued processes

Abstract: A stochastic partial differential equation (SPDE) is derived for the super Brownian motion regarded as a distribution function valued process. The strong uniqueness for the solution to this SPDE is obtained by a connection between SPDEs and backward doubly stochastic differential equations. Similar results are also proved for the Fleming-Viot process. We also extend the uniqueness result to processes with interaction.

# **List of Participants**

Banuelos, Rodrigo (Purdue University)
Barlow, Martin (University of British Columbia)
Bass, Richard (University of Connecticut)
Bogdan, Krzysztof (Wroclaw University of Technology)
Burdzy, Krzysztof (University of Washington)
Chen, Zhen-Qing (University of Washington)
Croydon, David (University of Warwick)
Deuschel, Jean-Dominique (Technische Universitat Berlin)
Eisenbaum, Nathalie (CNRS - University of Paris VI)
Evans, Steve (University of California, Berkeley)
Feng, Shui (McMaster University)
Fitzsimmons, P. J. (UC San Diego)
Fukushima, Masatoshi (Osaka University)
Gordina, Masha (University of Connecticut)

Hairer, Martin (University of Warwick) Hambly, Ben (University of Oxford) Hsu, Elton (Northwesthern University) Kajino, Naotaka (University of Bielefeld) Kassmann, Moritz (Bielefeld University) Khoshnevisan, Davar (University of Utah) Kigami, Jun (Kyoto University) Kim, Panki (Seoul National University) Kulczycki, Tadeusz (Polish Academy of Sciences) Kumagai, Takashi (RIMS Kyoto) Kwasnicki, Mateusz (Polish Academy of Sciences) Le Jan, Yves (Universite Paris Sud) Li, Xuemei (University of Warwick) Pal, Soumik (University of Washington) **Perkins, Ed** (University of British Columbia) Ren, Yanxia (Peking University) Rckner, Michael (Universitaet Bielefeld) Schilling, Rene (TU Dresden) Song, Renming (University of Illinois) Sturm, Karl-Theodor (University of Bonn) Swanson, Jason (University of Central Florida) Takeda, Masayoshi (Tohoku University) Uemura, Toshihiro (Kansai University) Vondracek, Zoran (University of Zagreb) Winter, Anita (UniversitLt Duisburg-Essen) Xiang, Kainan (Nankai University) **Xiong, Jie** (University of Tennessee)

# Chapter 30

# Almost periodic order: spectral, dynamical, and stochastic approaches (11w5062)

# Sep 25 - Sep 30, 2011

**Organizer(s):** Michael Baake (University of Bielefeld) David Damanik (Rice University) Daniel Lenz (Friedrich-Schiller-Universität Jena)

# **Overview of the Field**

Quasicrystals were discovered in early 1982 by Dan Shechtman (Haifa) in the form of an AlMn alloy that displayed a sharp Bragg type diffraction image with perfect icosahedral point symmetry. This challenged the understanding of solids at the time, and needed a while to be accepted for publication [16]. Ultimately, it led to a paradigm shift for what we understand as 'order' in a solid or in a more general structure. For this discovery, Shechtman was awarded the Nobel Prize in Chemistry in 2011, just a few days after our meeting took place.

The field of Aperiodic Order is the mathematical counterpart to the physics and chemistry of quasicrystals, and the meeting was concerned with all aspects of it that relate to almost periodicity. In fact, the experimental discovery by Shechtman had many precursors in mathematics, ranging from ornaments via Kepler's famous fivefold pattern and Penrose's tiling to modern tiling theory, or from Bohr's theory of almost periodic functions via Meyer's book [13] to the present day development of almost periodic measures.

# **Recent Developments and Open Problems**

The field has seen substantial recent developments in several directions. Specifically, we single out the following three:

- The theory of point processes has transformed the field of mathematical diffraction theory (see [18] for a recent review). This has allowed for treatment of various random models as well as a solution to homometry problem for pure point diffraction.
- In the spectral theory of associated Schrödinger operators, an in depth analysis of fractal spectral features of the Fibonacci Hamiltonian has been accomplished.
- Various methods from dynamical systems have provided new perspectives on old problems.

These topics have been a special focus of attention at the conference. They will be discussed in further detail in the next section.

# **Presentation Highlights**

#### Random Operators: A Short (Hi)Story (Peter Stollmann)

This review talk was about random Schrödinger operators and their history:

- The Anderson model.
- The metal-insulator transition in spectral terms.
- The general formalism of random operators.
- Models with aperiodic order.

While the first sections concentrated on random models and the localization phenomenon, we mentioned in the last section results that treat aperiodically ordered models.

In his celebrated article [1] from 1958, P.W. Anderson proposed a mathematical model to explain the phase transition from insulator to metal in disordered solids. This has prompted intensive research both in mathematics and physics. Despite great progress, the state of the mathematically rigorous understanding of the metal insulator transition is still unsatisfactory: while there are now methods to prove that typical random models exhibit an energy interval with localization (pure point spectrum with rapidely decaying eigenfunctions), there is no rigorous proof of delocalization so far.

The situation is even harder for Hamiltonians that might be used to model quasicrystals. Apart from onedimensional results, there is little understanding. It is expected that such models will have purely singular continuous spectrum.

# Geometric realization for hyperbolic substitution tilings and an *n*-dimensional Pisot substitution conjecture (Marcy Barge)

Suppose that  $\Phi$  is an *n*-dimensional substitution (non-periodic, primitive, FLC) with linear expansion  $\Lambda$  and tiling space  $\Omega_{\Phi}$ . We seek a *geometric realization*  $G : \Omega_{\Phi} \to \mathbb{T}^D$  that semi-conjugates the inflation-andsubstitution homeomorphism  $\Phi$  on  $\Omega_{\Phi}$  with a hyperbolic toral automorphism F restricted to an invariant set of the torus  $\mathbb{T}^D$ . G should be homologically essential and as nearly one-to-one as possible. To accomplish this, we restrict to the case that  $\Lambda$  is *hyperbolic* (no eigenvalue has an algebraic conjugate on the unit circle) and *unimodular* (every eigenvalue of  $\Lambda$  is an algebraic unit).

There is a finitely generated  $\mathbb{Z}$ -module  $GR \subset \mathbb{R}^n$  restricted to which  $\Lambda$  is a linear isomorphism. Let D denote the rank of GR and let A be a  $D \times D$  integer matrix representing  $\Lambda : GR \to GR$  in some basis. (A is hyperbolic.) There is then a rank D submodule of  $H^1(\Omega_{\Phi};\mathbb{Z})$ , say  $\langle \gamma_1, \ldots, \gamma_D \rangle$ , invariant under  $\Phi^*$ , restricted to which  $\Phi^*$  is represented by the transpose of A. We proceed as follows. Each  $\gamma_i$  can be considered to be a (homotopy class of a) map  $\gamma_i : \Omega_{\Phi} \to \mathbb{T}$ , and their product yields  $\Gamma : \Omega_{\Phi} \to \mathbb{T}^D$ . We have  $\Gamma \circ \Phi$  equals  $F_A \circ \Gamma$  in cohomology ( $F_A$  being the hyperbolic toral automorphism induced by A). By lifting  $\Gamma$  to an appropriate abelian cover and applying a standard global shadowing procedure from hyperbolic dynamics, we homotope  $\Gamma$  to G.

We have shown that the  $G : \Omega_{\Phi} \to \mathbb{T}^D$  so constructed is continuous and obeys  $G \circ \Phi = F_A \circ G$ . Furthermore, G is a.e. r-to-one for some  $r \in \mathbb{N}$  and G is homologically essential in that  $G^* : H^1(\mathbb{T}^D; \mathbb{Z}) \to H^1(\Omega_{\Phi}; \mathbb{Z})$  is injective.

Moreover, if in addition  $\Lambda$  is *Pisot family*, and the *generalized degree*,  $D(\Lambda)$ , of  $\Lambda$  equals the rank D of GR, then G is surjective and also semi-conjugates the  $\mathbb{R}^n$ -action on  $\Omega_{\Phi}$  with a Kronecker action on  $\mathbb{T}^D$ .

Thus the coordinate functions of G give D independent continuous eigenfunctions of the  $\mathbb{R}^n$ -action on  $\Omega_{\Phi}$ . Under these conditions, the eigenvalues of the  $\mathbb{R}^n$ -action are relatively dense in  $\mathbb{R}^n$  and the tilings in  $\Omega_{\Phi}$  have the Meyer property. We conjecture the following: If  $\Phi$  is a unimodular Pisot family substitution and  $rank(H^1(\Omega_{\Phi};\mathbb{Z})) = D(\Lambda)$  then the  $\mathbb{R}^n$ -action on  $\Omega_{\Phi}$  has pure discrete spectrum.

(Based on joint work with J.-M. Gambaudo, see [5]).

#### Fibonacci numbers and representations of quivers (Claus-Michael Ringel)

It is well-known that the entries of the dimension vectors of some distinguished 3-Kronecker modules are the Fibonacci numbers; the 3-Kronecker modules are triples of matrices with the same shape, thus representations M of the quiver Q with two vertices a, b and three arrows  $a \rightarrow b$ . Using covering theory, one may consider instead of Q its universal covering  $\tilde{Q}$ , which is the 3-regular tree with bipartite orientation. Thus, instead of M, we now deal with a representations  $\tilde{M}$  of  $\tilde{Q}$ , but this means that the two vector spaces given by M are written as direct sums of a large number of much smaller vector spaces  $M_i$ . In terms of dimensions, we exhibit in this way partition formulae for the Fibonacci numbers. The dimensions of the vector spaces  $M_i$  can be arranged to form two triangles, one for the even-index Fibonacci numbers, the other for the odd-index ones, and one may compare the triangles with the Pascal triangle of binomial coefficients. These distributions of numbers are additive functions on valued translation quivers, but also they may be constructed inductively by using some hook formula. The hook formula shows that the numbers along the inclined lines can be obtained by evaluating monic integral polynomials (but the actual coefficients of these polynomials are not known). One column of the first triangle has been identified by Hirschhorn (2008) as the number of Delannoy paths which do not horizontally cross the main diagonal. It seems astonishing that no other row or column had hitherto been recorded in Sloane's Encyclopedia of Integer Sequence.

There are intriguing relations between the two triangles: for example, differences along suitable arrows in one triangle are numbers which occur in the other triangle. Also, the left hand side and the right hand side of the odd-index triangle determine each other. All these results were found by looking at certain exact sequences involving Fibonacci modules, but they can be verified also recursively. There is another interpretation of the numbers in the triangles, namely as dimensions of some (subspace) representations of the 3-regular tree, now with a unique sink and no sources.

### Stationary spatial stochastic processes and the inverse problem in pure point diffraction (Robert V. Moody)

The inverse problem in diffraction is the problem of recovering the physical distribution of a material from knowledge of its diffraction. The diffraction is a positive, centrally symmetric translation bounded measure in the Fourier dual space of the native space of the material. The question we raise ere is whether or not we can find solutions to this problem no matter what positive, centrally symmetric translation bounded measure we begin with.

The fundamental issue that arises in attempting to answer this question is what sort of mathematical object should we be looking for in trying to model the potential physical distribution of material whose diffraction is to be the given measure? In this paper we show that in the case of pure point diffraction we can always find solutions to this problem. These solutions come in the form of a new type of mathematical object which we call a stationary spatial stochastic process. The talk discussed the motivation for this concept out of ideas from stochastic point processes, and showed how it arises both as an extension of the Halmos-von Neumann theory of dynamical systems with pure point spectra and by a Gel'fand construction based on the eigenfunctions of the system.

At the end of the talk we discussed open problems around the explicit nature of the solutions created by the process, how the wealth of solutions to the problem may be filtered through the use of moments, and the apparent potential for some sort of cohomological extension to the theory.

The work is joint work with Daniel Lenz [12].

#### **Generalised Thue-Morse systems (Uwe Grimm and Franz Gähler)**

These two consecutive, closely related talks covered spectral and topological aspects of generalised Thue-Morse systems.

The first talk briefly summarised the proof of the purely singular continuous diffraction of the classical Thue-Morse sequence in the balanced weight case; see [18] and references therein. It then introduced generalised Thue-Morse substitutions generated by substitution rules  $1 \rightarrow 1^k \bar{1}^\ell$ ,  $\bar{1} \rightarrow \bar{1}^k 1^\ell$  on the two-letter alphabet  $\{1, \bar{1}\}$ , where  $k, \ell \ge 1$  and  $k = \ell = 1$  corresponds to the classical Thue-Morse case. All these rules give rise to purely singular diffraction measures in the balanced case. Their distribution functions possess

uniformly converging Fourier series expansions with coefficients which are determined recursively, and the corresponding densities can be expressed as Riesz products. The pure point part of the dynamical spectra are recovered by factors which arise from the same sliding block map as in the classical case; the corresponding substitutions are generalisations of the period-doubling rule. The talk ended by showing how this approach generalises to bijective substitutions in higher dimensions, and explicitly considered the example of the squiral tiling. Again, it shows singular continuous spectrum, and a factor with maximal pure point spectrum can be constructed using a suitable block map.

In the second talk, topological invariants, in particular Cech cohomology groups, were computed for the whole series of generalised Thue-Morse and generalised period-doubling tiling spaces. For this purpose, each of the tiling spaces was constructed as an inverse limit using the Anderson-Putnam construction. A tiling space is approximated by a finite cell complex (the AP complex) in such a way that the inverse limit of the substitution acting on the AP complex is homeomorphic to the tiling space. As a consequence, the Cech cohomology is given by the direct limit of the substitution action on the Cech cohomology of the AP complex. The AP complexes could be chosen in such a way, that the sliding block map from the generalised Thue-Morse tilings to the generalised period-doubling tilings extends to the respective AP complexes, intertwining the substitution maps acting on them.

As a result, not only the cohomology of the respective tiling spaces is obtained, but also the embedding of the generalised period-doubling cohomology in the generalised Thue-Morse cohomology. All these computations could be carried out for the whole series of tiling spaces parametrised by the natural numbers k and  $\ell$ . Using results recently derived by Greg Maloney (also presented at the workshop), the number of different AP complexes could be reduced to three for each of the generalised Thue-Morse and generalised period-doubling tiling spaces. The remaining dependence on k and  $\ell$  is only in the substitution maps. For all choices of k and  $\ell$ , the substitution acts with eigenvalues  $k + \ell$ ,  $k - \ell$  and -1 on the cohomology of generalised Thue-Morse tiling spaces. From these results, also the dynamical zeta function for the substitution action on the continuous hull is readily derived.

(Based on joint work with Michael Baake).

# Three aperiodic questions and their (lack of) progress (Aernout C.D. van Enter and Jacek Miękisz)

In this presentation, the following three questions were discussed, based on an ongoing collaboration between 1988 and 2000, and also further progress on them in so far as that occurred.

Question 1: Aperiodic order as order. How should one describe long-range order, and give spectral characterisations thereof?

Question 2: Where does aperiodic order come from? Can one find models of quasicrystals or 'weak crystals' in which either ground states or Gibbs states display aperiodic order?

Question 3: Aperiodic order as disorder. Can one compute and obtain interesting aperiodic examples of the Parisi overlap distribution (which was introduced for the paradigmatic disordered model, spin glasses)?

As for Question 1, in [11] the authors investigated the distinction between what is now called "diffraction versus dynamical spectrum", with an interpretation in terms of of atomic versus molecular long-range order. It became well-known afterwards, based on work by Baake, Lee, Lenz, Moody, Scholttmann and Solomyak, that pure point diffraction and pure point dynamical spectrum, under some mild assumptions, are equivalent properties of dynamical systems of translation bounded measures. But this type of equivalence does not extend to systems with continuous spectrum, as the example of the Thue-Morse sequences showed [11]. The diffraction spectrum of the Thue-Morse system is purely singular continuous, while the dynamical spectrum has a non-trivial pure point part in form of the dyadic rationals. This spectral information is not reflected in the diffraction spectrum.

However, this 'missing' part can be extracted from the diffraction of a factor, the so-called period doubling sequences, which are Toeplitz sequences. In [4], an even simpler example of this phenomenon is presented for a one-dimensional system of random dimers, which can be of +- or -+ type, and which can be located on 2n, 2n + 1 or on 2n, 2n - 1 intervals. This system has absolutely continuous diffraction spectrum, but the long-range order associated to the location of the dimers provides an additional point in the dynamical spectrum. It thus appears that molecules can be more, but not less, ordered than their constituent atoms. A

completely general statement to this effect is not yet available, however.

About Question 2, one can construct aperiodic tilings which are ground states for nearest-neighbor (tiling) models, or as aperiodic sequences, which are ground states for long-range interactions. Some stability and intrinsic frustration properties for tiling models have been proved, but as for positive temperatures (Gibbs states), one is still restricted to one-dimensional aperiodic long-range order, which occurs for infinite-range interactions. This can occur for one-dimensional long-range models, or for exponentially decaying interactions which are stabilised in two other directions; compare [14, 15]. To prove the existence of a quasicrystalline state for a short-range model remains open.

About Question 3, it was observed in [10] that continuous diffraction spectrum implies a trivial overlap distribution, whereas the Fibonacci sequences provide an example with a continuous overlap distribution and the period-doubling Toeplitz sequences have a discrete, ultrametric overlap distribution. Recently, in [9], this was extended to show that continuous overlap distributions occur for general Sturmian sequences (= 'balanced words' = 'most homogeneous configurations'). Moreover, for paperfolding sequences, a discrete ultrametric overlap distribution with dense support was found. Although in the theory of spin glasses a huge progress has occurred for mean-field models of the Sherrington-Kirkpatrick type (due especially to Guerra and Talagrand), not much is known about short-range models. Aperiodic examples may thus play a useful role in illustrating various possibilities. For instance, the fact that the overlap distribution is disorder-independent becomes much more plausible once one realises that one does not need disorder at all to obtain nontrivial overlap distributions. It would be interesting to obtain examples also in higher dimensions, via tiling constructions.

#### **Random measures and diffraction (Matthias Birkner)**

This talk elaborated an observation (due to Jean-Baptiste Gouéré) that connects the autocorrelation of a random measure with its so-called Palm distribution, a well-studied object in the fields of random measures and in stochastic geometry: Let  $\Phi$  be a shift-ergodic signed random measure on  $\mathbb{R}^d$  with locally square integrable total variation. Then, the natural autocorrelation  $\lim_{n\to\infty} \frac{1}{\operatorname{vol}(B_n)} \Phi|_{B_n} * \Phi|_{B_n}$  exists almost surely and is non-random ( $B_n$  denotes the ball of radius n around the origin and  $\Phi|_{B_n}$  the restriction to that ball). It is given by the reduced second moment measure and can, in the case of a positive random measure, also be interpreted as the (scaled) intensity measure of the Palm distribution, Here, the latter has a natural interpretation as the configuration of  $\Phi$  viewed 'from a typical point drawn from  $\Phi$ '. The result was illustrated by explicitly computing the autocorrelation and the diffraction, its Fourier transform, for various cluster processes. These confirm the observation that additional randomness, coming from the independent clusters, modifies the diffraction of a given point process by adding an absolutely continuous component.

(This contribution is based on joint work with M. Baake and R. V. Moody [2]).

#### Dynamical methods in spectral theory of quasicrystals (Anton Gorodetski)

The Fibonacci Hamiltonian is a central model in the study of electronic properties of one-dimensional quasicrystals. It was shown by Süto that its spectrum is a zero-measure Cantor set for every non-zero value of the coupling constant. The question on the properties of the spectrum can be reduced to the question on dynamical properties of a so called trace map. In our joint work with David Damanik [7, 8], we studied the dynamical properties of the trace map and used them to describe the spectral properties of the Fibonacci Hamiltonian. In particular, we showed the following:

(i) For sufficiently small values of the coupling constant, the boundary points of a gap in the spectrum depend smoothly on the coupling constant. Moreover, the size of the gap tends to zero linearly as the coupling constant tend to zero;

(ii) For small values of the coupling constant, we have that the sum of the spectrum with itself is an interval. Therefore, the spectrum of the square Fibonacci Hamiltonian is an interval for small values of the coupling constant;

(iii) For small values of the coupling constant, the density of states measure of the Fibonacci Hamiltonian is exact-dimensional, the almost everywhere value of the local scaling exponent is a smooth function of the coupling constant, is strictly smaller than the Hausdorff dimension of the spectrum, and converges to one as coupling constant tends to zero.

#### **On Proximality (Johannes Kellendonk)**

Given a dynamical system  $(X, G, \alpha)$  where X is a compact metric space, G a locally compact,  $\sigma$ -compact, Abelian group and  $\alpha$  a minimal group action, we investigate the proximality relation  $P \subset X \times X$ . Two points  $x, y \in X$  are *proximal* if  $\inf_{t \in G} d(\alpha_t(x), \alpha_t(y)) = 0$ , where d is the metric on X. We are in particularly interested in tiling or Delone dynamical systems, because the nature of the diffraction spectrum of the Delone set is tightly related to the spectral type of the dynamical spectrum of the system, and the latter can be studied with the help of the proximal relation, as will be developed.

The continuous eigenfunctions determine what is called the maximal equicontinuous (or Kronecker) factor of the dynamical system and the factor map  $\pi$  gives rise to an equivalence relation  $R_{\pi} = \{(x, y) : \pi(x) = \pi(y)\}$  which contains P. The question is, how large are the typical equivalence classes of  $R_{\pi}$ , and in which way do they differ from the equivalence classes of P? This also leads to considering the minimal rank i.e. the smallest number of elements in an equivalence class of  $R_{\pi}$  and the set  $Y \subset X/R_{\pi}$  of equivalence classes which contain only pairwise non-proximal points.

(Based on joint work with Marcy Barge [6]).

#### Measuring the complexity of tilings with infinite local complexity (Lorenzo Sadun)

A standard assumption in studying tilings is that there should only be a finite number of connected 2-tile patterns, up to translation. This is called Finite Local Complexity, or FLC. However, many interesting tilings have Infinite Local Complexity (ILC), either because there are infinitely many tile types, or because the tiles can slide past one another in a continuous manner. Examples include the pinwheel tiling, Toeplitz flows (which can model solenoids), and many fusion tilings.

Adapting a construction from the topological entropy of flows, we define a complexity function  $C(\epsilon, L)$  at precision  $\epsilon$  and length scale L. The important question is how this function behaves as  $L \to \infty$  for fixed  $\epsilon$ , and whether this behavior (e.g., bounded, or polynomial growth, or exponential with a particular exponent) is the same for all small  $\epsilon$ . Such behavior is invariant under topological conjugacies. The behavior as  $\epsilon \to 0$  for fixed L is *not* invariant, and is far less meaningful.

### **Scientific Progress Made**

The main goal of the meeting was to bring people from the field of Aperiodic Order together and to exchange the recent advances, with some focus on spectral aspects. The field is developing rapidly, and expanding into a variety of directions. After several more specialized meeting (for instance on the topology of tiling spaces), this exchange was needed to keep track of the developments. We believe that this goal was fully reached.

Moreover, due to the different but related questions in neighbouring disciplines, it was a good opportunity to discuss with colleagues and start new collaborations. One notable instance emerged from the interaction between Aernout van Enter and two of the organisers (MB and DL), pointing a way to reach an equivalence result for dynamical versus diffraction spectrum beyond the pure point situation. Another instance is the realization that the work on tridiagonal matrices with Fibonacci diagonals and off-diagonals presented by William Yessen contains ideas that will be useful in a different context, namely orthogonal polynomials on the unit circle, where the obstacle of energy-dependence of a key quantity may be overcome by implementing those ideas in this context. This will be carried out in a collaboration between three of the workshop participants.

### **Outcome of the Meeting**

The mathematical theory of aperiodic order was systematically started with the NATO workshop in 1995 and the ensuing long-term program at the Fields Institute, both organised by Robert V. Moody and Jiri Patera. The field has seen a steady development since then, and is likely to get some further push now by the Nobel Prize to Shechtman. This meeting was central in the sense that it showed how diverse the questions are, yet how well the different mathematical disciplines worked and work together to further our knowledge and understanding. It is fair to say that the interactive atmosphere of the meeting was outstanding, and that important directions for future research could be identified.

In summary, for a field like this, there is no alternative to an attractive meeting place such as BIRS or Oberwolfach, and we are confident that particularly this meeting initiated quite a number of high quality cooperations and publications.

### **Participants**

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# Chapter 31

# **Proof complexity (11w5103)**

# Oct 02 - Oct 07, 2011

**Organizer(s):** Samuel Buss (University of California, San Diego) Stephen Cook (University of Toronto) Antonina Kolokolova (Memorial University of Newfoundland) Toni Pitassi (University of Toronto) Pavel Pudlak (Institute of Mathematics, Prague)

### **Overview of the Field**

Proof complexity is a research area that studies the concept of complexity from the point of view of logic. In proof complexity, an important question is: "how difficult is it to prove a theorem?" There are various ways that one can measure the complexity of a theorem. We can ask what is the length of the shortest proof of a theorem in a given formal system (size of the proofs) or how strong a theory is needed to prove the theorem (that is, how complex are the concepts involved in the proof). The former is studied in the context of proof systems (in particular, propositional proof systems), the latter in bounded arithmetic.

Naturally, the length of a shortest proof of a theorem very much depends on the type of proof system in which it is being proved. For a proof system, we also would like to know if there is an efficient algorithm that would produce a proof of any tautology, and whether it would produce a shortest such proof. These questions, besides their mathematical and philosophical significance, have practical applications in automated theorem proving.

From the computational point of view, the question of proving tautologies is a co-NP question: that is, a counterexample to a formula which is not a tautology would be short and easily verifiable. Moreover, it is known that the existence of a propositional proof system in which all tautologies have short proofs is equivalent to proving that NP is closed under complementation. This establishes an important link between proof complexity and a major open problem in computational complexity theory. There are other connections between computational and proof complexity (for example, circuit lower bounds and proof system lower bounds), although in some cases the proof complexity counterparts of computational complexity results are still unresolved.

A related, uniform side of proof complexity is the study of weak systems of arithmetic (in particular, bounded arithmetic). Here the complexity of a proof of a theorem is defined in terms of the complexity of concepts involved in that proof. For example, the weaker systems of arithmetic cannot operate with concepts such as the Pigeonhole Principle. A recent subarea of proof complexity, called bounded reverse mathematics, studies the complexity of reasoning needed to prove a given theorem: that is, what is the weakest theory in which a given mathematical theorem can be proven.

Proof complexity historically was developed during the 1960's and 1970's, as an outgrowth of research on computer-based theorem provers. At first, researchers in proof complexity concentrated primarily on lower bounds on proof size, and targeted lower bounds on computational complexity (for instance, Cook's characterization of the NP=?coNP problem in terms of proof complexity) and independence results in formal

theories such as bounded arithmetic (the theories  $I\Delta_0$  and PV at first, and later fragments such as  $S_2^i$  and  $T_2^i$ .) More recently, especially in the past 10-15 years, proof complexity has become increasingly concerned with problems in computer-based proof search again. This aspect was well-represented at the BIRS workshop, with talks on resolution, on SAT solvers, on linear programming, and on semi-definite programming. This renewed interest by the proof complexity community in practical computer-based theorem provers is a welcome development. Indeed, it is hoped that significant future developments will arise from these two strands of proof complexity, namely from the interplay between the lower bounds on proof complexity and computational complexity, and the upper bounds of improved algorithms for theorem proving.

### **Recent Developments**

Proof complexity is an active field of research. This interdisciplinary area is recognized as a respectable field both in computational complexity and in proof theory. The number of papers published, as well as the number of researchers working in proof complexity steadily increases. The present workshop documented the viability of this field.

There are many directions of research in proof complexity. A large part of these directions was represented in the workshop. Due to space limitations we mention only a few of them in this report.

#### **Resolution and SAT-solvers**

SAT solvers, or "satisfiability solvers" represent the state of the art in *practical* algorithms for determining the satisfiability of propositional formulas (usually given as sets of clauses). The solvers have been quite successful (indeed, unexpectedly successful) in solving large instances of SAT that arise in applications for software verification, hardware verification, and many other areas. The most successful solvers to date for these kinds of applications are based on the DPLL (Davis-Putnam-Logemann-Loveland) search procedures that use the clause learning method of Marques-Silva and Sakallah.

Resolution proof system was introduced in automated theorem proving. Thus the study of this system is motivated by practical problems. However, it is also a basic proof system in the theoretical study of proof systems. Resolution is also tightly connected with SAT-solvers. Namely, DPLL, the most commonly used tool in solving SAT is just one facet of the tree-like proofs based on Resolution. Recent advances in the study of Resolution were mostly motivated by connections with SAT-solvers. Lower bounds and trade-offs between various parameters of resolution proofs can explain why certain SAT-solvers are not efficient in certain situations. One set of such results was presented in the lecture of Jakob Nordström. These results are described in the section Highlights.

#### **Presentation highlights**

The main highlight of this topic of the workshop was a talk by Jakob Nordstrom (KTH) on "Understanding the Hardness of Proving Formulas in Propositional Logic". This was a survey talk, covering both the Resolution proof system and SAT solvers, and emphasizing the interplay between them. In particular, some new results on formula space complexity in the Resolution setting and their relation to SAT solver performance were discussed. The full description of the talk is below:

#### Jakob Nordstrom, Understanding the Hardness of Proving Formulas in Propositional Logic.

Abstract: Proving formulas in propositional logic is believed to be theoretically intractable in general, and the importance of deciding whether this is so has been widely recognized, e.g., by this being listed as one of the famous million dollar Millennium Problems. On the practical side, however, these days SAT solvers are routinely used to solve large-scale real-world SAT instances with millions of variables. This is in contrast to that there are also known small example formulas with just hundreds of variables that cause even state-of-the-art SAT solvers to stumble.

What lies behind the spectacular success of SAT solvers, and how can one determine whether a particular formula is hard or tractable? In this talk, we will discuss if proof complexity can say anything interesting about these questions.

In particular, we propose that the space complexity of a formula could be a good measure of its hardness. We prove that this would have drastic implications for the impossibility of simultaneously optimizing time and memory consumption, the two main resources of SAT solvers. Somewhat surprisingly, our results are obtained by relatively elementary means from combinatorial pebble games on graphs, studied extensively in the 70s and 80s.

Joint work with Eli Ben-Sasson.

#### Some other notable talks in this area<sup>1</sup>

Another problem recently studied in proof complexity concerns various modifications of DPLL that are used in SAT-solvers. In order to prove bounds on these proof system it is necessary to find corresponding modifications of Resolution. The most successful SAT-solvers use clause learning. Advantages and limits of this method were presented in two talks devoted to the analysis of clause learning:

#### Jan Johannsen, Lower Bounds for Width-restricted Clause Learning

Abstract: Clause learning is a technique used by propositional satisfiability solvers where some clauses obtained by an analysis of conflicts are added to the formula during backtracking. It has been observed empirically that clause learning does not significantly improve the performance of a solver when restricted to learning clauses of small width only. We survey several lower bound theorems supporting this experience.

Sam Buss, An Improved Separation of Regular Resolution from Proof Resolution and Clause Learning.

Abstract: We prove that the graph tautology principles of Alekhnovich, Johannsen, Pitassi and Urquhart have polynomial size pool resolution refutations using only input lemmas as learned clauses and without degenerate resolution inferences. Consequently, these can be shown unsatisfiable by polynomial size DPLL proofs with clause learning.

#### **Subsystems of Bounded Arithmetic**

In Bounded Arithmetic first order theories are studied that have close connection with complexity classes in computational complexity and proof systems in propositional logic. The research in this subarea focuses on the following problems:

- finding the weakest theory in which a given theorem from computational complexity can be proven,
- separating theories corresponding to complexity classes,
- characterizing low complexity theorems of a given theory.

There is a lot of interaction going on between bounded arithmetic and computational complexity. For instance, in recent years several characterizations of  $\forall \Sigma_1^b$  theorems of the theories  $T_2^n$  of the bounded arithmetic hierarchy have been found. These results introduced new classes of total polynomial search problems that were not known before.

#### **Presentation highlights**

In a videotaped lecture Stephen Cook presented a survey of first order theories associated with complexity classes. In the second part of the lecture he talked about formalizing matching algorithms.

#### Stephen Cook, Formalizing Randomized Matching Algorithms

Abstract: Using Jeřábek's framework for probabilistic reasoning, we formalize the correctness of two fundamental RNC2 algorithms for bipartite perfect matching within the theory VPV for polytime reasoning. The first algorithm is for testing if a bipartite graph has a perfect matching, and is based on the Schwartz-Zippel Lemma for polynomial identity testing applied to the Edmonds polynomial of the graph. The second algorithm, due to Mulmuley, Vazirani and Vazirani, is for finding a perfect matching, where the key ingredient of this algorithm is the Isolating Lemma.

Joint work with Dai Tri Man Le.

<sup>&</sup>lt;sup>1</sup>Due to space limitation we mention only two talks. The abstracts of other high quality talks can be found in the materials of the workshop. The same applies to the following sections.

#### Some other notable talks in this area

Theories for approximate counting appeared also in another lecture. Leszek Kolodziejczyk talked about the problem of separating these theories from theories  $T_2^n$ .

#### Leszek Kolodziejczyk, Fragments of approximate counting.

Abstract: We study the low-complexity consequences of Jerabek's theory of approximate counting, that is,  $T_2^1$  plus the surjective weak pigeonhole principle for  $P^N P$  functions, with the goal of showing that it does not prove all the  $\Sigma_1^b$  sentences provable in full bounded arithmetic. This is inspired by the question of whether the levels of the bounded arithmetic hierarchy can be separated by a sentence of fixed low complexity, and the related question of whether the CNFs provable in constant depth Frege systems form a hierarchy with depth. We give some partial results. Joint work with Sam Buss and Neil Thapen.

Emil Jeřábek talked about a problem that apparently does not have much to do with proof complexity. But in fact the problem is highly motivated by proof complexity and has an interesting consequence for first order theories studied in bounded arithmetic.

#### Emil Jeřábek, Root finding in $TC^0$ .

Abstract: We show that for any constant d, there is a uniform  $TC^0$  algorithm computing approximations of complex zeros of degree-d univariate rational polynomials (given by a list of coefficients in binary). Equivalently, the theory  $VTC^0$  + the set of all true  $\forall \Sigma_0^B$  sentences includes IOpen (for the string sort).

#### Proof systems for integer linear programing

Another important subarea of proof complexity is the study methods used in integer linear programing by means of propositional proof systems. For example, using a machinery developed in proof complexity it has been shown that there are instances of integer linear programing that cannot be solved in subexponential time by the well-known method of cutting planes. For most methods such lower bounds are not known yet, but some partial results have been obtained.

#### **Presentation highlights**

The most impressive lecture on this topic was given by Albert Atserias. He showed how to combine methods of finite model theory and integer linear programing to prove results about the graph isomorphism problem. Here is a more detailed description of the lecture.

#### Albert Atserias, Sherali-Adams Relaxations and Indistinguishability in Counting Logics.

Abstract: Two graphs with adjacency matrices **A** and **B** are isomorphic if there exists a permutation matrix **P** for which the identity  $\mathbf{P}^{T}\mathbf{A}\mathbf{P} = \mathbf{B}$  holds. Multiplying through by **P** and relaxing the permutation matrix to a doubly stochastic matrix leads to the linear programming relaxation known as fractional isomorphism. We show that the levels of the Sherali-Adams (SA) hierarchy of linear programming relaxations applied to fractional isomorphism interleave in power with the levels of a well-known color-refinement heuristic for graph isomorphism called the Weisfeiler-Lehman algorithm, or equivalently, with the levels of indistinguishability in a logic with counting quantifiers and a bounded number of variables. This tight connection has quite striking consequences. For example, it follows immediately from a deep result of Grohe in the context of logics with counting quantifiers, that a fixed number of levels of SA suffice to determine isomorphism of planar and minor-free graphs. We also offer applications both in finite model theory and polyhedral combinatorics. First, we show that certain properties of graphs, such as that of having a flow-circulation of a prescribed value, are definable in the infinitary logic with counting with a bounded number of variables. Second, we exploit a lower bound construction due to Cai, Fürer and Immerman in the context of counting logics to give simple explicit instances that show that the SA relaxations of the vertex-cover and cut polytopes do not reach their integer hulls for up to  $\Omega(n)$  levels, where n is the number of vertices in the graph.

Joint work with Elitza Maneva.

This was the other of the two videotaped lectures.

#### Another notable talk in this area

The study of the constraint satisfaction problem is a very active area in theoretical computer science. This is because many practical problems can be represented as a particular type of the constraint satisfaction problem. Therefore it is important to understand the computational complexity of constraint satisfaction problems for natural classes. Konstantinos Georgiou studied a particular form of the problem from the point of view of the Sherali-Adams method.

Konstantinos Georgiou, Refuting CSPs require Sherali-Adams SDPs of Exponential Size, due to Pairwise Independence.

Abstract: This work considers the problem of approximating fixed predicate constraint satisfaction problems (MAX k-CSP(P)). We show that if the set of assignments accepted by P contains the support of a balanced pairwise independent distribution over the domain of the inputs, then such a problem on n variables cannot be approximated better than the trivial (random) approximation, even after augmenting the natural semidefinite relaxation with  $\Omega(n)$  levels of the Sherali-Adams hierarchy. It was recently shown that under the Unique Game Conjecture, CSPs for predicates satisfying this condition cannot be approximated better than the trivial approximation. Our results can be viewed as an unconditional analogue of this result in a restricted computational model. Alternatively, viewing the Sherali-Adams SDP system as a proof system, our result states that a proof of exponential size is required in order to refute highly unsatisfiable instances. For our result we introduce a new generalization of techniques to define consistent local distributions over partial assignments to variables in the problem, which is often the crux of proving lower bounds for such hierarchies.

This is joint work with Siavosh Benabbas, Avner Magen and Madhur Tulsiani.

### **Other topics**

A very interesting lecture was given by a leading expert in computational and proof complexity Alexander Razborov. He developed a theory, which he calls *flag algebras*, for proving results in extremal combinatorics. His aim his to solve problems of the type of Turán's Conjecture from 1941 and the Cacceta-Häggkvist Conjecture. He did not prove any of these two conjectures, but made a substantial progress towards the solution. What is the most interesting aspect of his approach is that it is completely new. Here is the abstract of his talk.

#### Alexander Razborov (University of Chicago), Flag algebras.

Abstract: A substantial part of extremal combinatorics studies relations existing between densities with which given combinatorial structures (fixed size "templates") may appear in unknown (and presumably very large) structures of the same type. Using basic tools and concepts from algebra, analysis and measure theory, we develop a general framework that allows to treat all problems of this sort in an uniform way and reveal mathematical structure that is common for most known arguments in the area. The backbone of this structure is made by commutative algebras defined in terms of finite models of the associated first-order theory.

In this talk I will give a general impression of how things work in this framework, and we will pay a special attention to concrete applications of our methods.

# **Panel discussion**

During the workshop we had a panel discussion on the future of proof complexity. Due to the presence of most of the leading experts in the field it was a unique opportunity to discuss such strategic problems, and the panel discussion proved to be highly stimulating. Many participants proposed research directions for the field, as well as suggested open problems (see below). The panel discussion was viewed by most participants very positively — interesting and informative.

### Problems

During the workshop many open problems were suggested in the talks, as well during the panel discussion. Thus, we decided to make a compendium of open problems suggested by the participants and include it here in the report.

#### List of problems

- 1. Separate levels of  $T_2^k[R]$  hierarchy: We don't know a k such that sentences  $\forall \Sigma_k^b$  would separate levels. This corresponds to separating levels of bounded-depth Frege systems (a well-known problem). During the panel discussion Pavel Pudlák pointed out that, although the problem is hard, we probably do have means to solve it.
- 2. (Antonina Kolokolova, panel discussion) More connections between finite model theory and proof complexity, in the spirit of Albert Atserias and Yijia Chen's work.
- 3. (Oliver Kullmann, panel discussion) Look at single instances for SAT.
- 4. (Sam Buss, panel discussion) Look at SMT solvers and higher order setting: relax conditions at SMT setting, analyze counterexample guided abstraction refinement.
- 5. (Paul Beame, panel discussion) How to do an analog of clause learning in the integer programming setting (e.g., learning an equation)? What are the limitations of integer linear programming?
- 6. (Jan Johannsen, panel discussion) Algorithms vs proof systems question, e.g., DLL vs. tree resolution, DLL+CL vs. WRTC.
- 7. (Russell Impagliazzo, panel discussion)
  - (a) Dynamic programming analysis similar to resolution.
  - (b) Proof complexity of satisfiable instances. E.g., myopic searches. We can bound the time needed on unsatisfiable formulas, but can we do it also for satisfiable?
  - (c) Find problem solvable in B-ODI, but not in backtracking trees.
- 8. (Toni Pitassi, panel discussion) Lower bounds for stronger proof systems. Also, approximation algorithms vs. LS, Lasserre, etc.
- 9. (Alasdair Urquhart) What is the complexity of determining the minimum regular width of a set of clauses? (Conjecture: PSPACE-complete).
- 10. (Moshe Vardi via Alasdair Urquhart) What is the complexity of determining the resolution width of a set of clauses? (Conjecture: EXPTIME-complete).
- 11. (Alasdair Urquhart) Prove or disprove: The Tseitin graph tautologies always have a regular proof with minimal size. Same question for the pigeonhole principle.
- 12. (Alexander Razborov) Unconditional size lower bounds for "simple" proof systems like Cutting Planes (combinatorial, without interpolation) or Lovasz-Schrijver.
- 13. (Albert Atserias and Alexander Razborov) Prove that the integrality gap of 2 for Vertex Cover problem survives  $\Omega(n)$  rounds of Sherali-Adams without Unique Games conjecture.
- 14. (Toni Pitassi and Alexander Razborov) Remove restrictions in Pitassi/Patrascu's upper bound being close to optimal.
- 15. (Jakob Nordström and Alexander Razborov) Is there a tautology with superlinear lower bounds on (total) variable space? This problem was listed in 2002 paper by M. Alekhnovich, E. Ben-Sasson, A. Razborov and A. Wigderson "Space complexity in propositional calculus". In particular, are there polynomial-size *k*-CNF formulas with total refutation space  $\Omega((sizeof)F)^2$  in resolution?

- (Jakob Nordström and Alexander Razborov) Prove superconstant clause space lower bounds for PCR or Cutting Planes proofs for any bounded fan-in tautology. (The question for PCR also appears in ABRW'02 paper).
- 17. (Jakob Nordström) Is tractability captured by space complexity? That is, do theoretical trade-offs show up in real life for state-of-the-art SAT solvers run on pebbling contradictions?
- 18. (Jakob Nordström) Can the Substitution Theorem be proven for, say, Cutting Planes or Propositional Calculus (with or without Resolutions), thus yielding time-space trade-offs for these proof systems as well?
- 19. (Jakob Nordström) Are there superpolynomial trade-offs in resolution for formulas refutable in constant space? Can every proof be carried out in at most linear space?
- 20. (Stephen Cook) Use Emil Jerabek's techniques to formalize constructive aspects of fundamental theorems that require probabilistic reasoning. This includes theorems in cryptography, such as the Goldreich-Levin Theorem, and construction of pseudo-random number generators from one-way functions.
- 21. (Stephen Cook) A very recent paper by Pavel Hrubes and Iddo Tzameret proves that the 'hard matrix identities' (such as AB = I implies BA = I) over certain rings have quasi-polynomial size Frege proofs. The big open question here is: does this result have a uniform version? This would involve formalizing these identities in a suitable theory such as those introduced by Stephen Cook and Lila Fontes: "Formalizing Linear Algebra", CSL 2010.
- 22. (Edward Hirsch) Devise an "interesting" heuristic proof system, i.e., a heuristic proof system that makes an advantage over classical proof systems for a problem that possesses no known polynomially bounded heuristic acceptor.
- 23. (Leszek Kolodziejczyk) Can Jerabek's theory for approximate counting, i.e.  $T_2^1(\alpha)$  plus the surjective WPHP for  $PV_2(\alpha)$  functions, be separated from full  $S_2(\alpha)$  by an NP search problem?
- 24. (Leszek Kolodziejczyk) Is there a sequence  $\{A_n : n \ge 1\}$  of narrow (polylog width) CNFs, with  $size(A_n) = poly(n)$ , that does have short constant-depth refutations, but does not have quasipolynomial-size treelike "random Res(log) refutations". More precisely, this means that there should be no quasipolynomial-size treelike Res(log) refutations of  $A_n \wedge B_n$ , where  $B_n$  is any narrow CNF true under at least a 1 (1/n) fraction of all truth assignments.

### **Scientific Progress Made**

Participants of the workshop reported on many opportunities for collaborations, some just starting and some for which the resulting papers are already in preparation. In particular, Jan Johannsen and Sam Buss have obtained during the workshop new results about the provability of the obfuscated Stone tautologies in reg-WRTI and in DPLL with clause learning; a planned paper is in preparation. Albert Atserias and Moritz Müller reported that they made a significant progress on their joint work on general lower bounds for daglike Res(k) system during the workshop (in preparation). There was a discussion between Stephen Cook, Russell Impagliazzo, Valentine Kabanets and Antonina Kolokolova after Stephen Cook's talk which is leading to an ongoing collaboration on formalizing a more general version of Schwartz-Zippel lemma. Alasdair Urquhart said he made plans to continue collaboration with Oliver Kullmann; he also reported that his conversations with Toni Pitassi about clause learning should result in a joint publication. Another collaboration project was between Sebastian Müller, Jan Johannsen, Moritz Müller and Iddo Tzameret; they have arranged follow-up research visits. Many results presented at the workshop were work in progress and papers in preparations; participants commented on obtaining helpful feedback.

A solution to one of the problems suggested during the panel discussion was solved by a person who was not able to attend, Jan Krajíček, when student participants from the same research group recounted to him the workshop events. A note on this is written and available from Krajíček's website.

# **Participants**

Aehlig, Klaus (Universität München) Atserias, Albert (Universitat Politecnica de Catalunya) Beame, Paul (University of Washington) Beck. Chris (Princeton University) Beyersdorff, Olaf (Leibniz University Hannover) Buss, Samuel (University of California, San Diego) Cook, Stephen (University of Toronto) Edmonds, Jeff (York University) Galesi, Nicola (Università degli Studi di Roma La Sapienza) Gallagher, Jonathan (University of Calgary) Georgiou, Konstantinos (University of Waterloo) Ghasemloo, Kaveh (University of Toronto) Hirsch, Edward (Steklov Institute of Mathematics at St. Petersburg) Hrubes, Pavel (University of Calgary) Impagliazzo, Russell (University of California, San Diego) Jerabek, Emil (Mathematical Institute AS CZ) Johannsen, Jan (LMU Munich) Kabanets, Valentine (Simon Fraser University) Kolodziejczyk, Leszek (University of Warsaw) Kolokolova, Antonina (Memorial University of Newfoundland) Kullmann. Oliver (Swansea University) Kuroda, Satoru (Gunma Prefectural Women's University) Lauria, Massimo (Institute of Mathematics AS CR) Maciel, Alexis (Clarkson University) Mueller, Moritz (CRM Centre de Recerca Matemtica) Muller, Sebastian (Charles University) Nguven, Phuong (McGill) Nordstrom, Jakob (KTH Royal Institute of Technology) Pankratov, Denis (University of Chicago) Pich, Jan (Charles University) Pitassi, Toni (University of Toronto) Pollett, Chris (San Jose State University) Pudlak, Pavel (Institute of Mathematics, Prague) **Razborov, Alexander** (Institute for Advanced Study) Robere, Robert (Memorial University of Newfoundland) Soltys, Michael (McMasters University) Thapen, Neil (Mathematical Institute AS CR) Tzameret, Iddo (Tsinghua University) Urguhart, Alasdair (University of Toronto) Wang, Zi Chao (Charles University in Prague)

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# Chapter 32

# **High Dimensional Probability (11w5122)**

# Oct 09 - Oct 14, 2011

**Organizer(s):** Richard M. Dudley (Massachusetts Institute of Technology) Christian Houdr (Georgia Institute of Technology) David M. Mason (University of Delaware) Jan Rosinski (University of Tennessee) Jon Wellner (University of Washington)

# **Overview of the Field**

Problems in probability theory increasingly involve high dimensions either in the basic sample spaces or in the dimensionality of the classes of functions or sets involved. In statistical problems, this occurs via the vast and fast data collection made possible by new generations of instrumentation in areas as diverse as microarray data in genetics, cosmic background microwave radiation measurements in astronomy, and new imaging methods in medicine and biophysics. Similarly, real world problems of interest in combinatorial optimization are high-dimensional in nature.

High Dimensional Probability is an area of mathematical research with deep roots in the classical limit theorems of probability. The problems of major focus to researchers in this area initially arose from the study of limit theorems in infinite-dimensional spaces such as Hilbert spaces, Banach spaces and normed linear spaces. Interest and motivation for such results goes back at least to the work of Glivenko-Cantelli, Kolmogorov-Smirnov and Donsker on the large sample behavior of empirical distribution functions.

The desire to provide a rigorous framework for the derivation and understanding of results of this type was the primary impetus for the development of a general theory of limit theorems in infinite dimensions. This goal has in large part been achieved.

But the most remarkable feature of this program is that it has resulted in the creation of powerful new tools and perspectives, whose range of application has extended far beyond its original purpose, and with an increasing number of interactions with other areas of mathematics, statistics, and computer science. These include additive combinatorics, random matrix theory, nonparametric statistics, empirical process theory, statistical learning theory, strong and weak approximations, distribution function estimation in high dimensions, combinatorial optimization, and random graph theory. For example, lately we have seen surprising connections between high dimensional probability and dependent sequences in additive combinatorics, and between concentration of measure inequalities and statistics.

High dimensional probability theory continues to develop innovative new tools, methods, techniques and perspectives to analyze the increasingly manifold phenomena happening around us.

### **Outcome of the Meeting**

The primary objectives of this workshop were:

(1) To bring together experts in high dimensional probability and those in a number of the "areas of strong interaction" to discuss some of the major problems in this area and report on progress towards their solution.

(2) To facilitate interactions and communications between the experts actively involved in the development of new theory in high dimensional probability, and leading researchers in statistics, machine learning, and computer science. Our intention is to deepen contacts between several different communities with common research interests focusing on probability inequalities, empirical processes, strong approximations, Gaussian and related chaos processes of higher order, Markov processes, and applications of these methods to a wide range of problems in other areas of mathematics or to applications in statistics, optimization theory, and machine learning.

(3) To foster and develop interest in this area of research. There are many interesting and exciting problems, which can be formulated in a way that can be understood by graduate students, postdoctoral students, and new researchers.

Our goal was to focus on the following areas:

A. Applications of concentration of measure results and methods to random matrices.

B. Concentration of measure inequalities.

C. Interactions between small ball probabilities, approximation theory, prior distributions for nonparametric Bayes procedures, entropy bounds for high-dimensional function classes.

D. Applications of high dimensional probability methods to analysis and stochastic analysis.

E. Applications of modern empirical process and strong approximation methods to treat problems in machine learning, nonparametric estimation and inference, with a particular focus on high- and infinite-dimensional statistical models.

F. Identification of major problems and areas of potentially high impact for applications and use in other areas of mathematics, statistics, and computer science.

Based on the presented results and discussion at the meeting, we believe that we more met our goal. The followup proceedings volume of the meeting is planned to be completed in 2012.

# **Presentation Highlights**

Our participants presented talks on a wide variety of subjects, which stimulated a number of lively discussions that will likely lead to new research and collaborations. We have attached the their abstracts, as well as a division of them by subject.

# Division of Abstracts by Subject

#### **Random Matrices**

Adamczak: The Circular Law for random matrices with independent log-concave rows Eichelsbacher: Universal moderate deviations for the eigenvalue counting function of Wigner matrices

Mark Meckes: Concentration and convergence rates for spectral measures of random matrices

#### **Small Deviations**

Aurzada: Small deviation probabilities of Gaussian processes and path regularity Li: Recent Developments on Small Value Probabilities

#### **Infinitely Divisible and Related Processes**

Basse-O'Connor and Rosinski: On the uniform convergence of random series in Skorohod space and representations of cadlag infinitely divisible processes Figueroa-Lopez: Small-time expansions for local jump-diffusions models with infinite jump activity

#### Partial Sums, Self-Normalized Sums and Processes

Kevei and Mason: Self-Normalized Sums and Self-Normalized Levy Processes

Kevei and Mason: A More General Maximal Bernstein-Type Inequality Peligrad: Exact asymptotics for linear processes

#### **Central Limit Theorems and Density Function Estimation**

Deheuvels: Uniform-in-Bandwidth Functional Limit Laws for the Empirical Process and Applications Goetze: Asymptotic Approximations in the CLT in Free and Classical Probability and Applications Giné: Rates of Contraction for Posterior Distributions in  $L_r$ ,  $1 \le r < \infty$ . Kuelbs: A CLT for Empirical Processes and Empirical Quantile Processes

#### **Random Structures with Gaussian Components**

Hoffmann-Jorgensen: Slepian's Inequality and Stochastic Orderings Lifshits and Linde: Gaussian summation processes and weighted summation operators on trees Marcus: Permanental Processes Elizabeth Meckes: Projections of Probability Distributions: A Measure-theoretic Dvoretzky Theorem

#### **Tail Estimates**

Hitczenko: Tail Bounds and Extremal Behavior of Light-tailed Perpetuities Latała: Tail estimates for sums of independent log-concave random vectors

#### **Invariance Principles and Approximations**

Dedecker: *The almost sure invariance principle for unbounded functions of expanding maps* Merlevede: *On strong approximation for the empirical process of stationary sequences* Shao: *Stein's Method and Applications* 

#### **Convexity and Its Applications**

Gozlan: Concentration of measure and optimal transport Koldobsky: A hyperplane inequality for measures of convex bodies

#### Nonparametric Estimation and Inference

Koltchinskii: Complexity Penalization in Low Rank Matrix Recovery Radulovic: Direct Bootstrapping Technique and its Applications to Novel Goodness of Fit Test Reynaud-Bouret: Some Lasso procedure for multivariate counting processes and its particular link

#### **Problems motivated by Mathematics Physics**

Chen: Renormalization in the model of Brownian motions in Poissonian potentials Panchenko: Structure of the Gibbs measure in the Sherrington-Kirkpatrick model

#### **Special Processes**

de la Pena: *How Long will it Take?* Yukich: *Probabilistic Analysis of Large Geometric Structure* 

### Abstracts

The Circular Law for random matrices with independent log-concave rows Radosław Adamczak (University of Warsaw) I will show how the replacement principle by Tao and Vu together with Klartag's thin shell inequality and simple bounds for the smallest singular value allow for a relatively easy proof of the circular law for the class of matrices mentioned in the title.

#### Small deviation probabilities of Gaussian processes and path regularity Frank Aurzada (Technische Universität Berlin)

We study the sample path regularity of Gaussian processes and relate it directly to the theory of small deviations. For example, we show that if the path of a centered Gaussian process is *n*-times differentiable then the exponential rate of decay of its  $L_{\infty}$ -small deviations is at most  $\varepsilon^{-1/n}$ . We also show a similar result if *n* is not an integer. Further generalizations are given, which parallel the entropy method – which is recalled in this talk – to determine the small deviations.

# On the uniform convergence of random series in Skorohod space and representations of càdlàg infinitely divisible processes

#### Andreas Basse-O'Connor (Aarhus University)

Let  $X_n$  be independent random elements in the Skorohod space D([0, 1]; E) of càdlàg functions taking values in a separable Banach space E. Let  $S_n = \sum_{i=1}^n X_i$ . We show that if  $S_n$  converges in finite dimensional distributions to a càdlàg process, then  $S_n + c_n$  converges a.s. uniformly over [0, 1] for some  $c_n \in D([0, 1]; E)$ . This result extends the Itô-Nisio Theorem to the space D([0, 1]; E), which is surprisingly lacking in the literature even for  $E = \mathbf{R}$ . The main difficulties of dealing with D([0, 1]; E) in this context are its non-separability under the supremum norm and the discontinuity of the addition under Skorohod's  $J_1$ -topology.

We use this result to prove the uniform convergence of various series representations of càdlàg infinitely divisible processes. As a consequence, we obtain explicit representations of the jump process, and of related path functionals, in a general non-Markovian setting. Finally, we illustrate our results on an example of stable processes. To this aim we obtain criteria for such processes to have càdlàg modifications, which may be of independent interest.

#### Renormalization in the model of Brownian motions in Poissonian potentials Xia Chen (University of Tennessee)

The model of Brownian motion in Poissonian potential describes a typical trajectory of a Brownian particle surviving from being attracted by the obstacles randomly located in the space (think about the stars in the universe). In the existing literature, the random potential is defined as the convolution between a Poissonian field and a bounded and locally supported function. According to the Newton's law of universal attraction and some other related laws in physics, the most natural way of constructing the random potential is to define it as the Riesz potential of the Poissonian field. On the other hand, the Riesz potential of the Poissonian field blows up. In this talk, this problem will be fixed by the way of renormalization. In addition, some asymptotic patterns of our models will be established and more problems will be asked. Part of the talk is based on some collaborative works with Kulik and Rosinski and Xiong.

#### The almost sure invariance principle for unbounded functions Jérôme Dedecker (Université Paris Descartes)

We consider two classes of piecewise expanding maps T of [0, 1]: a class of uniformly expanding maps for which the Perron-Frobenius operator has a spectral gap in the space of bounded variation functions, and a class of expanding maps with a neutral fixed point at zero. In both cases, we give a large class of unbounded functions f for which the partial sums of  $f \circ T^i$  satisfy an almost sure invariance principle. This class contains piecewise monotonic functions (with a finite number of branches) such that:

- For uniformly expanding maps, they are square integrable with respect to the absolutely continuous invariant probability measure.
- For maps having a neutral fixed point at zero, they satisfy an (optimal) tail condition with respect to the absolutely continuous invariant probability measure.

This is a joint work with Sébastien Gouëzel (université Rennes 1) and Florence Merlevède (université Paris Est-Marne la vallée).

Uniform-in-Bandwidth Functional Limit Laws for the Empirical Process and Applications Paul Deheuvels (LSTA - Université Pierre et Marie Curie) The functional limit laws for increments of the uniform empirical process, due to Deheuvels and Mason (1992) and Deheuvels (1992), allow to describe the limiting behavior of maximal deviations of nonparametric functional estimators. Deheuvels and Ouadah (2011) have established the following uniform-in-bandwidth in probability version of these results. Denoting by  $\{\alpha_n(t) : 0 \le t \le 1\}$  the usual uniform empirical process, set  $\xi_n(h; t; u) := \alpha_n(t + hu) - \alpha_n(t)$ , for 0 < h < 1,  $0 \le u \le 1$  and  $0 \le t \le 1 - h$ . Set  $\log_+ v := \log(v \lor e)$ , and let, for each  $n \ge 1$ ,  $\mathcal{F}_n(h) := \{(2h \log_+(1/h))^{-1/2}\xi_n(h; t; \cdot) : 0 \le t \le 1 - h\}$ . Denote by  $\mathcal{S}$  the unit ball of the reproducing kernel Hilbert space pertaining to the Wiener process on [0, 1], and let  $\Delta(\cdot, \cdot)$  denote the Hausdorff set-distance induced by the sup-norm of bounded functions on [0, 1]. Set  $\mathcal{J}_n := [a_n, b_n]$ , where  $a_n \le b_n$  are such that

$$na_n/\log n \to \infty$$
 and  $b_n \to 0$ .

Deheuvels and Ouadah (2011) showed that, under these assumptions, as  $n \to \infty$ ,

$$\sup_{h \in \mathcal{J}_n} \Delta\left(\mathcal{F}_n(h), \mathcal{S}\right) \xrightarrow{\mathrm{IP}} 0.$$

We extend this result to multivariate empirical processes. As an example of application, we consider an i.i.d. sequence  $X_1, X_2, \ldots$  of  $\mathbb{R}^d$ -valued random vectors with continuous density  $f(\cdot)$  on a neighborhood of  $\mathcal{I} := \prod_{j=1}^d [c_j, d_j]$ , with  $c_j < d_j$  for  $j = 1, \ldots, d$ . Letting  $K(\cdot)$  denote a function of bounded variation, and bounded support, integrating to 1 on  $\mathbb{R}^d$ , we consider the kernel estimator of  $f(\cdot)$  defined by

$$f_{n,h}(x) := \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h^{1/d}}\right) \quad \text{for} \quad x \in \mathbb{R}^d.$$

We will show that our limit law implies that, under the assumptions above, as  $n \to \infty$ ,

$$\sup_{h \in \mathcal{J}_n} \left| \sup_{x \in \mathcal{I}} \left\{ \frac{nh}{2\log_+(1/h)} \right\}^{1/2} \pm \left\{ f_{n,h}(x) - E(f_{n,h}(x)) \right\} - \left\{ \sup_{x \in \mathcal{I}} f(x) \int_{\mathbb{R}^d} K^2(t) dt \right\}^{1/2} \right| \stackrel{\mathbb{P}}{\to} 0$$

#### How Long will it Take?

#### Victor de la Pena (Columbia University)

In this talk we introduce an approach to estimate the first hitting time of random processes. The approach provides a natural extension of the concept of boundary crossingby non-random functions to the case of stochastic processes. Two examples are provided: one motivated by cancer research, and the other on dealing with drought predictions for the Southwest US and the Mediterranian region. This is Joint work with Mark Brown, Yochanan Kushnir and Tony Sit.

#### Universal moderate deviations for the eigenvalue counting function of Wigner matrices Peter Eichelsbacher (Ruhr-University Bochum)

We establish a moderate deviation principle (MDP) for the number of eigenvalues of a Wigner matrix in an interval. The proof relies on fine asymptotics of the variance of the eigenvalue counting function of GUE matrices due to Gustavsson. The extension to large families of Wigner matrices is based on the Tao and Vu Four Moment Theorem and applies localization results by Erdös, Yau and Yin. Moreover we investigate families of covariance matrices as well. This is joint work with Hanna Döring.

#### Small-time expansions for local jump-diffusions models with infinite jump activity José E. Figueroa-López (Purdue University)

We consider a Markov process X with deterministic initial condition x, which is the solution of a stochastic differential equation driven by a Lévy process Z and an independent Wiener process W. Under some regularity conditions, including non-degeneracy of the diffusive and jump components of the process as well as smoothness of the Lévy density of Z, we obtain a small-time second-order polynomial expansion in time for the tail distribution and the transition density of the process X. The method of proof combines a recent approach by Figueroa-López and Houdré (2009) for regularizing the tail distribution of a Lévy process with classical results of Malliavin calculus for purely-jump processes, which have to be extended here to deal with the mixture model X. As an application, the leading term for out-of-the-money option prices in short maturity under a local jump-diffusion model is also derived. This is a joint work with Cheng Ouyang.

> Rates of Contraction for Posterior Distributions in  $L^r$ -metrics,  $1 \le r \le \infty$ Evarist Giné and Richard Nickl (University of Connecticut and University of Cambridge)

The frequentist behavior of nonparametric Bayes estimates, more specifically, rates of contraction of posterior distributions to shrinking  $L^r$ -norm neighborhoods of the unknown parameter,  $1 \le r \le \infty$ , are studied. A theorem for nonparametric density estimation is proved under general assumptions on the prior. The result is applied to a variety of common examples, including Gaussian processes and wavelet series. The rates of contraction are minimax-optimal for  $1 \le r \le 2$ , but deteriorate as r increases beyond 2. In the case of Gaussian nonparametric regression, a Gaussian prior is devised for which the posterior contracts at the optimal rate in all  $L^r$ -norms,  $1 \le r \le \infty$ . Modern theory of Gaussian processes, including lower bounds for small ball probabilities, is used.

#### Asymptotic Approximations in the CLT in Free and Classical Probability and Applications Friedrich Götze (Bielefeld University)

In the classical CLT expansions of the entropy distance to the class of normal distribution are shown assuming the existence of moments and entropy of sums only. This extends Barron's (1986) CLT in the entropic distance to higher order approximations assuming minimal conditions. Explicit bounds for the entropic distance of order  $O(n^{-1})$  (assuming four moments) are shown. Extensions to the multidimensional and stable case and relations to results e.g. by Rio using Wasserstein distances are discussed as well.

For comparison we discuss asymptotic approximations of first and second order in the CLT of free probability assuming four moments and a corresponding expansion of Voiculescu's free Entropy. This is joint work with G. Chistyakov and S. Bobkov.

#### Concentration of measure and optimal transport Nathael Gozlan (Université Paris Est - Marne la Vallée)

This talk is devoted to Talagrand's transport entropy inequality  $T_2$ . First we will recall its connection to Gaussian dimension free concentration of measure. Then we will present a new result showing that Talagrand's inequality is equivalent to a modified Log-Sobolev inequality. This latter result improves a celebrated result by Otto and Villani. Joint work with C. Roberto and P-M Samson.

#### Tail Bounds and Extremal Behavior of Light-tailed Perpetuities Paweł Hitczenko (Drexel University)

We study the tail and extremal behavior of a sequence of random variables  $(R_n)$  defined by the recurrence  $R_n = M_n R_{n-1} + Q_n$ ,  $n \ge 1$ , where  $R_0$  is arbitrary,  $(M_n, Q_n)$  are iid copies of a non-degenerate random vector (M, Q) satisfying  $0 \le M \le 1$ , and  $0 \le Q \le q$ . The imposed conditions guarantee that  $(R_n)$  converge in distribution to a random variable R, usually referred to as perpetuity. We provide an upper bound for the tail of a limiting random variable R. Our bound is similar in nature to a lower bound obtained under the additional assumption that  $Q \equiv q > 0$  by Goldie and Grübel (1996). Furthermore, we apply our result to obtain some information on the extremal behavior of the sequence  $(R_n)$ . Specifically, we show that when  $Q \equiv q > 0$  then under mild and natural conditions on M the suitably normalized extremes of  $(R_n)$  converge in distribution to a double exponential random variable. This partially complements a result of de Haan, Resnick, Rootzén, and de Vries (1989) who considered extremes of the sequence  $(R_n)$  under the assumption that P(M > 1) > 0.

#### Slepian's Inequality and Stochastic Orderings Jorgen Hoffmann-Jorgensen (University of Aarhus)

It is well-known that Slepian's inequality is of great importance in the theory of Gaussian processes. There exists many forms of Slepian's inequality in the literature. One of the most general versions can be found in Ledoux and Talagrand's book (Probability in Banach spaces), but theorem is wrong as it stands (this can be shown by easy counterexamples). It is well-known that Slepian's inequality is closely related to various stochastic orderings; for instance the supermodular ordering. Recall that  $f : R^k \to R$  is supermodular if  $f(x \lor y) + f(x \land y) \le f(x) + f(y)$  and if  $X = (X_1, \ldots, X_k)$  and if  $Y = (Y_1, \ldots, Y_k)$  are random vectors, we write  $X \le_{sm} Y$  if  $Ef(X) \le Ef(Y)$  for all supermodular functions f for which the expectations exist. In the modern literature it is generally stated that it suffices to verify this inequality for bounded supermodular functions. In the talk, I shall show that this is correct if  $k \le 2$  but wrong if  $k \ge 3$ . One commonly stated consequence of Slepian's inequality says that if X and Y are Gaussian vectors such that var  $X_i = \operatorname{var} Y_i \forall i$  and  $\operatorname{cov} (X_i, X_j) \le \operatorname{cov} (Y_i, Y_j) \forall i \ne j$ , then  $X \le_{sm} Y$ . However, this result relies on the wrong statement above. This means that the statement is correct if  $k \le 2$  but I suspect that it fails if  $k \ge 3$ . The correct versions of Slepian's inequality involves 3 types of conditions (a): Smoothness (twice or more times differentiability); (b): Growth conditions (polynomial or

exponential); (c): Regularity of the covariance matrix. In the talk I shall present a version of Slepian's inequality which covers all the correct versions I know, including Fernique's version (where covariance are replaced by intrinsic metric). The minimal conditions, under which I have been able to establish Slepian's inequality allows f(x) to grow as  $e^{ax^2}$  for some a > 0, it do not require differentiability (it allows f to be an indicator function) but it do requires a weak type of approximate, directional continuity together with a condition on the range of the covariance matrices (which becomes redundant if f is sufficiently directional continuous).

#### Self-Normalized Sums and Self-Normalized Lévy Processes Péter Kevei (University of Szeged)

Let  $X, X_1, X_2, \ldots$ , and  $Y, Y_1, Y_2, \ldots$  be iid random variables and non-negative iid random variables, respectively, independent of each other. Define the self-normalized sum  $R_n = \sum_{i=1}^n X_i Y_i / \sum_{i=1}^n Y_i$ . We investigate the possible limiting distributions of  $R_n$ along the subsequences of the natural numbers. In particular, we show that if Y is in the centered Feller-class and  $E|X| < \infty$ , then all the possible subsequential limits of  $R_n$  has a  $C^{\infty}$  density function. We also consider the process version of the problem. This is an ongoing joint work with David Mason.

#### A hyperplane inequality for measures of convex bodies Alexander Koldobsky (University of Missouri-Columbia)

The hyperplane problem asks whether there exists an absolute constant C so that for any origin-symmetric convex body K in  $\mathbb{R}^n$ 

$$|K|^{\frac{n-1}{n}} \le C \max_{\xi \in S^{n-1}} |K \cap \xi^{\perp}|,$$
(32.1)

where  $\xi^{\perp}$  is the central hyperplane in  $\mathbb{R}^n$  perpendicular to  $\xi$ , and |K| stands for volume of proper dimension. The problem is still open, with the best-to-date estimate  $C \sim n^{1/4}$  established by Klartag, who slightly improved the previous estimate of Bourgain. In the case where the dimension  $n \leq 4$ , the inequality (32.1) was proved with the best possible constant  $C = \left|B_2^n\right|^{\frac{n-1}{n}} / \left|B_2^{n-1}\right|$  (this constant is less than 1), where  $B_2^n$  is the unit Euclidean ball in  $\mathbb{R}^n$ . In this talk we show that the latter result can be extended to arbitrary measures in place of volume. Namely, if  $n \leq 4$ , K is an origin-symmetric convex body in  $\mathbb{R}^n$ , and  $\mu$  is a measure in  $\mathbb{R}^n$  with non-negative continuous density f (so that  $\mu(K) = \int_K f$ ) then

$$\mu(K) \le \frac{n}{n-1} \frac{\left|B_2^n\right|^{\frac{n-1}{n}}}{\left|B_2^{n-1}\right|} \max_{\xi \in S^{n-1}} \mu(K \cap \xi^{\perp}) |K|^{1/n}.$$

The constant is sharp, and the inequality holds true in higher dimensions under an additional assumption that K is an intersection body.

#### Complexity Penalization in Low Rank Matrix Recovery Vladimir Koltchinskii (Georgia Institute of Technology)

We will discuss a problem of estimation of a large Hermitian  $m \times m$  matrix A based on a finite number of measurements of randomly picked linear functionals of this matrix. In the noiseless case, the goal is to recover the target matrix exactly with a high probability based on the number of measurements of the order mrank(A) (up to constants and log-factors). Among the examples of this problem are the matrix completion (when the functionals are just the entries of the matrix) and the estimation of a density matrix in quantum state tomography. Recent results of Candes and Tao (2010) and Gross (2011) show that, in the case of matrix completion, such a recovery is possible provided that the target matrix satisfies certain "low coherence" conditions. The method is based on minimizing the nuclear norm over the affine space of matrices that agree with the data. We will be more interested in the case of noisy recovery (matrix or trace regression) where various versions of penalized least squares method can be used with complexity penalties based either on the nuclear norm, or on von Neumann entropy (in the case of quantum state tomography). We will discuss recent results of Koltchinskii (2010, 2011), Koltchinskii, Lounici and Tsybakov (2011) on oracle inequalities showing how the error of such estimators depends on the rank of the target matrix and other parameters of the problem. The proofs of these results are based on a variety of tools, including matrix versions of Bernstein inequalities and generic chaining bounds.

A CLT for Empirical Processes and Empirical Quantile Processes Involving Time Dependent Data James Kuelbs (University of Wisconsin-Madison) We establish empirical quantile process CLT's based on n independent copies of a stochastic process  $\{X_t : t \in E\}$  that are uniform in  $t \in E$  and quantile levels  $\alpha \in I$ , where I is a closed sub-interval of (0, 1). Typically E = [0, T], or a finite product of such intervals. Also included are CLT's for the empirical process based on  $\{I_{X_t \leq y} - \Pr(X_t \leq y) : t \in E, y \in R\}$  that are uniform in  $t \in E, y \in R$ . The process  $\{X_t : t \in E\}$  may be chosen from a broad collection of Gaussian processes, compound Poisson processes, stationary independent increment stable processes, and martingales.

#### Tail estimates for sums of independent log-concave random vectors Rafał Latała (University of Warsaw)

We will present new tail estimates for order statistics of sums of independent log-concave vectors and show how they may be applied to derive deviation inequalities for  $l_r$  norms and norms of projections of such vectors. Part of the talk is based on the joint work with Radosław Adamczak, Alexander Litvak, Alain Pajor and Nicole Tomczak-Jaegermann.

#### Recent Developments on Small Value Probabilities Wenbo Li (University of Delaware)

Small value probabilities or small deviations study the decay probability that positive random variables behave near zero. In particular, small ball probabilities provide the asymptotic behavior of the probability measure inside a ball as the radius of the ball tends to zero. In this talk, we will provide an overview on some recent developments, including symmetrization inequalities in high dimension, smooth Gaussian processes, and branching related processes.

Gaussian summation processes and weighted summation operators on trees M.A. Lifshits, W.Linde (St.Petresburg State University, F. Schiller University Jena)

We study Gaussian summation processes on trees

$$X(t) := \sigma(t) \sum_{s \preceq t} \alpha(s) \xi(s) \,, \quad t \in T$$

where T is a tree,  $\alpha$  and  $\sigma$  are given weights on T, and  $\xi(s)$  are independent standard Gaussian rvs. In some important cases, we provide necessary and sufficient conditions for boundedness of X.

In parallel, we investigate compactness properties of weighted summation operators  $V_{\alpha,\sigma}$  as mapping from  $\ell_1(T)$  into  $\ell_q(T)$  for some  $q \in (1, \infty)$ , defined by

$$(V_{\alpha,\sigma}x)(t) := \alpha(t) \sum_{s \succeq t} \sigma(s)x(s), \quad t \in T.$$

These operators are natural discrete analogues of Volterra operators. We introduce a metric d on T such that compactness properties of (T, d) imply two–sided estimates for the (dyadic) entropy numbers of  $V_{\alpha,\sigma}$  (recall that behavior of entropy numbers is directly related to small deviation probabilities of X). The results are applied to a large variety of trees and weights.

#### Permanental Processes Michael B. Marcus (CUNY)

An  $\alpha$ -permanental process  $\theta := \{\theta_x, x \in S\}$ , is a real valued positive stochastic process that is determined by a real valued kernel  $\Gamma = \{\Gamma(x, y), x, y \in T\}$ , in the sense that its finite joint distributions are given by

$$E\left(\exp\left(-\sum_{i=1}^{n}\lambda_{i}\theta_{x_{i}}\right)\right) = |I + \Lambda\widetilde{\Gamma}|^{-\alpha},$$
(32.2)

where I is the  $n \times n$  identity matrix,  $\Lambda$  is the  $n \times n$  diagonal matrix with entries  $(\lambda_1, \ldots, \lambda_n)$ ,  $\tilde{\Gamma} = {\Gamma(x_i, x_j)}_{i,j=1}^n$  is an  $n \times n$ matrix and  $\alpha > 0$ . When  $\Gamma$  is symmetric and positive definite and  $\alpha = 1/2$ ,  $\theta = {G_x^2, x \in S}$ , where  ${G_x, x \in S}$  is a mean zero Gaussian process with covariance  $\Gamma$ . However, the right-hand side of (32.2) can define a stochastic process for kernels  $\Gamma$  that are not symmetric. For example, when  $\Gamma$  is the zero potential density of a transient Markov process, that is not symmetric. Therefore, permanental processes are positive stochastic processes that generalize processes that are the squares of Gaussian processes.

In certain cases the squares of Gaussian processes are related by the Dynkin Isomorphism Theorem to the local times of symmetric Markov processes. The more general permanental processes are similarly related to the local times of Markov processes that need not be symmetric.

In this paper we discuss recent results about sample path properties of permanental processes obtained with Hana Kogan and Jay Rosen. In particular we identify permanental processes with kernels that are the potential densities of transient Markov processes as the loop soup local times of the Markov processes.

#### A More General Maximal Bernstein-Type Inequality Péter Kevei and David M. Mason (University of Szeged and University of Delaware)

We describe a new and unexpected general maximal Bernstein-type inequality, along with a number of interesting applications.

#### Projections of Probability Distributions: A Measure-theoretic Dvoretzky Theorem Elizabeth Meckes (Case Western Reserve University)

There is a widely studied phenomenon which can be described by saying that high-dimensional random vectors typically have Gaussian marginals. For example, for a probability measure on  $\mathbb{R}^d$ , under mild conditions, most one-dimensional marginals are approximately Gaussian if d is large. This fact has important implications in statistics, in particular for the procedure known as graphical projection pursuit. Natural questions are then, for example, how many projections typically have to be tried before finding something non-Gaussian, or in another direction one could ask how large k can be as a function of the ambient dimension for k-dimensional marginals to be approximately Gaussian. I will discuss a quantitative approach to this phenomenon which sheds light on both of these questions. In particular, I will give the main ideas of the proof that, under mild conditions, a probability measure on  $\mathbb{R}^d$  has mostly Gaussian marginals if k < 2log(d)/log(log(d)), and that this estimate is best possible in the metric considered.

#### Concentration and convergence rates for spectral measures of random matrices Mark W. Meckes (Case Western Reserve University)

I will discuss how a combination of concentration of measure and metric entropy techniques can be used to estimate the Wasserstein distance between the empirical spectral distribution of a random matrix and its mean. The techniques apply to several different models of random matrices, and allow us in particular to improve on previous results of Diaconis–Shahshahani, Hiai–Petz, Guionnet–Zeitouni, Chatterjee, and Kargin.

#### On strong approximation for the empirical process of stationary sequences Florence Merlevède (University of Paris Est)

In this talk, I shall present a strong approximation result with rate for the empirical process associated to a stationary sequence of real-valued random variables, under dependence conditions involving only indicators of half lines. This strong approximation result also holds for the empirical process associated to iterates of expanding maps with a neutral fixed point at zero as soon as the correlations decay more rapidly than  $n^{-1-\delta}$  for some positive  $\delta$ , which shows that our conditions are in some sense optimal. (Joint work with D. Dedecker and E. Rio).

#### Structure of the Gibbs measure in the Sherrington-Kirkpatrick model Dmitry Panchenko (Texas A&M University)

In the Sherrington-Kirkpatrick spin glass model, given i.i.d. standard normal r.v.s  $(g_{i,j})$ , one considers a Gaussian process

$$H_N(\vec{\sigma}) = \sum_{i,j=1}^N g_{i,j}\sigma_i\sigma_j$$

indexed by vectors  $\vec{\sigma} = (\sigma_1, \dots, \sigma_N) \in \{-1, +1\}^N / \sqrt{N}$  of length one and defines a random probability measure, called the Gibbs measure,

$$G_N(\{\vec{\sigma}\}) = \frac{\exp(\beta\sqrt{N}H_N(\vec{\sigma}))}{Z_N}$$

for some inverse temperature parameter  $\beta > 0$ . As the size of the system N goes to infinity, one would like to understand the geometry of the set on which the measure  $G_N$  concentrates or, in one possible interpretation, given an i.i.d. sample  $(\vec{\sigma}^l)$  from  $G_N$ , one would like

to find the asymptotic distribution of the Gram matrix  $(\vec{\sigma}^l \cdot \vec{\sigma}^{l'})_{l,l' \ge 1}$  under all the randomness involved,  $EG_N^{\otimes \infty}$ . This distribution was predicted by the Italian physicist Giorgio Parisi and the main feature of his theory is that the measure  $G_N$  in the limit must concentrate on an ultrametric set. I will review several results from recent years that partially confirm Parisi's predictions.

#### Exact asymptotics for linear processes Magda Peligrad (University of Cincinnati)

In this talk we present several new asymptotic results for linear processes. We shall address first the following question: giving a sequence of identically distributed random variables in the domain of attraction of a normal law, does the associated linear process satisfy the central limit theorem? We study this question for several classes of stationary processes. For independent and identically distributed random variables we show that the central limit theorem for the linear process is equivalent to the fact that the variables are in the domain of attraction of a normal law, answering in this way an open problem in the literature. Further, we present the convergence to the fractional Brownian motion and we also discuss the self-normalized version of this theorem. Then, we introduce the exact moderate and large deviation asymptotics in non-logarithmic form. We give an asymptotic representation for probability of the tail of the normalized sums and specify the zones in which it can be approximated either by a standard normal distribution or by the marginal distribution of the innovation process. Applications to fractionally integrated processes, regression models and computation of value at risk and expected shortfall are pointed out. Finally, we shall mention some open questions. The results presented are based on recent joint papers with Hailin Sang, Wei Biao Wu and Yunda Zhong.

#### Direct Bootstrapping Technique and its Applications to Novel Goodness of Fit Test Dragan Radulovic (Florida Atlantic University)

We prove a general theorem that characterizes situations in which we could have asymptotic closeness between the original statistics  $H_n$  and its Bootstrap version  $H_n^*$ , without stipulating the existence of weak limits. As one possible application we introduce a novel goodness of fit test based on modification of Total Variation metric. This new statistic is more sensitive than Kolmogorov Smirnov statistics, it applies to higher dimensions and it does not converge weakly; but we show that it can be Bootstrapped.

# Some Lasso procedure for multivariate counting processes and its particular link with some exponential inequalities for martingales

Patricia Reynaud-Bouret (CNRS and University of Nice Sophia-Antipolis)

Genomics and neurosciences produce a huge amount of high-dimensional data, where complex structures of dependence are involved. If one can infer those structures, the result may hint for particular synergy between neurons or transcription regulatory elements for instance. One of the natural model of such data is the multivariate Hawkes process, which is a particular case of counting process. The inference of the dependency structure in this set-up is a sparse non-parametric problem for which Lasso procedure is particularly adequate. However to obtain a full data driven procedure, some parameters of the procedure need to be calibrated in a full adaptive way. At this stage, sharp and particular exponential bounds for martingales are really useful. In those inequalities, the bracket of the martingale is estimated and plugged in the deviation bound. A discussion on the best way to perform this may follow. This is a joint work, still in progress, with N. R. Hansen (Copenhagen) and V. Rivoirard (Dauphine).

#### Stein's Method and Applications

Qi-Man Shao (Hong Kong University of Science and Technology)

Stein's method is a powerful tool in estimating accuracy of various probability approximations. It works for both independent and dependent random variables. It works for normal approximation and also for non-normal approximation. The method has been successfully applied to study the absolute error of approximations and the relative error as well. In this talk, we shall review the latest developments on Stein's method and its applications. The focus will be on Cramér type moderate deviation theorems under a general Stein's identity, for Studentized non-linear statistics as well as applications to Curie-Weiss models in statistical physics.

> Probabilistic Analysis of Large Geometric Structures Joseph E. Yukich (Lehigh University)

Fundamental questions pertaining to large random geometric structures often involve sums of spatially correlated terms having short range interactions but complicated long range dependence. This phenomenon arises in a range of fields, including (i) the statistical estimation of entropy and dimension via graphical methods, (ii) the study of functionals of the convex hull of an i.i.d. sample, (iii) models for random sequential packing, and (iv) random geometric graphs and networks. This talk will survey general methods for establishing limit theorems for geometric functionals of large random structures. It is shown that if the geometric functionals satisfy a spatial dependency condition known as stabilization then laws of large numbers, variance asymptotics, and central limit theorems follow, subject to appropriate scaling. The general theory is shown to answer questions in the areas (i)-(iv).

## **Participants**

Adamczak, Radoslaw (University of Warsaw) Aurzada, Frank (Technische Universitat Berlin) **Basse-O'Connor, Andreas** (University of Tennessee / University of Aarhus) Bryc, Wlodzimierz (University of Cincinnati) Chen, Xia (University of Tennessee) de La Pena, Victor (Columbia University) Dedecker, Jerome (University Paris-Descartes) Deheuvels, Paul (UPMC - LSTA) Dudley, Richard M. (Massachusetts Institute of Technology) Eichelsbacher, Peter (Ruhr-Universitaet Bochum) Figueroa-Lopez, Jose Enrique (Purdue University) Gao, Fuchang (University of Idaho) Gin, Evarist (University of Connecticut) Goetze, Friedrich (University of Bielefeld) Gozlan, Nathael (Universite Paris-Est Marne-la-Vallee) Hitczenko, Pawel (Drexel University) Hoffmann-Jorgensen, Jorgen (University of Aarhus) Houdr, Christian (Georgia Institute of Technology) Kevei, Peter (Szeged University) Koldobsky, Alexander (University of Missouri) Koltchinskii, Vladimir (Georgia Institute of Techology) Kuelbs, James (University of Wisconsin-Madison) Latala, Rafal (University of Warsaw) Li, Wenbo (University of Delaware) Lifshits, Mikhail (St-Petersburg State University) Linde, Werner (FSU-Jena) Lounici, Karim (Georgia Institute of Technology) Marchal, Philippe (Universite Paris 13) Marcus, Michael (CUNY) Mason, David M. (University of Delaware) Meckes, Elizabeth (Case Western Reserve University) Meckes, Mark (Case Western Reserve University) Merlevede, Florence (University Paris Est) Panchenko, Dmitriy (Texas A&M University) Peligrad, Magda (University of Cincinnati) Radulovic, Dragan (Florida Atlantic University) Reynaud-Bouret, Patricia (CNRS - Universite de Nice Sophia Antipolis) Rosinski, Jan (University of Tennessee) Shao, Qi-Man (Hong Kong University of Science and Technology) Wolff, Pawel (University of Warsaw) Yukich, Joe (Lehigh University)

## Chapter 33

## **Cycles on modular varieties (11w5125)**

Oct 30 - Nov 04, 2011

**Organizer(s):** Pierre Charollois (Institut de Mathématiques de Jussieu) Samit Dasgupta (University of California, Santa Cruz) Matthew Greenberg (University of Calgary) Benedict Gross (Harvard)

Finding solutions of polynomial equations using analytic and geometric methods is a classical and highly developed subject. On the other hand, methods for solving Diophantine equations, i.e., finding integer solutions of integral polynomial equations, are usually of an algebraic nature. Hinted at by Dirichlet's famous "class number formula", analytic methods for solving important mathematical equations, like those defining elliptic curves, have seen significant development in the second half of the twentieth century. The major tool allowing for this development is the theory of modularity, which connects the worlds of analysis, geometry and arithmetic. In this workshop, which attracted 44 participants from all over the world, explored a variety of state-of-the art modularity-based techniques for studying the solutions of diophantine equations.

The meeting began with a pair of lectures by Victor Rotger and Henri Darmon on the connections between three beautiful objects – the de Rham fundamental group of the modular curve, the triple product L-function, and diagonal cycles. Put together, these objects yield explicitly computable points on elliptic curves, as well as new cases of the Birch and Swinnerton-Dyer conjecture in ranks zero and one. The constructions of these lectures fit into the framework of the Gross-Prasad conjectures, which were discussed in lectures by Chung-Pang Mok, Shou-Wu Zhang, and Wei Zhang, where the case of unitary groups was emphasized.

Much of Tuesday was concerned with the zeta and L-functions. Colmez lectured on constructions and analysis of Shintani zeta functions. Denis Benois presented his results on exceptional zeroes of p-adic L-functions of modular forms at near central points, and Mijian Brakocevic presented deep theorems on the nonvanishing of Rankin Selberg L-functions, results in the spirit of the famous theorem of Cornut and Vatsal. The day ended with a lively problem session moderated by Jordan Ellenberg that resulted in a list of important open problems that would have significant impact on the field. A summary of this session is available on the workshops web site.

On Wednesday, we began with a lecture by Eyal Goren in which we took a step back and looked at the variety of cycle constructions that arise in different parts of the subject. The next two lectures, by Jan Bruinier and Tonghai Yang focused on the connections between the cycles discussed in Gorens lecture and Kudlas program relating Arakelov heights of cycles to derivatives of Eisenstein series.

Thursday morning was highlighted by lectures of Francois Brunault and Massimo Bertolini. Brunault discussed the connection between p-adic regulators and special values of p-adic L-functions of elliptic curves. Bertolini presented a p-adic Beilinson formula and made a connection between Katos Euler system and the results of Darmon and Rotger presented earlier in the conference. The theme of Katos Euler system was taken up again on Friday morning in Romyar Sharifis talk on cyclotomic units and the cohomology of modular curves.

The workshop had a fantastic vibe and all participants communicated their enthusiasm to the organizers:

The workshop was really excellent, with a focus that was narrow enough to provide real opportunities for research synergy but broad enough that one was not seeing "the same people, one always sees." The talks of Rotger and Darmon suggested a research project that I could undertake with them, and with a postdoctoral collaborator, Kirsten Wickelgren. (Jordan Ellenberg, University of Wisconsin)

The workshop has exceeded my expectations. The program was carefully thought out, balanced current results with some background material and was of exceptionally high level altogether. A mixture of current results and recent work were reported which informed me and broadened my understanding of the current state of the field. I returned home inspired by the great mathematics I have learned. The facilities and staff were, as always, superb. It remains to congratulate BIRS and the organizers for once again putting together a great workshop. (Eyal Goren, McGill University)

## **List of Participants**

Agashe, Amod (Florida State University) Agboola, Adebisi (University of California Santa Barbara) **Benois, Denis** (Universite Bordeaux I,) Berger, Laurent (Ecole Normale Supérieure de Lyon) Bertolini, Massimo (Universita' degli Studi di Milano) Brakocevic, Miljan (McGill University) Bruinier, Jan (TU Darmstadt) Brunault, Franois (ENS-Lyon (France)) Castella, Francesc (McGill University) Chapdelaine, Hugo (Laval) Charollois, Pierre (Institut de Mathématiques de Jussieu) Ciperiani, Mirela (The University of Texas at Austin) Colmez, Pierre (Institut de Mathématiques de Jussieu) **Cornut, Christophe** (CNRS) Darmon, Henri (McGill University) Dasgupta, Samit (University of California, Santa Cruz) de Shalit, Ehud (Hebrew University of Jerusalem) Ellenberg, Jordan (University of Wisconsin) Franc, Cameron (McGill University) Goren, Eval (McGill University) Greenberg, Matthew (University of Calgary) Howard, Benjamin (Boston College) Johnson-Leung, Jennifer (University of Idaho) Kudla, Stephen (University of Toronto) Kuehn, Ulf (Universitaet Hamburg) Longo, Matteo (Università di Padova) Masdeu, Marc (Columbia University) Mok, Chung Pang (McMaster University) Niziol, Wieslawa (University of Utah) Park, Jeehoon (POSTECH) Prasanna, Kartik (University of Michigan) Rapoport, Michael (Universitat Bonn) **Rotger, Victor** (Universitat Politècnica de Catalunya) Seveso, Marco Adamo (Università di Milano) Sharifi, Romyar (University of Arizona) Spiess, Michael (Univ. Bielefeld) Stevens, Glenn (Boston University) Trifkovic, Mak (University of Victoria) Vigni, Stefano (King's College London) Voight, John (University of Vermont)

Cycles on modular varieties

Yang, Tonghai (University of Wisconsin) Zhang, Wei (Columbia University) Zhang, Shou-Wu (Columbia University)

## Chapter 34

## WIN2: Women in Numbers 2 (11w5075)

## Nov 06 - Nov 11, 2011

**Organizer(s):** Chantal David (Concordia University) Matilde Lalin (Universite de Montreal) Michelle Manes (University of Hawaii)

This workshop was a unique effort to combine strong, broad impact with a top level technical research program. In order to help raise the profile of active female researchers in number theory and increase their participation in research activities in the field, this event brought together female senior and junior researchers in the field for collaboration. Emphasis was placed on on-site collaboration on open research problems as well as student training. Collaborative group projects introducing students to areas of active research were a key component of this workshop.

We would like to thank the following organizations for their support of this workshop: BIRS, PIMS, Microsoft Research, and the Number Theory Foundation.

## **Rationale and Goals**

Number theory is a fundamental subject with connections to a broad spectrum of mathematical areas including algebra, arithmetic, analysis, topology, cryptography, and geometry. This very active area naturally attracts many female mathematicians. Although the number of female number theorists is steadly growing, there are still relatively few women reaching high profile positions and visibility at international workshops and conferences. The lack of female leaders in the area is an issue that tends to perpetuate itself, since it has repercussions in attracting and training the next generation of female mathematicians.

In order to increase the number of active female researchers in number theory, a workshop on "Women in Numbers" (WIN 2008) was held at BIRS in November, 2008. This workshop was tremendously successful, surpassing even its stated goals. Several research collaborations—typically involving some senior and junior mathematicians, and in some cases advanced graduate students—began in the working groups of WIN 2008. Many of these collaborations have already proved fruitful in producing publishable research, and a few of the collaborations have continued long past the initial workshop.

For this momentum to continue, it is essential that WIN 2008 is not a single, isolated event, but rather the beginning of a long-term program to develop and support female number theorists. This workshop was designed continue and build upon the work started at WIN 2008. The specific goals were:

- 1. to highlight research activities of women in number theory;
- 2. to increase the participation of women in research activities in number theory;
- 3. to train female graduate students in number theory and related fields;
- to strengthen the research network of potential collaborators in number theory and related fields started by the WIN 2008 conference;

- 5. to enable female faculty at small colleges to participate actively with research activities including the training of graduate students; and
- 6. to provide information on women in number theory with an inclusive approach.

Participant testimonials, comments from (male and female) colleagues, and other feedback suggest that significant progress was made toward goals 1 through 4. In particular, the conference gave greater exposure to the research programs of active female researchers in number theory. Through collaborative projects, students participated in new research in the field, and faculty at small colleges were exposed to supervision activities. Some of the group projects will lead to new results and publications, and the conference organizers are currently exploring venues for publication of a conference proceedings volume.

A Women in Numbers listserv, a website, and a Facebook page have all been established. These will serve as the basis for the **WIN Network**, a network for female researchers in number theory. It is the sincere hope of the workshop organizers that progress was also achieved toward goals 5 and 6 above, but only time will tell.

### **Participants and Format**

The participants were 41 female number theorists — 12 senior and mid-level faculty, 14 junior faculty and postdocs, and 15 graduate students. About one-third of the participants, mostly faculty, were invited by the conference organizers. The remaining slots were intended for junior faculty, postdocs, and graduate students.

The organizers solicited applications, advertising via: the BIRS website, the *Association of Women in Mathematics* newsletter, and various mailing lists including the Number Theory listserv and the previous Women in Numbers 2008 participants.

Fifty-three applicants submitted a CV and a research statement (for postdocs and faculty) or a list of courses taken and letter of recommendation (for graduate students). After a careful and thorough review of these documents, the organizing committee selected what were deemed to be the strongest applicants for participation in the workshop.

Based on the participants' research interests and expertise, the organizers then divided the participants up into eight research groups of 4–6 members each; usually two senior members (group leaders) and 2–4 junior members. Group leaders chose a project for collaborative research during and following the conference. They provided materials and references for background reading ahead of time. The group leaders also gave talks during first three days of the meeting to introduce all participants to their respective group projects. During the last two days of the workshop, junior participants presented the progress made on the group projects. These presentations usually involved more than one presenter. As a result, essentially all workshop participants were able to give a talk at some point during the conference.

Each group also submitted a short written progress report on their project. These reports, along with the project title and the names of the group members, are included in Section 34. Collaboration on the research projects is on-going via electronic communication. Some of these projects will lead to new results and publications. The organizers also expect to publish a conference proceedings volume in the future.

### Schedule

The official schedule for the workshop appears below. Note that most nights, the project groups reconvened and continued working after dinner.

Sunday: 4pm Check-in begins 5:30 – 7:30 dinner 8:00 informal gathering

Monday: 7:00 – 8:45 breakfast 8:45 – 9:00 intro & welcome (BIRS Station Manager & Organizers)

- 9:00 10:30 presentation by Group 1 leaders: Marie-José Bertin and Matilde Lalín
- $10:30 11:00 \ coffee$
- 11:00 12:30 presentation by Group 2 leaders: Chantal David and Heekyoung Hahn
- 12:30 1:30 Lunch
- 1:30 2:30 BIRS tour
- 2:00-2:30 coffee
- 2:30 4:00 presentation by Group 3 leaders: Alina Bucur and Melanie Matchett Wood

4:00 – 6:30 work in project groups 6:30 dinner

#### **Tuesday:**

7:00 - 8:45 breakfast
8:45 - 9:00 announcements
9:00 - 10:30 presentation by Group 4 leaders: Alina Cojocaru and Alice Silverberg
10:30 - 11:00 coffee
11:00 - 12:30 presentation by Group 5 leaders: Wieslawa Niziol and Sujatha Ramdorai
12:30 - 1:30 Lunch
1:30 - 3:00 presentation by Group 6 leaders: Rachel Pries and Hui June Zhu
3:00 - 3:30 coffee
3:00 - 6:30 work in project groups
6:30pm dinner

#### Wednesday:

7:00 - 8:45 breakfast
8:45 - 9:00 announcements
9:00 - 10:30 presentation by Group 7 leaders: Ling Long and Gabriele Nebe
10:30 - 11:00 coffee
11:00 - 12:30 presentation by Group 8 leaders: Kristin Lauter and Bianca Viray
12:30 Lunch / Free afternoon

#### Thursday:

7:00 - 1:30pm breakfast / project groups / lunch
1:30 - 2:00 Group 1 report by team members
2:15 - 2:45 Group 2 report by team members
2:45 - 3:15 Coffee break
3:15 - 3:45 Group 3 report by team members
4:00 - 4:30 Group 4 report by team members
4:45 - 5:15 Group 5 report by team members
5:30 - 6:00 Group 6 report by team members
6:00 - 7:30 dinner
8:00 informal career discussion

### Friday:

7:00 – 8:45 breakfast 8:45 – 9 announcements 9:00 – 9:30 Group 7 report by team members 9:45 – 10:15 Group 8 report by team members 10:15 – 10:45 Coffee 10:45 – 11:30 closing discussion / future plans 11:30 – 1:30 lunch checkout by noon

## **Research Projects and Project Groups**

#### **Group 1: Elliptic Surfaces and Mahler measure**

**Participants**: Marie-José Bertin (Université Paris VI), Amy Feaver (University of Colorado Boulder), Jenny Fuselier (High Point University), Matilde Lalín (Université de Montréal), and Michelle Manes (University of Hawai'i at Mānoa).

The (logarithmic) Mahler measure of a nonzero multivariable Laurent polynomial  $P \in \mathbb{C}[x_1^{\pm 1}, \dots, x_n^{\pm 1}]$  is defined by

$$\mathbf{m}(P) := \frac{1}{(2\pi i)^n} \int_{\mathbb{T}^n} \log |P(x_1, \dots, x_n)| \frac{dx_1}{x_1} \dots \frac{dx_n}{x_n}.$$

This object has interesting connections to heights of polynomials and numbers, transcendence theory, volumes in hyperbolic space, knot invariants, ergodic theory, among others.

For a one-variable polynomial, one obtains a simple expression in terms of the roots of the polynomial. For multivariable polynomials there is no general formula, but there exist several examples of polynomials that yield special values of zeta and L-functions that are often associated to the geometric object defined by the zero set of the polynomial. For example, there are several examples were the polynomials correspond to an elliptic curve and the Mahler measure is related to L(E, 2). These formulas have been related to Beilinson's conjectures.

In this project, we considered a family of K3-surfaces  $Y_k$  (where k is a parameter) defined by the desingularization of  $P_k = 0$  where

$$P_k(x, y, z) = x + \frac{1}{x} + y + \frac{1}{y} + z + \frac{1}{z} - k.$$

The Picard number  $\rho(Y_k)$  is generically equal to 19, but for some special values of k,  $\rho(Y_k) = 20$ . In this case, the K3-surface is called singular and the transcendental lattice has dimension 2, analogous to the elliptic curve case. The cases of k = 0, 2, 10 fall into this category and were studied by Bertin [2, 3]. The goal of the project was to study the Mahler measures for the cases of k = 3, 6, 18 which are also known to correspond to singular K3-surfaces.

We were able to obtain

$$m(P_3) = \frac{15\sqrt{15}}{2\pi^3} L(f_{15},3) \stackrel{?}{=} \frac{|\det T(Y_3)|^{3/2}}{2\pi^3} L(Y_3,3)$$
$$m(P_6) = \frac{24\sqrt{24}}{2\pi^3} L(f_{24},3) = \frac{|\det T(Y_6)|^{3/2}}{2\pi^3} L(Y_6,3)$$
$$m(P_{18}) = \frac{120\sqrt{120}}{2\pi^3} L(f_{120},3) + \frac{21\sqrt{3}}{10\pi} L(\chi_{-3},2) \stackrel{?}{=} \frac{|\det T(Y_{18})|^{3/2}}{9\pi^3} L(Y_{18},3) + \frac{21\sqrt{3}}{10\pi} L(\chi_{-3},2),$$

where  $f_{15}$ ,  $f_{24}$ ,  $f_{120}$  denote newforms of levels 15, 24 and 120, and T denotes the transcendental lattice of  $Y_k$ . The question marks indicate conjectural formulas.

We used a formula of Bertin [1] to relate the Mahler measures to the L-functions of newforms. The other part of the proofs consists of relating the L-function of the newforms to the L-function of the surfaces. For this part, the main ingredient is Livné's modularity theorem. This was accomplished in the case of k = 6, but the k = 3, 18 cases are harder to attack because we use an elliptic fibration of the surface having an infinite section which requires the use of Néron's desingularization. We hope to complete theses proofs in the near future.

# Group 2: Square-free values of sequences related to reductions of elliptic curves over finite fields

**Participants**: Shabnam Akhtari (CRM, Montreal), Chantal David (Concordia University), Heekyoung Hahn (McGill University), Min Lee (Columbia University), and Lola Thompson (Dartmouth College).

Let *E* be an elliptic curve over  $\mathbb{Q}$ . For each prime *p* of good reduction, *E* reduces to a curve  $E_p$  over the finite field  $\mathbb{F}_p$  with  $\#E_p(\mathbb{F}_p) = p + 1 - a_p(E)$  where  $|a_p(E)| \leq 2\sqrt{p}$  (the Hasse bound).

There are many conjectures about properties of the various reductions as one varies over all the primes, for example, the Sato-Tate conjecture which was recently proven by Taylor, Harris and Shepherd-Barron. Or the Lang-Trotter conjecture about  $\# \{p \le x : a_p(E) = r\}$  for a given integer r, or the Koblitz conjecture about  $\# \{p \le x : \#E_p(\mathbb{F}_p) \text{ is prime}\}\)$ . Those last two conjectures are mostly completely open. The most important result known is perhaps the work of Elkies [5] who showed that there are infinitively many supersingular primes (i.e. primes such that  $a_p(E) = 0$ ) for any E over  $\mathbb{Q}$ . This is the only known lower bound for those questions.

Let  $f_p(E)$  be a sequence associated with the reductions of E over  $\mathbb{F}_p$ . The two cases that we have in mind are  $f_p(E) = p + 1 - a_p(E)$  and  $f_p(E) = a_p(E)^2 - 4p$ . The first sequence describes the order of the reduced groups  $E_p(\mathbb{F}_p)$  and the second one is related to the ring of endomorphisms of the reduced curve  $E_p$  over  $\mathbb{F}_p$ . We concentrate on the case where E does not have CM.

We want to count

$$\pi_{f,E}^{SF}(x) = \# \{ p \le x : f_E(p) \text{ is squarefree} \}.$$

It is easy to make a conjecture

$$\pi_{f,E}^{\rm SF}(x) \sim C_{E,f}^{\rm SF}\pi(x) \tag{34.1}$$

where

$$C_{E,f}^{\rm SF} = \sum_{d=1}^{\infty} \frac{\mu(d) |C_{E,f}(d^2)|}{|G_E(d^2)|}$$
(34.2)

with  $G_E(d^2)$  the Galois group of  $\mathbb{Q}(E[d^2])/\mathbb{Q} \subseteq \operatorname{GL}_2(\mathbb{Z}/d^2\mathbb{Z})$  and  $C_{E,f}(d^2) \subseteq G_E(d^2)$  a conjugacy class determined by  $f_p(E)$ .

There are some known results about the above conjecture. It was shown to hold under some standard conjectures in analytic number theory (namely the Generalized Riemann Hypothesis, the Artin Holomorphy Conjecture and the Pair Correlation Conjecture) by Cojocaru [4], and it as shown to hold on average by David and Jimenez Urroz [7].

As a first project, we will concentrate on writing an unconditional upper bound for  $\pi_{E,f}^{SF}(x)$  of the type

$$\pi_{E,f}^{\rm SF}(x) \le C_{E,f}^{\rm SF} \pi(x) \left(1 + \underline{o}(1)\right), \tag{34.3}$$

where  $C_{E,f}^{SF}$  is the conjectural constant of (34.2). In order to do so, we first write

$$\pi_{E,f}^{\rm SF}(x) \le \# \left\{ p \le x : \ell^2 \nmid f_p(E) \text{ for all } \ell \le z \right\},\tag{34.4}$$

and use the Cheboratev Density Theorem in the extension obtained by adjoining all  $\ell^2$ -torsion for  $\ell \leq z$ . One needs to deal with the error term by choosing z appropriately, and presumably, this can be done without assuming the GRH.

In the paper [7], the authors considered the problem of evaluating  $\pi_{E,f}^{SF}(x)$  on average over a family of curves. The main result of the paper can be restated by saying that for most curves,  $\left|\pi_{E,f}^{SF}(x) - C_{E,f}^{SF}\pi(x)\right|$  is very small, except possibly for a small exceptional set of curves. In a second project, we will concentrate on improving that result (i.e. improving the size of the exceptional set) by combining the use of the Cheboratev Density Theorem (for sieving small squares) and the average (for sieving large squares).

While in Banff, we wrote the details of the proof of (34.3), which involves only some straightforward applications of the Chebotarev Density Theorem, as a way to familiarise ourselves with the tools needed to study the conjecture (34.1). By using (34.4), and sieving for squares of primes up to  $z = \log \log x$ , we were able to get the correct upper bound, with the conjectural constant  $C_{E,f}^{SF}$ .

We then began to study the second project. Among other things, we are led to averages of the type

$$\sum_{E \in \mathfrak{C}} C_{E,f}^{\rm SF},$$

where  $C_E^{\text{SF}}$  is the constant defined in (34.2). Such averages were considered by Jones [6], under some hypothesis on the size of exceptional Galois groups in Serre's theorem, and more recently by Zywina [8] who was able to prove the results of Jones in some cases with any hypothesis, by using an effective result of Masser and Wüstholz. We are now investigating the generalisation of the results of Jones and Zywina to our setting.

#### Group 3: Statistics for D<sub>4</sub> curves over finite fields

**Participants**: Alina Bucur (University of California at San Diego), Jing Hoelscher (University of Illinois at Chicago), Renate Scheidler (University of Calgary), and Melanie Matchett Wood (American Institute of Mathematics and University of Wisconsin-Madison).

Algebraic curves over finite fields are basic objects in number theory that also happen to come up in many applications, e.g. cryptography, error-correcting codes. One of the fundamental properties of a curve of a finite fields is its number of rational points over the field of definition, or more generally over extensions of said field. For example, these numbers determine the zeta function of the curve, which exhibits behavior similar to zeta functions of number fields, with the added bonus that in the case of finite fields, the Riemann Hypothesis is a theorem of Weil.

Besides looking at a single curve, it is also interesting to look at average properties of the number of points over a family of curves. Traditionally, this has been done in situations where the finite field was allowed to vary, as in this case one can use powerful methods of Deligne. But more recently, attention has been focused on families over a fixed finite field  $\mathbb{F}_q$ , where things behave quite differently. For instance, Kurlberg and Rudnick have studied the family of hyperelliptic curves [14]; Bucur, David, Feigon, Lalín looked at the families of cyclic *p*-fold covers of  $\mathbb{P}^1$  [9, 11] and plane curves [10]; Bucur and Kedlaya computed the statistics for curves that are complete intersections of smooth quasi-projective subschemes of  $\mathbb{P}^n$  [12]; Wood has answered the same question about degree 3 (not necessarily cyclic) covers of  $\mathbb{P}^1$  [16]. In each of these cases, the statistics of the number of points on a curve in the given family turns out to be governed by a probabilistic model, i.e. they behave asymptotically like a sum of certain i.i.d. random variables. These random variables can be interpreted as the probabilities that the fiber over each point of the relevant projective space has a given number of points.

In the first three cases the average number of points on a curve in the family turns out to be exactly the same as the number of points on  $\mathbb{P}^1$  itself, namely q+1. But in the case of complete intersections, the average number of points is < q + 1, while in the last case it is > q + 1.

A natural extension of the case studied by Kurlberg and Rudnick in [14] is the case of the double covers of hyperelliptic curves. While this is an easy question to formulate, one stumbles at the first step since not even the number of curves in this family is known. In all the previous cases, the objects in the families studied were parametrized by a rational moduli space. However, in the present case, the parameter space for our curves is more complicated.

Counting isomorphism classes of double covers of a scheme S is equivalent to counting isomorphism classes of pairs (s, L) where L is a line bundle on S and  $s \in L^{\otimes -2}$  (e.g. see [15]). From Wood's previous work [15], we know that counting isomorphism classes of double covers of a scheme S with a line bundle on the double cover is equivalent to counting isomorphism classes of binary quadratic forms on S (as defined in [15]). These facts allow us to break the problem into two steps. First we will parametrize double covers  $D \xrightarrow{2} C$  of a specific hyperelliptic cover C with fixed genus  $g_D$ .

When we work out concretely what binary quadratic forms on  $\mathbb{P}^1$  are, it turns out that we need to count orbits of the action of a certain group G on  $\mathcal{O}(m-r)x^2 \oplus \mathcal{O}(m)xy \oplus \mathcal{O}(m+r)$  (where  $\mathcal{O}(i)$  denotes the usual sheaf on  $\mathbb{P}^1$ , whose global sections are binary degree *i* forms). During the week of the workshop, we reduced the problem to the count of these orbits. We proved that the main term is given by the case r = 0. We used Dickson's work on equivalence classes of pairs of binary quadratic forms [13] to compute an asymptotic for the r = 0 term. Using this computation, we proved that the main term in the number of double covers of double covers  $D \xrightarrow{2} C \xrightarrow{2} \mathbb{P}^1$  of a given genus  $g_D$  is given asymptotically as  $g_D \to \infty$  by

$$q^{2g_D+5}\frac{(2-q^{-1})(1-q^{-(2g_D+4)/3})}{(1-q^{-1})(1-q^{-2})} + O\left(q^{5g_D/3}\left(1-q^{-(g_D-1)/6}\right)\right).$$

Note that the result is for double covers of double covers, and not for  $D_4$  covers, which is our target. The next step is to sieve for the other possible Galois groups and get an asymptotic for all  $D_4$  covers of  $\mathbb{P}^1$ . Then we will need to sieve for various covers that have various desirable geometric properties, like reduced, irreducible and smooth.

#### **Group 4: Arithmetic Geometry**

**Participants**: Alina Carmen Cojocaru (University of Illinois at Chicago), Rachel Davis (University of Wisconsin), Antonella Perucca (Katholieke Universiteit Leuven), Alice Silverberg (University of California, Irvine), Katherine E. Stange (Stanford University), and Diane Yap (University of Hawai'i at Mānoa).

The group explored some problems relating to abelian surfaces over the field of rational numbers and over finite fields.

We began by studying some of the background on abelian varieties, especially the arithmetic aspects of abelian surfaces, including classification of the endomorphism ring, structure of torsion modules, properties of the associated Galois representations, splitting (simple vs. non-simple), and properties of the reductions modulo primes for abelian varieties over the rationals. See [17-46] for some of the papers we looked at.

We also formulated some problems to consider, and discussed various approaches we would take to solve them. We did some exploratory work and achieved a better understanding of the problems, what is known, and what obstacles remain.

#### Group 5: K-theory and Algebraic Number Theory

**Participants**: Veronika Ertl (University of Utah), Wieslawa Niziol (University of Utah), Bregje Pauwels (University of California at Los Angeles), Sujatha Ramdorai (University of British Columbia), and Ila Varma (Princeton University).

One of the fundamental open problems in arithmetic is the description of the Galois group  $G = \operatorname{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ . Class field theory affords a description of the Galois group  $G^{ab}$ maximal abelian extension of  $\mathbb{Q}$  and the decomposition groups, namely the Galois groups  $G_p^{ab}$ , of the maximal abelian extensions of the local fields  $\mathbb{Q}_p$ , as p varies over prime integer primes, are important constituents of the description of  $G^{ab}$ . Local class field theory affords a description of finite quotients of  $G_p^{ab}$  in terms of  $K^*$ , where K is a finite abelian extension of  $\mathbb{Q}_p$ , via the reciprocity map. Higher dimensional local fields of dimension > 1 have been studied by Kato, Saito, Vostokov, Fesenko and others. They have proved the existence of higher dimensional reciprocity maps which describes the Galois groups of abelian extensions of higher dimensional local fields F of dimension n, in terms of higher Milnor K-groups  $K_n^M(F)$ . Let F be any field. The Bloch-Kato conjecture asserts that there is an isomorphism

$$K_n^M(F)/p^n \simeq H^n(\operatorname{Gal}(F^{\operatorname{sep}}/F, A)).$$

Here  $F^{\text{sep}}$  is a separable closure of F, p a prime and A is the Galois module  $\mu_{p^m}^{\otimes m}$  if p is prime to the characteristic of F and the module of differentials  $\nu_n(F)$ ) otherwise. Thus, for higher dimensional local fields F, the higher Milnor K-groups  $K_n^M(F)$  occur as a common theme in studying higher dimensional reciprocity laws and the Milnor conjecture.

An important question in arithmetic geometry is the study of the Gersten sequence for Milnor K-theory which we describe below. Let X be a smooth (or more generally regular) scheme, over a local ring of mixed characteristic. Then the Gersten complex is the complex

$$0 \to K_n^M \to \bigoplus_{x \in X^0} i_x^* K_n^M(x) \to \bigoplus_{x \in X^1} i_x^* K_{n-1}^M(x) \to \dots$$

where  $X^k$  is the set of codimension k points on X,  $i_x : x \to X$  is the inclusion map and one considers pull backs of the Milnor K-sheaves. The Gersten conjecture is the assertion that this sequence is exact. We would like to think about two concrete problems:

1. Determine the structure of  $K_n^M(K)$  of complete discrete valuations fields of mixed characteristic. Check [49, 51] for what is known. Consult [52, 50] for basics on K-theory and Milnor K-theory. 2. Gersten's conjecture is open as stated, i.e., integrally. It is known mod-*l*, if *l* is different from the residue characteristic *p*. We will try to see whether we can prove it mod-*p*.

The problems as stated above are difficult problems and a review of literature on the questions was undertaken. Though no concrete progress was made towards the solution of the two problems, the possibility of using the existing techniques in describing the Milnor K-groups  $K_i^M(F)$  for special higher dimensional local fields, to understand the Milnor K-group  $K_1^M(R)$  for total quotient rings of noncommutative, Auslander regular Iwasawa algebras was explored. This would have implications for the study of *p*-adic *L*-functions arising in noncommutative Iwasawa theory.

### Group 6: Zeta functions of Artin-Schreier varieties and Hodge polygons of exponential sums

**Participants**: Rebecca Bellovin (Stanford University), Sharon Anne Garthwaite (Bucknell University), Ekin Ozman (University of Texas-Austin), Rachel Pries (Colorado State University), Cassandra Williams (Colorado State University), and Hui June Zhu (State University New York at Buffalo).

Let q be a power of a prime p. Given a variety V over the finite field  $\mathbb{F}_q$ , an important problem is to count the number of rational points of V over finite extensions of  $\mathbb{F}_q$ . This information is encoded in the zeta function of V. By works of Dwork [56] and Deligne [55] on the Weil conjectures [60], the zeta function of a smooth projective variety V is a rational function in  $\mathbb{Q}[T]$ . When V is a hypersurface of dimension n, the non-trivial information about the zeta function is encoded in an L-function  $L(V/\mathbb{F}_q;T)$ , whose roots are algebraic integers with complex absolute values equal to  $q^{n/2}$ , and  $\ell$ -adic absolute values equal to 1 for each prime  $\ell \neq p$ . It remains to know the distribution of the p-adic absolute values of these roots. This question is equivalent to determining the slopes of the p-adic Newton polygon NP(V) of the L-function.

On the other hand, it is a classical question in number theory to study the exponential sum of a Laurent polynomial  $f(x_1, \ldots, x_n)$  in  $\mathbb{F}_q[x_1^{\pm 1}, \ldots, x_n^{\pm 1}]$  by its *L*-function  $L(f/\mathbb{F}_q; T)$ . Write its normalized *p*-adic Newton polygon by NP(*f*). These two questions are related in the following way: Consider the affine toric Artin-Schreier variety  $V_f$  in  $\mathbb{A}^{n+1}$  defined by the affine equation  $y^p - y = f(x_1, \ldots, x_n)$ . The *p*-adic Newton polygon of  $L(f/\mathbb{F}_q; T)$  and the *p*-adic Newton polygon of  $L(f/\mathbb{F}_q; T)$  are the same after scaling by a factor of p-1, denoted by NP( $V_f$ ) = (p-1)NP(f).

Until recently the task of determining the *p*-adic Newton polygon of an Artin-Schreier variety or exponential sum was anything but easy; they were only accessible in very special cases, and estimation results of the Newton polygons were often case-by-case. However things have changed due to the work of [57, 54, 59].

For a Laurent polynomial f, the Hodge polygon  $\operatorname{HP}(f)$  of the L-function of the exponential sum of f is defined using weightings of lattice points in a polytope  $\Delta_f$  determined by the monomials in f. This combinatorial object encodes the essential topological (cohomological) data for the toric Artin-Schreier variety  $V_f$ . In this way  $\operatorname{HP}(f)$  guards the p-adic valuations of the roots of  $L(f/\mathbb{F}_q;T)$ , and hence it gives a lower bound of  $\operatorname{NP}(f)$  (see [59, 54]). This is analogous to the fact that the Hodge numbers of an algebraic variety over a finite field determine a Hodge polygon which is a lower bound for the Newton polygon [58]. For a prescribed Newton polytope  $\Delta$  in  $\mathbb{R}^n$ , and a Laurent polynomial  $f(x_1, \ldots, x_n)$  in  $\mathbb{F}_q[x_1^{\pm 1}, \ldots, x_n^{\pm 1}]$  with  $\Delta_f = \Delta$ , there are necessary and sufficient conditions for when  $\operatorname{NP}(f)$  coincides with the lower bound  $\operatorname{HP}(\Delta_f)$  (see [54, 59]).

The starting point of our group project was computing the *L*-function of  $f = x_1^m + \cdots + x_n^m$  over  $\mathbb{F}_q$ . This classical case has been studied in the literature, and the Newton polygon of f can be computed using Gauss sums and the Stickelberger theorem. The goal of our project is to study deformations of the classical diagonal case to cases closely related to the important Kloosterman forms. First, we found closed form formulae for the Hodge polygons of Laurent polynomials of the form

$$f = x_1^m + \dots + x_n^m + x_1^{-m} + \dots + x_i^{-m}.$$

Second, we found closed form formulae for the Hodge polygons of the generalized Kloosterman family given by

$$f = x_1^m + \dots + x_n^m + t(x_1 \cdots x_n)^{-1},$$

with parameter t varying in  $\mathbb{Q}^*$ . For each reduction modulo p of f, one arrives at a special fibre of a motive over the torus  $\mathbb{G}_m(\mathbb{F}_p)$ . In addition, we proved some original asymptotic results about the variation of the Newton polygon for fixed dimension n and m >> 0.

#### Group 7: Project Title: Ramanujan supercongruences and complex multiplications

**Participants**: Sarah Chisholm (University of Calgary), Alyson Deines (University of Washington), Ling Long (Iowa State University), Gabriele Nebe (RWTH Aachen University), and Holly Swisher (Oregon State University).

Ramanujan discovered 17 series of the form

$$\sum_{k\geq 0} \frac{(1/2)_k^3}{k!^3} (6k+1) \frac{1}{4^k} = \frac{4}{\pi}, \ (1/2)_k = 1/2 \cdot (1/2+1) \cdots (1/2+k-1)$$

which is related to elliptic curves with complex multiplications. These expansions of  $\frac{1}{\pi}$  admit *p*-adic analogues, called Ramanujan supercongruences, of the following form: for any prime p > 3

$$\sum_{k=0}^{(p-1)/2} \frac{(1/2)_k^3}{k!^3} (6k+1) \frac{1}{4^k} \equiv (-1)^{(p-1)/2} p \mod p^3.$$

The goal of the project is to give a geometric proof of Ramanujan supercongruences. To be more precise, for  $\lambda \in \overline{\mathbb{Q}}$  such that  $E_{\lambda} : y^2 = (x-1)(x^2 - \frac{1}{1+\lambda})$  admits complex multiplications, following Ramanujan's idea, there exist numbers  $a, b, \delta \in \mathbb{Q}(\lambda)$  such that

$$\sum_{k \ge 0} \frac{(1/2)_k^3}{k!^3} (ak+b)\lambda^k = \frac{\delta}{\pi}.$$

Correspondingly, we will like to prove that for any prime p > 7 such that  $\lambda \in \mathbb{Q}_p$  the following congruence hold

$$\sum_{k=0}^{(p-1)/2} \frac{(1/2)_k^3}{k!^3} (ak+b)\lambda^k = u(p) \cdot b \cdot p \mod p^2,$$

where u(p) is a root of unity depending on p that can be embedded in  $\mathbb{Q}_p$ .

The Picard-Fuchs equation of the family of elliptic curves  $E_{\lambda} : y^2 = (x-1)(x^2 - \frac{1}{1+\lambda})$  is an order 2 hypergeometric differential equation, whose symmetric square is the Picard Fuchs equation for the family of K3 surfaces  $X_{\lambda} : z^2 = xy(x+1)(y+1)(x+\lambda y)$ . We counted the  $\mathbb{F}_p$  points on  $X_{\lambda}$  modulo  $p^3$  for arbitrary  $\lambda$  over  $\mathbb{F}_p$  by using results of Ahlgren, Kilbourn, Ono, Pennisten and hope this will give insights for accomplishing our project.

#### **Group 8: Arithmetic Intersection Formulas**

**Participants**: Jackie Anderson (Brown University, Jennifer Balakrishnan (Harvard University, Kristin Lauter (Microsoft Research), Jennier Park (Massachusetts Institute of Technology), and Bianca Viray (Brown University).

The goal of our project was to prove equality between two arithmetic intersection formulas when the assumptions for both formulas are satisfied. We begin with some motivation. The *absolute Igusa invariants*  $i_1, i_2, i_3$  of a genus 2 curve can be defined by values of modular functions on the Siegel moduli space. They determine the isomorphism class of a genus 2 curve over  $\mathbb{C}$  when  $i_1 \neq 0$ . The *Igusa class polynomials*  $H_{j,K}$  of a primitive quartic CM field K are the minimal polynomials of Igusa invariants: for each j = 1, 2, 3,  $H_{j,K} = \prod (x - i_j(C))$ , where the product ranges over isomorphism classes of genus 2 curves C with CM by K (i.e. with an embedding of  $\mathcal{O}_K$  into End(Jac(C))), and the modular function is evaluated at the point in the Siegel upper half plane corresponding to the canonically polarized Jacobian of the curve C. The coefficients of these polynomials are rational but not necessarily integral. To compute them efficiently, it is important to understand the denominators appearing in the coefficients.

The first Igusa invariant can be defined by the following ratio of modular forms:  $i_1 := 2 \cdot 3^5 \frac{\chi_{12}^2}{\chi_{10}^6}$ . A prime  $\ell$  appearing in the denominator of  $i_1$  corresponds to a pole of  $i_1$  at a CM-point over  $\overline{\mathbb{F}}_{\ell}$ . Since the numerators are modular forms, there is a pole of  $i_1$  at a point P only if P is a zero of  $\chi_{10}$ . Away from 2, div $(\chi_{10}) = 2G_1$ , so  $12 (G_1.CM(K))_{\ell}$  gives a formula for the  $\ell$ -valuation of the denominators, up to cancellation.

Bruinier and Yang [61] gave a conjectural formula for this intersection number for primitive quartic CM fields K, under the assumption that the discriminant of K is  $D^2 \tilde{D}$ , where D and  $\tilde{D}$  are primes  $\equiv 1 \pmod{4}$ . Let K be a totally imaginary quadratic extension of  $F = \mathbb{Q}(\sqrt{D})$ ,  $D \equiv 1 \pmod{4}$  and prime, A and B such that  $K = F(\sqrt{A + B\sqrt{D}})$ .

**Theorem 34.0.13 (Bruinier-Yang Conjecture)** Let  $\widetilde{K}$  be the reflex field of K and  $\widetilde{F}$  be the quadratic subfield of  $\widetilde{K}$ . Then

$$\frac{(CM(K).G_1)_{\ell}}{\log(\ell)} = \sum_{\substack{\delta = \frac{D-x^2}{4} \in \mathbb{Z}_{\geq 0}}} \sum_{\substack{n \text{ s.t. } \frac{n+\delta\sqrt{\tilde{D}}}{2D} \in \operatorname{Disc}_{\widetilde{K}/\widetilde{F}}}} B_{\frac{n+\delta\sqrt{\tilde{D}}}{2D}}(\ell),$$

where

$$B_t(l) = \begin{cases} 0, \text{ if } \mathfrak{l} \text{ splits in } \widetilde{K} \\ (v_{\mathfrak{l}}(t)+1)\mathfrak{A}(t\mathcal{D}_{\widetilde{K}/\widetilde{F}}\mathfrak{l}^{-1})f(\mathfrak{l}/l), \text{ otherwise} \end{cases},$$

where  $\mathfrak{A}(t\mathcal{D}_{\widetilde{K}/\widetilde{F}}\mathfrak{l}^{-1})$  denotes the number of ideals in  $\mathcal{O}_{\widetilde{K}}$  whose relative norm in  $\widetilde{F}$  is  $t\mathcal{D}_{\widetilde{K}/\widetilde{F}}\mathfrak{l}^{-1}$ . It has been proved by Yang [64] when  $A^2 - DB^2 \equiv 1 \pmod{4}$  is prime and  $\mathcal{O}_K$  is generated over  $\mathcal{O}_F$  by an element of a special form.

More recently, Lauter and Viray [63] gave a formula for the intersection number that holds, away from a few primes, for all primitive quartic CM fields such that  $\mathcal{O}_K$  is principally generated over  $\mathcal{O}_F$ . We state it here in a simple case to emphasize its formal likeness to the formula given by Bruinier-Yang. Assume that  $\mathcal{O}_K$  is generated over  $\mathcal{O}_F$  by one element, say  $\eta$ , so  $\mathcal{O}_K = \mathcal{O}_F[\eta]$ . Let  $\widetilde{D}$  denote  $\operatorname{Norm}_{F/\mathbb{Q}}(\operatorname{Disc}_{K/F}(\mathcal{O}_K))$ and let  $\alpha_0, \alpha_1, \beta_0, \beta_1 \in \mathbb{Z}$  be such that

$$\operatorname{Tr}_{\mathrm{K/F}}(\eta) = \alpha_0 + \alpha_1 \frac{\mathrm{D} + \sqrt{\mathrm{D}}}{2}, \quad \operatorname{Norm}_{\mathrm{K/F}}(\eta) = \beta_0 + \beta_1 \frac{\mathrm{D} + \sqrt{\mathrm{D}}}{2}$$

**Theorem 34.0.14 (Lauter-Viray)** Assume that  $\ell \neq 2$ , D = 5 and that  $d_u(n)$  (defined below) is an odd fundamental quadratic discriminant prime to  $\ell$ , for every n that appears below.

$$\frac{(CM(K).G_1)_{\ell}}{\log(\ell)} = \sum_{\delta = \frac{D-\Box}{4} > 0} \sum_{\substack{n \text{ such that} \\ \frac{\delta^2 \frac{D-n^2}{4-D} \in \ell\mathbb{Z} > 0 \\ n \equiv -c(K) \pmod{2D}}} B(\delta, n)$$
$$B(\delta, n) = \frac{1}{2} \left( v_{\ell} \left( N \right) + 2 \right) \mathfrak{A}_{d_u(n)} \left( N \right) \rho_{d_u(n)} \left( N \right)$$

where

$$\begin{split} \mathfrak{A}_d(N) &:= \# \left\{ \mathfrak{b} \subseteq \mathbb{Z} \left[ \frac{d + \sqrt{d}}{2} \right] : \operatorname{Norm}(\mathfrak{b}) = N, \mathfrak{b} \text{ invertible} \right\} \\ \rho_d(N) &:= \left\{ \begin{matrix} 0 & \text{if } \left( \frac{d^*}{p} \right)^{a_p} \left( \frac{-\ell e_p}{p} \right) = -1 \text{ for some } p | d, \\ & \text{where } N = p^{a_p} e_p \text{ and } d^* = (-1)^{\frac{p-1}{2}} \frac{d}{p} \\ 2^{\#\{p:p|N \text{ and } p|d\}} & \text{otherwise} \end{matrix} \right. \\ c(K) &:= \delta \left( \alpha_0^2 + \alpha_0 \alpha_1 D + \alpha_1^2 \frac{D^2 - D}{4} - 4\beta_0 - 2\beta_1 D \right) \\ d_u(n) &:= (\alpha_1 \delta)^2 - 4 \frac{(n + c(K))\delta}{-2D}. \end{split}$$

Since the Lauter-Viray and Bruinier-Yang formulas both hold for primitive quartic CM fields under certain assumptions, we considered the fields where both hypotheses were satisfied and sought to prove a direct correspondence between the two statements. As a first step, we split the work into cases according to the form of the generator  $\eta$  (see [62]). During the WIN2 Workshop, we worked on the case where  $\eta = \frac{1+\sqrt{A+B\sqrt{D}}}{2}$ . This gives simplified formulas for  $\alpha_i, \beta_i, c(K), d_u(n)$ . Using this, we were able to prove that the Bruinier-Yang and Lauter-Viray formulas are equal and match term-by-term:

**Theorem 34.0.15 (ABLPV)** Assume that  $\left(\frac{\delta^2 \tilde{D} - n^2}{4Dl}\right)$  is coprime to  $(2\delta \ell d_u)$ , that  $\rho_{d_u(n)}\left(\frac{\delta^2 \tilde{D} - n^2}{4Dl}\right) \neq 0$  and that all the assumptions for BY and LV are satisfied (in particular, assume that  $(\ell, 2\delta d_u) = 1$ ). Then

$$\mathfrak{A}_{d_u(n)}\left(\frac{\delta^2\widetilde{D}-n^2}{4Dl}\right)\rho_{d_u(n)}\left(\frac{\delta^2\widetilde{D}-n^2}{4Dl}\right) = \mathfrak{A}\left(\frac{n+\delta\sqrt{\widetilde{D}}}{2D}\mathcal{D}_{\widetilde{K}/\widetilde{F}}\mathfrak{l}^{-1}\right).$$

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## Chapter 35

# **Diophantine methods, lattices, and arithmetic theory of quadratic forms** (11w5011)

## Nov 13 - Nov 18, 2011

**Organizer(s):** Wai Kiu Chan (Wesleyan University) Lenny Fukshansky (Claremont McKenna College) Rainer Schulze-Pillot (Universitaet des Saarlandes) Jeff Vaaler (University of Texas, Austin)

### **Overview of the Field and Recent Developments**

The study of equations over the integers or the rational numbers is the subject of diophantine geometry. This also includes generalizations to finite extensions of the rationals, their rings of integers, and also to function fields over a finite field, and the rings of polynomials therein. This is a vast subject, in which a variety of methods from geometry, analysis, and arithmetic are used. For our intended workshop we focus on problems involving height functions, methods from the geometry of numbers, and the arithmetic of lattices with quadratic and hermitian forms. In the sections to follow we present a brief overview of a few directions in the theories of *height functions* and of *quadratic forms*, in particular concentrating on the interplay of these two lively areas.

#### Height functions and Diophantine problems.

Height functions of various sorts have played a fundamental role in diophantine problems. Height functions are used to measure the complexity of an algebraic object such as a polynomial or a point on an algebraic variety. A comprehensive account of their role in the modern theory of diophantine equations is contained in the recent monograph "Heights in diophantine geometry" by E. Bombieri and W. Gubler. In addition to this, a new research direction has been stimulated by recent work of Allcock and Vaaler on the metric space structure induced by certain height functions. If  $h(\alpha)$  denotes the absolute Weil height on the nonzero algebraic number  $\alpha$ , then  $h(\alpha) = h(\zeta \alpha)$  for all roots of unity  $\zeta$ . It follows that the height h is well defined on the quotient group  $\overline{\mathbb{Q}}^{\times} / \operatorname{Tor}\{\overline{\mathbb{Q}}^{\times}\}$  denotes the multiplicative group of nonzero algebraic numbers, and  $\operatorname{Tor}\{\overline{\mathbb{Q}}^{\times}\}$  is its torsion subgroup. In fact  $\overline{\mathbb{Q}}^{\times} / \operatorname{Tor}\{\overline{\mathbb{Q}}^{\times}\}$  has the structure of a vector space over  $\mathbb{Q}$  (written multiplicatively), and h is a norm on this vector space. It follows that the metric completion is a Banach space over the real numbers. This Banach space has recently been investigated and shown to be isometric to a co-dimension one subspace of  $L^1$  of a certain explicitly given measure space.

measure that naturally arises is the unique invariant measure with respect to the action of the absolute Galois group of  $\overline{\mathbb{Q}}/\mathbb{Q}$ . Hence this group acts as a group of isometries on the Banach space. One expects that a similar but more elaborate structure will hold for the metric completion of elliptic curves, or more generally for abelian varieties, with respect to suitable height functions.

An important application of height functions to the study of diophantine equations arises from Northcott's finiteness property: there are only finitely many projective points over an algebraic number field with height bounded from above by a given constant. Hence, if one can prove that a given diophantine equation has a non-trivial solution of explicitly bounded height, then finding such a solution is reduced to a finite search. Therefore such bounds on heights are often referred to as *search bounds* for solutions of diophantine equations. This idea is frequently used in diophantine geometry when looking for points on varieties over number fields. In fact, in recent years there have been a number of results by a variety of authors on counting the number of points of bounded height on varieties, in particular in the direction of influential conjectures of R. Heath-Brown and Y. Manin.

On the other hand, one cannot expect the existence of explicit search bounds for diophantine equations of arbitrary degree in an arbitrary number of variables: This would provide an algorithm for deciding whether an equation has a solution, thus contradicting Matiyasevich's famous undecidability result for Hilbert's tenth problem. The only hope to obtain such search bounds for equations in a large number of variables is by restricting the degree, and it is known that even for a single equation of degree four search bounds already cannot exist. The two extensively studied situations here are that of a system of linear equations and of one quadratic equation. The first of these is addressed by Siegel's lemma and its many different generalizations, while the second stems from the work of J. W. S. Cassels on small-height zeros of quadratic forms. Cassels' theorem, proved in 1955, states that any isotropic rational quadratic form has a non-trivial rational zero of small height, where the explicit bound on height depends on the height of the coefficient vector of the form and its number of variables. There has been a large amount of work done by many authors ever since 1955 on various generalizations and extensions of Cassels' theorem. The investigation of height bounds for zeros of quadratic, hermitian, and bilinear forms, as well as the effective structure of corresponding bilinear spaces, not only carries independent number theoretic interest, but also contributes to our understanding of the boundary of Diophantine undecidability.

Another active direction of research closely connected to the above discussion is the study of classical and generalized Hermite constants, as well as related extensions of the classical geometry of numbers. Hermite's constant for a lattice  $\Lambda$  in  $\mathbb{R}^N$  is defined to be

$$\gamma(\Lambda) = \frac{\min_{\boldsymbol{x} \in \Lambda \setminus \{\boldsymbol{0}\}} \|\boldsymbol{x}\|^2}{\det(\Lambda)^{1/N}} = \frac{\min_{\boldsymbol{y} \in \mathbb{Z}^N \setminus \{\boldsymbol{0}\}} Q_{\Lambda}(\boldsymbol{y})}{\det(Q_{\Lambda})^{1/2N}},$$

where  $Q_{\Lambda}$  is a positive definite quadratic form on  $\Lambda$ . Hermite's constant is fundamental in lattice theory and discrete optimization problems, in particular in connection with sphere packing. In recent years new generalizations of the classical Hermite constant using height functions have been defined in adele spaces and algebraic groups over number fields. Hermite's constant in the non-commutative setting of central simple algebras has also been investigated, for instance in the works of J. Thunder and T. Watanabe. The study of generalized Hermite constants is a promising new direction, emphasizing the interplay of the arithmetic theory of quadratic forms with the theory of height functions.

#### Quadratic forms.

The arithmetic theory of quadratic (and hermitian) forms is on the one hand a subfield of the theory of diophantine equations, dealing with a particularly simple class of equations whose zero sets are also simple from the point of view of algebraic geometry. It has special features since the orthogonal group of a rational quadratic form provides a large group of automorphims which allows to bring group theoretic, representation theoretic, and ergodic methods into play. A recent spectacular success of these methods is the theorem of

Ellenberg and Venkatesh on representation of quadratic forms by quadratic forms. A more classical but still very active group theoretic aspect (the oscillator representation and the theta correspondence) is at the basis of the use of the theory of modular forms for the investigation of quadratic forms, yet another group theoretic connection is the construction of lattices (or equivalently integral quadratic forms) using the theory of finite groups, as shown for example in Griess' recent work on the Barnes-Wall lattice. These aspects give the arithmetic theory of quadratic forms a special status in the larger field of diophantine equations.

The subject has seen dramatic progress in the twentieth century through the work of Siegel, Witt, Eichler, Kneser, Tamagawa, and it continues to flourish. The local-global principle for rational quadratic forms together with the strong approximation theorem for the spin group allows to reduce many (though by no means all) questions about integral quadratic forms to computations over the integers of a local field. Most of these local problems have been well understood in the case of odd residue characteristic for quite some time; the case of residue characteristic 2 (the dyadic case) presents, especially if 2 is ramified, considerable technical and conceptional difficulties. Remarkable progress has been obtained here by Nicu Beli in 2004, completing the determination of the spinor norm groups of lattices over the integers of general dyadic local field and of similar local groups arising in connection with the representation problem.

The global representation problem of integral quadratic forms is dealt with by a variety of methods, some of which have already been mentioned above. In 2009 Colliot-Thélène and Xu Fei showed that some of the difficulties arising here can be interpreted as an analogue of the well known Brauer-Manin obstruction in arithmetic geometry. Brüdern, Fouvry, Greaves, Heath-Brown, Blomer and Dietmann used new refinements of the classical Hardy-Littlewood circle method in conjunction with other arithmetic methods to prove results about representation of integers as sums of squares with restricted variables. Remarkably, classical analytic techniques, such as Hardy-Littlewood circle method, were also successfully used by Heath-Brown, Dietmann, Browning, and others to obtain new height search bounds for diophantine equations extending the classical results of Cassels and Siegel and their generalizations, as well as in the direction of Manin's conjecture. Hence investigations in the theory of heights frequently appeal to techniques quite similar to those commonly used in the arithmetic theory of quadratic forms. Moreover, many problems of diophantine geometry involve at some point arguments from the classical geometry of numbers and from the study of the arithmetic of particular definite or indefinite rational or integral quadratic forms, e.g. in the study of the Néron-Tate height on abelian varieties. More recently, in 1990s and 2000s, such classical ideas and techniques played an important role in the development of the deep and influential general theory of heights as seen in the works of: J.-B. Bost, H. Gillet, and C. Soulé; S. Zhang; S. David and P. Philippon; M. Sombra; E. Bombieri, D. Masser, and U. Zannier, and many others. A combination of theoretically obtained bounds for the size or number of solutions or for existence of representations for sufficiently large integers or forms and a computer assisted search below those bounds have in several cases proven to be extremely successful, for example in forthcoming work of Bhargava and Hanke on the 290-conjecture of Conway and in work of Jenkins and Rouse on the computation of minima of high-dimensional lattices.

Important progress has also been obtained recently in the area of reduction theory and construction of lattices with special properties (e. g. large minimum, specified automorphism group), where again often combinations of theoretical and computer assisted methods are successful. As examples we mention work of Schürmann, Watanabe, Gunnells, Yasaki on perfect forms and on Voronoi reduction and the construction of an extremal lattice in dimension 72 by Nebe.

## **Outcome of the Meeting and Scientific Progress Made**

The goal of this workshop was to bring together people working in the following areas:

- 1. Classical arithmetic theory of quadratic forms and lattices.
- 2. Diophantine problems and the theory of height functions.

In spite of the close connections between these areas, it is quite rare for mathematicians working in these

subjects to meet altogether for a joint workshop. Our workshop provided such a unique opportunity, which has certainly resulted in fruitful mathematical communication and will hopefully lead to significant future progress. There is a variety of prominent research directions that lie in the intersection of these two areas. Here are just a few of them:

1. Representation problems for quadratic forms and lattices over global fields and rings; finding representatives of small height in orbits of representation under the automorphism group of the form and counting representations of bounded height.

2. Small zeros (with respect to height) of individual quadratic forms and of systems of quadratic forms, originating in the work of Cassels and Siegel, its various generalizations, and related Diophantine problems with the use of heights.

3. Classical Hermite constant, geometry of numbers, and various generalizations with the use of height functions, explicit reduction theory of definite and indefinite quadratic forms.

Diophantine methods with the use of height functions are usually based on geometry of numbers and ideas from lattice theory. The target of these methods often lies in the realm of quadratic forms theory.

A proceedings volume of our workshop will be published in the AMS Contemporary Mathematics series. We feel that we met our goals of bringing together two mathematical communities and helping to start some new research directions. We include below comments from a few of our participants about the usefulness of the workshop from their perspective.

#### From Tim Browning (University of Bristol):

Of all the lectures at the conference I found the one by Colliot-Thelene the most inspiring. It deals with a problem that is right at the limit of what analytic number theory can handle and I plan to look at papers of Hooley from 2006 to see whether one can use the circle method to handle strong approximation for q(x,y,z)=P(t) when q is positive definite. The meeting was also very useful in that it gave me the opportunity to talk to Colliot-Thelene about the "state of affairs" for conic bundle surfaces with many split degenerate fibers, which has given me very useful motivation about a problem that I've recently started looking at (from the point of view of additive combinatorics) with a student of Ben Green (Lilian Matthiesen a postdoc at Bristol). Generally I greatly enjoyed meeting people that I don't normally encounter on the conference circuit and some of interactions led to useful and quite unexpected conversations about different aspects of quadratic forms and Thue type inequalities.

#### From Juan Marcos Cervino (University of Heidelberg):

Besides the fact, that being invited to a Workshop at BIRS is already a great pleasure (as one speaker mentioned: is one of the things a mathematician should do, as in normal life one should plant a tree..), I am very glad having had the opportunity to attend it. I would like to summarize my experience in the following items.

- It is always a pleasure to be in a place, where one feels oneself welcomed. This is the case for the whole BIRS (installations, personnel, et cetera). This being naturally the basis of a pleasant stay of any kind, which in our particular case certainly contributed to the effectiveness of the Workshop.

- The not so compressed schedule enabled us, the participants, to speak about our research interests in a less rigid atmosphere than within the talks themselves (the given schedule being certainly the "golden ratio", since on the other hand I would have liked to give a talk, as certainly others). For example, I got to know Prof. R. Coulangeon, who got interested in part of my research and is going to invite me to Bordeaux (France) to talk more precisely about the relations between his and my work. I discussed also with Prof. G. Nebe on a problem which was already pointed out to me by Prof. B. Venkov some weeks ago in Aachen. We will pursue this investigation further.

- Specialized Conferences or Workshops help younger mathematicians, I mean 'not so experienced mathematicians' (as is my case), to extract the main problems in the area, which may orient ideas and research. Despite the mixture of the two main groups in the Workshop, this was certainly possible in my case. These

two groups were, in my eyes, not too far away from each other, so that the mixture was in the end somehow homogeneous.

#### From Rainer Dietmann (Royal Holloway, University of London):

I found it very good to bring together people from many different areas. For example for me, it was an excellent opportunity to talk to Lenny Fukshansky and Jeff Vaaler about small zeros of pairs of quadratic forms, to people from Analytic Number Theory (Tim Browning and Roger Heath-Brown), to algebraists such as David Leep, to modular forms people such as Rainer Schulze-Pillot who gave me some very useful references on the problem of representing quadratic forms by quadratic forms, and to other "point-counting" number theorists such as Martin Widmer. In fact, this meeting has been the most fruitful one for me for a long time.

#### From Roger Heath-Brown (Oxford University):

I have some thoughts on the workshop. Firstly, I felt it was the most successful meeting I've attended in the past 3 years (at least). I had been concerned that, coming from a more analytic background than most of the participants, I would find nothing of interest. In fact I came away inspired with 2 or 3 different ideas for future investigation - with most meetings the count is 0.

#### From David Leep (University of Kentucky):

This conference was incredibly useful to me because people from a number of different areas came together. It is always useful and wonderful to see people I already know. For example, I had excellent discussions with Jean Louis Colliot Thelene, a colleague with whom I have discussed mathematics for several decades. At this conference I explained a new theorem I proved that extended some of his work. I plan to include this theorem in the paper I will submit to the proceedings of this conference.

Besides seeing long time colleagues and acquaintances, I was able to meet a number of new people. This included people with whom I have already been in e-mail contact, but had never met, and other people with whom I have never been in contact. For example, I was quite pleased to meet Tim Browning. We had already been in e-mail contact (along with Colliot Thelene) about a paper that one of his PhD students had written. It was wonderful to meet him in person. That makes future e-mail contact much better and much more pleasant. It also makes a future visit more likely.

Perhaps the highlight of the conference for me was finally meeting Roger Heath-Brown. We have exchanged e-mail before on several topics. Roger was already familiar with some of my work. (Obviously I was already familiar with his work.) So it was a great pleasure to have conversations with him concerning some topics of mutual interest to both of us.

It was also fun meeting a number of new people, mostly younger people, and having discussions with them. I knew some of their names previously (for example Ben Kane and others) while some of their names were completely new to me. I thoroughly enjoyed the conference.

## **Presentation Highlights**

Our participants presented 6 hour-long plenary talks and 16 invited 30-minute talks, which stimulated a number of lively discussions that will likely lead to new research and collaborations. The goal of some plenary talks was to survey a given subarea, while most invited talks reported on specific recent developments. We have attached the abstracts below.

#### Hour-long talks

Eva Bayer-Fluckiger (École Polytechnique Fédérale de Lausanne)

Title: Galois algebras, Hasse principle and induction-restriction methods

**Abstract:** Let k be a field of characteristic  $\neq 2$ , and let L be a Galois extension of k with group G. Let us denote by  $q_L : L \times L \to k$  the *trace form*, defined by  $q_L(x, y) = \text{Tr}_{L/k}(xy)$ . Let  $(gx)_{g \in G}$  be a normal basis of L over k. We say that this is a *self-dual normal basis* if  $q_L(gx, hx) = \delta_{g,h}$ . If the order of G is odd, then L always has a self-dual normal basis over k (cf. [3]). This is no longer true in general if the order of G is even; some partial results are given in [4].

If k is an algebraic number field, then it is natural to ask whether a local–global principle holds for this problem. In order to make this question precise, we have to consider G–Galois algebras and not only field extensions. Moreover, it is useful to note that  $q_L$  is a G–quadratic form, in other words  $q_L(gx, gy) = q_L(x, y)$  for all  $x, y \in L$  and  $g \in G$ . The G–Galois algebra has a self–dual normal basis if and only if the G–form  $q_L$  is isomorphic to the unit G–form. We have the following:

**Theorem.** Suppose that k is a global field of characteristic  $\neq 2$ . Let G be a finite group, and suppose that the fusion of the 2-Sylow subgroups of G is controlled by the fusion. Let L and L' be two G–Galois algebras such that for all places v of k, the G–forms  $q_{L_v}$  and  $q_{L'_v}$  are isomorphic over  $k_v$ . Then the G–forms  $q_L$  and  $q_{L'}$  are isomorphic over k.

**Corollary.** Suppose that k and G are as above. Then a G-Galois algebra has a self-dual normal basis over k if and only if such a basis exists over all the completions of k.

The proof uses a result concerning induction and restriction for arbitrary G-quadratic forms, which is of independent interest. This is a joint work with Parimala.

#### J.-L. Colliot-Thélène (CNRS, Université Paris-Sud, France)

**Titre de l'exposé:** Sur l'équation q(x, y, z) = P(t) en entiers **Résumé:** Travail en commun avec Fei XU (Capital Normal University, Beijing, Chine).

#### **Définition :** Approximation forte hors de S

Soit X une variété algébrique sur un corps de nombres k. Soit  $S \subset T$  avec T ensemble fini de places contenant les places archimédiennes et  $\mathcal{X}/O_T$  un modèle de X/k sur l'anneau des T-entiers, puis pour chaque  $v \in T \setminus S$ , un ouvert  $U_v \subset X(k_v)$ . Dans toute telle situation, si l'ensemble

$$\prod_{v \in S} X(k_v) \times \prod_{v \in T \setminus S} U_v \times \prod_{v \notin T} \mathcal{X}(O_v) \subset X(\mathbf{A}_k)$$

est non vide, il contient l'image diagonale d'un point de X(k).

Lorsque ceci vaut, on a un principe local-global pour les points S-entiers.

Cas classiques d'approximation forte : la droite affine (reste chinois); équation  $q(x_1, \ldots, x_n) = a$  avec  $n \ge 4, q$  isotrope en une place  $v \in S$ . (Eichler, Kneser); groupe algébrique semisimple simplement connexe G/k sous une hypothèse forte de non compacité pour  $\prod_{v \in S} G(k_v)$  (Kneser, Platonov).

L'approximation forte peut être en défaut. De nombreux exemples ont été interprétés (CT-Xu, 2005–2009) en terme de l'obstruction de Brauer-Manin (qui jusque là avait plutôt été considérée dans l'étude des points rationnels).

On utilise le groupe de Brauer des schémas et l'accouplement

$$X(\mathbf{A}_k) \times \operatorname{Br}(X) \to \mathbb{Q}/\mathbb{Z}$$
  
 $(\{M_v\}, A) \mapsto \sum_v \operatorname{inv}_v A(M_v),$ 

qui est nul sur  $X(k) \times Br(X)$  (loi de réciprocité de la théorie du corps de classes). On note

$$X(\mathbf{A}_k)^{\mathrm{Br}(X)}$$

le noyau à gauche. On a donc  $X(k) \subset X(\mathbf{A}_k)^{\mathrm{Br}(X)}$ .

Définition : Approximation forte hors de S avec condition de Brauer-Manin )

On suppose  $X(\mathbf{A}_k) \neq \emptyset$ . Soit  $S \subset T$  avec T ensemble fini de places contenant les places archimédiennes et  $\mathcal{X}/O_T$  un modèle de X/k, puis pour chaque  $v \in T \setminus S$ , un ouvert  $U_v \subset X(k_v)$ . Dans toute telle situation, si l'ensemble

$$[\prod_{v \in S} X(k_v) \times \prod_{v \in T \setminus S} U_v \times \prod_{v \notin T} \mathcal{X}(O_v)]^{\operatorname{Br}(X)} \subset X(\mathbf{A}_k)^{\operatorname{Br}(X)}$$

est non vide, il contient l'image diagonale d'un point de X(k).

**Théorème** L'approximation forte hors de S avec condition de Brauer-Manin vaut pour tout X/k espace homogène d'un groupe algébrique G/k linéaire connexe, avec stabilisateurs géométriques connexes, et une hypothèse convenable de non compacité aux places de S.

Références : CT et Xu 2005-2009 (G semisimple simplement connexe); Harari 2008 (G commutatif connexe); Demarche 2011 (groupes quelconques); Borovoi et Demarche 2011 (espaces homogènes, cas général).

## Que dire sur les points entiers en dehors du cadre des espaces homogènes de groupes linéaires connexes ?

Penser à la situation analogue pour l'étude du principe local-global et l'approximation faible sur les points *rationnels*. Le cas des espaces homogènes de groupes algébriques linéaires connexes (avec stabilisateur connexe) a été beaucoup étudié (Eichler, Kneser, Harder, Chernousov, Sansuc, Borovoi). On a ensuite étudié l'extension à d'autres types de variétés, en particulier les variétés X avec une fibration  $\pi : X \to \mathbf{A}_k^1$  dont la fibre générale est un tel espace homogène.

Soient k un corps, q(x, y, z) une forme quadratique ternaire sur k, non dégénérée, et  $P(t) \in k[t]$  non nul. Notons X/k la variété affine

$$q(x, y, z) = P(t).$$

Si P(t) est séparable, X est lisse. Soit  $U \subset X$  l'ouvert complémentaire de x = y = z = 0. C'est une variété lisse. Soit  $\tilde{X} \to X$  une résolution des singularités de X, avec  $U \subset \tilde{X}$ .

Théorème principal de l'exposé (JLCT et Fei XU, 2011)

Pour k un corps de nombres et  $v_0$  une place de k telle que q est isotrope sur  $k_{v_0}$ , l'approximation forte hors de  $S = \{v_0\}$  avec condition de Brauer-Manin vaut pour tout ouvert Zariski V de X avec  $U \subset V \subset \tilde{X}$ .

La condition Brauer–Manin est nécessaire, mais l'approximation forte hors de S vaut si  $P(t) \neq c.(r(t))^2$  avec  $c \in k^{\times}$ .

#### Sinnou David (Université Pierre et Marie Curie - Paris 6)

#### Title: A journey through heights: the Lehmer problem

**Abstract:** After a brief description of the original Lehmer problem and the work that has been done around it till the seventies, we shall concentrate on the last decade. We shall show how the Lehmer problem can now be seen in a general geometric setup, how it interacts with aspects of global analysis, how the variation of the base field can be taken into account. We shall describe a few general conjectures that contain the original Lehmer problem as a special case and present a few recent results.

#### Roger Heath-Brown (University of Oxford)

**Title:** *p*-adic zeros of systems of quadratic forms

**Abstract:** This is a survey talk concerning the following problem. Let K be a field and let  $r \in \mathbb{N}$ . Define  $\beta(r; K)$  to be the largest integer n for which there exist quadratic forms

$$q_i(x_1,\ldots,x_n) \in K[x_1,\ldots,x_n] \quad (1 \le i \le r)$$

having only the trivial common zero over K. What can one say about  $\beta(r; K)$ , particularly in the case  $K = \mathbb{Q}_p$ ? It is conjectured that  $\beta(r; \mathbb{Q}_p) = 4r$  for all p and all r. This is known for r = 1 and r = 2.

Two lines of attack are sketched. The first uses reduction to  $\mathbb{F}_p$ , looks for a non-singular zero, and then applies Hensel's Lemma. This requires the use of a suitable "minimal model" for the system. The approach is successful when p is large in terms of r, and has been used by Leep to show that  $\beta(1; K) = 2^{t+2}$  when  $K = \mathbb{Q}_p(t_1, \ldots, t_k)$ , irrespective of p. However in the case  $K = \mathbb{Q}_p$  a counterexample shows that the method, at least in its simplest form, fails for p = 2.

The second approach uses induction on r. It provides results for all r but produces upper bounds for  $\beta(r; \mathbb{Q}_p)$  which are larger than 4r as soon as  $r \ge 3$ . The two methods can be made to interact, and it may be shown, using Leep's result, that  $\beta(3; \mathbb{Q}_p) \le 16$ .

#### Gabriele Nebe (RWTH Aachen University)

#### Title: Extremal lattices and codes

**Abstract:** Using invariant theory of finite complex matrix groups, Andrew Gleason has shown in his ICM talk in Nice 1970, that the minimum distance of a doubly-even self-dual binary code of length n cannot exceed  $4 + 4\lfloor \frac{n}{24} \rfloor$ . A similar bound has been proven by Siegel for even unimodular lattices of dimension n, where the minimum of the regular integral quadratic form is always  $\leq 1 + \lfloor \frac{n}{24} \rfloor$ . Lattices and codes achieving equality are called **extremal**. Of particular interest are extremal lattices and codes in the "jump dimensions" - the multiples of 24.

Number of extremal lattices L and codes C.

n	8	16	24	32	48	72	80	$\geqslant 3952$	$\geqslant 163,264$
C	1	2	1	5	1	?	$\geq 4$	0	0
L	1	2	1	$\geqslant 10^7$	$\geqslant 3$	$\geqslant 1$	$\geqslant 5$	?	0

A very intensively studied question is the existence on an extremal code of length 72. This survey talk reports on recent progress in the study of possible automorphism groups of such a code. I will also give a construction of the extremal even unimodular lattice  $\Gamma$  of dimension 72 I discovered in summer 2010. The existence of such a lattice was a longstanding open problem. The construction that allows to obtain the minimum by computer is similar to the one of the Leech lattice from  $E_8$  and of the Golay code from the Hamming code (Turyn 1967). With Richard Parker we showed that the lattice  $\Gamma$  is indeed the unique extremal even unimodular lattice that can be obtained from the Leech lattice with this Turyn construction.  $\Gamma$  can also be obtained as a tensor product of the Leech lattice (realized over the ring of integers R in the imaginary quadratic number field of discriminant -7) and the 3-dimensional Hermitian unimodular R-lattice of minimum 2, usually known as the Barnes lattice. This Hermitian tensor product construction shows that the automorphism group of  $\Gamma$  contains the absolutely irreducible rational matrix group (SL<sub>2</sub>(25)×PSL<sub>2</sub>(7)) : 2. It also reveals an additional structure of  $\Gamma$  as a lattice over  $\mathbb{Z}[\frac{1+\sqrt{5}}{2}]$ . This leads to a 1-parametric family of quadratic forms on  $\Gamma$  giving rise to even ( $n^2 + 5n + 5$ )-modular lattice of minimum 8 + 4n.

#### Jeffrey Thunder (Northern Illinois University)

#### Title: Counting certain points of given height in the function field setting

Abstract: Fix a dimension n and a degree d. It is a well-known result of Northcott that there are only finitely many points of bounded height in projective n-space that generate a number field of degree d over the rationals (or any other number field, for that matter). The question then becomes to estimate the number of such points. Such estimates essentially all amount to some sort of elaboration on counting lattice points in some region of Euclidean space.

If one replaces the field of rational numbers with a field of rational functions in one variable over a finite field, then the analog of Northcott's result is equally valid, and again one may try to estimate the number of such points. We will explain how one can go about counting points in this situation, how the Riemann-Roch

theorem can replace the lattice point estimates above, how that makes some things much simpler than the number field case, and what aspects are perhaps less clear. We will also discuss how the estimates change qualitatively depending on the relative sizes of the dimension and degree.

#### **30-minute talks**

#### Ricardo Baeza (Universidad de Talca)

#### Title: Levels and sublevels of Dedekind rings

**Abstract:** We prove a representation result for quadratic forms over polynomial rings and we apply it to show, that there exist Dedekind rings A with level s(A) = s(K) + 1, where K is the quotient field of A. This is joint work with Jon Arason.

#### Tim Browning (University of Bristol)

#### Title: Square-free hyperplanes on quadrics

**Abstract:** Given a polynomial with integer coefficients, the problem of determining whether or not it takes infinitely many square-free values has long been a central concern in the analytic theory of numbers. We ask what one can say when one restricts attention to polynomials whose arguments run over the integral points on an affine quadric.

For  $n \ge 3$  let  $f \in \mathbb{Z}[X_1, \ldots, X_n]$  be a non-zero polynomial, let  $Q \in \mathbb{Z}[X_1, \ldots, X_n]$  be a non-singular indefinite quadratic form and let m be a non-zero integer, with  $-m \det Q$  not equal to a square when n = 3. Let  $Y \subset \mathbb{A}^n$  be the affine quadric Q = m. We seek to exhibit conditions on f under which there exist infinitely many points  $\mathbf{x} \in Y(\mathbb{Z})$  for which  $f(\mathbf{x})$  is square-free. In fact we are able to obtain an asymptotic formula when f is linear, as follows.

**Theorem 1.** Assume that deg f = 1. Then there exist constants  $c_Y \ge 0$  and  $\delta > 0$  such that

$$#\{\mathbf{x} \in Y(\mathbb{Z}) : |\mathbf{x}| \leq X, \ f(\mathbf{x}) \text{ is square-free}\} = c_Y X^{n-2} + O_{\delta,f,Y}(X^{n-2-\delta}).$$

For comparison, when  $n \ge 4$ , Baker [1, 2] has used a variant of the Hardy–Littlewood circle method to study asymptotically the density of  $\mathbf{x} \in Y(\mathbb{Z})$  for which each coordinate  $x_i$  is square-free. The first step in the proof of Theorem 1 uses the indicator function

$$\sum_{k^2 \mid N} \mu(k) = \begin{cases} 1, & \text{if } N \text{ is square-free,} \\ 0, & \text{otherwise,} \end{cases}$$

where  $\mu$  is the Möbius function. For a fixed integer k this leads us to count  $\mathbf{x} \in Y(\mathbb{Z})$  with  $|\mathbf{x}| \leq X$  for which  $k^2 \mid f(\mathbf{x})$ . The argument bifurcates according to whether or not k is small. If k is small we use work of Gorodnik and Nevo [6], based on dynamical systems and mixing, to analyze the relevant counting problem. If k is large we transform the problem into one that involves counting integral points on suitable affine quadrics.

Suppose we are given a non-zero quadratic polynomial  $q \in \mathbb{Z}[T_1, \ldots, T_{\nu}]$ , with quadratic part  $q_0$ , for  $\nu \ge 2$ . Consider the counting function

$$M(q;B) = \#\{\mathbf{t} \in \mathbb{Z}^{\nu} : q(\mathbf{t}) = 0, \ |\mathbf{t}| \leqslant B\},\$$

for any  $B \ge 1$ . We will require an upper bound for M(q; B) which is uniform in the coefficients of q and which is essentially as sharp and as general as possible. A trivial estimate is  $M(q; B) = O_{\nu}(B^{\nu-1})$ , which is as good as can be hoped for when q is reducible over  $\mathbb{Q}$ . Assuming that q is irreducible over  $\mathbb{Q}$ , a result of Pila [7] reveals that  $M(q; B) = O_{\varepsilon,\nu}(B^{\nu-3/2+\varepsilon})$ , for any  $\varepsilon > 0$ . Again this is essentially best possible when rank $(q_0) = 1$ , as consideration of the polynomial  $T_1 - T_2^2$  shows. For the remaining cases we establish the following improvement.

**Theorem 2.** Assume that q is irreducible over  $\mathbb{Q}$  and that  $\operatorname{rank}(q_0) \ge 2$ . Then we have  $M(q; B) = O_{\varepsilon,\nu}(B^{\nu-2+\varepsilon})$ , for any  $\varepsilon > 0$ .

The most important feature of Theorem 2 is its uniformity in the coefficients of the quadratic polynomial q. It reflects the rough order of magnitude of M(q; B) when  $q = q_0$ . The result is proved by induction on  $\nu$ , the case  $\nu = 2$  essentially going back to work of Estermann. This is joint work with A. Gorodnik.

#### **Renaud Coulangeon (University of Bordeaux)**

#### Title: The unreasonable effectiveness of tensor product

**Abstract:** An extremal even unimodular lattice in dimension 72 was recently constructed by Gabriele Nebe, elaborating on ideas of Robert Griess. This lattice appears rather naturally as a tensor product over an imaginary quadratic ring of two lattices of lower dimension. Similar tensor constructions of extremal modular lattices in dimension 40 and 80 had already been proposed by Christine Bachoc and Gabriele Nebe in 1998. In this talk, I will first explain why one should not expect, in general, to produce dense lattices using tensor product and try then to analyze the very special features of the above mentioned constructions which explain their "unreasonable effectiveness". In a different direction, I will also report on an intriguing conjecture by Jean-Benoît Bost which predicts a very rigid behavior of so-called semi-stable lattices with respect to tensor product.

#### Rainer Dietmann (Royal Holloway, University of London)

#### Title: Weyl's inequality and systems of forms

**Abstract:** Whereas for one single quadratic form or a pair of quadratic forms a variety of approaches from areas such as modular forms or arithmetic geometry have been successfully applied, for systems of more than two quadratic forms Hardy-Littlewood's circle method still seems to be the most powerful tool. In our talk we explained how one can give the basic form of Weyl's inequality in Birch's seminal work ([5]) on forms in many variables a more efficient interpretation for systems of forms. As an application, we can improve results by W.M. Schmidt ([9], [10]) on systems of quadratic and systems of cubic forms, replacing  $2r^2 + 3r$  by  $2r^2 + 2r$  and  $10r^2 + 6r$  by  $8r^2 + 8r$ , respectively.

**Theorem 1.** Let  $Q_1, \ldots, Q_r \in \mathbb{Z}[X_1, \ldots, X_s]$  be quadratic forms, such that each form in their rational pencil has rank exceeding  $2r^2 + 2r$ . Then if  $\mathfrak{N}(P)$  denotes the number of common integer zeros of  $Q_1, \ldots, Q_r$  in an expanding box of size P, then

$$\mathfrak{N}(P) = \mathfrak{J}\mathfrak{S}P^{s-2r} + O(P^{s-2r-\delta})$$

holds true, where  $\mathfrak{J}$  and  $\mathfrak{S}$  are the singular integral and the singular series, respectively. Likewise, if  $C_1, \ldots, C_r \in \mathbb{Z}[X_1, \ldots, X_s]$  are cubic forms, such that each form in their rational pencil has h-invariant exceeding  $8r^2 + 8r$ , then

$$\mathfrak{N}(P) = \mathfrak{J}\mathfrak{S}P^{s-3r} + O(P^{s-3r-\delta}).$$

Moreover, we discussed the closely related problem of representing quadratic forms by quadratic forms: Let A be a non-singular positive definite symmetric integer  $n \times n$ -matrix, and B be a positive definite symmetric integer  $m \times m$ -matrix, and let N(A, B) be the number of integer solutions X of the matrix equation

$$X^{t}AX = B. (35.1)$$

Using Siegel modular forms, Raghavan ([4]) obtained an asymptotic formula for N(A, B) if n > 2m + 2, min  $B \gg (\det B)^{1/m}$  and det B is large enough. Writing (35.1) as a system of quadratic equations, this problem can also be attacked by the circle method. The following preliminary result (work in progress) has been obtained in joint work with Michael Harvey.

**Theorem 2.** Let c > 0 and suppose that

$$\min B \ge (\det B)^c.$$

Then there exists  $N(c) \in \mathbb{N}$  such that if  $n \ge N(c)$  and det  $B \gg_c 1$ , then

$$N(A, B) = \Im \mathfrak{S}(\det B)^{(n-m-1)/2} + O((\det B)^{(n-m-1)/2-\delta}).$$

The assumption on the dimension n now has become worse than in Raghavan's result, but the interesting feature here is that the assumption on the right-hand side B is less restrictive, showing that the circle method and the modular forms approach each have their strengths and weaknesses for this problem and yield complementary results.

#### Jonathan Hanke (University of Georgia)

#### Title: Understanding the (total) mass of quadratic forms of fixed determinant

**Abstract:** The mass of a genus of quadratic forms is a very useful invariant that is closely related to the class number, but can also be computed by purely local methods. In this talk we describe the structure of the somewhat coarser invariant called the total mass

$$\operatorname{TMass}_{n}(D) := \sum_{\substack{\operatorname{classes}[Q] \text{ with } Q > 0, \\ \operatorname{det}_{H}(Q) = D \text{ and } \operatorname{dim}(Q) = n}} \frac{1}{\#\operatorname{Aut}(Q)} = \sum_{\substack{\operatorname{pos. def. genera } G \text{ with} \\ \operatorname{det}_{H}(G) = D \text{ and } \operatorname{dim}(G) = n}} \operatorname{Mass}(G)$$

which is defined to be the sum of all masses of genera G of positive definite integer-valued quadratic forms of Hessian determinant D in n variables, and give an exact formula for  $\text{TMass}_n(D)$  when n = 3. The total mass is closely related to the asymptotics of certain arithmetic parametrizations of Bhargava which count the classes of ternary quadratic forms by their unique polynomial invariant (the discriminant!).

#### Ben Kane (University of Cologne)

#### Title: Representations by triangular, square, and pentagonal sums

Abstract: Fermat claimed that all positive integers are represented by 3 triangular numbers, 4 squares, 5 pentagonal, ..., and m m-gonal numbers. Its determination in the cases m = 4 (resp. m = 3) was celebrated work of Lagrange (resp. Gauss) and the full conjecture was finally resolved by Cauchy in 1813. In this talk, we will discuss the related question of which "weighted sums" represent all but finitely many positive integers, with a focus on complications which first arise in the m = 5 case. This is based on ongoing joint work with W.K. Chan and A. Haensch.

#### Abhinav Kumar (Massachusetts Institute of Technology)

#### Title: Energy minimization for lattices and periodic configurations, and formal duality

**Abstract:** Closely related to the sphere packing problem is the energy minimization problem for discrete sets of points in Euclidean space, which can be reformulated as an optimization problem for the (average) theta function. I will describe some numerical experiments (joint work with Henry Cohn and Achill Schuermann) which gives evidence for the energy minimizing periodic configurations in low dimensions, for Gaussian potential energy. Surprisingly, the putative optimizers are not necessarily lattices, but appear in families exhibiting formal duality.

#### Byeong-Kweon Oh (Seoul National University)

Diophantine methods, lattices, and arithmetic theory of quadratic forms

#### Title: Class numbers of ternary quadratic forms

Abstract: Let L be a positive definite ternary z-lattice. We define

$$\Lambda_p(L) = \{ x \in L \mid Q(x+z) \equiv Q(z) \pmod{ep} \text{ for all } z \in L \},\$$

where e = 2 if L is even and p = 2, otherwise e = 1. The z-lattice  $\lambda_p(L)$  is the primitive z-lattice obtained from  $\Lambda_p(L)$  by a suitable scaling. Let K be a ternary z-lattice. If a z-lattice L satisfies  $K = \prod_{p_i|2dL} \lambda_{p_i}^{m_i}(L)$ for some suitable  $m_i$ , we say L is lying over K. In this case we define

$$\operatorname{gen}^{K}(L) := \{ L' \in \operatorname{gen}(L) : \prod_{p_i \mid 2dL} \lambda_{p_i}^{m_i}(L') \simeq K \}.$$

We denote by  $h^{K}(L)$  the number of equivalence classes in gen<sup>K</sup>(L). Note that  $h(L) = \sum_{K' \in \text{gen}(K)/\sim} h^{K'}(L)$ . Let M be a ternary z-lattice. If  $\sigma = \tau_x \in O(M)$  for a primitive vector  $x \in M$ , we define  $\pi(\sigma, M) := Q(x)$ . If  $\sigma_1, \ldots, \sigma_t$  are all symmetries in O(M), we define **the signature of** M as follows:

$$\operatorname{sgn}(M) = \langle o(M); \pi(\sigma_1, M), \pi(\sigma_2, M), \dots, \pi(\sigma_t, M) \rangle.$$

Assume that  $\lambda_p(L) = K$  and p is an odd prime. In this talk we prove the following theorem:

**Theorem.** The number of equivalence classes in  $gen^{K}(L)$  having an isometry group with given order, and the signature of each lattice in  $gen^{K}(L)$  are completely determined by the signature of K (also the structure of  $L_p$  and  $K_p$ ).

From the above theorem, we can inductively compute  $h^K(M)$  for any lattice M lying over K if we only know the signature of K. For example, let  $K = \mathbf{z}x_1 + \mathbf{z}x_2 + \mathbf{z}x_3$  be ternary z-lattice such that

$$(B(x_i, x_j)) = \begin{pmatrix} 2 & 0 & -1 \\ 0 & 2 & -1 \\ -1 & -1 & 7 \end{pmatrix}.$$

Note that the class number of K is one. Define  $K(7^n) = \mathbf{z}x_1 + \mathbf{z}x_2 + \mathbf{z}(7^nx_3)$ . If we use the above theorem, we can easily compute  $h(K(7^n)) = 3 \cdot 7^{2n-2} + 2 \cdot 7^{n-1} - \frac{3}{8}(7^{2n-2} - 1)$ . This is a joint work with W. K. Chan from Wesleyan University.

#### Bruce Reznick (University of Illinois at Urbana Champaign)

Title: Linear dependence among powers of quadratic forms

Abstract: Let  $\Phi(d)$  be the smallest r so that there exist r pairwise non-proportional complex quadratic forms  $\{q_i\}$  with the property that  $\{q_i^d\}$  is linearly dependent.

**Problem:** compute  $\Phi(d)$  and characterize the minimal sets. Any set of  $2r + 2 q_i^d$ 's is dependent, so  $\Phi(d) \leq 2d + 2$ , but a "general" set of  $2r + 1 q_i^d$ 's is linearly independent.

The Pythagorean parameterization gives the unique minimal set up to change of variable:  $\Phi(2) = 3$  and  $(x^2 - y^2)^2 + (2xy)^2 = (x^2 + y^2)^2$ . Liouville's proof of Fermat's Last Theorem for non-constant polynomials implies that for  $d \ge 3$ ,  $\Phi(d) \ge 4$ . A deep theorem of Mark Green implies that  $\Phi(d) \ge 1 + \sqrt{d+1}$ . In the other direction, many 19th century examples show that  $\Phi(3) = \Phi(4) = \Phi(5) = 4$ . New results: a characterization of the minimal sets for  $d \le 5$ ; if  $d \ge 6$ , then  $\Phi(d) \ge 5$ ,  $\Phi(6) = \Phi(7) = 5$ ,  $\Phi(14) \le 6$ ;  $\Phi(d) \le 2 + |d/2|$  if  $d \ge 4$ .

My work on this was motivated by a 1999 seminar of Bruce Berndt about an question of Ramanujan, who wanted a generalization of the identity of the form  $f_1^3 + f_2^3 = f_3^3 + f_4^3$  for four specific quadratic forms in  $\mathbb{Z}[x, y]$ . Neither Ramanujan, nor Narayanan, who solved his question, noted that there existed other quadratic

forms  $f_j$  so that  $f_1^3 + f_2^3 = f_3^3 + f_4^3 = f_5^3 + f_6^3$  and  $f_1^3 - f_4^3 = f_3^3 - f_2^3 = f_7^3 + f_8^3$ , but nothing further for  $f_1^3 - f_3^3 = f_4^3 - f_2^3$ . This is typical. For  $\alpha \in \mathbb{C}$ ,

 $(\alpha x^{2} - xy + \alpha y^{2})^{3} + \alpha (-x^{2} + \alpha xy - y^{2})^{3} = (\alpha^{2} - 1)(\alpha x^{3} + y^{3})(x^{3} + \alpha y^{3}),$ 

and if  $y \mapsto \omega y$ , where  $\omega^3 = 1$ , then the right-hand side is unchanged, hence there are two other pairs of quadratic forms whose cubes which have the same sum. Up to change of variable, these are *all* the minimal solutions of degree 3. In some cases, solutions coalesce:  $x^6 + y^6$  is a sum of two cubes in four different ways and  $xy(x^4 + y^4)$  in six ways. There are three different minimal solutions of degree 4 and one of degree 5, but no families of solutions, as there are in degree 3.

Felix Klein promoted the idea of associating each linear form  $x - \alpha y$ ,  $\alpha \in \mathbb{C}$  with the image of  $\alpha$  on the Riemann map from  $\mathbb{C}$  to the unit sphere (and y to the north pole.) We associate quadratic forms to the *pairs* of points of their factors. In this way, the Pythagorean parameterization corresponds to antipodal pairs of the vertices of an octahedron, the unique solution for d = 5 corresponds to antipodal pairs of the vertices of a cube and the example for d = 14 corresponds to antipodal pairs of the vertices of a regular icosahedron. This cannot be an accident. In every known minimal solution  $\{q_j\}$ , there is a change of variables after which,  $|\alpha_j| = |\gamma_j|$  in each  $q_j(x, y) = \alpha_j x^2 + \beta_j x y + \gamma_j y^2$ .

It's useful to consider sums of the form  $\sum_{k=0}^{m-1} (\zeta_m^k x^2 + \beta xy + \zeta_m^{-k} y^2)^d$  where  $\zeta_m = e^{2\pi i/m}$  and m > 2d; the sum on roots of unity kills the coefficient of all terms but  $x^{d\pm m}y^{d\mp m}$  and  $x^d y^d$ , and  $\beta$  is chosen to leave a multiple of  $(xy)^d$ . In this way, one can show that  $\Phi(d) \leq 2 + \lfloor d/2 \rfloor$  if  $d \geq 4$ , although this is not best possible for d = 14. These sets of quadratic forms have a Klein correspondence with a polyhedron whose vertices are the two poles and two antipodal horizontal *m*-gons.

#### Damien Roy (University of Ottawa)

#### **Title:** On rational approximation to real points on plane quadratic curves defined over $\mathbb{Q}$

Abstract: A point  $(\xi_1, \xi_2)$  with coordinates in a subfield of  $\mathbb{R}$  of transcendence degree one over  $\mathbb{Q}$ , with  $1, \xi_1, \xi_2$  linearly independent over  $\mathbb{Q}$ , may have a uniform exponent of approximation by elements of  $\mathbb{Q}^2$  that is strictly larger than the lower bound 1/2 given by Dirichlet's box principle. This appeared as a surprise, in connection to work of Davenport and Schmidt, for points of the parabola  $\{(\xi, \xi^2); \xi \in \mathbb{R}\}$ . The goal of this talk is to show that this phenomenon extends to all real conics defined over  $\mathbb{Q}$ , and that the largest exponent of approximation achieved by points of these curves satisfying the above condition of linear independence is always the same, independently of the curve, namely  $1/\gamma \cong 0.618$  where  $\gamma$  denotes the golden ratio.

#### Rudolf Scharlau (Universität Dortmund)

#### Title: Automorphism groups of lattices in large genera

Abstract: In fixed dimension n, almost all lattices (with primitive integral quadratic forms) of determinant d have trivial automorphism groups when  $d \to \infty$ . This is a well known, classical consequence of reduction theory. The lattices of any given dimension and determinant split into genera, and in the thesis of J. Biermann (Göttingen, 1981) it had been shown that the result also holds for the lattices of any genus. Since the mass and the class number of genera tend to infinity also with the dimension n, one might expect that the result more sharply holds if  $\max(n, d) \to \infty$ . That is, only finitely many genera might exceed a specified proportion of lattices with non-trivial group. This is far from being proved. In the talk, we shall be more modest and report on explicit, computational results on the automorphism groups actually occurring for arithmetically interesting genera of dimension up to 20 and small level. Roughly speaking one observes that for these parameters (the level seems to be more appropriate than the absolute size of the determinant), automorphism groups are still a good invariant. On the other hand, when the level 1,2,3,4,5,6,7,11 goes up, the quick increase of the mass is mostly caused by a quick increase of the number of lattices with very small, eventually trivial automorphism group.

#### Achill Schürmann (Universität Rostock)

#### Title: Strictly periodic extreme lattices

**Abstract:** A lattice is called periodic extreme if it cannot locally be modified to yield a better periodic sphere packing. It is called strictly periodic extreme if it gives an isolated local optimum among periodic sphere packings. We derive sufficient conditions for periodic extreme and strictly periodic extreme lattices. We hereby in particular show that the root lattice  $E_8$ , the Coxeter-Todd lattice  $K_{12}$ , the Barnes-Wall lattice  $BW_{16}$  and the Leech lattice  $\Lambda_{24}$  are strictly periodic extreme.

#### **Cameron Stewart (University of Waterloo)**

#### Title: Exceptional units and cyclic resultants

Abstract: Let a be a nonzero algebraic integer of degree d over the rationals. Put  $K = \mathbb{Q}(a)$  and let  $\mathcal{O}(K)$  denote the ring of algebraic integers of K. We shall discuss estimates for the number of positive integers n for which  $a^n - 1$  is a unit in  $\mathcal{O}(K)$  and for the largest positive integer n for which  $a^j - 1$  is a unit for j from 1 to n.

#### Takao Watanabe (Osaka University)

#### Title: Polyhedral reduction of Humbert forms over a totally real number field

Abstract: Let k be a totally real number field and o the ring of integers of k. We write  $\mathbf{k}_{\mathbf{R}}$  for  $\mathbf{k} \otimes_{\mathbf{Q}} \mathbf{R}$ . Let  $H_n(\mathbf{k}_{\mathbf{R}})$  be the space of all  $n \times n$  symmetric matrices with entries in  $\mathbf{k}_{\mathbf{R}}$  and  $P_n(\mathbf{k}_{\mathbf{R}}) = \{ {}^{t}gg \mid g \in GL_n(\mathbf{k}_{\mathbf{R}}) \}$  be an open cone in  $H_n(\mathbf{k}_{\mathbf{R}})$ . The rational closure  $\Omega_k$  of  $P_n(\mathbf{k}_{\mathbf{R}})$  is defined to be the cone generated by  $\{x^tx \mid x \in \mathbf{k}^n \setminus \{0\}\}$  in  $H_n(\mathbf{k}_{\mathbf{R}})$ . Our purpose is to study polyhedral reduction of  $\Omega_k/GL(\Lambda)$  for a given projective o-module  $\Lambda \subset \mathbf{k}^n$  of rank n.

We define the  $\Lambda$ -minimum function  $\mathsf{m}_{\Lambda} : P_n(\mathsf{k}_{\mathbf{R}}) \longrightarrow \mathbf{R}_{\geq 0}$  by

$$\mathsf{m}_{\Lambda}(a) = \inf_{0 \neq x \in \Lambda} \operatorname{Tr}_{\mathsf{k}_{\mathbf{R}}/\mathbf{R}}({}^{t}xax) \,.$$

The domain  $K_1(\mathsf{m}_\Lambda) = \{a \in P_n(\mathsf{k}_{\mathbf{R}}) \mid \mathsf{m}_\Lambda(a) \ge 1\}$  gives an analog of Ryshkov polyhedron. Indeed,  $K_1(\mathsf{m}_\Lambda)$  is a locally finite polyhedron. Let  $\partial^0 K_1(\mathsf{m}_\Lambda)$  be the set of all vertices of  $K_1(\mathsf{m}_\Lambda)$ . By extending Voronoï's algorithm to  $K_1(\mathsf{m}_\Lambda)$ , we obtain a complete set  $\{b_1, \dots, b_t\}$  of representatives of  $\partial^0 K_1(\mathsf{m}_\Lambda)/GL(\Lambda)$ .

For  $a \in \partial^0 K_1(\mathsf{m}_\Lambda)$ , the perfect cone  $D_a$  is defined to be the closed cone in  $H_n(\mathsf{k}_{\mathbf{R}})$  generated by  $\{x^t x \mid x \in S_\Lambda(a)\}$ , where  $S_\Lambda(a)$  stands for the set of minimal vectors of a in  $\Lambda$ . Then we can show that the set of all perfect cones gives a polyhedral subdivision of  $\Omega_k$ , and hence the domain

$$\bigcup_{i=1}^{t} D_{b_i} / \Gamma_i$$

gives a fundamental domain of  $\Omega_k/GL(\Lambda)$ , where  $\Gamma_i$  denotes the stabilizer of  $b_i$  in  $GL(\Lambda)$ .

If n = 1 and  $\Lambda = o$ , then this result may be regarded as a precise form of Shintani's unit theorem for the square  $E_k^2$  of the unit group  $E_k = GL_1(o)$ . In the case that k is a quadratic field,  $K_1(m_o)$  is a polygonal region in  $\mathbf{R}_{\geq 0}^2$  with infinite vertices. We see that there are many real quadratic fields such that the number of elements of  $\partial^0 K_1(m_o)/E_k$  is equal to one.

#### Mark Watkins (University of Sydney)

#### Title: Indefinite LLL and solving quadratic equations

**Abstract:** This talk reviews work on modifying the LLL algorithm so that it would apply to indefinite symmetric matrices, and noted Simon's attempts (dating from 2005) to further apply this to solve quadratic equations (thus generalizing the 3-variable conic case known to Gauss). The question of finding a solution space of maximal dimension was also considered, as was the generality of an idea of Cassels (adapted by

Simon) in various circumstances. The practicality of the algorithms appears evident, with only the factorizing of the determinant preventing the algorithm from running in polynomial time. The quite recent work of Castel on solving an indefinite form of dimension 5 *without* factorizing the discriminant was also mentioned briefly.

#### Martin Widmer (Graz University of Technology)

#### Title: Integral points of fixed degree and bounded height

**Abstract:** In Jeff Thunder's talk we have considered the number of algebraic points of bounded height and of fixed degree over a given global field k. By Northcott's Theorem it is known that these points are finite in number, and the emphasis of Thunder's talk was to find the asymptotics as the height bound becomes large. In this talk we consider a closely related problem. Let k be a number field, let n and e be positive rational integers, and let X > 1 be real. We consider the algebraic points  $(\alpha_1, ..., \alpha_n)$  of affine Weil height at most X such that each coordinate is an algebraic integer, and such that they generate an extension  $k(\alpha_1, ..., \alpha_n)$  of k of degree e.

We present a precise asymptotic estimate for their number (as X tends to infinity) involving several main terms of decreasing order. We outline the proof in the much simpler special case e = 1 where one has to count lattice points in an unpleasant shaped subset S of the Euclidean space  $\mathbb{R}^m$ . Here a crucial ingredient of the proof is a gap principle for the successive minima of a lattice under a certain subgroup  $\mathcal{M}$  of the diagonal endomorphisms. Loosely speaking it says that we can replace our set S by  $\Phi(S)$  for any element  $\Phi$  of  $\mathcal{M}$ , essentially without changing the number of lattice points. This principle might have applications to other counting problems.

# **List of Participants**

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# Chapter 36

# **Black Holes: New Horizons (11w5099)**

# Nov 20 - Nov 25, 2011

**Organizer(s):** Valeri Frolov (University of Alberta) Sang Pyo Kim (Kunsan National University) Don Page (Institute of Theoretical Physics, University of Alberta) Misao Sasaki (Yukawa Institute for Theoretical Physics, Kyoto University)

This meeting was a joint activity of 3 theoretical physics institutes: Institute of Theoretical Physics of the University of Alberta (Canada), Asia Pacific Center for Theoretical Physics (Korea), and Yukawa Institute of Theoretical Physics (Kyoto, Japan). The meeting attracted leading experts in the field from 10 countries. As a result we had very fruitful and informative discussions of the exciting and intriguing problems of the physics and mathematics of black holes.

# **Overview of the Field**

Black holes are one of the most amusing predictions of the Einstein's General Relativity. A first solution of the Einstein equations describing a black hole was obtained by Schwarzschild in 1916, soon after these equations were formulated. A prediction that the gravitational collapse of a massive star may produce a black hole was first made by Oppenheimer and Snyder (1939). However till the beginning of seventies of the past century there were no astrophysical confirmation of the existence of black holes. During this long period a lot of work was done by theoretical physicists and mathematicians which results in very deep understanding of properties of black holes.

A mathematical model of a physical spacetime adopted in the General Relativity is a differential manifold. Points of this manifold are identified with events. The (pseudo-) Riemannian metric on the spacetime manifold is used to determine an interval between a pair of near-by events. Directions generated by null vectors at a given point form a local null cone. Particle worldlines are represented by timelike smooth curves, with a tangent vectors (velocity) inside future directed local null cones, while light propagates along null geodesics. A spacetime is asymptotically flat if it has a distant region similar to the Minkowski space where the curvature becomes small. A black hole is a region in an asymptotically flat spacetime from where no information carrying signals propagating along causal (timelike and/or null) curves can reach infinity. Existence of a black hole indicated that the global causal structure of the spacetime is non-trivial. The boundary separating 'visible' and 'invisible' regions is called the event horizon. From mathematical point of view study of black holes and their properties is study of global and causal properties of spacetime manifolds with metrics obeying the Einstein equations. The Einstein equations is a set of coupled non-linear second order partial differential equations for 10 functions of four variables, the metric components. The global analysis of this system is quite complicated. However, now there exist quite good understanding of its solutions describing black holes.

An important breakthrough at the end of sixties – beginning of seventies was application of a global geometrical analysis to the black hole theory, which not only allowed one to give a covariant definition of a black hole but also to prove several fundamental theorems. The now-classical theorems stating that black holes have no hair (that is, no external individual attributes except mass, angular momentum, and charge), that a black hole contains a singularity inside it, and that the black hole area cannot decrease were proved during this period. It was demonstrated that black hole solutions are classically stable. However, in 1974 it was shown by Hawking that black holes are unstable with respect to quantum process of particle creation. Black holes emit particles with (practically) thermal spectrum and black holes obey the laws similar to the laws of thermodynamics. In particular they have entropy proportional to their surface area. All these and other results made it possible to construct a qualitative picture of the formation of black holes, to describe their possible further evolution and interaction with matter and other classical physical fields.

During next 30 years the status of black holes changed dramatically. Many stellar mass black holes were discovered in the X-ray binaries. Moreover, it is now believed that centers of many galaxies (including our) contain supermassive black holes with the mass of millions and billions of the solar mass. Gamma-ray bursts, the most powerful sources of high frequency electromagnetic radiation in the Universe, are explained by a model, where a center engine producing the energy is a black hole.

More recently another aspect of black hole physics became very important for astrophysical applications. The collision of a black hole with a neutron star or coalescence of a pair of black holes in binary systems is a powerful source of gravitational radiation which might be strong enough to reach the Earth and be observed in a new generation of gravitational wave experiments (LIGO and others). The detection of gravitational waves from these sources requires a detailed description of the gravitational field of a black hole during the collision. In principle, gravitational astronomy opens remarkable opportunities to test gravitational field theory in the limit of very strong gravitational fields. In order to be able to do this, besides the construction of the gravitational antennas, it is also necessary to obtain the solution of the gravitational equations describing this type of situation. Until now there exist no analytical tools which allow this to be done. Under these conditions one of the important tasks is to study colliding black holes numerically.

For many years, black holes have been considered as interesting solutions of the theory of General Relativity with a number of amusing mathematical properties. Now, after the discovery of astrophysical black holes, the Einstein gravity has become an important tool for their study [1]. Black holes are considered now as the most powerful sources of the gravitational radiation in the Universe. Black holes play also an important role of probes of new physical concepts, such as the modern string theory and recent models with large extra dimensions. Study of different aspects of black hole physics requires developed mathematical tools. (A more detailed discussion of the modern status of black holes can be found in a recent book [2]).

## **Recent Developments and Open Problems**

(1) LIGO and other gravitational observatories search now for gravitational waves. Black holes in binary systems are considered as the most probable powerful sources of the strong gravitational radiation. Theoretical modeling of the black hole coalescence requires solving Einstein equations in the regime of extremely strong field and fast evolution. Numerical relativity is the only available 'final resource' for obtaining detailed description of such phenomena. The computational aspects of black holes, such as study of black hole coalescence and gravitational radiation, is important and rapidly developing area of research (see e.g. [3]).

(2) To identify black holes as astrophysical objects one uses theoretical results concerning light and particle propagation in the close vicinity of black holes. From mathematical point of view this is a problem of

#### Black Holes: New Horizons

study highly non-linear ODEs for geodesic motion and solutions of partial differential equations for fields in the given metric. A lot of work has been done in this area. Now, when the General Relativity provides tools in the modern astrophysics, different aspects of these 'old' problems require new more detailed consideration. For example, for study polarized light propagation near rotating black holes one needs to develop WKB methods for multi-component fields (such as electromagnetic and gravitational ones) in a curved spacetime, which gives correct long-time asymptotics of the solution of the wave equations.

(3) One of the most important new development of the black hole theory is connected with higher dimensional gravity. The idea that spacetime may have more that 4 dimensions is rather old. The existence of extra dimensions in the string theory is required for consistency this theory. Models with large extra dimensions became popular in the brane world theories. In such theories the matter is confined to 4-dimensional spacetime submanifold embedded in the higher dimensional bulk space, while gravity can propagate in extra dimensions. Black holes, which are solitonic type solutions of the Einstein equations, play the role of natural probes of extra dimensions in these theories.

(4) A lot of work was done recently in study of black hole solutions in asymptotically anti-deSitter spacetime in connection with AdS/CFT correspondence. In this approach it is possible to relate conformal quantum field, 'living in the AdS 4D boundary, with the properties of the classical solutions of the gravitational equations in the bulk spacetime. In this approach bulk black hole solutions correspond to the quantum field at finite temperature.

(5) Recently it was demonstrated that there exists a large variety of black hole solutions in higher dimensional Einstein theory of gravity. These solutions differ by the topology of their event horizons. Explicit stationary black hole solutions were obtained in 5 dimensions. There are indications that similar and more complicated black hole solutions exist in 6 and higher dimensions [4]. Important problems, which require developed mathematical tools are: to prove the existence of such solutions and to find and classify them. Another open problem is dynamical stability of higher dimensional black holes.

(6) It has been known for a long time that geodesic equations in the Kerr metric, describing a 4-dimensional rotating black hole, are completely integrable. Recently it was discovered that the complete integrability is a characteristic common property of ALL higher dimensional black holes with the spherical topology of the horizon. The geodesic motion in the spacetime of higher dimensional rotating black holes is a new physically interesting case of completely integrable systems. There exists a number of interesting mathematical problems, such as construction of Lax pairs for such systems and application of KAM method for study general properties of such dynamical systems. It was also shown that the same hidden symmetries, which are responsible for the complete integrability of geodesic equations, also imply complete separation of variables in the physically interesting field equations. ODE obtained by such a separation are second order linear equations with polynomial coefficients. The power of these polynomials grows with increasing the number of the spacetime dimensions. Study of the Sturm-Liouville problem for 'angular' eigen-modes and general properties of the 'radial equations' is practically open problems, interesting for the physical applications (see e.g. a review [5]).

(7) Another interesting problem is study of 'different phases' in a space of higher dimensional black-hole solutions in a spacetime with compact extra dimensions, and transition between these phases (see e.g. a review [6]).

(8) An interesting subject is study of black holes in non-Einstein gravity.

The purpose of the workshop was to discuss physical and mathematical aspects of black holes, recent progress in this area, and its open problems.

# **Presentation Highlights**

#### **Black string instability**

Several quite interesting talks were devoted to the problem of higher dimensional black holes. Some of new results were obtained in this area by combination of numerical and analytical results.

A simplest example of higher dimensional object with non-trivial topology of a horizon is a black string (brane). Such solutions exist in a spacetime with large compact extra dimensions. Any space which is a direct sum of a Ricci flat 4D black hole metric and flat torus is again Ricci flat and, hence, it is a higher dimensional black hole solution of vacuum Eintein equations. It has been known for a long time that such solutions become unstable when the size of flat extra dimensions become sufficiently large as compared with the gravitational radius. This so called Gregory-Laflamme instability discovered in 1993 [7] later was studied in details in the linearized regime. But there remained an open question: what is the final state of such instability. At the present meeting there were demonstrated results of recent numeric simulations, performed by Luis Lehner and Frank Pretorius [8], which finally allow one to make definite conclusions concerning the dynamics of unstable black string solutions. There simulations show that at first stage the long black string looses its homogeneity in the flat z-direction and a single black hole is formed, with a black string attached to it. Later the string becomes thinner, its energy is partly absorbed by the black hole. When thickness of the string reaches the critical value, new smaller size black holes are formed. This process continues in time with formation of a self-similar discrete structure, containing smaller and smaller size black holes.

#### **Merger transitions**

Another interesting subject discussed at the meeting is the phase transitions of black objects in a space with large compact extra dimensions. In this approach one studies condition of coexistence of black hole solutions with different topology in the parameter space and focuses on stationary critical (maybe unstable) solutions when the topology of the black object changes. Barak Kol [9] proposed a conjecture that horizons during the phase of reconstruction has the structure of conefolds. Roberto Empharan at his talk demonstrated a simple analytical model which describes merges of the horizons. Namely, he considered a higher dimensional rotating black hole in a spacetime with the cosmological constant. Such black holes allow arbitrary large rotation parameters. When this parameter is large enough the black hole horizon crosses the cosmological horizon. At this point the global horizon changes its topology. The results presented in the talk show that the Kol's conefold conjecture is valid in this case. This result opens an interesting possibility for search of the analytical proof of this conjecture in more general cases.

#### **Black holes in Randall-Sundrum model**

Randall-Sundrum model is another approach with large extra dimensions. In this model the bulk space is a higher-dimensional Universe described by warped geometry, while four dimensional submanifold (brane) describes our 'visible' world. Finding black hole solutions in such spacetimes, and even proof of their existence is a rather complicated problem. Recently the progress was achieved in the work of the group of Wiseman [10]. Using the numerical methods based on the Ricci-flow approach, they succeeded to obtain 5 dimensional regular black hole solutions attached to the brane. Don Page and collaborators presented at the meeting a new independent proof of the existence of the large black holes in the Randall-Sundrum model. Instead of solving numerically the 5D Einstein equations, they used numerical tools to find a minimum of

the positive definite integral, which vanishes when such equations are satisfied. Since the problem is quite complicated this independent result obtained by a different method is quite important. However, there still exists an unsolved puzzle connected with black holes solutions in the Randall-Sundrum model. Sometime ago, using arguments based on the ideas of AdS/CFT correspondence, several scientists arrived to a conclusion that such static solutions are impossible because of the emission by the black hole quantum radiation of conformal fields. The obtained numerical solutions (at least for large black holes) do not have indication on the existence of such radiation. Possible resolutions of this paradox were discussed in the talk by Takahiro Tanaka.

#### Black hole solutions with reduced symmetry

Most of the known higher dimensional black hole solutions possess rather high symmetry. Robert Mann demonstrated the existence of higher dimensional black hole solutions in the presence of scalar complex fields with reduced symmetry [11]. This is a generalization of recent 4 dimensional results by Gary Horowitz and collaborators [12]. Numerical simulations of black hole solutions with axion hairs and gravitational collapse in such systems were presented by Hirotaka Yoshino.

#### **Black hole numerics**

Review of recent progress in numerical study of black hole merger and collisions was given by Matt Choptuik and Masaru Shibata. Namely, Choptuik presented recent results of the numerical simulation of higher dimension black hole collisions and new results on the gravitational critical collapse of the matter. Shibata and his collaborators focused of 'real' processes of a 4D black hole formation in the neutron-star–neutron-star and neutron-star–black-hole binaries and in the stellar core collapse. They presented an updated estimation of the rate of the gravitational waves emission and its dependence on the equation of state of the matter in the neutron stars.

#### **Black holes in non-Einstein gravity**

Quite large number of talks were devoted to black hole solutions in different generalizations of the Einstein gravity. There exist at least two reasons why such solutions are important:

- In order to apply the methods similar to AdS/CFT correspondence for the description of usual quantum systems in the strong coupling regime the modification of bulk gravity equations are required.
- Low energy gravity equations in the string theory contain higher in curvature corrections and other fields.

The popular now modifications of the first type form a class of so called Horava-Lifshitz gravity theories. Recent results concerning existence of black hole and cosmological solutions in these theories were presented and summarized in the talks by Ruth Gregory and Shinji Mukohyama.

An example of the second kind of non-Einstein theory is a so called Gauss-Bonet gravity. In 4 dimensions there exists a special linear combination of quadratic in curvature invariants which is a total derivative and the corresponding action is a topological invariant. Adding such a term to the Einstein action in 4 dimensions does not affect the Einstein equations. However, in 5 and higher dimensions adding of the Gauss-Bonet term to the action modifies the Einstein equation. A similar modifications also occurs in 4 dimensions if there exists an additional scalar (dilaton) field and the Gauss-Bonet contribution to the action contains a prefactor depending on this field. A special property of these theories is that the dynamical equations do not contain metric derivatives higher than the second order.

Asymptotically AdS solutions of the Gauss-Bonet gravity in 5 dimensional spacetime were discussed in the talk by Rong-Gen Cai, who demonstrated how these solutions might be used for description of holographic superconductors in the related AdS/CFT description. The talk of Jutta Kunz summarized recent numerical results of study black holes in the dilaton Gauss-Bonet gravity in 4 dimensions. A new unexpected result obtained in this work is the existence of static spherically symmetric wormhole solutions [13]. It was argued that these solutions are stable.

#### Hidden symmetries of black holes

During recent years a lot of work was done in study of hidden symmetries of higher dimensional black hole. The main result obtained in this area is the proof of the complete integrability of the geodesic particle and light motion in the background of arbitrary higher dimensional rotating black hole with spherical topology of the horizon. This result and similar results on the complete separability of the Hamilton-Jacobi, Klein-Gordan and some other relativistic field equations is based on the existence of the closed conformal rank 2 Killing-Yano tensors in such spaces. Moreover, it was also demonstrated that the most general solutions describing higher dimensional rotating black holes in asymptotically AdS spacetime do possess this property. New development presented at the meeting was demonstration that the complete integrability property is also valid for the motion of particles with internal (spin) degrees of freedom (talk by Pavel Krtous, see also [14, 15]). Another important development was presented by Claude Warnick. He demonstrated how the notion of the closed conformal rank 2 Killing-Yano tensors can be generalized to the case of the connections with torsion and described interesting applications to Kerr-Sen black hole solutions.

#### Spinoptical effects in rotating black holes

Application of the geometrical optics approximation for the light propagation in a curved spacetime has quite long story. The well known statement is that in the high-frequency approximation light propagates along null geodesics and if it is linearly polarized, its polarization vector is parallel transported (see e.g. [16]). In the talks by Valeri Frolov and Andrey Shoom it was demonstrated that this conclusion seams to be oversimplified. It should be emphasized that the geometrical optics approximation (as well as similar WKB approximation) are well defined locally. To reduce solution of the wave equations in the high frequency limit one constructs a Lagrangian submanifold of the phase space satisfying the eikonal equation. However, even small change of this equation can modify long time behavior of the Lagrangian submanifold, and, hence, the asymptotic form of the solution. In the talk it was proposed to improve the standard geometrical optics approach in order to take care of this problem. For this purpose from the very beginning the Maxwell equations are written as two independent sets of the equations: one for right-polarized and the other for left-polarized light. Geometric optics is constructed as a high frequency approximation in each of the independent sectors and the lowest order polarization dependent corrections are included in the eikonal equations. As a result, right and left polarized beams of light have slightly different trajectories, while a beam with initial linear polarization splits in two spatially separated circular polarized beams. Possible application of this effects to the polarized light propagation near a rotating black hole was discussed.

#### **Black hole entropy**

Two talks devoted to the problem of black hole entropy gave brief review of the problem and recent developments. Steve Carlip focused on the idea of using effective conformal description of black hole entropy [17]. He demonstrated that many of the adopted now approaches are based on the idea that the microscopic constituents responsible for the black hole allows description in terms of 2D conformal fields. He also formulated main generic features of these approaches. An alternative explanation of the black hole entropy in the loop gravity was presented by Hanno Sahlmann.

#### Visualization problem

There exist several different methods that are used to visualize properties of special solutions in the General Relativity. Examples are Carter-Penrose conformal diagrams and different embedding diagrams for specially chosen 2D slices of the metric. Kayll Lake presented a new interesting approach which allows one to get better qualitative understanding of global properties of the spacetime. Namely, he proposed to use gradient flows constructed for curvature invariants. He demonstrated that at least in the simplest cases (including interesting black hole solutions) the number and characteristics of the singular points of such flows contain important information concerning global properties of the solution.

#### **Black hole analogues**

In the conclusion, we need also to mention a talk by Bill Unruh. He described a recent experiment performed at UBC. In this experiment amplification of the surface waves in a container with moving water was studied. The profile of the container was chosen so that the water flux in some region moves faster than the speed of waves. Such a system is a liquid analogue of a white hole. It was demonstrated that the amplification coefficient is practically frequency independent in a wide frequency range. This behavior is consistent with theoretical predictions, and might be considered as an experimental evidence for the Hawking effect in the condensed matter analogues of black- and white-hole.

## Scientific Progress Made and Outcome of the Meeting

It is difficult to expect that during this short period of 5 days of the meeting fundamental problems could be solved. The main result of the workshop is that several of the problems of modern 'mathematical physics of black holes' were identified, formulated and discussed. This subject covers wide spectrum of physical properties of systems containing black holes. Numerical methods developed for simulation of black hole coalescence, are now used for calculation of the cross-section for higher dimensional black hole collision. These results are used in the discussion of possibility of black hole production in colliders. Similar methods allowed one to describe the non-linear stage of the instability of black string in the spacetime with large compact extra dimensions. Combination of numerical and analytical results is important for other black hole problems, such as black holes in non-Einstein gravity and black holes in Randall-Sundrum models. The latter subjects are closely connected with the string theory. Black holes are used in the AdS/CFT correspondence as important component of the construction. At the same time the ideas of this approach play an important role in the explanation of the mechanism of black hole entropy. This close interconnection between different problems of black holes is an important new element of the modern 'state of art'. For this reason an exchange of ideas between experts in different areas of 'mathematical physics of black holes' and using different, both analytical and numerical, tools was very timely, important and productive. In the long term perspective this is the main result of the present event.

There were a number of 'immediate' proposals and 'short term projects', that arose as a result of the talks and discussions. To be more concrete let us give some examples.

The talk of Andrey Zelnikov discussed the self-energy of particles in the vicinity of black holes. At the talk Barak Kol posed a question: Why an additional gravitational force acting on a charged particle is repulsive? This question generated an interesting discussion after the talk. As a result of joint discussions it was proposed a simple mechanism, explaining not only the sign of the effect, but also (at least in the weak field limit) giving a correct numerical factor. The discussion of the question how generic this mechanism is and what might be its applications to other cases continued after the conference by the exchange of e-mails. This may finally results in a joint publication of some participants of the meeting. In any case this discussion clarified a fundamental problem of the self energy of classical charged objects in the external gravitational field.

Another immediate result of the discussion after the talk of Don Page was the following. At the past BIRS Black Hole meeting Hirotaka Yoshino presented arguments, based on his numerical simulations that there do not exist static black hole solutions in the Randal-Sundrum model. Independent arguments in favor of such conclusion based on the AdS/CFT arguments were given earlier. More recently Wiseman and collaborators numerically found such solutions. This result was confirmed by independent calculations of the group of Don Page at the University of Alberta and presented at the meeting. As a result of the discussions during the meeting, Hirotaka Yoshino decided to repeat his old calculations with higher accuracy in order to find a possible solution of this puzzle. Takahiro Tanaka was also stimulated in development of his critical analysis of the AdS/CFT arguments.

One of us (V.F.) may add one, more personal example. Some of our colleagues from Japan expressed high interest in the new results on spinoptics in a curved spacetime presented in our with Andrey Shoom talks. As a results, after my return to Kyoto, where I am staying as a visiting professor, I was invited to give extensive lectures on this subject at Yukawa Institute of Theoretical Physics and at Osaka City University. This illustrates another result: Fresh new ideas presented at the meeting immediately became available to experts from 10 different countries. This demonstrates how effective was a chosen format of the meeting.

To summarize, we would like to say that the BIRS meeting "Black Holes: New Horizon" was very successful. It combined high quality of the talks, and warm friendy atmosphere of discussions. The staff of the BIRS helped us a lot both at the stage of preparation of the meeting, as well as during its work. All the participants enjoyed very much a friendly atmosphere of Banff Center and BIRS. We would like to thank BIRS for the cooperation and help.

(Prepared by Valeri Frolov on the behalf of the organizers.)

## **List of Participants**

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# Chapter 37

# **Approximation algorithms and the hardness of approximation (11w5117)**

# Nov 27 - Dec 02, 2011

**Organizer(s):** Chandra Chekuri (University of Illinois Urbana-Champaign) Joseph Cheriyan (University of Waterloo) Ryan O'Donnell (Carnegie Mellon University) Mohammad R. Salavatipour (University of Alberta) David Williamson (Cornell University)

# **Overview of the Field**

Most of the many discrete optimization problems arising in the sciences, engineering, and mathematics are NP-hard, that is, there exist no efficient algorithms to solve them to optimality, assuming the  $P \neq NP$  conjecture. The area of approximation algorithms focuses on the design and analysis of efficient algorithms that find solutions that are within a guaranteed factor of the optimal one. Loosely speaking, in the context of studying algorithmic problems, an approximation guarantee captures the "goodness" of an algorithm – for every possible set of input data for the problem, the algorithm finds a solution whose cost is within this factor of the optimal cost. A hardness threshold indicates the "badness" of the algorithmic problem – no efficient algorithm can achieve an approximation guarantee better than the hardness threshold assuming that  $P \neq NP$  (or a similar complexity assumption). Over the last two decades, there have been major advances on the design and analysis of approximation algorithms, and on the complementary topic of the hardness of approximation, see [33], [34].

The long-term agenda of our area (approximation algorithms and hardness results) is to classify all of the fundamental NP-hard problems according to their approximability and hardness thresholds. This agenda may seem far-fetched, but remarkable progress has been made over the last two decades. Approximation guarantees and hardness thresholds that "match" each other have been established for key problems in topics such as:

- covering and partitioning (the set covering problem [11]),
- algebra (overdetermined system of equations [14])
- graphs (clique, colouring [35]),

- combinatorial optimization (maximum cut [13],[17]),
- constraint satisfaction (maximum sat problems [13],[14]), etc.

Even more significant than these specific successes is the impact of the results and techniques from this area on related areas of mathematics. We list a few instances.

• Combinatorial Optimization: Combinatorial optimization is a mature body of research that has been developed by some of the leading researchers in discrete math over more than five decades; it has many deep mathematical results as well as many "real world" applications. The technique of iterative rounding has been developed in our area (starting with Jain [15]) to give remarkably good results for problems beyond the reach of classical combinatorial optimization. Recently, iterative rounding combined with the uncrossing technique has been used to give new proofs for several of the classic results in combinatorial optimization, including Edmonds' matching polyhedron theorem, which is one of the keystone results of the area; see the manuscript by Lau, Ravi and Singh [20].

• Metric Embeddings: Structure-preserving embeddings between various geometric spaces have been studied intensively for decades, in fields like differential geometry and functional analysis. Starting with the work of Linial, London, and Rabinovich [22], many applications of metric embeddings have been found in computer science, especially in the area of approximation algorithms. Moreover, the interaction between these fields has increased in recent years, with techniques developed in our area leading to the solution of open problems in non-linear functional analysis, e.g., the work of Brinkman and Charikar [9] solving the problem of dimension reduction in  $L_1$ , and the work of Arora, Rao, Vazirani [5] and Arora, Lee, Naor [4] leading to the near-solution of the Euclidean embedding problem for finite subsets of  $L_1$ .

• Analysis of Boolean Functions: Recent progress on hardness of approximation has come with the development of new tools in the area of "analysis of Boolean functions". This area combines techniques from harmonic analysis, probability theory, and functional analysis to study basic properties of Boolean functions. One recently developed tool, the Invariance Principle (Mossel-O'Donnell-Oleszkiewicz [25]), allows transfer of results from Gaussian probability spaces to results on Boolean probability spaces. This has led to fruitful connections between hardness of approximation and the geometry of Gaussian space. Although the original motivation for the Invariance Principle was proving matching hardness thresholds, it has also led to the solution of problems in other areas of mathematics and computer science. For example, in the mathematical theory of Voting and Social Choice, the Invariance Principle was used to prove: the "Majority Is Stablest Conjecture" and the "It Ain't Over Till It's Over Conjectures" regarding the optimality of Majority voting (Mossel-O'Donnell-Oleszkiewicz [25]); new results on the predictability of voting in many-party elections (Mossel [26]); and new quantitative bounds for Arrow's Theorem (Mossel [28]). Recently developed methods in the analysis of Boolean functions have also led to intractability results in the areas of property testing and learning theory, as well as positive results in the area of derandomization.

The goals of the workshop are as follows:

- 1. To bring together researchers in the fields of approximation algorithms (who work on finding algorithms with good approximation guarantees) and complexity theory (who work on finding hardness thresholds), and to stimulate the exchange of ideas and techniques between the two groups.
- 2. To highlight some of the new technical/mathematical directions in approximation guarantees (hierarchies of linear programming and semidefinite programming relaxations, uses of convex programming) and hardness thresholds (boolean functions, noise stability). These directions will be the subject of either survey or focus talks.
- 3. One specific topic on which we will focus is the status of the "Unique Games Conjecture", which states that unless P is equal to NP, there is no efficient algorithm to distinguish whether one can satisfy almost all constraints or almost no constraints of a particular type of constraint satisfaction problem

(Khot [16]). It is not currently known whether Unique Games Conjecture is true. However, several quite exciting results have been shown by assuming the truth of the Unique Games Conjecture; in particular, matching hardness thresholds have been shown for several fundamental problems in combinatorial optimization, such as the maximum cut problem and the minimum vertex cover problem (Khot-Kindler-Mossel-O'Donnell [17], Khot-Regev [19]). There has been significant work on the Unique Games Conjecture both on the part of algorithms researchers and complexity theorists. The algorithms researchers are finding approximation algorithms for the Unique Games Problem; approximation algorithms with particular approximation guarantees will disprove the conjecture. The complexity theorists have been using the Unique Games Conjecture to find additional hardness thresholds for fundamental problems. As part of the workshop, we will survey the current status of the conjecture, and devote time to approaches to resolve the conjecture, as well as further applications of it.

- 4. Another focus topic for the workshop is the hierarchy of LP (linear programming) and SDP (semidefinite programming) relaxations. The key idea here is to start from an LP relaxation of an NP-hard problem, and then obtain a series of tighter and tighter LP or SDP relaxations, by adding auxiliary variables and linear or semidefinite constraints. These methods were developed by Balas [7], Sherali and Adams [32], Lovasz and Schrijver [23], Lasserre [21], etc., and capture most of the known LP and SDP relaxations that have been exploited in the design of approximation algorithms. A stream of exciting research starting from the work of Arora, Bollobas and Lovasz [2], [3] has developed techniques to prove lower bounds on the approximation guarantees achievable by these methods. An important direction is to capture the relationship between hardness thresholds and the lower bound results on hierarchies of convex relaxations.
- 5. To include many younger researchers, and foster a relaxed interaction with established researchers. Our goal is to have a third of the workshop participants from this group.
- 6. To allow groups of Canadian researchers working in this area to meet, and either initiate or renew collaborations.

The workshop will present an opportunity to bring together some of the experts in related fields with the hope of initiating collaboration on some of the major open problems, and to explore the wider ramifications of the evolving body of powerful results and techniques from our area.

## **Recent Developments and Open Problems**

The study of approximation algorithms and the hardness of approximation is one of the most exciting areas among researchers in theoretical computer science; every major conference in the field has several papers on these topics. Significant progress is being made. We give two examples of recent, dramatic innovations:

(1) Raghavendra [30] has recently shown that there is a fixed efficient semidefinite programming algorithm which achieves the best approximation guarantee for all constraint satisfaction problems – assuming the Unique Games Conjecture.

(2) Asadpour, Goemans, Madry, Oveis Gharan, and Saberi [6] recently achieved the first significant improvement on the approximation guarantee of the asymmetric traveling salesman problem in over twenty five years. Shortly after, Mömke and Svensson [24] obtained a 1.461-approximation algorithm, for the graphic TSP, based on a novel use of matchings. The analysis of this algorithm has been further improved by Mucha [29] who shows an approximation ratio of 13/9.

# **Presentation Highlights**

#### Lift and Project

Konstantinos (Costis) Georgiou gave a tutorial presentation on the Lift and Project method, on the first day of the workshop. He introduced all popular lift-and-project systems deriving LP and SDP hierarchies, including the Lovasz-Schrijver LP and SDP system, the Sherali-Adams system, and the Lasserre system. The goal of his talk was to describe in a crystal-clear way the definitions of the systems, with many examples, as well as the proof of convergence to the integral hull – the proof illustrates some of the essential features of lift-and-project systems.

#### **Routing in Undirected Graphs with Constant Congestion**

The first plenary talk was given by Julia Chuzhoy, on a result that was acclaimed as a breakthrough by experts on the subject, [10]. The Maximum Edge Disjoint Paths Problem (MEDP) is a fundamental routing problem in Combinatorial Optimization. The input consists of an undirected graph G = (V, E) and k node pairs  $(s_1, t_1), (s_2, t_2), \ldots, (s_k, t_k)$ . The goal is to maximize the number of node pairs that can be connected by edge-disjoint paths. Let n denote the number of nodes in the graph. The approximability of MEDP in undirected graphs is still not well understood: the best known approximation ratio is  $O(\sqrt{n})$  while the best known hardness of approximation threshold is  $\Omega(\log^{1/2-\epsilon} n)$ , assuming that NP is not contained in randomized quasi-polynomial time. An impediment to improving the approximation ratio is that almost all algorithms are based on a multicommodity flow relaxation for the problem. A grid-like example shows that the maximum fractional (multicommodity) flow can be  $\Omega(\sqrt{n})$  times the maximum integral flow even in planar graphs. This topological obstruction goes away if we consider a relaxation of MEDP, namely, the MEDP with congestion problem (MEDPwC): here we allow the paths for the pairs to use an edge up to c times for an integer c.

Chuzhoy presented an efficient randomized algorithm to route  $\Omega(OPT/\text{polylog}(k))$  source-sink pairs with congestion at most 14, where OPT is the maximum number of pairs that can be simultaneously routed on edge-disjoint paths. The best previous algorithm that routed  $\Omega(OPT/\text{polylog}(n))$  pairs required congestion poly(log log n), and for the setting where the maximum allowed congestion is bounded by a constant c, the best previous algorithms could only guarantee the routing of  $\Omega(OPT/n^{O(1/c)})$  pairs. The key technical result of the paper shows that a graph has a large "routing structure" if it has a large well-linked set; this is proved by embedding an expander graph in any graph that has a large well-linked set.

Chuzhoy's result resolves an important open problem, though much work still remains to be done to get a full understanding of MEDPwC and related problems.

#### **The Traveling Salesman Problem**

The Traveling Salesman Problem (TSP) is one of the most well-studied problems in combinatorial optimization. Given a set of cities  $\{1, 2, ..., n\}$ , and distances c(i, j) for traveling from city *i* to *j*, the goal is to find a tour of minimum length that visits each city exactly once. An important special case of the TSP is the case when the distance forms a metric, i.e.,  $c(i, j) \leq c(i, k) + c(k, j)$  for all i, j, k, and all distances are symmetric, i.e., c(i, j) = c(j, i) for all i, j. If the distances are not symmetric, they are said to be asymmetric.

For thirty years, a  $\frac{3}{2}$ -approximation algorithm due to Christofides has been the best known approximation algorithm for the TSP when edge costs are symmetric and obey the triangle inequality. Only in the past year has there been any significant progress in improving the state-of-the-art in approximating this important problem, and we had an entire day of talks dedicating to discussing the progress that has been made.

A sub-case of the TSP is the *graphic* TSP. In this case, the distances c(i, j) are derived from an undirected graph G given as input, with  $\{1, 2, ..., n\}$  as its vertex set. The cost c(i, j) is the number of edges on the

shortest path between i and j in G.

In a plenary talk, Amin Saberi described his December 2010 result with his student Shayan Oveis Gharan and with Mohit Singh which gave a  $(\frac{3}{2} - \epsilon)$ -approximation algorithm for the graphic TSP, in which  $\epsilon \approx 10^{-12}$ , [27]. The analysis of the algorithms builds on a variety of ideas such as properties of strongly Rayleigh measures from probability theory, graph theoretical results on the structure of near minimum cuts, and the integrality of the T-join polytope from polyhedral theory. It is worth noting that this result also bounds the integrality gap of the Held-Karp linear programming relaxation (worst case ratio between integer and linear programming relaxation solution) of the graphic TSP by the same ratio.

In a second plenary talk, Ola Svensson described his 1.461-approximation algorithm (April 2011), jointly with Tobias Mömke, for the graphic TSP, based on a novel use of matchings, [24]. Traditionally, matchings have been used to add edges in order to make a given graph Eulerian, whereas their approach also allows for the removal of certain edges. For the TSP on graphic metrics (graph-TSP), the approach yields a 1.461-approximation algorithm with respect to the Held-Karp LP lower bound. For graph-TSP restricted to a class of graphs that contains degree three bounded and claw-free graphs, they show that the integrality gap of the Held-Karp relaxation matches the conjectured ratio 4/3. The framework allows for generalizations in a natural way and also leads to a 1.586-approximation algorithm for the traveling salesman path problem on graphic metrics where the start and end vertices are prespecified. Later, Mucha [29] improved on one part of the analysis (but not the algorithm) to achieve an approximation guarantee of  $\frac{13}{9}$ .

In the afternoon, we then had a sequence of three 30 minute talks about TSP-related problems. David Shmoys gave a talk about the traveling salesman path problem. In this problem, in addition to the usual input for the TSP, one is also given two cities *s* and *t*. The goal is to find the minimum-cost that starts at *s*, ends at *t*, and visits all the other cities in-between. For nearly 20 years, the best known approximation algorithm for this problem has been a  $\frac{5}{3}$ -approximation algorithm due to Hoogeveen, which is simply an adaptation of Christofides' algorithm. Shmoys described his work with his student Hyung-Chan An and with Robert Kleinberg to obtain a  $\frac{1+\sqrt{5}}{2}$ -approximation algorithm for the problem, [1].

Anke van Zuylen gave a talk on "A proof of the Boyd-Carr conjecture." A long-standing conjecture related to the TSP concerns the ratio of the cost of an optimal tour to the solution of a well-known linear programming relaxation of the TSP. It is known that this ratio is always at most  $\frac{3}{2}$ , and is for some instances at least  $\frac{4}{3}$ , but the exact worst-case ratio is unknown. Boyd and Carr considered the minimum-cost cycle cover problem; a tour is a cycle cover, but there can be cheaper cycle covers than a tour. Boyd and Carr conjectured that the ratio of the minimum-cost cycle cover to the linear programming relaxation for the TSP is always at most  $\frac{10}{9}$ . Van Zuylen described her proof of this conjecture in work together with Frans Schalekamp and David Williamson, [31].

Finally, Zachary Friggstad described his work on the asymmetric traveling salesman path problem with multiple salesmen, [12]. In addition to the input given for the traveling salesman path problem described above, there is a number k of salesman who can be sent to visit the cities. All k salesman start at s and end at t, and the union of their paths must visit all the cities. Friggstad described his bicriteria algorithm for this problem that in one extreme case uses k salesmen and has cost at most  $O(k \log n)$  times the optimal, and in the other extreme uses 2k salesman and has a cost only  $O(\log n)$  times the optimal.

#### Semidefinite Programming Hierarchies and the Unique Games Conjecture

David Steurer, in a plenary talk, presented his new results, jointly with Boaz Barak and Prasad Raghavendra, on the Unique Games Conjecture, [8].

Semidefinite programming (SDP) relaxation are a form of convex relaxation that found many uses in algorithms for combinatorial optimization. In the early 1990's several researchers proposed stronger forms of SDP relaxation known as SDP hierarchies. Steurer presented a new way of taking algorithmic advantage of these hierarchies to solve constraint satisfaction problems for 2-variable constraints such as Label-Cover, Max-Cut, and Unique-Games. Specifically, he described an algorithm based on an SDP-hierarchy that pro-

vides arbitrarily good approximation to all these problems in time poly(n) \* exp(r), where r is the number of eigenvalues in the constraint graph larger than some constant threshold (depending on the accuracy parameter and type of constraint used). In particular, quasi-polynomial-time algorithms are obtained for instances whose constraint graph is hyper-contractive, as is the case for all the canonical "hard instances" for MAX-CUT and UNIQUE-GAMES. This result gives more reason to consider relatively low levels of an SDP hierarchy as candidate algorithms for refuting Khot's Unique Games Conjecture.

#### The Sliding Scale Conjecture From Intersecting Curves

In another plenary talk, Dana Moshkovitz discussed the Sliding Scale Conjecture; this conjecture was posed by Bellare, Goldwasser, Lund and Russell in 1993 and has been open since. It says that there are PCPs with constant number of queries, polynomial alphabet and polynomially small error. She showed that the conjecture can be proved assuming a certain geometric conjecture about curves over finite fields. The geometric conjecture states that there are small families of low degree curves that behave, both in their distribution over points and in the intersections between pairs of curves from the family, similarly to the family of all low degree curves.

#### Hardness of Approximating the Closest Vector Problem (with Pre-Processing)

The final plenary talk was given by Nisheeth Vishnoi, on results obtained jointly with Subhash Khot and Preyas Popat, [18].

In the Closest Vector Problem (CVP) one is given as input a basis B for a lattice and a target vector t, and the goal is to find the lattice point closest to t, say in the  $l_2$  norm. This problem is NP-hard; the best approximation algorithm achieves roughly  $2^{O(n)}$  while the best hardness is  $2^{\log n/\log \log n}$ . It is an outstanding open problem to close this gap.

An easier sounding version of this problem, motivated from cryptography, is the Closest Vector Problem with Pre-processing (CVPP): Here B can be pre-processed arbitrarily and the input consists just of t. Could CVPP be much easier than CVP? For instance, one can compute the shortest vector in the lattice generated by B, a NP-hard problem, for free. Indeed, it was shown by Ahoronov and Regev how to approximate CVPP to within about  $\sqrt{n}$  factor!

Vishnoi first surveyed the approximability of lattice problems and then showed that, as far as the best known hardness of approximation results are concerned, they can almost close the gap between CVP and CVPP: CVPP is hard to approximate to within a factor of  $2^{(\log n)^{(1-\epsilon)}}$  unless NP is contained in quasi-poly time.

## 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, the plenary talks, and the tutorial (on lift-and-project methods) were very well received.

There is a growing number of new results that are obtained using the lift and project method. It appears that several interesting new results could be obtained using LP and SDP hierarchies, perhaps with running times that are slightly super-polynomial (such as quasi-polynomial). Some very recent results (such as results on directed Steiner trees) are evidences of this.

Some interesting questions in this direction were also raised at the end of the tutorial. In particular, a number of researchers have started looking into approximation algorithms for some of the classical problems

(e.g., set cover) that beat the hardness thresholds obtained so far if one allows the algorithm to run in superpolynomial time. More specifically, they have devised a  $(1 - \epsilon) \ln n + O(1)$ -approximation for set cover with running time  $2^{\tilde{O}(n^{\epsilon})}$  that is based on exploiting the Lovasz-Schrijver hierarchy of relaxations.

One of the participants reports that lift-and-project methods gave an SDP with an integrality gap of  $O(\log n)$  for the unsplittable flow problem on a path. This does not match the recent constant factor approximation, but it is another demonstration that hierarchies can be used to improve integrality gaps.

Another group of researchers have started working on a promising approach toward subexponential constant-factor approximations for Sparsest Cut. More specifically, they have a conjecture on the existence of certain random walks on vertex expander graphs whose stationary distribution is approximately uniform. One of their results – discovered at the BIRS Workshop – uses  $n^{O(\delta)}$ -rounds of the Lasserre SDP hierarchy to achieve a relaxation that appears to be significantly stronger than the Goemans-Linial SDP.

Following the plenary talk on the "sliding scale conjecture from intersecting curves" there were several discussions among workshop participants regarding what would be needed from the family of intersecting curves in order to prove the sliding scale conjecture. Discussions continued also shortly after the workshop, with additional participants. The outcome is a manuscript clarifying some of the obstacles that one would need to overcome. In particular, a certain property that may have appeared to be desirable for the family of intersecting curves, termed in the manuscript as "well mixed", was proved to conflict with the sliding scale conjecture. As a possible remedy, the manuscript suggests a notion of "well separated" intersecting curves, that (if it exists) may potentially resolve the sliding scale conjecture.

At the end, we mention that the above are only a few examples of the research progress made during or after the workshop, and there could be several other ongoing projects that started at the workshop.

**Acknowledgment**: It is a pleasure to thank the BIRS staff for their support; this contributed to the success of the workshop. In particular, we thank Wynne Fong, Brenda Williams, and Brent Kearney.

## **List of Participants**

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# Chapter 38

# Mathematics: Muse, Maker, and Measure of the Arts (11w5070)

# Dec 04 - Dec 09, 2011

**Organizer(s):** Ingrid Daubechies (Duke University) Shannon Hughes (University of Colorado at Boulder) Robert Moody (University of Victoria) Daniel Rockmore (Dartmouth College) Yang Wang (Michigan State University)

## **Overview of the Field**

Mathematics and arts have a long historical relationship. Tile mosaics since the early civilizations combine both artistic beauty and mathematical complexity. The ancient Egyptians and ancient Greeks knew about the golden ratio, regarded as an aesthetically pleasing ratio, and incorporated it into the design of monuments including the Great Pyramid, the Parthenon, the Colosseum. There are many examples of artists who have been inspired by mathematics and studied mathematics as a means of complementing their works. The Greek sculptor Polykleitos prescribed a series of mathematical proportions for carving the ideal male nude. Renaissance painters developed the theory of perspective, and many, including Piero della Francesca, became accomplished mathematicians themselves. The interplay of mathematics and art has continued to flourish throughout our history. Mathematics had greatly inspired artists as M. C. Escher, Picasso, Salvador Dali and artistic movements such as the minimalist and abstract art. Conversely, the art of tiling had contributed to the discovery of Penrose tiles and the study of aperiodic structures such quasicrystals, one of the most important areas in mathematics.

The study of geometry and advent of digital age have sown the seeds for a revolution in the arts. The processing power of modern computers allows mathematicians and non-mathematicians to visualize complex mathematical objects such as the Mandelbrot set and other fractal sets. The artistic beauty of such sets had attracted many mathematicians to discover fundamental properties they play in dynamical systems and chaos. In the modern industry of computer animation, fractals play a key role in modeling mountains, fire, trees and other natural objects. Fractals are an example of the growing field of generative art, which refers to ways to systematically and autonomously generating artwork in an algorithmic way using a computer. The workings of systems in generative art often rely on various fundamental scientific theories such as Complexity theory and Information theory. Generative art is not limited to abstract art. By combining it with Learning Theory it

is even possible to artificially generate paintings and music that mimic known masters. While generative art refers to an autonomous system for generating artwork, artists today are increasingly relying on mathematics and computers to aide their creative work. Besides painting and music, the intricacy of origami highlights the fusion of mathematics and art. Modern computing has allowed us to make complex geometric designs that have led to the design and creation of origami figures whose complexity and delicacy cannot even be imagined in the past.

Mathematics is increasingly making its impact in the study of stylometry in art. The term stylometry was coined in 1897 by the historian of philosophy, Wincenty Lutaslowski, as a catch-all for a collection of statistical techniques applied to questions of authorship and evolution of style in the literary arts. The advent of high definition digitization for works of art may have opened up a whole new venue for art authentication. With scans of paintings capturing minute details that even human experts can easily miss it is hoped that more sophisticated mathematical and statistical tools can be developed to shed light on the question of provenance. It is also hoped that these new mathematical and statistical techniques will become valuable tools of research for art historians. Indeed, increasingly, huge treasuries of visual works are being digitized for the purposes of art historical education and research as well as restoration and conservation. Several research projects in this direction, such as the study of Jackson Pollock by Richard Taylor et al, the restoration of digital imagery of medieval draperies by the Chudnovsky brothers and the recent Van Gogh Project, had received headline media coverage.

## **Recent Developments and Challenges**

The intended purpose of the workshop is to bring together leading mathematical researchers whose work pertain to arts. In doing so we hope to promote the application of mathematics to the study of arts, and to develop some coherent frameworks for moving this area of research further ahead. Given the diversity of the research activities this area spans it is impossible to cover all topics comprehensively. The workshop focused on two growing areas of research: visual stylometry analysis and mathematical techniques for art making. These selected topics will highlight how mathematical and statistical techniques can be valuable tools for the study of arts.

The evaluation of a work of art for attribution has historically relied on the techniques of connoisseurship, a process by which a questioned work is subjected to the evaluation by a few experts who are steeped in the work and life of the artist in question. The analyses are usually based on their extensive visual experience and encyclopedic knowledge of the career of the would-be artist, as well as other kinds of art historical data. The advent of high definition digitization for works of art has opened up a whole new venue for stylometry analysis. Powerful mathematical and statistical techniques are now available for the study of art, literature and music in terms of authentication and style analysis, motion capturing and more.

Stylometry analysis of literary style has its origins dating back to the mid 1800s. It is Augustus de Morgan, an English logician who first suggested to his friend in a letter in 1851 that questions of authorship might be settled by determining the length of words "*if one text does not deal in longer words than another.*" This technique and later more sophisticated ones have been used on stylometric analysis of works attributed to Shakespeare. Today, stylometric analysis of literature is already a field that has truly come into its own. Although stylometric analysis of art has lagged and is undoubtedly more challenging, time is ripe for it to take off. More importantly, stylometric analysis of art calls for a more diverse and (perhaps more sophisticated) repertoire of mathematical and statistical techniques. The stylometric study by Taylor et al (1999) of Jackson Pollock is based on the fractal property of Pollock's drip paintings, which shows that Pollock paintings have rather unique fractal signatures. Another pioneer work on stylometry of art was the analysis of drawings that had been attributed to the great Flemish artist Pieter Bruegel the Elder by Lyu et al (2004). In it the use of multiscale wavelet analysis was proposed as a tool for visual stylometry. Beside the Bruegel paintings the technique was also used to analyze a large altarpiece generally attributed to the workshop of the Renaissance

master Perugino. The results of these experiments provided evidence indicating that the wavelet coefficients could be used as a source of information identifying the artist. More recently, in a comprehensive effort to study stylometry of art, several research teams had been put together to study the paintings of Vincent Van Gogh using high resolution digital scans in the "Van Gogh Project (VGP)." The research by these teams focused on the brush stroke analysis of these paintings using a variety of techniques such as wavelets, hidden Markov trees, sparse coding, c.f. a survey in Johnson et al (2008). A study by Hughes et al (2010) focuses on the use of Empirical Mode Decomposition for stylometry analysis. Wendt, Roux, Abry and Jaffard (2009) have and analyzed provenance and authorship of paintings by the analysis of multifractals. The results of these studies provide evidence that the mathematical study of stylometry of art is a fertile field.

Nevertheless challenges remains in the field of visual stylometry. Aside from the obvious challenge of obtaining high quality digital imageries for stylometric analysis, there are a number of mathematical challenges as well. For example, the style of a particular artist is no static, and there are a great deal of subject-dependent variations in style even from an artist whose style remained rather constant over the years. The mathematical techniques used for stylomery analysis mostly focus on brush strokes, by doing so some important defining qualities of an artist are not taken into account. Furthermore, the mathematical techniques used so far are based mostly on multiscale decomposition techniques such as wavelets and Empirical Mode Decomposition. More techniques must be developed for the field to truly take off.

Another important topic of this workshop is to bring experts in these areas to discuss the latest mathematical techniques for art making. The advances in the study of geometry, dynamical systems, information theory, learning theory, and others have led to rapid advances in many areas of art making. And conversely, the pursue of new ideas and trends in art such as tiling, origami, computer graphics and abstract art has contributed greatly to the advances in some areas of mathematics. The visually stunning Mandelbrot set and many other fractal sets come from nonlinear dynamical systems, from which the study of chaos was born. Today fractals have been used not only as a generative tool for making beautiful pictures but also a tool for modeling natural objects and physical phenomena such as rough surfaces in material science. The discovery of Penrose tiles has led to the study of aperiodic orders and the study of quasicrystals, and has inspired the Escheresque artistic aspirations of many mathematicians, artists and students.

Today generative art is an active and broad area of research and practice. Generative art aims for the creation of artwork using algorithms (both deterministic and random). While Mandelbrot set and fractals represent a typical generative art, the field has gone far beyond it. Sophisticated mathematical and statistical techniques are now available to create a wide array of intricate artworks. For example, the texture model by Gousseau, Morel and others have led to exquisite abstract paintings that could often mimic those of the masters. The work by Robert Lang and John Montroll have developed geometrical and computational techniques that have taken origami to a state that was unimaginable just a few years ago. Some of these techniques in origami are now found applications in robotics. The study of ancient mosaics has led to new insights on how geometry was used in the making of patterns and tilings in the ancient time. Realistic modelling and rendering of textures and complex systems such as water waves has taken computer graphics to a new level that it becomes a vital part of film making. The advent of digital photography has opened up a whole new frontier of interplay between mathematics and arts. With the explosive growth of digital photography comes many challenging mathematical problems. Today "computational photography" is an extremely active research area in mathematics and computer science, which has also led to an attempt by mathematicians and computer scientists to generate artificial "photographs" that are realistic and artistic in its rendering. Mathematical models have also been used to evaluate the "artistry" of photographs with some degree of success. Mathematical techniques have also been used to enhance and to restore artwork. The work by Chudnovsky brothers on the digital archiving of medieval draperies and the digital restoration and enhancement of old films are also such examples. There are enormous challenges ahead in these areas. For example, although there is a model to evaluate artistry for digital photos, it is still relatively primitive at this stage. While we have been able to build more and more sophisticated mathematical models to generate arts, artistry rarely figures into the generating process. How to integrate it into the process remain one of the great

challenges in mathematical arts.

## **Presentation Highlights and Outcomes**

The workshop is characterized by many excellent presentations. They include very detailed overviews of key related areas of research and cutting edge researches. The workshop kicked off with a beautiful presentation by Ingrid Daubechies, who is a leading researcher in the area of stylometry analysis for visual arts. She gave a very in-depth overview of the field and highlighted many challenges in the area. In particular, she has gone into details about how the ongoing Van Gogh Project has shaped the field and has lead to many novel new techniques. Her talk had set the tone for many subsequent talks. David Mumford gave a beautiful overview on random models for image synthesis, drawing from both his earlier work in the 90's on image statistics and latest work by him and many others such as the Paris Group. Jim Coddington from MoMA spoke about the latest technological advances in analyzing arts that allow us to detect a painting underneath another one, and the mathematical challenges to restore such a painting. Craig Kaplan illustrated the use of computer graphics techniques in the generation of arts.

Several speakers have presented their findings in stylometry analysis, which are among the latest advances in this new field. Shannon Hughes presented the Hidden Markov model for authentication. James Wang developed a brush stroke model that is significantly different from the conventional wavelet based approach, and it can be applied effectively to Chinese watercolor paintings and calligraphy. James Hughes (joint with Dan Rockmore and Yang Wang) showed that the latest advances in Empirical Mode Decomposition (EMD) present a powerful tool for stylometric analysis. An exciting new development is presented by Patrice Abry and Stephan Jaffard, who showed that multifractal analysis, commonly used in the study of statistical mechanics and nonlinear dynamics, can be an effective tool for the study of brushstrokes and hence for visual stylometry. In one of the highlighted presentations, Jason Brown showed how he used Fourier analysis to unravel the mystery of the Beetle's *A Hard Day's Night*, a feat that has been featured in a number of media outlets.

beside the presentations in stylometry there are a number of engaging talks in other areas related to mathematics and arts. Reza Sarhangi spoke about the polyhedral modularity for the creation of artistic geometric patterns, and show how the idea was used for making patterns in the Near East. George Hart presented various beautiful geometric constructions for the making of artistic and intriguing geometric objects. Robert Moody gave a beautiful presentation on aperiodic tiling and Penrose tiles, and how the research blends in with physics and arts. Both Robert Schneider and Luke Wolcott illustrated the interplay of mathematics and music. Alice Major showed how mathematics is an integral part of her beautiful poems. The presentations by James Wang and James Hughes also included a very intriguing but relatively undeveloped concept: the measurement of artistic beauty. In particular, James Wang developed a system that ranks digital photos. His presentation has sparked a lively discussion on how and whether mathematics can or should be used to evaluate the *artistry* of an art.

This workshop is the first major meeting on stylomtery, and it will not be the last as the field gains more and more attention. Our hope is that from this experience we will be able to share our ideas and latest findings to move the research further ahead. The fact that there are experts in arts and mathematics (including accomplished artists such as Robert Moody, David Mumford, Jim Coddington, George Hart, Jason Brown, Robert Schneider, Alice Major) in attendance will provide a great boost for the field.

The workshop has been memorable for many participants because of the interactions between mathematicians and those who have strongly established record in art making (e.g. those aforementioned participants). To many of the participants whose primary specialty is mathematical research, it has open their eyes on many intriguing possibilities. The workshop has already spurred several ongoing and potential collaborations, which would not have happened without it. Sarhangi and Wang have already submitted an NSF proposal for the upcoming BRIDGE conference, which will for the first time include a session on stylometry. Daubechies, Hughes, Kaplan and Wang are contemplating a proposal for the next Banff meeting. S. Hughes have discussed collaborating with P. Abry and S. Jaffard. Coddington has generously offered to help researchers with digital images in the MoMA collection. Brown and Y. Wang are looking into a deeper study of music and stylometry using the latest mathematical and machine learning techniques.

# **List of Participants**

Brown, Jason (Dalhousie University) Coddington, Jim (Museum of Modern Art) Daubechies, Ingrid (Duke University) Hart, George W. (Museum of Mathematics) Hughes, Shannon (University of Colorado at Boulder) Hughes, James (Dartmouth College) Jaffard, Stephane (Université Paris est Créteil) Kaplan, Craig (University of Waterloo) Major, Alice (Independent) Moody, Robert (University of Victoria) Mumford, David (Brown University) Sarhangi, Reza (Towson University) Schneider, Robert (University of Kentucky) Wang, Yang (Michigan State University) Wang, James (Penn State University and NSF) Wolcott, Luke (University of Washington)

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# Chapter 39

# **Current challenges in statistical learning** (11w5051)

# Dec 04 - Dec 09, 2011

**Organizer(s):** Hugh Chipman (Acadia University) Xiaotong Shen (University of Minnesota) Robert Tibshirani (Stanford University) Joseph Verducci (The Ohio State University) Mu Zhu (University of Waterloo) Ji Zhu (University of Michigan)

# **Overview of the Field**

In recent years, statistical learning has seen rapid growth within statistics and computer sciences. This growth has been driven primarily by the need to analyze data of complex structures and process massive amounts of data from scientific investigations. In a discovery process, statistical uncertainty is usually high, given the limited amount of information contained in the data. In gene function prediction, for example, data may be structured, and contain features whose size greatly exceeds the sample size. This imposes major challenges to statistical learning, which demands powerful statistical tools to efficiently and accurately extract information of scientific interest from high-dimensional (or massive) data of complex structures.

In statistical learning, challenges arise from real applications, which require the processing of complex combinations of thousands of potential features to make reliable and valid generalizations. As a result, developing efficient and accurate methods has become of paramount importance for large-scale and high-dimensional problems. For instance, support vector machines were designed to optimize estimated margins between distributions for classification rules, bypassing the estimation of distributions for efficiency and accuracy. Emerging issues in applications continue to be a driving force in the development of statistical learning.

Statistical learning analyzes statistical aspects of general types of relations, for data expressed in terms of video sequences, text documents, gene and social networks and web-pages, among others. Areas of interest include unsupervised, semisupervised and supervised learning, rankings, text and web mining, network analysis, genomics, drug discovery, intrusion and fraud detection. In what follows, we list several specific research areas and directions that have broad interest among potential workshop participants. Kernels Methods and Large Margin Classification: Through the concept of margins, kernel methods [7] classify objects of interest by mapping data onto a feature space, with each coordinate corresponding to one feature of the data. This mapping is efficiently computed through kernels for various types of data. One advantage of kernel methods is that a nonlinear problem is treated linearly after kernel mapping, permitting an efficient treatment of large-scale problems. Kernel methods, known as kernel machines, have been rapidly developing. For kernel methods, several websites have been constructed to communicate recent developments, e.g., www.kernel-machines.org). Despite the extensive successes of kernel-based large margin theory [3], issues remain with regard to its relationship with distribution-based classification theory, as well as how to account for biases in model selection when estimating generalization error. In addition, early attempts at designing a universal kernel have been only modestly successful, and criteria for choosing an appropriate kernel remain a topic of practical interest.

## **Recent Developments and Open Problems**

This workshop provided a unique opportunity for researchers to explore the filed of statistical learning in depth; discussed pros and cons of the existing methods. In addition, the workshop identified new research directions from different, but related, areas. Emerging areas for statistical learning include: (a) Ensembles methods for massive high-dimensional data, (b) Regularization, (c) High-dimensional feature selection, and (d) Graphical and network models, and (e) Genomic analysis and data mining.

#### Ensembles

One of the key developments for ensembles utilizes the notion of combining multiple predictors to form a single accurate predictor. Such ensemble methods take many forms and have resulted in remarkably flexible and efficient tools for prediction. One ensemble method that has generated significant interest is the Boosting [5] family of algorithms such as AdaBoost. Boosting was motivated from the PAC model of learning, which successively puts more weight on misclassified objects until they become correctly classified. These methods have been recently reformulated in the context of additive or logistic models with specialized loss functions. Although the empirical evidence is strong for combining different representations, theoretical understanding of these methods remains lacking. For example, the Winnow algorithm, a kind of perceptron that uses a multiplicative weight-update scheme, performs especially well when many dimensions are irrelevant. In this case it has generalized better than its large margin counterpart. Thus the principles of large margins and low generalization error may, and do, lead to different assessments of classifiers.

#### Regularization

In statistical learning, regularization [9] introduces additional information to regression; usually related to the complexity of a solution, which is incorporated as a penalty. For example, in linear regression, a penalty penalizes an increase in a models size through individual regression coefficients; in nonlinear regression a penalty is imposed for lack of smoothness. Regularization with different penalties can lead to solutions to a variety of problems, which is interpretable from the Bayesian perspective. In high-dimensional data analysis, issues continue to arise with respect to how to design suitable penalties and how to tune regularization parameter(s) for predictive accuracy.

#### **High-dimensional Feature Selection**

Feature selection is a fundamental tool for data analysis. One focus of recent research has been centered on feature selection in high-dimensional situations, to respond to the pressing need to process large amounts of data of complex structures. In high-dimensional situations, data analysis often involves a large number of features, which may greatly exceed the sample size. In the past, feature selection has been extensively investigated mainly for low-dimensional situations, where many information criteria such as AIC [1] and BIC [6] have been proposed for model selection. For high-dimensional situations, however, developing efficient computational tools becomes extremely important. Recent developments of Lasso [8] and Lars [4] for feature selection have demonstrated the need for efficient computation. Moreover, various methods have been proposed and studied for achieving high predictive accuracy as well as for accuracy of selection. The focus in this area has been on developing efficient computational tools leading to desired statistical properties.

#### Graphical and network models

Graphical models [2] are useful to analyze and visualize conditional independence relationships between interacting units, in addition to their structural implications. For instance, in dynamic network analysis, a structural change is often a result of certain events or experimental conditions. In Gaussian graphical models, precision matrices are estimated to describe dependencies among interacting units through maximum likelihood. In the past, the research effort has concentrated on reconstruction of a *single* sparse graph. It is known that existing methods may not perform well when the dimension of a matrix is larger than the sample size. For multiple graphical models, detection of structural changes over graphs has been one focus. However, this is challenging due to the enormous size of candidate graphs, which is super-exponential in the total number of nodes over multiple models.

#### **Genomic Applications and Data Mining**

Various statistical learning methods have been widely used in genomics analysis, including clustering for microarray analysis, hierarchical classification and semisupervised learning for gene function prediction and gene network analysis, among others. Various emerging issues from biomedical applications are activated in the presence of structured data from various gene networks, where mining the structures of a problem becomes critical.

#### **Presentation Highlights**

**Tensor data analysis.** Art Own, Professor of Statistics, at Stanford University, opened the week with an overview of tensor data analysis, where he focused on when and why the bootstrap method breaks for a tensor of three or more. As he indicated, no proper bootstrap can exist in such a situation. He then modified a resampling scheme, which has showed to perform well for the famous Netflix data, which is a sparsely sampled table with rows for customers and columns for movies, or vice versa. His central message is that care is necessary for tensor data analysis. There was also be a case study discussed by Dean Eckles, who presented challenges in analyzing consumer behavior data collected at Facebook, from a practitioner's point of view.

**High-dimensional feature selection.** High-dimensional feature selection remained to be a focus of this workshop. Wonyul Lee, a graduate student at North Carolina at Chapel Hill, presented results on consistent feature selection in high-dimensional situation. Yongdai Kim, Seoul National University, presented results on feature selection and parameter estimation for nonconvex regularization, and argued that nonconvex regularization with suitably designed regularizers is advantageous over its convex counterpart statistically. Then he discussed the issue of local versus global solutions for nonconvex regularization. Marina Vannucci, Rice University, presented a class of Bayesian models, for feature selection. The models incorporate additional information such as gene functions and gene-gene relations.

**Classification and clustering.** There were several technical talks on classification and clustering. Yichao Wu, North Carolina State University, proposed weighted learning methods in the context of support vector machines, which aims to solve a nonconvex problem through weighted learning. Ruben Zamar, University of British Columbia, presented a classification method that is robust not only to outliers in the training and also in the test data. This is achieved through an ensemble of robust classifiers based on mixture models. Alejandro Murua presented statistical models behind algorithms for biclustering analysis, which may have nice Bayesian interpretations. Matias Salibian-Barrera, University of British Columbia, presented their results on sparse-K-means clustering algorithms, which have a nice sparseness property, in addition to robustness.

**Graphical and network models.** Estimation of high-dimensional network structures has become one active area of research recently, which arises naturally in the analyses of many physical, biological and socioeconomic systems. Of particular interest is learning the structure of a network over time. George Michailidis, University of Michigan, presented network Granger causal models for exploration of sparsity of its edges and inherent grouping structure among its nodes. George proposed interesting algorithms based on a variant of Group Lasso to discover the Granger causal interactions among the nodes of the network. Of course, there are issues in estimation of relevant covariance and precision matrices. Junhui Wang, University of Illinois at Chicago, argued that positivity of covariance and precision matrices need to be reinforced. He presented results based on gradient descent algorithms to generate positivity matrices.

**Applications.** There are several exciting application talks. David van Dyk, Imperial College, London, presented massive data-analytic and data-mining challenges for statistical analysis of astronomic data. Hongzhe Li, University of Pennsylvania, focused on a problem of segment identification. This arises in in studying copy number variants that are alternations of DNA of a genome that results in the cell having a less or more than two copies of segments of the DNA. The problem under consideration is ultra-high dimensional. Li and his collaborator proposed methods for robust identification. In addition, Annie Qu talked about selecting correlation structure for large cluster size data. Identifying correct correlation structure is very important to improve the efficiency of parameter estimation. In their approach, they transformed a correlation structure model selection problem to be a covariate model selection problem, which is capable to handle the increasing cluster size as the sample size increases.

### **Publication of Papers**

A poll was taken at the meeting to see if there were substantial interest in publishing papers from the workshop in some sort of proceedings, and a majority were in favor. An on-line survey asked each participant for a level of interest, ranging from not interested (the work has already been submitted elsewhere), to uncertain (need to check with co-authors), to definite intent. With more than half the participants showing some interest, and about 10 stating definite intent, a vote was taken on the exact form of publication. By majority vote it was decided that all interested participants should submit their workshop-related papers for publication in a special issue of Statistical Analysis and Data Mining, a leading journal in this field, which is co-published by the American Statistical Association and Wiley-Blackwell Publishers. One of the co-organizers, Joe Verducci, is Editor-in-Chief of this journal, and he obtained unanimous consent from his Editorial Board in favor of the special issue. A deadline of April 30, 2012 has been set for submission. All papers will undergo the usual review process of the journal, and a special introduction will be written to acknowledge the support from BIRS. Publication is expected in early 2013.

### **Outcome of the Meeting**

About 40 people, including statisticians, computer scientists, mathematicians, graduate students, and a broad range of scientists, participate in the week-long workshop. Group discussions, formal and informal, were interleaved with presentations, making for lively exchanges and a creative learning environment.

A very tangible outcome of the meeting, and an indication of the high quality of scientific presentations, was the decision to have a special issue of the journal *Statistical Analysis and Data Mining* devoted to papers presented at the conference. All articles will be subjected to the usual peer-review process for the journal. Additional details are provided in a separate section below.

Most of the respondents thought that having attended this workshop positively impacted their experience in collaboration and research. Some comments on this impact include:

"I am discussing with Prof. Xiaoming Huo from Georgia Tech a possible project in the near future. He will visit York in March, 2012." *Steven Wang, York University.* 

"Yes. Art Own presented an interesting talk on analysis of tensor data, on which I am currently working on." *Junhui Wang University of Illinois at Chicago*.

"[I received an] Invitation to be an AE for Statistical Analysis and Data Mining, which I accepted." Bertrand Clarke, University of Miami. "Stan Young and I talked about a new method of controlling False Discovery Rate that could be used in conjunction with the Tau-Path procedure that I presented. A student of mine is investigating this further." *Joseph Verducci, The Ohio State University.* 

"The workshop was very useful to learn about current developments in data mining which are very relevant to my own research. The presentations and discussions with other participants were very inspiring. I also appreciated the immediate feedback I had from other researchers regarding my own current research." *Ruben Zamar, University of British Columbia.* 

"Wrote the paper "Robust and Sparse k-means" with Matias Salibian and Yumi Kondo, and Started the new research project "Robust and sparse kernel k-means" with Alejandro Murua, Matias Salibian and Yumi Kondo." *Ruben Zamar, University of British Columbia.* 

"I have obtained commitments from several participants at the workshop to submit their latest research to the journal Statistical Analysis and Data Mining (jointly published by Wiley and the American Statistical Association) for which I am currently Editor-in-Chief." *Joseph Verducci, The Ohio State University.* 

"I consulted Wenbo Li on a number of results in probability theory. It helped to clarify several technical issues. I am ready to finish up a paper because of this." *Jiahua Chen, University of British Columbia.* 

"I've opened a new front in text network models, based on feedback from the meeting; this is joint work with Jacopo Soriano and Justin Gross on models for political blogs." *David Banks, Duke University.* 

"David Banks invited me to a SAMSI / SIAM workshop on computational advertising." Dean Eckles.

"This workshop has been one of the most positive research experiences I had in the last 5 years! I wish to thank the organizers and the BIRS staff for making this possible." *Ruben Zamar, University of British Columbia.* 

### Wrap-up

The workshop focused on recent developments of machine learning and data mining. Participants of the workshop rated the workshop a success, admitting that many questions have been raised, yet with only a fraction of them have been answered. They all agree that further collaborations are necessary to address a number of emerging issues. First, there are substantial statistical differences between the study of high-dimensional problems and that of conventional problems. Second, efficient algorithms are needed, for performing scale-up data analysis for existing scientific and engineering problems, as well as well those yet to be discovered.

In particular, the workshop identifies several emerging research areas which would be most challenging yet extremely important since they are fundamental problems in machine learning and data mining. One important area is on optimization for high-dimensional non-convex problems. It is urgent to develop feasible algorithm to obtain the global solution. Most of existing theoretical properties are established based on the knowledge that the global solution can be achieved. However, in practice, it is an extremely challenging problem to find the global solution for high-dimensional data. Another important area is to extract important signals from very noise data through matrix decomposition. This is equivalent to obtain low rank approximation from a very high-dimensional matrix. This research area has many applications such as image process, data compression and storage for extremely large data sets in genomics and astronomy studies. The third important area is on high-dimensional network data which are applicable for social network and gene network. Developing fast and efficient algorithm for network data is very challenging since there are typically no replicates available but the number of parameters involved could be very high. Finally, it is also very important to develop a dynamic model for network data in order to evaluate the dynamic changes of network associations over time.

### **List of Participants**

Ahmed, S. Ejaz (U. of Windsor) Banks, David (Duke University) Bondell, Howard (North Carolina State University) Chen, Jiahua (University of British Columbia) Chipman, Hugh (Acadia University) Ciampi, Antonio (McGill University) Clarke, Bertrand (University of Miami) Cutler, Adele (Utah State University) Eckles, Dean (Stanford University) Huo, Xiaoming (Georgia Institute of Technology) Jeon, Jong-June (Seoul National University) Kim, Yongdai (Souel National University) Kondo, Yumi (The University of British Columbia) Li, Hongzhe (University of Pennsylvania) Li, Wenbo (University of Delaware) Liu, Yufeng (The University of North Carolina at Chapel Hill) Michailidis, George (University of Michigan) Murdoch, Duncan (University of Western Ontario) Murua, Alejandro (Universite de Montreal) Owen, Art (Stanford University) Peng, Wang (Bowling Green State University) **Qin, Steve** (Emory University) Qu, Annie (University of Illinois at Urbana Champaign) Salibian-Barrera, Matias (University of British Columbia) Shen, Xiaotong (University of Minnesota) Stenning, David (University of California at Irvine) Thierry, Chekouo Tekougang (University of Montreal) van Dvk, David (Imperial College London) Vannucci, Marina (Rice University) Verducci, Joseph (The Ohio State University) Wang, Junhui (University of Illinois at Chicago) Wang, Steven (York University) Wonyul, Lee (The University of North Carolina at Chapel Hil) Wu, Yichao (North Carolina State University) Young, Stanley (National Institute of Statistical Sciences) Zamar, Ruben (University of British Columbia) Zhang, Helen (University of Arizona) Zhu, Mu (University of Waterloo) Zhu, Ji (University of Michigan)

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# Two-day Workshop Reports

Two-day Workshop Reports

### Chapter 40

# High-performance numerical methods supporting radiation therapy treatment planning (11w2035)

### Mar 11 - Mar 13, 2011

**Organizer**(s): Yuriy Zinchenko (University of Calgary)

### **Overview of the Field**

The projected increase in the incidence and mortality of thoracic and abdominal cancers is an important health concern for Canadians. For many diseases, radiation therapy is a proven treatment modality, and nearly half of all cancer patients receive radiation therapy, either as the sole treatment or combined with surgery and/or systemic pharmaceutical agents, e.g. chemotherapy. Important technological advances, such as Intensity Modulated Radiation Therapy (IMRT), have solidified or expanded the role of radiation therapy in improving control of cancers, notably for head and neck cancers and prostate cancer. For disease in the thorax and abdomen –in aggregate terms, cancers with the highest mortality rate– however, the effectiveness of radio-therapy has been drastically limited by the sensitivity of non-tumour lung and liver tissues, and confounded by the technical challenges due to breathing-related organ movement and patient setup uncertainty. Thus, there is a marked need for improving state-of-the-art radiotherapy planning and delivery methods.

Since the state-of-the-art radiation therapy treatment planning process typically involves highly complex computer-assisted mathematical modeling to support near-optimal decision making, it is impossible to address such a need without adequate advancements in associated mathematical models and high-performance numerical methods, carefully integrating those with existing and emerging radio-therapeutic technologies.

### **Recent Developments and Open Problems**

Of particular interest is minimizing negative effects of uncertainties that are inherently present during the radiation treatment planning phase. As we improve our medical imaging capabilities, highly tailored to the shape and position of the cancer treatments minimize the radiation dose to healthy tissue, but also create a

greater risk of a geometric miss of the disease if cancer moves. So, without effective targeting and adequate accounting of these uncertainties during the mathematical modeling and treatment planning phases, there is a risk of damaging healthy tissues indiscriminately, thus failing to control the disease, especially using high-precision technologies like IMRT, which in turn nowadays become almost ubiquitously present in clinics.

The above mentioned uncertainties may be targeted at several distinct phases of treatment planning and delivery, for example, by developing novel medical imaging techniques that provide more accurate biological information to planners (e.g., PET/CT combination), by providing information on present organ and tumor locations and consequently allowing for real-time intervention during the treatment delivery (e.g., gating), and finally, by informing the underlying numerical models about the anticipated uncertainties a-priori during the treatment planning phase to enable the delivery of *robust* near-optimal radiation treatment (e.g., robust optimization of IMRT plans).

As the radiation treatment modalities become more advanced and complex, a concurrent treatment planning challenge is to formulate the associated treatment planning model that carefully captures the desired clinical objectives and yet remains computationally tractable, that is, possible to optimize over in short time alloted under clinical planning scenario and with limited computational and human resources.

All of the above provides both challenges and excellent opportunities to develop a truly collaborative scientific framework that would ultimately enhance state-of-the-art standards for cancer treatment and management.

#### **Presentation Highlights**

Radiation therapy treatment planning, besides acquiring the initial medical imaging data and setting proper clinical objectives, involves formulating a mathematical model for treatment delivery, and, subsequently, exploring the model's control variable space (numerically) in search of a (near) optimal treatment plan. The workshop was focused on the following principal components of this process: (1) (clinically) adequate modeling, (2) numerical optimization methods, and (3) implementation.

The workshop led participants on a guided tour of state-of-the-art radiation therapy, opening with some clinical insights into the problem (presented by a radiation oncologist, Princess Margaret Hospital, and the chair of medical physics, Memorial Sloan-Kettering Cancer Center – two world-leading cancer treatment and research centers). The opening was followed by presentations given by a number of distinguished applied mathematicians and computer scientists primarily working in the area of optimization. An important component of the workshop was a presentation by an industrial research scientist from Elekta, one of the commercial leaders in radiation therapy products, on the challenges in the field as seen by the product developers.

In addition, the first day of the workshop was concluded by a networking and poster session where some of the more junior attendees had a chance to present their work and the floor was opened to a more informal discussions.

### **Scientific Progress Made**

During the workshop, primarily, during the panel discussion, a number of concrete projects were proposed for collaborative research, and potential research groups were identified; these include

- 1. GPU-supported Monte-Carlo-based accurate dose computation engine,
- 2. data-mining for clinically "good" and "bad" treatment plans,
- 3. constructing and exploring the Pareto-space of non-dominated treatment plans,
- 4. real-time GPU-supported treatment plan re-optimization.

Presently, we are investigating the viability of these research directions.

### **Outcome of the Meeting**

This was a first event within the envisioned series of once-in-two-years workshops on high-performance numerical methods supporting radiation therapy treatment planning. The intent is to grow these workshops into regular series of intense collaborative research events that bring together a diverse group of applied mathematics, medical physics and radiation oncology researchers, as was reconfirmed during the BIRS workshop in March of 2011. First and foremost we target a creation of a truly active, interdisciplinary and sustainable research framework addressing the problems in the field of optimal radiation therapy treatment planning.

The main goal of the proposed workshop series is to determine and regularly update a set of integrated strategic directions for development and collaboration in high-performance numerical methods and models that support optimal radiation therapy treatment planning – an interdisciplinary area that brings together researchers and practitioners in applied mathematics and operations research, medical physics, and radiation oncology. We believe that the goal may be achieved by bringing together leading experts in the area and a selected group of post-doctoral fellows and graduate students in the collaborative environment. Consequently, 2011 BIRS workshop served an important milestone towards radical advancement in the state-of-the-art standards of radiotherapy treatment planning.

#### **List of Participants**

Aleman, Dionne (University of Toronto) Apte, Aditya (Memorial Sloan Kettering Cancer Center) Chan, Timothy (University of Toronto) Deasy, Joseph (Memorial Sloan-Kettering Cancer Center) Eskicioglu, Murat (University of British Columbia Okanagan) Ferris, Michael C. (University of Wisconsin) Ghobadi, Kimia (University of Toronto) Goez, Julio (Lehigh University) Hare, Warren (UBC Okanagan) Hope, Andrew (Princess Margaret Hospital / University of Toronto) Jiang, Steve B. (University of California, San Diego) Lee, Taewoo (University of Toronto) Li, Yuying (University of Waterloo) Long, Troy (University of Michigan) Lucet, Yves (University of British Columbia Okanagan) Men, Chunhua (Elekta) Milette, Marie-Pierre (BC Cancer Agency-Centre for the Southern Interior) Ramakrishnan, Jagdish (MIT) Romeijn, Edwin (University of Michigan) Shirvani Ghomi, Poovan (University of Calgary) Terlaky, Tamas (Lehigh University) Unkelbach, Jan H. (Massachusetts General Hospital (MGH)) Wright, Stephen (University of Wisconsin) Zinchenko, Yuriy (University of Calgary)

### Chapter 41

# Data Analytics Research Workshop (11w2167)

### May 27 - May 29, 2011

**Organizer(s):** Denilson Barbosa (University of Alberta) Leslie Dolman (NSERC BIN/University of Toronto) Annette Mayer (University of Toronto)

### **Overview of the Field**

Business intelligence (BI) is the commercial term for using information within organizations to make informed decisions, and to run operations effectively based on available data. It has numerous application areas in critical domains including health, energy and infrastructure planning. Broadly speaking, BI is directly related to the areas of computer science, modeling, analysis and forecasting. As a research field, it encompasses data and knowledge management, management of digital media, modeling of processes and policies, data quality, data privacy and security, data integration, data exchange, data cleaning, inconsistency management, information retrieval, data mining, analytics, and decision support.

The goal of the workshop was to provide an in-depth review of the research underway in the NSERC Business Intelligence Network (BIN), a national network currently completing the second of a five year research program. BIN comprises 15 PIs at 7 universities (University of Alberta, University of British Columbia, Carleton University, Dalhousie University, University of Ottawa, University of Toronto and University of Waterloo). Investigators are working in partnership with researchers at a number of organizations including SAP, IBM, iAnywhere, Palomino and Zerofootprint. Over 55 graduate students and post-docs are currently involved in the network.

The industry partners in BIN, all of which have strong presence in the Canadian Information Technology industry, are currently developing expertise around these technologies and incorporating them into their products. In this setting, our network is involved in creating the next generation of software tools that will drive data analytics and management is all areas, and is therefore strongly related the Canadian government's research priorities.

### **Recent Developments and Open Problems**

BI is an area rich in open problems, both from a conceptual point of view as well as from the various application areas in which BI is used. Currently, BI solutions have been proposed for addressing large-scale challenges in modern societies, in areas related to health, energy and the environment, urban planning, etc. One common theme in such applications is that they are too complex to be fully modeled in advance, and they produce an abundance of data which are automatically gathered in a multitude of independent systems. This is in part due to the commoditization of computer hardware, which has opened up the possibility of applying massive computing infrastructure to tackle such applications and workloads.

The NSERC BIN network was formed with the goal of developing knowledge as well as expertise within Canada in the area of BI. Broadly speaking, BIN is thematically organized into four main research areas: Strategy and Policy Management, Capitalizing on Document Assets, Adaptive Data Cleaning for BI, and Business-driven Data Integration.

The Strategy and Policy Management theme aims at providing higher-level modelling tools to BI, thus helping bridge the gap between the worlds of business and data. To accomplish this objective, BIN is developing novel concepts and tools for modeling social, organizational and intentional settings (e.g., virtual organizations, organizational structures and actors, strategic and tactical business objectives, government laws, policies and regulations, etc.) as well as linking such models to actual computer systems where the data resides.

The research under the Business-driven Data Integration theme aims at completing the link from the higher-level view of BI into the operational level of data management. Among other goals, this research aims at changing the current paradigm of warehousing all available data into a single repository before it can be processed, integrated, cleaned, understood, and only then used in BI models. Instead, the vision proposed by BIN is to derive and automate all the necessary steps to feed the data into a BI model from the higher-level descriptions of the business and their goals.

The work under Capitalizing on Document Assets aims primarily at enabling the use of information residing in documents to be used seamlessly with or without structured data (residing in databases) in support of decision making. More precisely, this work is aimed at automatically extracting, organizing, cleaning and integrating data expressed in textual form, and originating from both formal documents (e.g., regulations, legal and technical documents, patents, customer reviews, etc.) and informal documetns (e.g., customer comments and complaints, blogs, emails, news articles, etc.).

Also in the spirit of providing higher-level BI tools, the research under the Adaptive Data Cleaning area is building a general framework that includes specification languages for data quality and cleaning; it also includes the development of tools that, based on these languages, allow for the specifications of models of data quality that can be used to assess data, and also to specify and apply data cleaning solutions. Within such a model it will be possible to express, in terms of quality measures, desirable quality properties that can be checked and evaluated with the concrete data at hand.

### **Presentation Highlights**

The meeting had two sets of presentations. The project presentations gave an overview of the state of ongoing research, introducing recent results and setting the tone for the network-wide discussion:

- A1 One challenge for a network such as BIN is the need for relevant use cases in which real data and expertise is used to can guide the development and evaluation of this kind of research. Dr. Topaloglous presented his efforts and results towards bringing a real use case to BIN researchers, originating from running the Rouge Valley Health System.
- A2 Prof. Yu presented, in a sense, a coherent and concise tutorial on the vision for the Next generation BI

technologies using strategic business modelling, advanced adaptive software technology and enterprise architecture modelling to create BI-enabled Adaptive Enterprise Architecture. He also pointed out future research avenues, focusing on applying the solutions developed to date to one or more industries, building a business case and creating prototypes for concept demonstration.

- A3 Prof. Tompa described ongoing work on compiling high-level (enterprise-level) policies into actionable database constraints, to be defined over the actual production database systems. His approach consists in (1) mapping business policies into constraints on database states and state transitions, (2) capturing policies as constraint diagrams, and (3) produce efficient routines for checking such constraints automatically.
- A4 One issue within BI is that business processes must adapt to the content imposed by the specifics of the relevant data, the users, and the stakeholders. Prof. McIlraith discussed an AI approach to alleviate such problems based on (1) developing business process modelling formalisms that support specification of abstract business processes and (2) developing computational machinery to customize, verify, and optimize business processes and data with respect to stakeholder needs.
- A5 The a need for dynamic location-aware methods for constructing data cubes that allow scalable, faster access to data was the theme of Prof. Viktor's address. She outlined ongoing work that relies on finding the minimal set of attributes that correlate with a specific user and her locations of interest. Her goal is to have both the data cube creation and the subsequent data mining model construction location-aware. One challenge to accomplish this goal is to unambiguously identify data items for seemingly disparate sources, which is a problem researched within BIN as well.
- A6 Prof. Aboulnaga presented his architecture for "pay-as-you-go" data integration, which enables "situational applications" to access structured data from diverse data sources on the Web at low cost. Furthermore, he outlined an incipient research project geared towards providing scalable support for the complex analytics workloads in a cloud computing environment, with emphasis on performance optimization.
- A7 The next presentation described the work of Prof. Amyot and his team, on managing patient flows in health care organizations driven by BI principles. Their approach was to validate the expressive power of current tools by actually modelling the process of cardiovascular care and other patient flows with the tools being developed by the BIN team. One particular difficulty that was discussed was the need for more (real) data in order to effectively conduct this research.
- A8 An architecture for data integration driven by (high-level) conceptual models was described by Prof. Kiringa. This work represents substantial steps towards achieving a core goal of the BIN research program: bridging the gap between conceptual and database models. Their approach resulted in the mappings being compiled, which leads to substantially better performance, and also led to clean semantics for MDX.
- A9 Prof. Pottinger discussed system where users can coordinate data between two databases where changes in a base database *B* should be reflected in the contingent database *C*. Her system is based on the idea of data coordination, which she explained. Another project discussed concerned the design and study of a conceptual language and framework for top-down creation and population of warehouses.
- A10 The next presentation, by Prof. Miller, outlined how to use business context and business requirements to guide the construction of database mappings. Two key novel aspects of the approach consists in augmenting basic mapping rules with causality knowledge derived from the business schema, and dealing with incompleteness by using preference rules that define constraints over the set of preferred business schema instances.

- A11 The TARgeTEd Social Event Summarization (TARTESES) system was described next by Prof. Lakshmanan. The proposed system would be able to detect events/signals about a specific target within the realm of online social networks and report important events across all social media. Moreover, instead of simply filtering raw data of interest, the system should be able to report its results in a summarized form, and also provide a comparison of the summarise against crowd opinion from different communities.
- A12 Prof. Milios described ongoing work that combines interaction and visualization with state-of-the-art machine learning methods and natural language processing tools to enable users to explore and analyze the information enclosed in large document collections. Among the challenges discussed are choosing the appropriate set of text features to be used in the text analysis. The presentation also included results of ongoing work.
- A13 One research problem address by Prof. Ng and his team is that of how to perform next-level natural language summarization, abstraction (generate new text). Their focus is on informal conversational data (e.g., emails, blogs, reviews, meeting notes, etc.). The presentation covered recent results in using natural language processing tools to provide abstractive summaries of conversations, in which a new text (the summary) is synthesized from the summary. This technique has been shown superior to extractive summarization (in which fragments of the original text are used as the summary).
- A14 Machine reading, which aims at extracting valuable data, information, knowledge automatically from text, is the central theme of the work presented by Prof. Barbosa. He described recent results from this team on focused information extraction from blogs concerning the identification of direct and indirect relations among recognizable entities in the text corpus. Directions for future work include using relation extraction for question answering and narrative-based summarization of the information extracted.
- A15 In the work of Prof. Bertossi and his team, the vision for a general theory of context for data cleaning, in particular for applications in data management, is that (1) a logical theory T is the one that has to be "put in context"; (2) the context is another logical theory, C; and (3) the connection between T and C is established through connection (possibly shared) predicates and mappings. The presentation also discerned about different notions of context and how they are used in practice.
- A16 Prof. Özsu presented results and ongoing work of two BIN-related projects. The first, led by Prof. Ilyas uses uncertain data management techniques (possible worlds, consistent query answering) to address the data cleaning problem (entity de-duplication, and removing integrity constraint violations). The other project, led by the presenter, aims at addressing the issue of how to perform multi-query processing over uncertain data streams.

The second round of presentations were led by the industrial partners in BIN, with the goal of bringing perspectives and practical challenges of actual customers and providers of BI solutions deployed today. These discussion were organized by themes:

- I1 Social computing: as we move to empower the individuals we need to interact with them within their social context. Most decisions in business are made collectively, this ensures that all alternatives are explored, that experience is leveraged and that all parties are bought into the decision. Challenges in this area include: involving others in our decision processes by engaging them with insight around information, being able to draw insight from the Opinion being expressed internally and externally to the organization, and everaging the wisdom of the crowd to the improve quality of information.
- 12 **Cloud computing applied to BI**, with the goal of enabling Analytics as a Service. The need for such solutions stem from the fact that cloud deployment is increasingly relevant. The challenges in enabling this infrastructure for BI are: (1) providing cloud-optimized solutions supporting multi-tenancy,

resource sharing, scaling in/out and up/down, sharding, workload optimization, license/cost optimization, business and regulatory constraints; (2) understanding whether the cloud infrastructure itself introduces new analytical workflows or makes existing ones no longer intractable; and exploiting new data/access models enabled by this infrastructure.

- 13 Compliance: as BI providers empower users, they also have to consider the risks represented by distributed decision making. With hundreds of regulatory bodies placing constraints on business, often multiple overlapping any decisions, it is essential that we empower our users to be aware of their risks and to understand if, when and why they are out of compliance. Key observations on the issue are: (1) compliance remains the first priority from the IT management perspective, even as the bodies of regulations continue to expand. Reducing the cost of managing compliance is essential to IT success; (2) Business Users need to be notified when they are in or out of compliance, and how they can mitigate their risks; (3) organizations as a whole need to better understand and more accurately measure risks so they can make informed decisions.
- I4 Consumable Analytics, which is the view that BI should focus is on the business end user. Key observations in this regard from current experience are that new analytics demand new user experiences, and visualizations, and that novel interactive visualizations and discovery tools will lead to a new set of query-generation gestures. Moreover, the goal of this effort is to provide consumable for all (i.e., attention should be paid to accessibility, globalization, etc.) and everywhere (i.e., not just the office).
- I5 Geospatial and Temporal Analytics: as the number and diversity of data sources increase, we need finer tools to glean intelligence from such data. This includes ways to address: context, disambiguation, time and space.
- 16 Mobility: decisions are being made everyday in the organization, and providing users with information to empower them, that information must be present when those decisions are being made. Since the decision makers all have mobile technology, and rely on it as a portal to resources, we must leverage these devices to deliver rich, effective and timely information. Enabling mobility in BI solutions will require solving pressing issues w.r.t. geospatial and temporal analytics.
- I7 Big Data: 90% of the data in the world today has been created in the last two years. Everyday, we create 2.5 quintillion bytes of data. Such "Big Data" data sets are too large (and often too unstructured), so much so that they defy conventional analytic techniques and/or can not produce outcomes in tolerable time frames. Effective BI will not be achieved unless we solve this problem.
- 18 User-driven integration and mapping of data: given the complexity of the BI applications, eliminating the human from the loop will not be feasible for many years, if not decades. Instead, we should focus on making the BI process (particularly the data integration and mapping) more accessible to knowledge workers. Challenges towards this goal include: (1) making the user experience more intuitive; (2) supporting multiple heterogeneous data sources; (3) performance.
- 19 Unstructured data: a vast amount of information and corporate memory is hidden inside documents on file shares, email servers, web sites, etc. We must convert this to a usable form and make it consumable. Discover knowledge, not find documents. Challenges include: (1) solutions must work on Web-scale, with big data; (2) solutions must work in real-time, on live streams, enabling interactive exploration; (3) solutions must turn knowledge workers into consumers: make sense, make connections, reason, discover, visualize; (4) there must be notions of quality and reliability of the facts extracted: measure, feedback, improve.
- 110 **Real time and Streaming Business Analytics**. BI-relevant data not only comes in large quantities, they are also time-sensitive. Effective BI solutions must be capable of more than just event handling,

they also need complex aggregate and rule processing on the fly. Further, the relationship between between data volatility and query performance must be understood. Some implications for the modern database architectures include: data partitioning; incremental updates for aggregates; and concurrent writes & consistent reads.

### **Scientific Progress Made**

This meeting had two main goals: (1) congregating a large and representative fraction of the network for technical discussions, and (2) enabling the network to identify further collaboration opportunities. In both regards the meeting was an astounding success. The audience represented a substantial subset of the network, and ranged from graduate students to members of the board of directors.

**Towards a better understanding of "Core BI".** The meeting was the first network-wide opportunity for a deeper discussion of foundational aspects and state-of-the-art in core themes within the network research program. Such discussion was particularly useful in the context of the Strategy and Policy Management Theme, which is concerned with developing usable models and tools for business intelligence end users. Thus, in many ways the success of the network hinges on these models as well as on successfully integrating all other pieces of the research with them. Prof. Yu's presentation started this discussion and set the tone for the subsequent presentations and discussions, resulting in a very productive debate. Dr. Topaloglou's remarks, derived from real-life experiences in deploying a BI solution, were also instrumental in shaping the debate and focusing the research team.

On a similar tone, the meeting allowed the network to gather a broader perspective on the state of state of business intelligence research from other research groups, in the keynote presentation by Dr. Dayal from HP Labs. In particular, the keynote offered a glimpse of new tools and techniques, as well as several success stories of applying these tools to real-life problems in various industries.

**BI curriculum development.** This deeper understanding of BI enabled further a discussion within BIN into developing reference material on BI, to be used as the basis of introductory texts at the undergraduate level for the field. The need for such a text has been originally articulated as a longstanding and major need from the industrial partners.

**Strengthening collaboration.** During the meeting several research opportunities were identified, covering all research themes and groups. Novel directions for collaborative research identified during the meeting include: (1) sharing data/expertise from the health care use case (P1, P3, P10, I3); (2) combining efforts in data integration (P6, P9, I8); integrating information extraction techniques (P12, P13, P14, I4, I9); exploring social computing (P11, I1); linking high-level business concepts with operational data management tools (P3, P7, P8, I8); addressing system scalability issues (P6, I2, I7, I10); incorporating mobile and spatio-temporal data into BI solutions (P5, I1, I5, I6).

#### Acknowledgements

The entire BIN team, and particularly the meeting organizers, would like to acknowledge all the support provided by the Banff International Research Station and its staff, who provided BIN with an ideal setting in which to have a focused and productive meeting. Thank you.

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### Chapter 42

### **Alberta Number Theory Days (11w2169)**

### Jun 17 - Jun 19, 2011

**Organizer(s):** Amir Akbary (University of Lethbridge) Brandon Fodden (University of Lethbridge)

### **Overview**

The fourth installment of the Alberta Number Theory Days was held in BIRS on the weekend of June 17 to 19. 29 people participated in this event, including 12 faculty members, 13 graduate students, and 4 postdoctoral fellows. A total of nine 45-minutes lectures were given. Three of the lectures were delivered by postdoctoral fellows from Alberta and British Columbia and the remaining six lectures were given by professors from Alberta.

The nine lectures covered a wide variety of areas in number theory. The break down of the lectures in terms of topics was as follows:

- 1. Analytic Number Theory, three lectures
- 2. Algebraic Number Theory, two lectures
- 3. Diophantine Approximation, one lecture
- 4. Computational Number Theory, two lectures
- 5. Representation Theory of *p*-adic Groups, one lecture

### **Summary of Lectures**

**Nathan Ng** started his talk by asking the question "what is an *L*-function?". He then described a possible answer to this important question given by Selberg [14] in 1989 at Amalfi's conference. The so called "Selberg class" is a family of Dirichlet series that satisfy certain analytic properties (analytic continuation, functional equation, Euler product, and Ramanujan bounds) similar to the classical Riemann zeta function. After describing the concept of a primitive element of the Selberg class, Ng stated the conjecture that all non-real zeros of any primitive element in the Selberg class are simple. After reviewing the known results of Levinson [7] and P. Bauer [1] on this conjecture for the degree one *L*-functions, Ng discussed his recent joint work with Milinovich where they investigated simple zeros of degree two *L*-functions (modular *L*-functions).

Habiba Kadiri discussed an explicit estimation on the error term in the celebrated Prime Number Theorem. After reviewing the classical method due to Rosser and Schoenfeld [10], [11] on this problem, she explained her recent work with Faber where they use smooth functions and an explicit estimate for the density of zeros of the Riemann zeta function to generalize and improve upon the previous results.

Tim Trudgian gave a lively talk on Skewes' Number. The Prime Number Theorem asserts that  $\pi(x)$ , the number of primes not exceeding x, is asymptotic to li(x), the logarithmic integral. It is known that, for all  $2 \le x \le 10^{14}$ , the inequality  $\pi(x) < li(x)$  is true. That there are infinitely many x for which this inequality does not hold was proved by Littlewood in 1914. In 1954 Skewes [16] proved that the inequality  $\pi(x) < li(x)$  will be violated for a number less than  $10^{10^{10^{10^{3}}}}$ . In his talk Trudgian gave an account of the work done on reducing this bound. The latest result on this problem is due to Demichel and Saouter [12] where they reduced the Skewes bound to  $1.397116701 \times 10^{316}$ . Finally, after describing Lehman's work on this problem, Trudgian commented on the possibility of reducing Lehman's bound [6] by employing the recent result [17] of himself on a sharp upper bound for the function S(T), the argument of the Riemann zeta-function along the critical line.

Al Weiss's talk entitled "What do Artin L-functions know about Galois module structure?" gave an account of Weiss's impressive work (joint with Gruenberg and Ritter) ([5], [8], [9]) on the so called "lifted root number conjecture". This conjecture, which is stronger than Chinburg's root number conjecture, is related to the Galois module structure of S-units of a number field. It is also related to Stark's conjecture which can be considered as a generalization of the analytic class number formula to Artin L-functions.

By describing Stark's conjecture and the lifted root number conjecture for a special class of number fields, **Paul Buckingham**'s talk nicely complemented Al Weiss's lecture. After giving an overview of these conjectures and describing them in a baby example of real quadratic fields, Buckingham provided a description of his work on these conjectures for multiquadratic extensions of an arbitrary number field.

A polynomial-exponential Diophantine equation is an equation in the form  $f(x) = y^n$  where f(x) is a polynomial with integer coefficients and y is a fixed positive integer. **Mark Bauer's** talk was centered around finding the solutions of such equations (i.e. pairs (x, n) where x and n are both integers). He explained that while many Diophantine equations can be attacked using variants of Wiles' approach in proving Fermat's Last Theorem [18], polynomial-exponential Diophantine equations do not usually yield to such techniques. In this lecture Bauer reported on his joint work with Mike Bennett where they use restricted (and unrestricted) irrationality measures to find all possible solutions of equations of the type  $x^3 + D = y^n$ , where n is in the form 3k + 1.

**Renate Scheidler**'s lecture was on "Infrastructure of Function Fields". The infrastructure concept was proposed by Shanks in 1972 in the case of indefinite binary quadratic forms and later was further explored by Williams for the ideals of real quadratic fields and orders (see [15] and [2]). The infrastructure is a mathematical system that "just barely" fails associativity; however it is suitable for the baby step giant step framework found in many algorithms of computational number theory. In her lecture, Scheidler described her work [13] and the recent work of Adrian Tang on the extension of this important framework to function fields.

An important application of infrastructure is in the computing of the class number and regulators of quadratic fields. This was the subject of talk by **Michael Jacobson**, where he discussed recent efforts to extend existing, unconditionally correct tables of both imaginary and real quadratic fields. Such tables are used to provide valuable numerical evidence in support of a number of unproven heuristics and conjectures, including those due to Cohen and Lenstra [3], [4]. Jacobson also described an unconditional verification algorithm based on ideas of Booker (that verifies the truth of the table generated under the assumption of the Riemann hypothesis) which surprisingly uses the trace formula of Maass forms.

**Masoud Kamgarpour** lectured on his joint work with Clifton Cunningham on Geometrization of characters of the multiplicative group of local fields. He described in several concrete example (such as the case of multiplicative group and the truncated Witt ring over the finite field of p elements) how one can consider

sheaves on these algebraic varieties as proper generalizations of characters of local fields of characteristic zero.

### **Concluding Remarks**

A number of participants commented that Alberta Number Theory Days 2011 was a success. It helped to strengthen the bonds (both academic and personal) and forge new links between number theorists in Alberta. The meeting allowed number theorists working in a wide variety of areas to share knowledge and discuss recent progress in their fields.

The organizers would like to thank BIRS and the Banff Centre for their hospitality and helpful staff. We would also like to acknowledge PIMS for their generous support. Finally, we would like to thank the speakers for their excellent talks.

### **List of Participants**

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### Chapter 43

# **Automated Deduction and its Application to Mathematics (11w2170)**

### Jun 19 - Jun 26, 2011

**Organizer(s):** R. Padmanabhan (The University of Manitoba) Robert Veroff (University of New Mexico)

### **Overview**

The goal of researchers in automated deduction is to develop methods and tools to assist mathematicians, scientists, and engineers with some of the deductive aspects of their work. In contrast to other symbolic computation systems, the core methods in automated deduction focus on searching for proofs and counterexamples. Automated deduction can be applied to wide-ranging problems in nearly any formal language. However, for problems in abstract mathematics and logic, it has been most successful to date when applied to problems stated in first-order and equational logic.

This workshop was the continuation of a series of yearly workshops that began in the summer of 2001 (http://www.cs.unm.edu/~veroff/ADAM/). The workshops have provided an opportunity to bring together researchers and students from both the mathematics and automated deduction communities to consider the application of automated deduction to problems in mathematics and logic. The objectives of the workshops include: collaborations on specific math and logic problems; expanding the community of mathematicians interested in applying automated deduction methods to their own research problems; and the continued development of automated deduction tools and strategies.

This year's workshop was dedicated to the memory of Bill McCune, whose untimely passing in May 2011 shocked and saddened his many friends and colleagues. Bill is perhaps best known for his expertise in the design and implementation of automated reasoning programs. His programs, including Otter [8], Prover9 and Mace4 [9], have been used to solve numerous open questions in mathematics and logic and continue to be used by researchers from various disciplines. Indeed, many of the presentations and discussions in this workshop were directly or indirectly influenced by Bill's work.

### **Presentation Highlights**

The unifying theme of the workshop was the application of automated deduction methods to research problems in mathematics. One consequence is that the presentations—especially those that focused on the math applications—were disparate in nature. The presentations can roughly be put into two categories, those focusing on automated deduction methods and tools and those focusing on the math applications themselves.

#### **Automated Deduction Methods and Tools**

*The TPTP Typed First-order Form with Arithmetic* (Sutcliffe). The TPTP World [15] is a well established infrastructure that supports research, development, and deployment of Automated Theorem Proving (ATP) systems. The TPTP World is based on the Thousands of Problems for Theorem Provers (TPTP) problem library [14], and includes the TPTP language, the SZS ontologies, the Thousands of Solutions from Theorem Provers (TSTP) solution library, various tools associated with the libraries, and the CADE ATP System Competition (CASC). This infrastructure has been central to the progress that has been made in the development of high performance first-order ATP systems—most state of the art systems natively read the TPTP language, many produce proofs or models in the TSTP format, much testing and development is done using the TPTP problem library, and CASC is an annual focal point where developers meet to discuss new ideas and advances in ATP techniques.

Originally the TPTP supported only first-order problems in clause normal form (CNF) [13]. Over the years support for full first-order formulae (FOF) [14] and typed higher-order formulae (THF) [16] has been added. In this talk, we introduce simply typed first-order formulae (TFF) into the TPTP World. TFF in turn is used as the basis for supporting arithmetic. Problems that use these new features have been added to the TPTP problem library. This will provide the impetus for the corresponding development of ATP systems. In particular, the integration of arithmetic capabilities into ATP systems will answer a long-standing demand from ATP users.

The key steps of these developments have been:

- The design of the TPTP TFF language.
- The choice and design of arithmetic features to be written in TFF.
- Collection of problems in TFF, especially problems with arithmetic.
- Building and adapting ATP systems to solve TFF problems.
- Extending the TPTP software infrastructure.

Our presentation described these developments, with the aim of publicizing the developments to working mathematicians, who might then be able to use these new capabilities in their mathematical endeavours.

A Syntactic Approach to Automated Deduction (Ernst). The best strategies for solving open problems in mathematics using first-order theorem-provers rely upon the practitioner having domain specific knowledge of the problem. For example, if it is possible to identify lemmas that are likely to appear in a proof, or if the theory is part of a well-understood hierarchy of related theories, then those facts can be leveraged to guide the proof search. However, it is often the case—especially for difficult open problems—that such information is unknown or unavailable. For this reason, it is necessary to consider search strategies that rely only upon the syntax of the problem representation, because that is the only information that practitioners are guaranteed to have. This talk outlined one approach for using the syntax of the problem to guide the proof search and presented two cases in which significant increases in efficiency were obtained without deploying any domain-specific knowledge of the problem.

Working Our Way Up a Theory Hierarchy (Veroff). We discussed two automated deduction methods for using theory hierarchies to help search for proofs of a theorem t in a target theory T. Using semantic guidance,

we consider models that falsify t in a simplified theory—that is, with one or more axioms deleted from T. Using the method of *proof sketches* [17], we consider proofs of t in an extended theory—that is, with extra assumptions added to T. In both cases, we use the additional information—models and proofs—to guide the search for a proof of t in the original target theory T.

We also summarized results for a successful application of these methods to a set of problems in loop theory, including the solution to some open questions. Some of the found proofs are several thousand steps long. See [5] for general background on the problem.

#### **Math Applications**

*Normal Forms in Graded Lie Algebras* (Churchill). The success of Prover9 in establishing particular cases of Jacobson's  $x^n = x \Rightarrow$  commutativity theorem in ring theory led us to suspect that such techniques could be applied to normal form problems which can be formulated in a graded Lie algebra context. To communicate these ideas to the other participants we delivered a general background lecture in that area, focusing for simplicity on the case of upper triangular matrices. Following that talk, we had one-on-one discussions with several participants on more complicated problems which also fit that perspective. See [1, 2, 4] for general background on the problem.

*Group Embeddings of Configurations with Prover9* (Ens and Padmanabhan). A configuration is a finite set of elements (called "points" just to have a guiding analogy with the plane geometry) and a finite set of blocks (again, we call them "lines") such that each point is incident with the same number of lines and each line is incident with same number of points. Motivated by the geometric definition of a group law on non-singular cubic curves, we define the concept of group embeddability of (n, k) configurations and classify the set of all (11, 3) configurations that can be embedded into abelian groups in such a way that whenever {P,Q,R} is a line in the configuration points of a complex cubic turns out to be isomorphic to the abelian group Z[3]  $\times$  Z[3]. In this paper we employ Prover9—a first-order theorem prover developed by William McCune—to determine the embeddability of (11,3) configurations. Naturally, there are two kinds of theorems we need to prove: for a given configuration, we have either a concrete group representation or else a proof that no such representation exists. Prover9 is successfully employed to get the proofs of both kinds. Finally, we apply the positive results to obtain a concrete geometric realizability (over a projective plane) of these configurations.

*Commutativity Theorems in CL-Semirings* (Padmanabhan and Zhang). There are many conditions known which force a ring to be commutative. Such theorems are known as "commutativity theorems". Here we generalize some of the commutativity theorems to cancellative semirings, i.e., semirings in which the addition is cancellative. We use Prover9 to give first-order proofs without actually going through the quotient construction.

*Bol-Moufang Groupoids of "Group-like" Type* (Phillips). An identity involving one binary operation is of *Bol-Moufang type* if it contains three variables, two which of which occur once, one of which occurs twice, on both sides of the equal sign, and in the same order. These include the well-known Moufang and Bol laws, whence the name. They have been widely investigated. In this talk, we investigate conditions under which Bol-Moufang groupoids axiomatized as algebras of type < 2, 1, 0 > (i.e., with two-sided identity and inverses, in the manner of groups), are, in fact, loops. We also look at "localized" versions of the Moufang laws in groupoids of this type. See [5, 10, 12].

*Model Builders, Automated Deduction and Automorphic Loops* (Vojtechovsky). A set Q with a binary operation  $\cdot$  and an element  $1 \in Q$  is a *loop* if  $1 \cdot x = x \cdot 1 = x$  for every  $x \in Q$ , and if for every  $x, y \in Q$  there are unique  $u, v \in Q$  such that  $x \cdot u = y, v \cdot x = y$ . A loop is *automorphic* if all its inner mappings are automorphisms.

The structural theory of automorphic loops emerged in the last three years, in large part thanks to automated provers and model builders. It presents a sweeping generalization of some classical results of group theory. In this talk we (i) prove the Odd Order Theorem and Lagrange Theorem for commutative automorphic loops, pointing to a crucial lemma obtained with Prover9, and (ii) construct a class of automorphic loops of order  $p^3$  with trivial center, all originating from a single example of order 27 obtained with Mace4.

See [3, 6, 7] for basic information on loops and automorphic loops.

#### **Outcome of the Workshop**

Our yearly workshops are workshops in the truest sense. Although presentations help establish some context, the most significant value is in the many group and one-on-one discussions that are motivated by the presentations. In this regard, the workshop was very successful. The mathematicians collaborated on their specific research problems; the computer scientists worked with the mathematicians on specific applications; and there was substantial discussion defining and designing new features for automated deduction tools. For one example, there was some discussion about adding support for the inference rule gL for cubic curves [11] to Prover9. There was a working prototype for the added functionality shortly after the end of the workshop.

### **List of Participants**

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Yang, Qiduan (University of British Columbia)
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### Chapter 44

# CanQueue 2011: 13th Annual Conference for Canadian Queueing Theorists and Practitioners (11w2154)

### Aug 26 - Aug 28, 2011

**Organizer(s):** Winfried Grassmann (University of Saskatchewan) Javad Tavakoli (University of British Columbia, Okanagan)

### **Overview of the Field**

Queueing theory is concerned with developing and investigating mathematical models of systems where customers wait for service. The terms customers and servers are generic. Customers could, for example, be humans waiting in a physical line or waiting on hold on the telephone, jobs waiting to be processed in a factory, or tasks waiting for processing in a computer or communication system. Examples of service include a medical procedure, a phone call, or a commercial transaction. Queueing theory started with the work of Danish mathematician A. K. Erlang in 1905, which was motivated by the problem of designing telephone exchanges. The field has grown to include the application of a variety of mathematical methods to the study of waiting lines in many different contexts. The mathematical methods include Markov processes, linear algebra, transform theory, and asymptotic methods, to name a few. The areas of application include computer and communication systems, manufacturing systems, and health care systems. Introductory treatments of queueing theory can be found, for example, in [1] and [2].

### **Recent Developments and Open Problems**

Many recent developments in queueing theory have been driven in large part by a greater interest in applications that involve human customers, for example in the rapidly growing call centre sector (see [3]). Humans behave in less predictable ways than, say, jobs in a factory or tasks in a computer system. For example, they may renege (abandon the queue), and retry later. The needs of human customers are likely to be heterogeneous (motivating the use of skills-based routing to connect different customers to different servers) and to vary with time (sometimes requiring transient rather than steady-state solutions). All of these complications lead to interesting mathematical challenges. The interest in modeling reneging has led to a substantial literature by now, for example see [5]. Asymptotic analysis, which in the past typically considered situations where the arrival rate approached the capacity of a system with fixed number of servers, has been rejuvenated by a focus on situations where the arrival rate and the number of servers approach infinity simultaneously (see [4] for the first such analysis). Such many-server asymptotic analysis has resulted in a collection of simple-to-use formulas for recommended staffing, consisting of a linear term (minimum staffing for stability) and a square root term (safety staffing, to protect against random fluctuations). In addition to the focus on the call centre sector, applications in health care are becoming increasingly important, for example see [6]. Successful health care applications are likely to require further extensions to the queueing theory toolkit to accommodate customers that are given different priorities and have different needs and servers that may group together to work on one service and then move on to other tasks. Typical queue performance measures, such as average wait or average cost, will also need to be re-examined, and a greater focus on measuring equity as well as quantification of the medical consequences of waiting may be necessary.

### **Objectives**

The objective of the CanQueue workshops, held annually since 1999, is to promote research and application of queueing theory. The workshops emphasize discussion of research projects in their early stages, to facilitate feedback from colleagues and collaboration while the direction of the project can still be influenced. It provides a venue for graduate students to present their work (in process or completed) in a supportive environment and it introduces interesting application areas. In this way, it strengthens the community of researchers in queueing theory in Canada.

This year, the meeting was held at the BIRS center in Banff, and as usual, it was a great success. The sessions were well attended, and there was often a lively discussion. We also appreciate the help we got from the center for organizing this meeting. Their effort greatly contributed to the success of CanQueue 2011.

### **Presentation Highlights**

The meeting started on Friday with three interesting talks on queueing in health care. Sherry Weaver, from the University of Calgary discussed how a model for a finite queue that can be used to accommodate urgent patients for knee replacement. Of course, when giving urgent patients priority, the wait of non-urgent patients may become unduly long. Problems of an unduly long wait for non-urgent patients is quite general in health care. To counteract this problem, David Stanford, University of Western Ontario, suggested increasing the priority as the waiting-time increases The results of his study were provided in a number of graphs. A similar problem arises in transplant queues where the transplants can become more urgent as time passes. This problem was discussed in detail by Steve Drekic, University of Waterloo in a paper co-authored by David Stanford and Dough Woolford, Wilfrid Laurier University.

A number of talks dealt with the application of queueing theory to radio networks. In particular, the following problem was addressed. The wireless spectrum has traditionally been assigned statically to licensed users. However, it is known that less than 5% of the assigned spectrum is typically used, and as the availability of the spectrum is getting more scarce and demand for radio access is increasing, it has become clear that unlicensed users have to gain access to the unutilized portions of the assigned spectrum. This situation gave rise to a number of research projects that were investigated by Attahiru Alfa, University of Manitoba, and his students, including Samitha Umwiththige, Sofia Alvarenga, Chamara Devanarayana, Charith Gunasekara, Samitha Wijedasa, and Nkouatchah Ngatched. They analysed cognitive radio, a technology to assist with dynamic spectrum sharing between licensed users, also known as primary users, and unlicensed users, also

known as secondary use. Coognitive radio can be adopted based on underlay or overlay approaches. Based on the overlay approach, secondary users seek idle channels for use when they are free of licensed users. However, in order to do this, secondary users have to detect the availability of idle channels. The durations of busy and idle periods are correlated random variables followong a general distribution. Some of the projects presented developped stochastic models for describing the states a radio channel. Based on these models, it is possible for an secondary user to develop a sensing strategy. A sensing strategy involves determining how frequently to sense a channel. If the sensing is too frequent an secondary user spends too much resource (e.g. battery power); on the other hand infrequent sensing leads to possible missed opportunities of channel idle times.

An interesting application of queueing theory is to predict the time between yellow alerts for ambulances, that is, the time when the number of available ambulances falls below a certain level k. Mathematically, this corresponds to a k-partial busy period and can be solved as such. This was explained in a talk by Armann Ingolfsson, University of Alberta, and his two students Amir Rastpour and Bora Kolfal. Another contribution of Armann Ingolfsson, with co-authors Mohammend Delassay, Bora Kolfal, and Z. George Zhang (Professor with Simon Fraser University) involved a two-dimensional Markov chain to solve queueing systems where servers adjust their service rate in response to system load.

There are close relationships between queueing and inventory as shown by Zhe George Zhang, Simon Fraser University. His queueing model dealt with switching from MTO (Work-To-Order) to MTS (Make-To-Stock). Another area having a close relation to queueing is the ruin problem in insurance as highlighted in a talk by David Landiault, University of Waterloo. A third area related to queueing theory is scheduling, as shown by two talks, both given by Tony Tran, Dara Terekhov (University of Toronto) and Douglas Down (McMaster University) and Christopher Beck.

The workshop included a number of more theoretical talks, reflecting the mix of mathematical developments and practical applications that has been a hall mark of the CanQueue workshops. A talk by Attahiru Alfa and V. Ramaswami showed that the number in the system in a Geo/G/ $\infty$  queue does not lead to simple expressions, quite in contrast to the M/G/ $\infty$  queue, where the number in the system follows a Poisson distribution. Percy Brill (University of Windsor) and Mei Ling Huang (Brock University) applied level crossing analysis to a bulk queue. A problem of great practical interest is how the tails of queue length distributions behave. In most, but not all cases, the distributions in question show a exponential decay. Two talks dealt with the tail behaviour of distributions observed in queueing theory. One was given by Hui Li (Mount Saint Vincent University), Javad Tavakoli (University of British Columbia Okanagan) and Yiqiang Zhao (Carleton University), and it dealt with singular cases, that is, cases where the decay is not exponential. The other one, given by Zafar Zafari, a student of Javad Tavakoli, University of British Columbia Okanagan, analysed as to when the number in a shorter queue system is singular. Another student of Javad Tavakoli analysed when to interrupt and restart a finite queueing system with server breakdowns.

For practical applications, time-varying arrival rates to queues are very important. Such arrivals where explored by numerical methods by Barbara Margolius, Cleveland State University. Numerical experimentation was also discussed in a talk by Winfried Grassmann, University of Saskatchewan (coauthored by Javad Tavakoli). who showed that the speed of modern computers, even laptops, allows for experimentations impractical in the past. However, not all problems benefits equally form higher speeds. In particular, in queueing networks, non-simulation methods increase exponentially with the number of queues in the network, and even if the speed of computers increases 100 fold, only networks with a limited number of queues can reasonably be solved numerically.

### **Scientific Progress Made**

As at past CanQueue meetings, the unique feature that facilitates progress on research is that these workshops attract both queuing theorists, who focus on developing new methodology, and researchers who apply queueing theory in various settings. Thus, it provides opportunities for theorists to learn about new application areas and the types of models that are needed for these areas and opportunities for researchers with a more applied bent to get suggestions from queueing theory specialists on potentially useful methodologies or approaches. As well, the 2011 workshop brought together theorists with different foci, for example those that focus on asymptotic analysis versus those that focus on matrix analytic methods, and the interchanges between these groups brought valuable insights on what each of these fields can add to the other.

CanQueue 2011 ended with a business meeting, and it was decided to create a special interest group within CORS. The name for this groups is still to be determined. It was also decided to hold the next CanQueue in London, Ontario. This ended the very successful meeting at BIRS in Banff.

### **A Note of Appreciation**

The organizers would like to thank BIRS staff for their very competent assistance in organizing this workshop. Many participants commented favourably on the superb BIRS facility. The location and the amenities made it considerably easier for us to attract the group of distinguished researchers that attended the workshop. We thank again for the excellent help of the staff of BIRS which greatly contributed to the success of CanQueue 2011.

### **List of Participants**

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### Chapter 45

### **Modeling and Simulation** (11w2017)

### Sep 02 - Sep 04, 2011

**Organizer(s):** Zhangxin John Chen (University of Calgary) Dong Liang (York University) Yanping Lin (University of Alberta)

### **Overview of the Field of Modeling and Simulation**

Computational Science has been called a third branch of science, along with theory and experiment. In truth, it is part of theory and part of experiment, but it is different from either. Many theoretical problems can only be solved using a high performance computer. Modeling and simulation, the major component of computational science, is much more than simply elaborating pure theory. In the last two decades there have been rapid developments of computer power and sophisticated computational techniques. These advances have permitted the application of high performance computing to modeling and simulation with unprecedented accuracy and scope. These sophisticated processes are now being applied to a wide range of important engineering and science problems that require a thorough understanding of the underlining principles of physics, chemistry, mathematical modeling, numerical solution techniques, and computing infrastructure. The effect is to create a more comprehensive understanding of emerging issues. These developments have profound implications in mathematics, science, engineering, and industry. Modeling and simulation is a critical tool for analyzing many different types of important phenomena such as flow and transport, weather prediction, wave propagation, novel material design, computational chemistry, and genome sequencing and analysis.

### **Recent Developments and Open Problems of Modeling and Simulation**

Our living environment, economic development, natural resource management, and national security are all influenced by our understanding of complex physical and chemical processes occurring in and around the earth. Groundwater contamination, oil and gas reservoir production, discovering new oil reserves, ocean hydrodynamics, CO2 storage and sequestration, and air quality control are all vital to our economic and social well being. Modeling and simulation research is driven by the rapid changes worldwide in each of these capacities.

Energy and environmental modeling and simulation require the observation of natural scientists, the tech-

nical expertise of engineers, the modeling and numerical skills of mathematicians, and the modern techniques of computer scientists. The engineering and science problems in these areas tend to culminate in coupled systems of nonlinear, time-dependent partial differential equations (PDEs). Numerical solutions of these PDEs are very challenging due to the multiple temporal and spatial scales presented, the nonlinear effects, and the large scale and unusually long duration simulations required [1, 2, 3].

### **Workshop Presentation Highlights**

The workshop themes include: (A) Mathematics of Multiphase Fluid Flow and Transport; (B) High-Quality Discretization of Flow and Transport; (C) Computational Modeling of Multiscale Phenomena; (D) Parallel Computing; (E) Nonlinear Effects on Propagation Properties of Numerical Models.

20 presentations in this workshop have dealt with these topics. Speakers have been carefully selected to ensure that a range of modeling and simulation techniques can be explored. This diversity is necessary in order to address various phenomena arising from emerging issues in the energy and environment sectors. Many of our speakers are world class, such as Todd Arbogast, Jim Douglas, Jr., Ismael Herrera, and Kirk Jordan. Four female participants and five young graduate students attended the workshop. A feature of this workshop is the opportunity provided for interactions between the participants. Workshop organizers have facilitated round-table sessions in which questions and answers have been shared, and lively discussions have been encouraged. Invited participants are from diverse interdisciplinary background and top in their field. Such a combination of ideas and perspectives has been beneficial to all attendees. The workshop presentations, discussion in the round-table sessions, and possible future collaborations amongst participants have created the opportunity for significant progress in the field of energy and environment modeling and simulation.

### Scientific Progress Made in Modeling and Simulation

The objective of this workshop is to bring together the worlds top active researchers (and their more junior counterparts) who study energy and environmental modeling and simulation to discuss past, recent, and prospective advances in this area. The speakers have summarized important advances from the past two decades and have discussed the current understandings, the state-of-the-art techniques, and the current major challenges. Each session of this workshop has provided a vehicle for participants to learn novel techniques and new advances in this area of work. The content has been academic in nature while addressing the many significant applications for industry.

The ultimate goal of the workshop is to expose workshop participants (in particular, junior researchers) to the latest developments in the field of modeling and simulation, while emphasizing the impact of this field on science, engineering, and industry.

The study of the diverse topics presented in the workshop through laboratory experiments, mathematical theory, and computational techniques requires interdisciplinary collaboration between engineers, mathematicians, computational scientists, and researchers working in industry, government laboratories, and academy. The collaborative work of researchers in this workshop will create meaningful progress in predicting, understanding, and optimizing many complex phenomena. The rational for this two-day BIRS workshop is to hold lectures that pull together the major ideas and recent research results, chart future directions, and address newly emerging issues for energy and environment modeling and simulation. It is anticipated that the participants have left the workshop knowing the future research directions and the needed potential applications.

### **Outcome of the Workshop**

The Banff International Research Station is a beautiful location for learning and building relationships. Its common areas have supported our goals to have researchers engaged in discussion throughout the workshop event. We have brought researchers from around the world to share their perspectives, test ideas, and create new connections both intellectually and socially while exploring the latest developments in modeling and simulation. This workshop has promoted, enhanced, and stimulated cross-continental research interactions and collaborations in mathematical sciences and will shape changes in the research work completed with modeling and simulation.

### **List of Participants**

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### Calculus 11x11x11 (11w2178)

#### Nov 11 - Nov 13, 2011

**Organizer(s):** Manny Estabrooks (Red Deer College) Pamini Thangarajah (Mount Royal University)

#### **Overview of the workshop**

During the May 2011 North-South Dialogue Meeting and the Alberta College Conference ongoing issues concerning introductory calculus were discussed. It was apparent that there were many common issues facing post secondary institutions in Alberta, and an initiative to organize a meeting at the Banff International Research Station (BIRS) was undertaken. Some of the challenges arising:

- Concern about standards varying from instructor to instructor and institution to institution both with regards to curriculum and assessment.
- Perceived pressure on mathematics departments and individual mathematics faculty both by administration and other departments to meet some success rate in the introductory calculus classes.
- Questioning of the value of calculus and its aims by other departments and administration.
- Stress and anxiety felt by students who are taking or are planning to take Introductory Calculus.

There is need for leadership in the province in meeting these challenges in the age of technology and the prevalence of the internet. Related to these issues mentioned above is the notion of where technology fits, what should be the role of the calculator in a calculus course, what role does/can/should the internet play in addressing some of the issues outlined above. The plan was to address many of these outstanding issues in a coordinated way and consequently increase the student satisfaction and success rates at the various institutions in their introductory calculus courses.

The outcome of all this was the 2-day workshop "Calculus  $11 \times 11 \times 11$ ," held November 11-13, 2011, at the BIRS. All six Alberta universities were present and many of the Alberta post secondary colleges, plus one college from BC. The primary focus was the teaching of calculus in the high schools, colleges, and universities in Alberta. It also included representatives from Alberta Education, and two students who presented valuable insights from their point of view.

#### **Objectives**

The objectives of this workshop were to identify all the common challenges faced by Alberta post secondary institutions with regards to their introductory calculus courses and look for common solutions. Ideally participants would leave with a summary document to be disseminated among all the participating post secondary institutions. Consequently, some of the principal items for discussion were:

- Decide if a common core curriculum is needed and if so what is it going to be.
- Decide whether it is appropriate to have common assessment criteria and if so what the criteria should be.
- Decide on the role of technology in calculus.

Introductory Calculus is an important course both to students and post secondary institutions, and is taken by many thousands of students in Alberta every semester. Any improvements that can be made should be made. This has been studied throughout the years ( for example see [1], [2]). British Columbia has had a core calculus curriculum document [3] for several years now; it is both timely and relevant that we consider this approach as well.

#### **Presentation Highlights**

The workshop was started Friday Nov. 11 at 6:30 pm with a splendid presentation from representatives from University of Alberta. On Saturday morning presentations from Alberta Education about the new high school curriculum were given. Saturday afternoon reports from all the other institutions present regarding calculus: #Sections, success rates, tests & exams, assignments, use of calculators, on-line usage, marking schemes, common tests/exams, diagnostic tests, pre-calculus review efforts etc. Also, Cathleen Sullivan from Pearson Canada discussed the correlation between instructors' attitudes and students' performance (MAA survey 2010, David at UBC, 212 post-secondary institutes in US), and the use of technology for assignments.

#### **Progress Made**

Sunday was spent addressing several issues including: i) a Calculus stream for commerce & social sciences, ii) assessment & diagnostic instruments & how we might share these, iii) various other issues identified during the previous session. We outlined a plan for the development of a document on our 'findings' (see Section 5 below).

#### **Outcome of the Meeting**

A document about the meeting and the recommendations it arrived at is being produced, and should hopefully appear by February 2012. We are hoping to organize a future workshop to update and finalize this document.

#### **List of Participants**

Aiffa, Mohammed (University of Calgary) Chanasyk, Donna (Edmonton Highschools(Paul Kane High School)) Chisholm, Sarah (University of Calgary) Connolly, Dennis (University of Lethbridge) Davis, Tyler (Univerity of Calgary) de Vries, Gerda (University of Alberta) Estabrooks, Manny (Red Deer College) Freed, Bill (Concordia University College) Gale, Susan (Memorial Composite High School) Hackborn, Bill (University of Alberta, Augustana campus) Henzel, Christine (Alberta Education) Hlede, Tony (Alberta Education) Hohn, Tiina (Grant MacEwan University) Kooistra, Remkes (The Kings University College) Martinig, April (University of Calgary) McNeilly, David (University of Alberta) Nosal, Eva (PIMS, University of Calgary) Peschke, Julie (University of Athabasca) Roettger, Eric (Mount Royal University) Sullivan, Cathleen (Pearsons) Thangarajah, Pamini (Mount Royal University) Tomoda, Satoshi (Okanagan College, BC) Torres, Maria (University of Athabasca) Zvengrowski, Peter (University of Calgary)

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Calculus 11x11x11

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# Focused Research Group Reports

Focused Research Group Reports

# **Eventually Nonnegative Matrices and their Sign Patterns (11frg149)**

#### May 15 - May 22, 2011

**Organizer(s):** Minerva Catral (Xavier University) Craig Erickson (Iowa State University) Leslie Hogben (Iowa State University) Dale Olesky (University of Victoria) Pauline van den Driessche (University of Victoria)

#### **Overview of the Field**

A matrix  $A \in \mathbb{R}^{n \times n}$  is eventually nonnegative (respectively, eventually positive) if there exists a positive integer  $k_0$  such that for all  $k \ge k_0$ ,  $A^k \ge 0$  (respectively,  $A^k \ge 0$ ). Here inequalities are entrywise and all matrices are real and square. An eigenvalue of A is *dominant* if its magnitude is equal to the spectral radius of A. A matrix A has the strong Perron-Frobenius property if A has a unique dominant eigenvalue that is positive, simple, and has a positive eigenvector. It is well known (see, e.g., [10]) that the set of matrices for which both A and  $A^T$  have the strong Perron-Frobenius property coincides with the set of eventually positive matrices. Eventually nonnegative matrices and eventually positive matrices have applications to positive control theory (see, e.g., [13]).

A sign pattern (matrix) is a matrix having entries in  $\{+, -, 0\}$ . For a real matrix A,  $\operatorname{sgn}(A)$  is the sign pattern having entries that are the signs of the corresponding entries in A. The idea of studying sign patterns was introduced by the economist Paul Samuelson to model certain problems in economics for which the signs (but not the magnitudes) of the matrix entries are known. If A is an  $n \times n$  sign pattern, the sign pattern class of A, denoted Q(A), is the set of all  $A \in \mathbb{R}^{n \times n}$  such that  $\operatorname{sgn}(A) = A$ . If P is a property of a real matrix, then a sign pattern A requires P if every real matrix  $A \in Q(A)$  has property P, and A allows P or is potentially P if there is some  $A \in Q(A)$  that has property P. Numerous properties have been investigated from the point of view of characterizing sign patterns that require or allow a particular property (see, e.g., [5, 9] and the references therein).

Sign patterns that require eventual positivity or eventual nonnegativity are characterized in [7]. Potentially eventually positive (PEP) sign patterns are studied in [1], where several necessary or sufficient conditions are given for a sign pattern to be PEP, and PEP sign patterns of order at most three are characterized. Much less is known about whether a sign pattern is potentially eventually nonnegative (PEN) as compared with whether

it is PEP, although there have been numerous papers on eventually nonnegative matrices (see for example [2, 3, 6, 8, 11, 12, 13, 14]).

#### **Recent Developments and Problems Investigated**

The study of PEP sign patterns utilizes the Perron-Frobenius eigenstructure of a positive matrix, and irreducible nonnegative matrices retain significant Perron-Frobenius properties. Motivated by this, we define a matrix to be *strongly eventually nonnegative* (SEN) if it is an eventually nonnegative matrix that has an irreducible nonnegative power. We also define a matrix to have the *semi-strong Perron Frobenius property* if its dominant eigenvalues are simple and nonzero, and its spectral radius has positive left and right eigenvectors. The class SSPF is those matrices A such that both A and  $A^T$  have the semi-strong Perron Frobenius property, so an SEN matrix is in SSPF.

Investigation of the classes of matrices SEN and SSPF led to consideration of additional classes, such as *r*-cyclic matrices. Our primary goal for the week at BIRS was to investigate sign patterns that allow matrices in SEN and/or SSPF and related classes. The requires problems for SEN and SSPF were not addressed because they have already been solved: It is shown in [7] that if an irreducible sign pattern  $\mathcal{A}$  requires eventual nonnegativity, then  $\mathcal{A}$  is nonnegative. Since an SSPF matrix must be irreducible, a sign pattern requires SSPF (or SEN) if and only if it is an irreducible nonnegative sign pattern.

#### **Scientific Progress Made**

Numerous results about PSEN and PSSPF sign patterns were established. The paper [4], which has been submitted, contains the details. The main results of our work are summarized below.

#### **Theorem** If A is PSEN, then A is either PEP or r-cyclic.

**Theorem** For  $n \leq 3$ , an  $n \times n$  sign pattern A is PSEN if and only if A is PSSPF, and these sign patterns are characterized.

We identified the following question as a significant open problem for PSEN and PSSPF sign patterns.

#### **Question** *Is every* $n \times n$ *PSSPF sign pattern PSEN?*

Examples of matrices in SSPF that are not eventually nonnegative are known, but in each case the sign pattern of the matrix is PSEN (and in some cases PEP). If there is a PSSPF sign pattern that is not PSEN, then it must have order at least 4 (by the theorem above).

The diagram in Figure 47.1 below shows the relationship between classes of sign patterns studied, including 1) potentially eventually positive sign patterns (PEP), 2) potentially strongly eventually nonnegative sign patterns (PSEN), 3) sign patterns that have a realization A that has a simple positive dominant eigenvalue with positive right and left eigenvectors (PSSPF), 4) irreducible sign patterns (irreducible), 5) potentially eventually nonnegative sign patterns (PEN), 6) r-cyclic sign patterns (r-cyclic), 7) potentially nilpotent sign patterns (PN), and 8) nonnegative sign patterns (nonnegative). The regions marked with ?? would be empty if every PSSPF sign pattern were PSEN, i.e., if the answer to the Question were yes. For each of the other regions in the diagram, an example of a matrix in that region is provided in [4].

4 irreducible $\mathcal{A}_4$	$\mathcal{A}_{46}$	??	3 PSSPF	??
$\mathcal{A}_{45}$	$\mathcal{A}_{456}$	??		- 00
7 PN A <sub>457</sub>		??	??	??
		$\mathcal{A}_{234567}$	$\mathcal{A}_{123457}$	
		2 PSEN	1 PEP	
	$\mathcal{A}_{4567}$	$\mathcal{A}_{23456}$	$\mathcal{A}_{12345}$	
		$\mathcal{A}_{234568}$	$\mathcal{A}_{123458}$	
$\mathcal{A}_{578}$	$\mathcal{A}_{5678}$	$\mathcal{A}_{568}$	A <sub>58</sub> 8 nonnegative	
$\mathcal{A}_{57}$	$\mathcal{A}_{567}$	$\mathcal{A}_{56}$	5 PEN A5	
	6 <i>r</i> -cyclic $A_6$		$\mathcal{A}_{\mathfrak{g}}$	

Figure 47.1: An Euler diagram of potentially eventually nonnegative sign patterns and related classes for patterns of order at least 2. The symbol  $A_{xyz}$  appearing in a region signifies we have an example of a pattern in this region. We do not have examples for the regions with a ?? in them. Those regions are empty if PSEN = PSSPF.

#### Acknowledgement

We thank BIRS for providing a wonderful environment in which to conduct mathematical research.

#### **List of Participants**

Catral, Minerva (Xavier University) Erickson, Craig (Iowa State University) Hogben, Leslie (Iowa State University) Olesky, Dale (University of Victoria) van den Driessche, Pauline (University of Victoria)

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# **Quantum Information for Quantum Chemistry (11frg014)**

#### Jun 05 - Jun 12, 2011

Organizer(s): Alan Aspuru-Guzik (Harvard University) Sabre Kais (Purdue University)

The development and use of quantum computers for chemical applications has potentially revolutionary impact opportunities to change the way computing is done in future generations. The workshop brought to-gether leading scientists from the fields of quantum information, quantum computing and quantum chemistry to exchange ideas and discuss ways to develop quantum algorithms and experimental realization and to push forward the quantum information revolution in the field of chemistry.

The main Objectives of meeting are:

- To advance our understanding of chemical processes using theoretical concepts and frameworks from quantum information. To build bridges between the communities of chemical physics and quantum information.
- To create a chain of tools for mapping quantum chemistry calculations onto a quantum algorithm. To develop calculations suitable for current and near-term quantum information processors but extendable to future devices.
- To overcome the challenges of experimental quantum simulation by developing new methods to suppress errors due to faulty controls and noisy environments. To create a toolbox of decoupling pulses and optimized error correction for integration with quantum algorithms for chemical systems.

At the meeting, Kais present an overview of the field of quantum information and computation in chemistry, discussed recent developments and open problems with emphasis on scientific progress made in this field. Presentation from the participants highlights the following topics:

 Implementation of adiabatic quantum optimization at D-Wave: D-wave has developed a hardware platform which implements an adiabatic quantum optimization algorithm[1]. The past few years have been spent characterizing this hardware tool, obtaining experimental data from the computer, and describing these experimental results using open quantum system models. The results have been extremely promising and now the quantum nature of the building blocks of the processor are well understood, focus has turned to using the hardware for real world applications. One of these applications is in the field of quantum simulation. At the workshop, Gildert and Rose presented an overview of the hardware in order to inform the other participants of the capability of this tool as a simulator[1]. Three presentations were given, the first describing the underlying Ising physics of the system, the second gave an introduction to the topology, processor architecture and fabrication processes. The final presentation covered characterizing and controlling an adiabatic quantum processor. The presentation and subsequent discussion session also included some very recent results suggesting how their system may be of use in quantum chemistry, and quantum random walks and the modeling of specific processes such as those occurring in photon capture in photosynthetic compounds. In particular Aspuru-Guzik discussed the first experimental realization of a quantum annealing protocol towards the study of lattice folding instances. Moreover, the challenges to be overcome are: Efficient mapping of lattice-folding free-energy functions into a spin-glass classical Hamiltonian and fully programmable device able to implement arbitrary coupling define each computational instances.

#### • Experimental quantum photonics:

One of the main objectives of the experimental quantum photonics is to build a photonic quantum simulator that is capable of exploring new physical phenomena in quantum chemistry, solid-state physics and other physical systems[2]. Quantum simulations are attracting much attention as it seems that the controlled manipulation of a few tens of qubits is already sufficient to provide insight into quantum systems that cannot be treated with classical computers. The main challenge, however, is the necessary level of coherent quantum control of individual qubits for the physical realization of quantum simulators. Walther group at Vienna[2] use the particular advantage of photons, the single particle quantum control and tunable measurement-induced interaction, to accomplish efficient quantum simulation of novel physical phenomena. This work aims to go significantly beyond state-of-the-art in developing new techniques for the generation and manipulation of multi-photon entanglement to break the ground for unimagined quantum control of ten or more individual photons. The results of these experiments will be crucial to demonstrate the feasibility of quantum simulation as a new promising application for optical quantum computers. In particular, Aspuru-Guzik and Walther discussed the demonstration of valence bond theory in chemical binding of conjugated chemical systems.

#### • Decoherence, correlation and quantum annealing:

Kyriakidis has focused on two topics. One is on the controlled creation and manipulation of correlated states whose decoherence and relaxation times are, by virtue of their physical correlation, much greater than the more commonly used states for quantum information processing. He identified two such promising states. One is the formation meron spin textures [3] in quantum dots. These textures were previously thought to exist only in bulk 2D electron systems, and only bound in pairs. He has shown that both these assumptions are false. In fact, isolated merons can condense into the ground states of multi-electron strongly interacting quantum dots. The advantage in terms of quantum information processing is that these states possess a topological degree of freedom – the winding number; these can be used as logical qubits that may be impervious to local decohereing fluctuations.

The second such state is a fermionic Fock state [4], again in quantum dots. Certain finite quantum systems can be open to particle exchange with a reservoir. In this case, the particle number of the system is not a good quantum number and one can speak of a coherent superposition of states with different particle numbers. He has shown [4] that these states, if they can be formed, will possess a coherence impervious to \*any\* single particle perturbation of the system – bosonic scattering (i.e., phonons, or lattice vibrations), particle exchange with the bath, etc.

The second focus of his work concerns adiabatic quantum computation and its efficacy for quantum simulation of physical systems and processes. He look in particular at how the choice of interpolation function affects the performance of the computation. He has developed heuristics to derive optimal

trajectories and have applied these to the factoring problem. His preliminary results indicate that optimizing the trajectories can dramatically and qualitatively improve the scaling of the computation with system size. It is currently an open question over how many decades this improved scaling can be maintained. It is also an open question as how transferable these promising results are to other important problems in quantum simulations.

• Lie theory of unitary group and quantum information:

In this talk Love discussed the Cartan decomposition of the unitary groups  $SU(2^n)$  with applications in quantum information theory. Sequences of Cartan decompositions have been used to prove bounds on the number of non-trivial entangling two qubit gates required to synthesize an arbitrary unitary operator on n qubits. He described a particular alternating sequence of Cartan decompositions that reproduce the best known results on synthesis of quantum circuits over CNOT gates: the quantum shannon decomposition. Concomitant with the existence of a Cartan decomposition is the existence of a Cartan involution that enables one to constructively obtain the factors at each stage of the decomposition, and ultimately to obtain the entire circuit for an arbitrary unitary matrix. Also, he described an implementation of the best-known sequence of Cartan decompositions for this purpose, and give performance data. Factorization of 8 qubit circuits is feasible with desktop computing resources, but of course the exponential scaling of the dimension of the group with the number of qubits sets sharp limits on applying these techniques to larger circuits.

These decompositions of unitary operators may be viewed as parameterizations - and may be used in quantum information in contexts outside the circuit model. He described one such application, the computation of mixed state entanglement by a convex roof optimization over the space of ensembles realizing the mixed state density matrix. Applications of this technique include the calculation of entanglement in FMO complexes and in the recently available D-Wave superconducting quantum annealing processors.

#### • Quantum algorithms and their implementation:

Papageorgiou review recent work at Columbia University concerning quantum algorithms and their quantum circuit implementation to study the simulation of a system evolving with Hamiltonian H. They are interested in the cost of quantum algorithms approximating  $e^{-iHt}$ , with error  $\varepsilon$ . They consider algorithms based on high order splitting formulas. These algorithms approximate  $e^{-iHt}$  by a product of exponentials and obtain upper bounds for the number of required exponentials with significant speedups relative to previously known results. They also study the estimation of the ground state energy of a system with relative error  $\varepsilon$ . Deterministic classical algorithms have cost that grows exponentially with the system size. The problem depends on a number of state variables d. They exhibit a quantum algorithm that achieves relative error  $\varepsilon$  using a number of qubits  $C'd\log\varepsilon^{-1}$  with total cost  $Cd\varepsilon^{-(3+\delta)}$ , where  $\delta > 0$  is arbitrarily small. This is joint work of A. Papageorgiou, I. Petras, J. F. Traub and C. Zhang[5]. Improving the cost estimates for Hamiltonian simulation the ground state energy estimation is an open problem. They anticipate improved estimates by taking into account the initial state. Their technique for deriving an approximate ground state can be extended to other eigenvalue estimation problems. Characterizing these problems and deriving cost of the respective algorithms is another open problem. Finally Papageorgiou discuss very recent work of A. Aho and J. Briceno on the design of QuID, a high-level programming language for describing quantum circuits, and a QuID compiler. QuID contains high-level features (modular code, looping, branching) and uses Dirac notation when possible. QuID outputs "quasm" (quantum assembly language) code but the design of the compiler is target agnostic. It uses an abstract internal representation of the quantum circuit. Currently QuiD can express basic quantum circuits, the quantum Fourier transform and diagonal operators. The compiler outputs quasm code with Pauli, single qubit rotations, Hadamard, CNOT and Toffoli gates. Extensions of the language will include other unitary operators and libraries. Extensions of the compiler will include the ability to select the set of elementary quantum gates and quantum circuit templates. Code optimization and error correction are parts of the future work.

#### **List of Participants**

Aspuru-Guzik, Alan (Harvard University) Gildert, Suzanne (D-Wave Systems Inc.) Kais, Sabre (Purdue University) Kyriakidis, Jordan (Dalhousie University) Love, Peter (Haverford) Papageorgiou, Anargyros (Columbia University) Rose, Geordie (D-Wave Systems Inc.) Walther, Philip (University of Vienna)

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# Mixed Boundary Value Problems in Nonsmooth Domains (11frg158)

#### Jun 12 - Jun 19, 2011

**Organizer(s):** Irina Mitrea (University of Minnesota) Katharine Ott (University of Kentucky)

#### **Overview of the Field**

The purpose of this Focused Research Group (FRG) was to consider several open problems regarding elliptic boundary value problems in domains with nonsmooth boundaries and with mixed boundary conditions of Dirichlet and Neumann type. The questions considered were motivated in part by recent progress on the mixed problem or Zarema's problem for the Laplacian in Lipschitz domains with  $L^p$  data,  $1 . If <math>\Omega$ is a bounded Lipschitz domain in  $\mathbb{R}^n$ ,  $n \ge 2$ , the mixed problem for the Laplacian reads

$$\begin{cases}
\Delta u = 0 & \text{in } \Omega, \\
u |_{D} = f_{D} \in L_{1}^{p}(D), \\
\frac{\partial u}{\partial \nu} \Big|_{N} = f_{N} \in L^{p}(N), \\
(\nabla u)^{*} \in L^{p}(\partial \Omega),
\end{cases}$$
(49.1)

where  $\partial\Omega = D \cup N$  and D and N are disjoint,  $\nu$  is the outward unit normal vector to  $\partial\Omega$ , and where for a given set E,  $|_E$  denotes the restriction to E. Hereafter, for  $E \subseteq \partial\Omega$  measurable, and  $1 , <math>L^p(E)$  stands for the Lebesgue space of p-integrable functions on E with respect to the surface measure on  $\partial\Omega$  and  $L_1^p(E)$  is the  $L^p$ -based Sobolev space of order one on E. Also, for any function  $v : \Omega \to \mathbf{R}$ ,  $v^*$  stands for the non-tangential maximal function of v given by

$$v^*(x) := \sup_{y \in \Gamma_\kappa(x)} |v(y)|, \qquad x \in \partial\Omega,$$
(49.2)

where for  $x \in \partial \Omega$  and some fixed  $\kappa >> 1$ , we have set

$$\Gamma_{\kappa}(x) := \{ y \in \Omega : |x - y| \leqslant \kappa \operatorname{dist}(y, \partial \Omega) \}$$
(49.3)

to be the non-tangential approach region with vertex at x. The study of the mixed problem (49.1) in Lipschitz domains is listed as open problem 3.2.15 in Kenig's CBMS lecture notes [6].

During the past thirty years there has been a great deal of interest in the classical Dirichlet and Neumann boundary value problems for the Laplacian in domains with varying degrees of smoothness, and especially Lipschitz domains (see [2] and [5] for two fundamental papers). The Lipschitz setting is significant in terms of both applications and theory. Mixed boundary value problems naturally model the behavior of several physical quantities arising in the modeling of heat transfer, metallurgical melting, stamp problems in elasticity, wave phenomena, etc., and since nonsmooth regions arise in nature, we want to understand how the geometry of a region is related to the solution of boundary value problems posed on the region. From a theoretical standpoint, the equations under consideration are constant coefficient, homogeneous differential operators and the family of solutions to such an operator is preserved by the dilations  $x \to rx$  on  $\mathbb{R}^n$ . The class of Lipschitz domains is also preserved by these dilations and includes domains with interesting features at all length scales. Thus, the analysis of boundary value problems in Lipschitz domains is a natural area of study and it involves fundamentally new problems as compared to smoother domains.

Under appropriate conditions on D and N, recent work of J. Taylor and FRG participants K. Ott and R. Brown [8, 9] shows that there exists  $p_0 > 1$ , with  $p_0$  depending on the Lipschitz constant of the domain and the dimension n, so that the boundary value problem (49.1) is well-posed for  $p \in (1, p_0)$ . In other words, it has been proved that (49.1) has a solution and this solution is unique in the class of functions satisfying  $(\nabla u)^* \in L^p(\partial \Omega)$ . In the case p = 1, the authors prove results for the mixed problem with data from Hardy spaces. Except for the exact value of  $p_0$ , simple examples show that this is the best possible result. Even in a smooth domain, we are not able to solve (49.1) in the case p = 2.

#### **Outcome of the Meeting**

#### The mixed problem for elliptic equations in Lipschitz domains with $L^p$ data

The first open problem that the participants addressed was to find appropriate conditions on the domain, the boundary, and the data, which guarantee that the gradient of the solution of

$$\begin{cases} \mathcal{L}u = 0 \quad \text{in } \Omega, \\ u \mid_{D} = f_{D} \in L_{1}^{p}(D), \\ \frac{\partial u}{\partial \nu} \Big|_{N} = f_{N} \in L^{p}(N), \\ (\nabla u)^{*} \in L^{p}(\partial \Omega), \end{cases}$$

$$(49.4)$$

lies in  $L^p(\partial\Omega)$  for some  $1 \leq p < \infty$ . Here  $\mathcal{L}$  is a second order elliptic differential operator with constant coefficients and  $\frac{\partial}{\partial\nu}$  generically denotes a conormal derivative associated with  $\mathcal{L}$ . When  $\mathcal{L} = \Delta$  then (49.4) becomes (49.1) and in the latter situation, J. Taylor, K. Ott, and R. Brown established  $L^p$  estimates for the solution of (49.1) as discussed in the previous section. A key ingredient of their proof is Hölder estimates at the boundary for the Green function associated to the mixed boundary value problem. Obtaining these estimates when  $\mathcal{L}$  is a matrix-valued differential operator (as in the case of systems), rather than a scalar operator, is a challenge and a problem that the participants confronted during the stay in Banff.

As a first step in approaching this problem, FRG participant S. Kim outlined his recent work on the Green functions for boundary value problems for elliptic systems. Kim had not previously considered mixed boundary conditions, but his work with collaborators [3, 4] seems applicable. The methods presented by Kim will provide a new and simpler approach to the Green function estimates used in the work of Taylor, Ott and Brown. We are currently working to use these techniques to prove the well-posedness of the mixed problem for the Lamé system of elasticity in a large class of two-dimensional Lipschitz domains with data in  $L^p$  for p

near 1.

#### Scattering for the Helmholtz equations

In this research direction, FRG participant F. Reitich discussed the problem of scattering for the Helmholtz equation in the complement of a compact obstacle,  $\overline{\Omega}$ , where we impose Dirichlet boundary conditions on part of the boundary of the obstacle and Neumann boundary conditions on the remainder of the boundary. Thus, for  $k \in \mathbb{R}^n$ , we are interested in the boundary value problem

$$\begin{cases} (\Delta + |k|^2)v = 0 & \text{in } \mathbf{R}^n \setminus \overline{\Omega}, \\ v|_D = e^{ik \cdot x}, \\ \frac{\partial v}{\partial \nu}|_N = \frac{\partial}{\partial \nu} e^{ik \cdot \cdot}, \\ v \text{ satisfies the outgoing radiation condition.} \end{cases}$$
(49.5)

Unpublished computational experiments for this problem motivated several questions which were addressed by the participants.

To begin, there are several boundary integral formulations of the scattering problem (49.5) that are used for computations. I. Mitrea and K. Ott [7] have successfully employed Mellin analysis techniques for the treatment of transmission boundary value problems for second order elliptic partial differential equations. These techniques have also been applied to the treatment of (49.1) in the case where  $\Omega$  is a polygon and the solution is given by a single layer potential representation. Other singular integral representations of the solution of (49.1), and in turn (49.5), are currently being studied.

A second question related to the scattering problem arises from the following convention. To simplify computations of solutions to the mixed problem, Reitich has found it convenient to replace the sharp discontinuity in the boundary by a smooth transition. This regularization gives a family of Robin problems depending on a parameter. Two natural questions to ask are do the solutions of these Robin problems converge to the mixed problem, and can we give estimates for the rate of convergence?

To give a concrete form of this question, consider the case of homogeneous boundary conditions,

$$\begin{cases} \Delta u = F \quad \text{in } \Omega, \\ \chi_{\epsilon} u + (1 - \chi_{\epsilon}) \frac{\partial u}{\partial \nu} ) = 0 \quad \text{on } \partial \Omega. \end{cases}$$
(49.6)

If we let  $\chi_0 = \chi_D$  be the indicator function of D and  $\chi_{\epsilon}$  be a family of smooth approximations to  $\chi_D$ , then a natural question to ask is if the solutions of the boundary value problem with  $\epsilon > 0$  converge to the solution of the mixed problem corresponding to  $\epsilon = 0$ . Another interesting question is to find a similar regularization of the boundary integral equations for the mixed problem with inhomogeneous boundary conditions and to establish that solutions of the regularized problem converge to the solution of the mixed problem. The coefficient of the normal derivative for the Robin problem vanishes and such problems do not seem to be widely studied.

#### **Open Problems**

During our time in Banff several additional, and promising, avenues for future research were identified. Building on the recent progress of studying the mixed problem for the Lamé system of elastostatics in twodimensional Lipschitz domains, an important open problem for future research is to consider other systems such as the stationary Stokes system of fluid flow. M. Wright has a great deal of experience with the Stokes system [1, 11]. The Focused Research Group allowed Wright to become familiar with the techniques used to attack the mixed problem and he is currently working on adapting these techniques to the study of boundary value problems with mixed boundary conditions for the Stokes system. A second interesting problem that arose out of discussions in Banff is to find the optimal range of p values for which the mixed boundary value problem with  $L^p$  data is well-posed. This would be of interest in even when the domain is smooth. We conjecture that the optimal range is p in the interval (1, 2). This question may be approached in the context of the polygonal domains where the Mellin transform methods used by FRG participants I. Mitrea and K. Ott should give a complete answer in two dimensional curvilinear polygons.

Another area that bears further investigation is the use of layer potential methods for the mixed problem. G. Verchota [10] established well-posedness for the Dirichlet and Neumann problems for the Laplacian by establishing the invertibility of classical layer potentials on the boundary. It is not known if we can attack the mixed problem by layer potentials. However, it was observed during our discussions that the well-posedness of the mixed problem implies that solutions may be represented by layer potentials. Such results are of interest as the representation provides a foundation for numerical schemes to compute solutions to the mixed problem.

#### Conclusion

This Focused Research Group brought together six mathematicians who had not previously worked together, but who shared a common interest in mixed boundary value problems. One unique aspect of this FRG is that it addressed both theoretical and numerical problems related to the topic. Several promising areas of research were identified and new collaborations were begun to attack these problems.

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# **Extending Properties of Tournaments to k-Traceable Oriented Graphs (11frg171)**

### Jul 31 - Aug 07, 2011

**Organizer(s):** Ortrud Oellermann (University of Winnipeg)

#### **Overview of the Field, Recent Developments and Open Problems**

A graph or digraph is *hamiltonian* if it contains a cycle that visits every vertex, and *traceable* if it contains a path that visits every vertex. A (di)graph is *k*-traceable if each of its induced subdigraphs of order k is traceable. A digraph D is strong if for every pair u, v of vertices in D there is a directed path from u to v and a directed path from v to u.

A digraph D obtained by assigning directions to the edges of a graph G is called an *oriented graph*. We say that D is an orientation of G. A *tournament* is an orientation of a complete graph and a *multipartite tournament* is an orientation of a complete multipartite graph.

Our interest in k-traceable oriented graphs stems from the following conjecture, which is stated in [2].

**The Traceability Conjecture (TC)**: For  $k \ge 2$ , every k-traceable oriented graph of order at least 2k - 1 is traceable.

The TC was motivated by the OPPC, an oriented version of the Path Partition Conjecture, which can be formulated as follows.

**OPPC:** If D is an oriented graph with no path of order greater than  $\lambda$  and a is a positive integer such that  $a < \lambda$ , then V(D) contains a set A such that the oriented graph induced by A has no path of order greater than a and D - A has no path of order greater than  $\lambda - a$ .

If the TC is true, it would imply that the OPPC is true for every oriented graph whose order is exactly one more than the order of its longest paths.

Apart from their connection to the OPPC, k-traceable oriented graphs are a natural generalization of the well-studied class of tournaments, these being the 2-traceable oriented graphs. As such they are of interest in their own right. It is thus natural to investigate to what extent the properties possessed by tournaments extend to k-traceable oriented graphs.

Moon [6] showed that strong tournaments have a very rich cycle structure. In particular he showed that every strong tournament is *vertex-pancyclic*, i.e., in every strong tournament on  $n \ge 3$  vertices every vertex

belongs to a cycle of length l for every  $3 \le l \le n$ . Thus all strong tournaments have a hamiltonian cycle.

One generalization of tournaments are the multipartite tournaments. The cycle structure of strong multipartite tournaments has been studied by several authors. For example, it is shown by Goddard and Oellermann [4] that every vertex of a strong *p*-partite tournament *D* belongs to a cycle that contains vertices from exactly *m* partite sets for each *m*,  $3 \le m \le p$ . Moreover, it is shown by Guo, Pinkernell and Volkmann [5] that if *v* is a vertex in a strong *p*-partite tournament, then *v* lies on some longest cycle and if  $p \ge 3$ , then *v* belongs to an *m* or (m+1)-cycle for every *m*,  $3 \le m \le p$ . More results on paths and cycles in multipartite tournaments appear in an extensive survey of Volkmann [7].

For small values of k the k-traceable oriented graphs share many properties that tournaments possess. For example, it is well-known that every strong tournament is hamiltonian. In [2] it is shown that strong k-traceable oriented graphs are hamiltonian for k = 3 and 4. However, when  $k \ge 5$  the situation changes dramatically. It was shown in [2] that for every  $n \ge 5$  there exists a strong nonhamiltonian oriented graph of order n that is k-traceable for every  $k \in \{5, ..., n\}$ . Thus for  $k \in \{2, 3, 4\}$  there are no strong nonhamiltonian k-traceable oriented graphs of order greater than k, while for each  $k \ge 5$  there are infinitely many.

Let n and t be integers such that  $3 \le t \le n$ . We say that a digraph D of order n is t-pancyclic if D contains a cycle of length r for every r,  $t \le r \le n$  and it is vertex-t-pancyclic if every vertex is contained in a cycle of every length r for  $t \le r \le n$ . Moreover, D is weakly (vertex-)pancyclic if it contains cycles of every length from g(D) to c(D) (through each vertex). It was shown in [1] that for k = 2, 3, 4 all strong k-traceable oriented graphs of order at least k + 1 are vertex-(k + 1)-pancyclic. In the same paper it was observed that this results does not extend to k-traceable graphs for  $k \ge 5$ . Nevertheless strong k-traceable oriented graphs with girth at least k are girth-pancyclic. The cycle spectrum of a (di)graph is the set of the lengths of the cycles in the (di)graph.

**Question 1:** Is a strong *k*-traceable oriented graph weakly pancyclic?

**Question 2:** If the answer to Question 2 is negative is it true that if D is a strong k-traceable oriented graph and m is an integer with  $g(D) \le m \le c(D)$  that there is D has a cycle of length m or m + 1? **Question 3:** What is the cycle spectrum of a strong k-traceable oriented graph?

A graph is G is *locally* k-traceable if for every vertex v and every set S of k vertices in N[v],  $\langle S \rangle$  is traceable. Every k-traceable graph is obviously locally k-traceable, but not vice versa, since a k-traceable graph of order n has minimum degree at least n-k+1, while local k-traceability does not require a minimum degree condition.

Question 4: Under what conditions are locally k-traceable graphs of order n, satisfying the minimum degree condition  $\delta(G) \ge n - k + 1$ , also k-traceable?

#### **Outcome of the Focussed Research Workshop**

Questions 1 and 2 were answered in the negative. For Question 3 it was shown that for every pair of integers n, k such that  $5 \le k < n$  and each subset S of  $\{n - k + 4, ..., n\}$ , there exists a strong k-traceable oriented graph of order n with cycle spectrum  $\{3, ..., n\} - S$ .

For Question 4 it was shown that if G is a locally k-traceable graph of order  $n \ge k^2 - 5k + 9$  and  $\delta(G) \ge n - k + 1$ , then G is k-traceable. The requirement on n cannot be relaxed because, for every  $k \ge 4$ , there exists a locally k-traceable graph of order  $k^2 - 5k + 8$  that is not k-traceable.

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# New methods for analysing metastable structures in closed, open or non-autonomous dynamical systems (11frg168)

#### Oct 23 - Oct 30, 2011

**Organizer(s):** Wael Bahsoun (Loughborough University) Arno Berger (University of Alberta) Chris Bose (University of Victoria) Gary Froyland (University of New South Wales) Cecilia González Tokman (University of Victoria) Rua Murray (University of Canterbury - New Zealand)

#### **Overview of the Field**

Dynamical systems  $\hat{T} : I \to I$  typically model complicated deterministic processes on a phase space I. The map  $\hat{T}$  induces a natural action on probability measures  $\eta$  on I via  $\eta \mapsto \eta \circ \hat{T}^{-1}$ . Of particular interest in ergodic theory are those probability measures that are  $\hat{T}$ -invariant; that is,  $\eta$  satisfying  $\eta = \eta \circ \hat{T}^{-1}$ . By Birkhoff's Ergodic Theorem, if  $\eta$  is ergodic and invariant, then it describes the time-asymptotic distribution of orbits of  $\eta$ -almost-all initial points  $x \in I$ . This picture is part of a well established classical mathematical understanding of dynamical systems.

From an applications point of view, it is desirable to find the invariant measures  $\eta$ , and analyse the way that typical orbits are "mixed" to the consequent equilibrium distribution. When the space I is equipped with a natural "smooth" measure m (such as the Lebesgue measure on subsets of  $\mathbb{R}^d$ ), the action of  $\hat{T}$  on  $\eta \ll m$  can be studied via the so-called *Frobenius–Perron* (transfer) operator:

$$\mathcal{L}\frac{d\eta}{dm} = \frac{d(\eta \circ \hat{T}^{-1})}{dm}$$

(see [32] for an introductory account). Numerical representation of  $\mathcal{L}$  can be accomplished via *Ulam's method* [39]—a Galerkin type projection onto the space of piecewise constant functions on partitions of *I*. As the underlying partitions are refined, the fixed points of Ulam's method are known to converge to densities of

interesting  $\hat{T}$ -invariant measures in a variety of settings [34, 15, 16, 18, 20, 17, 3, 37]. The quality of approximation is determined in part by the speed at which orbits are "mixed" by  $\hat{T}$ , and the speed of mixing is often controlled by the gap between the leading eigenvalue, and the rest of the spectrum of  $\mathcal{L}$  (on a suitable Banach space of test functions). Although the behaviour of this *spectral gap* can be well-behaved under Ulam-type approximations [29, 11], the gap is often small, frustrating efforts to control approximation errors. It has recently become clear [21, 19, 27, 25, 26, 22] that small spectral gaps are actually associated with *metastable structures*—subsets of phase space I which exchange mass very slowly. Moreover, these structures crop up in a variety of real applications (*eg*, molecular conformation dynamics [14], spacecraft orbits [12], large-scale ocean circulation [13]).

Consequently, the development of computational tools for identifying metastable states is interesting and important. A particularly fruitful idea is to regard a (closed) dynamical system is a union of interacting open subsystems. Essentially arbitrary *open systems* can be obtained from  $(\hat{T}, I)$  by excising a "hole"  $H_0$ from I. Orbits are computed as normal on  $X_0 := I \setminus H_0$ , but are lost to the system when they fall into  $H_0$ . Because trajectories are being lost to the hole, in many cases, there is no T-invariant probability measure. One can, however, consider *conditionally invariant* probability measures, which satisfy  $\eta \circ T^{-1} = \rho \eta$  for some  $\rho \in (0, 1)$ . This idea has a long history [38, 9, 8, 10], and has seen an explosion of interest in recent years [35, 36, 30, 23, 7], with many of the aforementioned references being focussed on the existence (or analytical approximation) of conditionally invariant probability measures. Very recently, attention has focussed on practical means of calculating these measures numerically [1, 2] and connecting them with metastable behaviour in dynamical systems [28, 22].

#### Scientific progress made and open problems

Our activities at BIRS were in two main directions:

- 1. Rigorous analysis of the application of Ulam's method [39] to the calculation of conditionally invariant probability measures for Lasota-Yorke type maps [33] into which "large" holes have been put. Using an analytical setup similar to that of Liverani and Maume-Deschamps [35], we proved that Ulam's method produces a sequence of density functions which converge (in  $L^1$ ) to the density of the (unique) absolutely continuous conditionally invariant probability measure for the open system, as well as a sequence of measures which converge weak\* to the conformal measure of the open system (concentrated on the surviving repelling Cantor set). Unlike previous work [1, 2] these results are not based in spectral perturbation theory [29, 30], so are not limited to "small" holes. A manuscript containing these results will shortly be submitted for publication [5]. Open problems include: generalising the setup to higher dimensions; controlling rigorously the rate of convergence; and using the method to study the interaction between multiple metastable states within a closed system (as in [28, 22]).
- 2. Investigating alternatives to Ulam's method for computation of invariant measures, conditionally invariant measures and metastable states [6, 4, 31, 24]. This work threw up many questions, which will form the basis of future projects by the group participants.

#### Acknowledgements

All four of us thank BIRS for the splendid working and living conditions provided. The work in [5] would not have happened without this meeting. CB is supported by an NSERC grant. GF was partially supported by the UNSW School of Mathematics and an ARC Discovery Project (DP110100068). CGT thanks the Pacific Institute for the Mathematical Sciences (PIMS) and the University of Victoria for financial support. RM thanks the College of Engineering (University of Canterbury) for funding to attend the workshop, and the Department of Mathematics and Statistics (University of Victoria) for hospitality during an adjacent visit.

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# Research in Teams Reports

Research in Teams Reports

# Heights on moduli space for post-critically finite dynamical systems (11rit155)

#### Mar 06 - Mar 13, 2011

**Organizer(s):** Matthew Baker (Georgia Institute of Technology) Patrick Ingram (Colorado State University) Rafe Jones (College of the Holy Cross) Joseph Silverman (Brown University)

#### **Overview of the Field**

The purpose of this Research In Teams event was to consider the arithmetic properties of post-critically finite (PCF) rational maps. In the study of complex holomorphic dynamics, it is a general theme that the dynamical properties of a holomorphic map are largely determined by the behaviour of the critical points. In studying the dynamics of a rational map, then, one is lead to consider the orbits of the critical points, and maps for which these critical orbits are all finite gain special prominence. These are the PCF maps. Let  $\mathcal{M}_d$  denote the moduli space of degree-d endomorphisms of  $\mathbb{P}^1$ , up to change of variables. If  $d = m^2$ , certain PCF elements of  $\mathcal{M}_d$  stand out, namely the so-called Lattès examples. These are maps  $f : \mathbb{P}^1 \to \mathbb{P}^1$  such that there is an elliptic curve E and an integer m, such that f is the action induced from [m] by viewing  $\mathbb{P}^1$  as the Kummer surface of E. If  $\mathcal{L}_d \subseteq \mathcal{M}_d$  is the locus of these Lattès examples, then one expects PCF maps to be somewhat sparse in  $\mathcal{M}_d \setminus \mathcal{L}_d$ . A deep result of Thurston makes this more concrete.

**Theorem 52.0.10 (Thurston [3], see also [4])** The PCF points in  $\mathcal{M}_d \setminus \mathcal{L}_d$  is contained in a countable union of 0-dimensional subvarieties.

Note that, since  $\mathcal{M}_d \setminus \mathcal{L}_d$  and the subvarieties in Thurston's result are all defined over  $\mathbb{Q}$ , all non-Lattès PCF maps have (up to change of coordinates) algebraic coefficients. Thurston's result, on the other hand, does not preclude the possibility of most (or even all) rational functions over  $\overline{\mathbb{Q}}$  being PCF, however unlikely this eventuality might seem.

From an arithmetic perspective, a refinement of the theorem above would be given by the following.

**Conjecture 52.0.16** For some height function  $h_{\mathcal{M}_d}$  relative to an ample class, the set of PCF points in  $\mathcal{M}_d \setminus \mathcal{L}_d$  is a set of bounded height.

Note that Theorem 52.0.10 would follow from Conjecture 52.0.16. Although Thurston's results in [3] contain more information than the statement of Theorem 52.0.10, the methods of proof involve a deep examination of iteration on Teichmuller space, and it would be of interest to have an algebraic proof of Theorem 52.0.10 Indeed, Conjecture 52.0.16 implies something much stronger than Theorem 52.0.10: that given any constant C, the set of PCF rational maps of degree d and coefficients of algebraic degree at most C is, up to change of variables, finite and effectively computable. This is a far cry from the possibility of all algebraic maps being PCF, which is not precluded by Theorem 52.0.10, or the more subtle results of Thurston given in [3].

Silverman has proposed a refined version of Conjecture 52.0.16. We define the *critical height* on  $\mathcal{M}_d(\overline{\mathbb{Q}})$  by

$$h_{\rm crit}(f) = \sum_{\beta \in \mathbb{P}^1} (e_f(\beta) - 1)\hat{h}_f(\beta),$$

where  $e_f(\beta)$  is the index of ramification of f at  $\beta$ , and  $\hat{h}_f(\beta)$  is the canonical height (as defined in [1]). As  $\hat{h}_f(\beta)$  vanishes precisely if  $\beta$  has a finite forward orbit under f, it follows that  $h_{crit}$  vanishes precisely on PCF points. What is not clear is that the critical height is in any way related to any height function on  $\mathcal{M}_d$ , in the usual sense.

**Conjecture 52.0.17** For some height function  $h_{\mathcal{M}_d}$  relative to an ample class, there exist constants  $c_1, ... c_4$  such that

$$c_1 h_{\mathcal{M}_d}(f) - c_2 \leqslant h_{\operatorname{crit}}(f) \leqslant c_3 h_{\mathcal{M}_d}(f) + c_4.$$

Conjecture 52.0.16 is equivalent to the assertion that  $h_{\mathcal{M}_d}$  is bounded on the subset defined by  $h_{\text{crit}} = 0$ , and so is clearly weaker than Conjecture 52.0.17. Although both of these conjectures are quite strong, there is some hope of progress. In particular, one of the participants proved Conjecture 52.0.17 for the moduli space of polynomials [2] in 2010. Simultaneously, Epstein [5] used related arithmetic techniques to prove various results on PCF polynomials which, while not as strong as the results in [2] from the perspective of Conjecture 52.0.17, allowed a proof of some of the more subtle parts of Thurston's work omitted in the statement of Theorem 52.0.10 above.

#### **Scientific Progress Made**

The main goal of the Research in Teams workshop was to extend some of the earlier work, most notably the results in [2], to the context of rational functions. This seems somewhat difficult, as the theory of local heights (used extensively in [2]) is greatly simplified in the case of polynomial dynamics. Employing geometric results of McMullen [6], we were able to reduce Conjecture 52.0.16 to the following plausible conjecture in non-archimedean dynamics

**Conjecture 52.0.18** Every sufficiently attracting fixed point of a rational map is the accumulation point of a critical orbit. Specifically, if  $|\cdot|_v$  is a norm on  $\overline{\mathbb{Q}}$  extending the p-adic norm on  $\mathbb{Q}$ , then there is a constant  $C_{p,d} \leq 1$  such that if  $f(z) \in \overline{\mathbb{Q}}(z)$  has degree d, if  $f(\gamma) = \gamma$ , and if  $|f'(\gamma)|_v < C_{p,d}$ , then  $\gamma$  is the accumulation point of critical orbit. We further require, for each fixed  $d \ge 2$ , that  $C_{p,d} = 1$  for all but finitely many primes p.

The analogue of Conjecture 52.0.18 for complex dynamics has been known since the time of Fatou, and so it seems reasonable to posit the same claim for *p*-adic dynamics. Moreover, we were able to establish this conjecture, and hence Conjecture 52.0.16, in several restricted contexts.

**Theorem 52.0.11** Conjecture 52.0.18 holds for rational maps of degree 2, and rational maps of degree 3 with a ramified fixed point. In particular, Conjecture 52.0.16 holds for  $M_2$ .

While it might appear that the above theorem also proves Conjecture 52.0.16 for certain maps of degree 3, this is not quite true; one requires a result for maps of degree 9 to obtains this. It should be noted that the restriction to a certain subvariety of  $\mathcal{M}_3$  was largely a practical concern, and in discussions with Alon Levy since the conclusion of the workshop, we seem to have eliminated this restriction. It is not clear that the argument generalizes, but we remain hopeful that Conjecture 52.0.16 will be proven eventually (and recent work with Levy make this seem increasingly likely). It is also interesting to note that we were able to establish the conjecture in another context.

#### **Theorem 52.0.12** Conjecture 52.0.18 holds for the moduli space of polynomials of degree d, for any $d \ge 2$ .

Although this result is of lesser interest, since Conjecture 52.0.16 (and, indeed, the much stronger Conjecture 52.0.17) is already known in this context, the proof in [2] is of a very different nature, unrelated to Conjecture 52.0.18. Theorem 52.0.12, then, provides further evidence for the veracity of Conjecture 52.0.18, as well as allowing for several new results in the *p*-adic dynamics of polynomials, analogous to some classical results in complex dynamics. Although the main conjecture addressed at the workshop remains open, we expect that these results will lead to a significant publication, and the progress made has brought us closer to our ultimate goals of proving Conjectures 52.0.16 and 52.0.17.

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Ingram, Patrick (Colorado State University) Jones, Rafe (College of the Holy Cross)

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# Chapter 53

# **Problems in Pluripotential Theory** (11rit157)

# May 29 - Jun 05, 2011

**Organizer(s):** John Anderson (College of the Holy Cross) Joseph Cima (University of N. Carolina) Norm Levenberg (Indiana University) Thomas Ransford (Laval University)

### **Overview of the Field**

Let K be a compact set in  $\mathbb{C}^n$ . A central object of study in potential theory (n = 1) and in pluripotential theory (n > 1) is the *pluricomplex Green function*:

$$V_K(\mathbf{z}) := \sup\{\frac{1}{\deg(p)} \log |p(\mathbf{z})| : ||p||_K \leq 1, \ p \text{ (holomorphic) polynomial}\}.$$

The uppersemicontinuous regularization  $V_K^*(\mathbf{z}) := \limsup_{\zeta \to \mathbf{z}} V_K(\zeta)$  is either identically  $+\infty$ , if K is pluripolar; i.e.,  $K \subset \{\mathbf{z} : u(\mathbf{z}) = -\infty\}$  for some  $u \not\equiv -\infty$  which is plurisubharmonic on a neighborhood of K, or else  $V_K^*$  is plurisubharmonic in  $\mathbb{C}^n$ . For  $K \subset \mathbb{C}^n$  compact, the *polynomial hull of* K is the set

$$\hat{K}_P := \{ \mathbf{z} \in \mathbf{C}^n : |p(\mathbf{z})| \leq ||p||_K \text{ for all polynomials } p \}$$

$$= \{ \mathbf{z} \in \mathbf{C}^n : V_K(\mathbf{z}) = 0 \}$$

(thus  $V_K = V_{\hat{K}_P}$ ) while the projective hull of K (cf. [3]) is the set

$$\hat{K} := \{ \mathbf{z} \in \mathbf{C}^n : \exists C_{\mathbf{z}} \text{ with } |p(\mathbf{z})| \leqslant C_{\mathbf{z}}^{\deg p} ||p||_K \text{ for all polynomials } p \}$$
$$= \{ \mathbf{z} \in \mathbf{C}^n : V_K(\mathbf{z}) < +\infty \}.$$

Wermer [7] showed that if  $\gamma$  is a real-analytic curve in  $\mathbb{C}^n$ , then  $\hat{\gamma}_P \setminus \gamma$  is a one-dimensional, complexanalytic subvariety of  $\mathbb{C}^n \setminus \gamma$ . The projective hull is a notion which, *a priori*, is defined for closed subsets K of  $\mathbb{P}^n$ ; if  $K \subset \mathbb{P}^n$  is contained in an affine  $\mathbb{C}^n \subset \mathbb{P}^n$ , then the portion of this more general notion of the projective hull for subsets of  $\mathbb{P}^n$  that lies in  $\mathbb{C}^n$  coincides with our definition of the projective hull for subsets of  $\mathbb{C}^n$ . Harvey and Lawson [3] conjectured that if  $\gamma$  is a real-analytic curve in  $\mathbb{P}^n$ , then  $\hat{\gamma} \setminus \gamma$  is a one-dimensional, complex-analytic subvariety of  $\mathbb{P}^n \setminus \gamma$ .

Clearly the projective hull is interesting only if K is pluripolar. Since there exist  $C^{\infty}$  curves  $\gamma$  in  $\mathbb{C}^n$  which are *not* pluripolar [2], the Harvey-Lawson assumption that  $\gamma$  be real-analytic is natural. The projective hull is a subtle object. For example, a fascinating result of Sadullaev [5] implies that if A is a connected, pure m-dimensional complex-analytic subvariety of  $\mathbb{C}^n$ ,  $1 \leq m \leq n-1$ , and if  $K \subset A$  is compact and not pluripolar in  $A^{reg}$  (the regular points of A), then  $A \subset \hat{K}$  if and only if A is algebraic.

Unwinding the definitions, the condition that  $\mathbf{z}_0 \in \hat{K}_P$  says that  $|p(\mathbf{z}_0)| \leq ||p||_K$  for all polynomials  $p(\mathbf{z})$  while the condition that  $\mathbf{z}_0 \in \hat{K}$  says that

$$|p(\mathbf{z}_0)| \leqslant C_{\mathbf{z}_0}^{\deg p} ||p||_K \tag{53.1}$$

for all polynomials  $p(\mathbf{z})$  where  $C_{\mathbf{z}_0} = e^{V_K(\mathbf{z}_0)}$ . These growth estimates provides some motivation for the results and questions below.

## **Recent Developments and Open Problems**

An old result of Rudin [4] can be paraphrased as follows: let  $\Delta := \{z \in \mathbf{C} : |z| < 1\}$  denote the unit disk in  $\mathbf{C}$  and let  $\phi \in C(\overline{\Delta})$ , i.e.,  $\phi$  is a continuous, complex-valued function on  $\overline{\Delta}$ . Consider the vector space

$$\mathcal{M} := \{a + b\phi : a, b \text{ (univariate, holomorphic) polynomials}\}.$$
(53.2)

Suppose for all  $z_0 \in \Delta$ ,

$$|f(z_0)| \leq ||f||_T := \max_{|\zeta|=1} |f(\zeta)| \text{ for all } f \in \mathcal{M}$$

Then  $\phi$  is holomorphic in  $\Delta$ . Wermer considered a weak version of this maximum principle hypothesis:

For all 
$$z_0 \in \Delta$$
, there exists  $C_{z_0}$  such that  $|f(z_0)| \leq C_{z_0} ||f||_T$  for all  $f \in \mathcal{M}$ . (53.3)

Under the additional assumption that  $\phi|_T$  be real-analytic, he reached the same conclusion as Rudin. Note that in the setting of (53.2), condition (53.3) becomes

$$|a(z_0) + b(z_0)\phi(z_0)| \leqslant C_{z_0} ||a + b\phi||_T \text{ for all polynomials } a, b.$$
(53.4)

Now suppose  $\phi \in C(\Delta \setminus \{0\})$ . We let

$$\gamma := \{ (z, \phi(z)) : |z| = 1 \}$$

and

$$\Sigma := \{ (z, \phi(z)) : 0 < |z| < 1 \}.$$

Consider the condition that  $\Sigma \subset \hat{\gamma}$ . This says that for each  $0 < |z_0| < 1$ , there exists a constant  $C_{z_0}$  with

$$|p(z_0, \phi(z_0))| \leqslant C_{z_0}^{\deg p} ||p(\cdot, \phi(\cdot))||_T = C_{z_0}^{\deg p} ||p||_{\gamma}$$

for all polynomials p = p(z, w). Wermer [8] observed that if  $\phi$  is meromorphic in  $\Delta$  then  $\Sigma \subset \hat{\gamma}$ . He conjectured that the following converse-type result was true: given  $\phi \in C(\overline{\Delta} \setminus \{0\})$  with  $\phi$  real-analytic on T, if  $\Sigma \subset \hat{\gamma}$ , then  $\phi$  is meromorphic in  $\Delta$ . The real-analyticity of  $\phi$  on T was assumed to ensure that  $\gamma$  be pluripolar. Note that (53.4) is related to this projective hull hypothesis in the sense that (53.4) is (53.1) at the point  $(z_0, \phi(z_0))$  for polynomials p(z, w) which have degree at most one in w and with  $C_{z_0}$  to the first power.

## **Presentation Highlights**

Since this was a "Research in teams" assembly there were no formal presentations.

## **Scientific Progress Made**

We proved a generalization of the existing version of the Rudin and Wermer results.

**Theorem**. Let *F* be a finite subset of  $\Delta$  and let  $\phi \in C(\overline{\Delta} \setminus F)$ . The following are equivalent:

- 1.  $\phi$  is meromorphic on  $\Delta$ ;
- 2. for each  $z_0 \in \Delta \setminus F$  there exists  $C_{z_0}$  such that  $|a(z_0)+b(z_0)\phi(z_0)| \leq C_{z_0}||a+b\phi||_T$  for all polynomials a, b.

A deep result of Shcherbina [6] states that if  $\Omega \subset \mathbf{C}$  is a domain and  $f : \Omega \to \mathbf{C}$  is a continuous function with  $\{(z, f(z)) : z \in \Omega\} \subset \mathbf{C}^2$  pluripolar, then f is holomorphic. Using this, we can show:

**Proposition**. Let  $\phi \in C(\overline{\Delta} \setminus \{0\})$ . Suppose  $\gamma$  is pluripolar and  $\Sigma \subset \hat{\gamma}$ . Then  $\phi$  is holomorphic on  $\Delta \setminus \{0\}$ .

A deeper problem is to conclude that  $\phi$  has at worst a pole at the origin. A sufficient condition ensuring this is that  $\Sigma = \hat{\gamma} \cap ((\Delta \setminus \{0\}) \times \mathbf{C})$ . This allows us to easily show that  $V_{\gamma}$  is harmonic on  $\Sigma$ . We suspect this extra hypothesis is unnecessary.

To motivate a future look at some pluripotential-theoretic questions, we considered the classic univariate setting of complex potential theory. Let  $\mathcal{M}(K)$  denote the convex set of probability measures supported in a given nonpolar compact set  $K \subset \mathbb{C}$ . For  $\mu \in \mathcal{M}(K)$ , let

$$p_{\mu}(z) := \int_{K} \log \frac{1}{|\zeta - z|} d\mu(\zeta) \text{ and } I(\mu) := \int_{K} \int_{K} \log \frac{1}{|\zeta - z|} d\mu(\zeta) d\mu(z)$$

denote the logarithmic potential and logarithmic energy of  $\mu$ . Define

$$C_{K} := \{\mu \in \mathcal{M}(K) : p_{\mu} \text{ is continuous}\};$$
$$E_{K} := \{\mu \in \mathcal{M}(K) : I(\mu) < +\infty\};$$
$$P_{K} := \{\mu \in \mathcal{M}(K) : \mu(P) = 0 \text{ for all polar } P\}.$$

Clearly  $C_K \subset E_K \subset P_K \subset \mathcal{M}(K)$ . We verified:

**Proposition.** Suppose K is not polar at each of its points; i.e., for each  $z \in K$  and each r > 0,  $K \cap B(z, r) = \{z' \in K : |z - z'| < r\}$  is not polar. Then  $C_K$  is dense in  $\mathcal{M}(K)$  in the weak-\* topology.

A key element of the proof of the proposition is the following: if  $K \subset \mathbf{C}$  is not polar, then there exists a positive measure  $\mu$  with support in K such that  $p_{\mu}$  is continuous. A deep theorem of Ancona [1] gives a stronger result: if  $K \subset \mathbf{C}$  is not polar, then there exists a compact set  $K' \subset \mathbf{C}$  with  $V_{K'}$  continuous. The proof in [1] is difficult; we discussed a different approach to a possible proof beginning with the measure  $\mu$ .

### **Outcome of the Meeting**

We are in the process of writing up and submitting for publication an article which will include our generalization of the Rudin/Wermer/projective hull results. We will continue to work on eliminating the extra hypothesis  $\Sigma = \hat{\gamma} \cap ((\Delta \setminus \{0\}) \times \mathbf{C})$ . Future projects may include a possible Rudin/Wermer theorem on the polydisk in  $\mathbf{C}^n$ , n > 1. Questions related to Ancona's theorem [1] and analogues of the subsets  $C_K$ ,  $E_K$ ,  $P_K$  of  $\mathcal{M}(K)$  for  $K \subset \mathbf{C}^n$ , n > 1 will require more thought.

# **List of Participants**

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# Chapter 54

# The SU(3) Casson invariant for spliced sums (11rit159)

# Jun 19 - Jun 26, 2011

**Organizer(s):** Hans U. Boden (McMaster University) Chris Herald (University of Nevada - Reno) Benjamin Himpel (Aarhus University)

## **Overview of the Field**

Taubes [11] laid the groundwork for new topological invariants motivated by Chern-Simons theory by showing that the SU(2) Casson invariant of a homology 3–sphere M has a gauge theoretical interpretation as the Euler characteristic of  $\mathcal{A}/\mathcal{G}$  in the spirit of the Poincaré-Hopf theorem, where he views the Chern-Simons invariant

$$cs(A) = \frac{1}{8\pi^2} \int_M \operatorname{tr}(A \wedge dA + \frac{2}{3}A \wedge A \wedge A)$$

as a  $S^1$ -valued Morse function on  $\mathcal{A}/\mathcal{G}$ ,  $\mathcal{A}$  being the space of SU(2) connections on M and  $\mathcal{G}$  the group of gauge transformations. Taubes realized that the Hessian of the Chern-Simons invariant and the odd signature operator coupled to the same path of SU(2) connections have the same spectral flow.

Using Taubes's point of view, an SU(3) Casson invariant  $\tau$  was introduced by [1] and later refined by [3], where suitable correction terms needed to be incorporated to make the invariant independent of perturbations. In the process of understanding this new invariant, a connected sum formula was found [2], and computational tools were developed for Dehn surgeries on (2, q)-torus knots [6] as well as for Brieskorn spheres [10, 4, 5]. These papers provide calculation methods for homology spheres obtained by several different cut and paste methods, and the families of examples for which these have yielded calculations show intriguing patterns; they have not, however, led to a conjectural formula for a general Dehn surgeries. It is therefore important to continue exploring the behavior of the invariant under further cut and paste constructions.

# **Recent Developments and Open Problems**

More recently, some results were obtained concerning the behavior of  $\tau$  under the spliced sum construction. Given knots  $K_1$  and  $K_2$  in homology 3-spheres  $M_1$  and  $M_2$ , respectively, the spliced sum of  $M_1$  and  $M_2$  along  $K_1$  and  $K_2$  is the homology 3-sphere obtained by gluing the two knot complements along their boundaries matching the meridian of one knot to the longitude of the other. This operation is a generalization of connected sum; indeed when  $K_1$  and  $K_2$  are trivial knots, the spliced sum of  $M_1$  and  $M_2$  along  $K_1$  and  $K_2$ is none other than the connected sum  $M_1 \# M_2$ .

Casson's invariant  $\lambda_{SU(2)}$ , which is additive under connected sum, is also additive under the more general operation of spliced sum by Boyer and Nicas [8] and independently Fukuhara and Maruyama [9]. Recently, the SU(3) Casson invariant for spliced sums of a (2, p) and (2, q) torus knot  $K_1$  and  $K_2$  in the 3–sphere was computed in [7] as

$$\tau(M) = 16\,\lambda'(K_1)\,\lambda'(K_2),\tag{54.1}$$

where  $\lambda'(K)$  is the SU(2) Casson knot invariant normalized to be 1 for the trefoil.

In this Research in Teams project we set out to extend these splice sum computations to splice sums of arbitrary (p, q) torus knots. The flat moduli spaces of these knot complements, when  $p, q \neq 2$ , is more complicated, having a stratified structure. For this reason, the flat moduli space of such a splice sum is necessarily degenerate, and requires perturbation to obtain a finite collection of points to count to evaluate the invariant.

### **Scientific Progress Made**

To reach our goal for *Research in Teams* of extending formula (54.1) to splice sums of arbitrary torus knots, the following steps were necessary:

- 1. Analyzing the SU(3) representation varieties of the knot complements,
- 2. Determining suitable perturbations and the resulting perturbed moduli spaces, and
- 3. Computing the spectral flow between the perturbed components.

We have completed the first step, both for (p,q) torus knots and for complements of a singular fiber in a 3-fiber Brieskorn sphere. To be more precise, we determined not just the representation varieties but also the restriction maps from the knot group representation varieties for  $X_1$  and  $X_2$  to the representation variety of their common boundary  $T^2$ 

$$R(X_1, \mathrm{SU}(3)) \xrightarrow{r_1} R(T^2, \mathrm{SU}(3)) \xleftarrow{r_2} R(X_2, \mathrm{SU}(3)).$$

In the cases being considered, the maps  $r_i$  are not generally one to one, but have the form of slightly singular fibrations above their images, which are smooth submanifolds of  $R(T^2, SU(3))$ , and the fibration structure only breaks down along a codimension one subset of the image. We verified that the images of  $r_1$  and  $r_2$  meet transversely, for arbitrary torus knots.

Suppose  $r_1$  and  $r_2$  have transverse images in a small neighborhood of  $[\alpha_0] \in R(T^2, SU(3))$ ., and suppose  $\alpha = \alpha_1 \cup_{\alpha_0} \alpha_2$  is nontrivial with  $Stab(\alpha_0) \neq T^2$ ,  $\alpha_i \in R(X_i, SU(3))$ . Set

$$C = \{ [\beta] \in R(M, SU(3)) \mid \beta = \beta_1 \cup \beta_2 \text{ with } \beta_i \in r_i^{-1}(\alpha_0) \text{ and in same component as } \alpha_i \}.$$

We showed that  $C \subset R^*(M, SU(3))$  and C is diffeomorphic to a fiber product of  $r_1^{-1}(\alpha_0) \times r_2^{-1}(\alpha_0)$ with  $S(U(2) \times U(1))/\mathbb{Z}_3$ , and  $\chi(C) = 0$ . This shows that many of the fiber products associated to many intersections contribute zero to  $\tau$ .

A more complicated situation occurs when  $\alpha_0$  is a singular point for one or both of the fibrations  $r_i$ . C is a product of two 2-spheres, at least one of which has a reducible representation on it and is not cut out transversely. This makes it more difficult to determine how this component contributes to  $\tau$  after perturbation.

We verified that, when this happens, we could perturb so that the perturbed moduli space is obtained as a fiber product is taken along smooth fibers, because, after perturbation, the singular points of  $r_1$  don't hit the image of  $r_2$ , and vice versa. We therefore expect the components to resolve into 4 components in the specific case of (2, q) torus knots. This prelimary work demonstrates that the current methods are sufficient to calculate the value of  $\tau$  on fiber sums of arbitrary (p, q) torus knots. To complete the calculation, we must do some book keeping (counting the number of intersections, of the different types), and do complete the spectral flow computations necessary to evaluate the signs and the correction terms. Again, our preliminary work during the week at BIRS indicates that the current methods will handle the needed spectral flow computations.

It had been observed in [5] that the representation variety of the complement of a singular fiber in a Brieskorn sphere has a similar stratified structure to that of the representation variety for a torus knot. In the course of our work, we realized that property that the images of  $r_1$  and  $r_2$  are transverse holds as well in this context. We were able to determine that most of the types of representation variety components for a splice sum of Brieskorn spheres can be handled by the same techniques as we developed for splice sums of torus knots, under a mild restriction on the Seifert invariants. (Unfortunately, the restriction on Seifert invariants precludes our treating 4-fiber Brieskorn spheres as splice sums of singular fibers in 3-fiber Brieskorn spheres, so this class of 3-manifolds remains a wide open challenge, but the allowable Seifert invariants still give many examples of interesting graph manifolds.) Unfortunately, splice sums of knots in nontrivial homology spheres give rise to additional types of fiber product components (involving different orbit types of  $\alpha_1$ ,  $\alpha_2$  and  $\alpha_0$ ) in the flat moduli space, so these Brieskorn sphere examples will require more analysis.

# **Outcome of the Meeting**

In summary, our meeting provided the three participants, who bring three distinct areas of expertise to the problem, the chance to develop common notation, and bring each other up to speed on the different aspects of the problem. Our collaboration has led to dramatic progress on all three steps identified above in calculating the SU(3) Casson invariant for splice sums of arbitrary torus knots. We are currently in the process of writing up a paper with the results on splice sums of torus knots using the workshop notes as a basis.

The meeting also allowed us to understand much more deeply the steps that will be necessary to extend our calculations to splice sums of Brieskorn spheres. Because of different orbit types of the representations that show up in this case, more advanced transversality and spectral flow techniques will be necessary to complete this project, but this line of research was also advanced significantly by our meeting.

### **List of Participants**

**Boden, Hans U.** (McMaster University) **Herald, Chris** (University of Nevada - Reno) **Himpel, Benjamin** (Aarhus University)

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# Chapter 55

# **Universal Higher Extensions (11rit174)**

# Jun 26 - Jul 03, 2011

**Organizer(s):** George Peschke (University of Alberta) Tim Van der Linden (Université catholique de Louvain)

We benefited greatly from the *Research in Teams* workshop at the Banff International Research Station. To explain this, we outline below the before/after-effect which resulted from the opportunity to meet face-to-face and to devote ourselves entirely to the task at hand for the duration of the visit.

# The Situation Before the Visit

In one stream of development, one partner in the project had just achieved an interpretation of group cohomology or Lie-algebra cohomology in terms of higher-dimensional central extensions, as developed by Rodelo–Van der Linden [14, 15]. It extends the classical interpretation of the second group cohomology in terms of equivalence classes of short exact sequences with central kernel. This development builds upon the notion of *semi-abelian category* as in Janelidze–Márki–Tholen [11], and the concept of *higher central extension* developed within the framework of categorical Galois theory based on the work of Janelidze et al. (See [2, 5, 9, 10].) In addition, methods from the theory of simplicial groups are used.

In a parallel and complementary stream of development, the second partner in the project had just achieved a proof of existence of universal *n*-step extensions of modules over an arbitrary unitary ring [12]. This development involves certain higher torsion theories, some potentially noncommutative. It immediately has several applications ranging from

- a torsion theoretic conceptual hindsight explanation for existing computational results about the effect of plus-constructions on the homotopy groups of a space, to
- identifying those groups, respectively Lie-algebras, which have a universal central *n*-extension in the sense of Rodelo–Van der Linden, to
- speculation about probable analogues in other non-abelian categories, notably the category of Πalgebras.

While already a superficial interface between these two developments gives rise to exciting insights, a lot of questions remained unanswered (e.g. how about a constructive description of these abstractly existing

universal central *n*-extensions?). Moreover, as hinted above, a number of further developments appeared promising, but there seemed to be no natural occasion for collaboration. It is this situation which lead us to apply for a *Research in Teams* workshop at BIRS.

# **Scientific Progress Made**

The workshop provided the opportunity for a blend of mutual education and extensive brain storming. As a consequence we now have clear outlines of several projects which are motivated by the two separate developments outlined above. Here is a brief description of these projects.

#### Comonad derived coefficient functors in semi-abelian varieties

A coefficient functor on a semi-abelian variety  $\mathcal{B}$  is detemined by a Birkhoff subcategory  $\mathcal{A}$  and its reflector  $I: \mathcal{A} \to \mathcal{B}$ . We describe these derived functors uniformly using a composite of 'abelianization', followed by 'tensoring over a solid ring'. We hope to describe the composite using a suitable generalization of the non-abelian tensor product introduced by Brown and Loday [3]; the work of Hartl [6] will be helpful here.

### A Quillen model structure for categorical Galois theory?

Here we use categorical Galois theory to define higher order central extensions. We discovered a mechanism by which this kind of categorical Galois theory interfaces with an associated Quillen model category structure [13]. This interface itself is quite unexpected and exciting. At a technical level it provides a nice conceptual context for recent work on the long exact homology sequence of a extension in a purely semi-abelian setting; see Everaert [4]. – Work on the relationship between this long exact sequence and the Serre spectral sequence of the extension is in progress.

#### Homological looping in semi-abelian categories

... is possible via projective presentations. The only problem is that such a projective presentation itself does not lie in the same category as the original object. When the context is suitably enlarged though, the concept makes sense and acts as it should.

#### The derived Yoneda lemma

In module categories Yoneda's lemma has derived versions; see [16, 7, 8]. This result is essential in characterizing higher torsion modules associated to a right exact reflector and, hence, in identifying those modules which are covered by a higher order universal extension; see [12].

However, it is clear that the validity of derived versions of Yoneda's lemma is not restricted to module categories at all. We are expecting such higher versions in more general settings as well, including settings of semi-abelian varieties, where the resulting Ext-groups should classify *higher central extensions* as discussed in [15].

### **Outcome of the Meeting**

We are extremely grateful for the opportunity to work in the *Research in Teams*-setting which BIRS offers to the mathematical community. We found the working environment at the Banff Centre to be ideal; it allows a

period of complete devotion to scientific investigation and collaboration—which is precisely what we needed to get our joint project started.

As explained above, the impact of the week at BIRS on our work is huge. It enabled us to reach far beyond our initial scope, and to develop more of the combined potential of previous works and quite dissimilar backgrounds. We were able to build the foundation for a fruitful collaboration, and this collaboration already gave rise to important new insights in our field.

# **List of Participants**

**Peschke, George** (University of Alberta) **Van der Linden, Tim** (Université catholique de Louvain)

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# Chapter 56

# Approximation theory and harmonic analysis on spheres and related domains (11rit156)

# Jul 17 - Jul 24, 2011

**Organizer(s):** Feng Dai (Department of Mathematical and Statistical Sciences, University of Alberta) Yuan Xu (University of Oregon)

# **Overview of the Field**

There have been continuing researches in approximation theory and harmonic analysis on the unit sphere throughout the last century. For approximation theory, one of the historical highlights is the complete characterization of best approximation by polynomials on the sphere in terms of a modulus of smoothness defined via the spherical means, the accumulation point of decades of works by many authors and finally materialized in [13, 1994]. For harmonic analysis on the sphere, besides the general results that hold for the homogeneous spaces, including the sphere, the essential results are those on multiplier theorems and convergence of projection operators and the Cesàro means in [1, 1972] and [14, 1986].

In recent years analysis on the sphere has been revitalized by applications in applied mathematics, such as earth sciences, computational mathematics and statistics. The topics have fruitful connections with many branches of mathematics, such as numerical integration, computer tomography, coding theory, data fitting, special functions, group representation, spectral theory, random matrices, and differential equations.

# **Recent Developments and Open Problems**

In recent years, there have been several significant development in these two fields:

1. The first significant progress is the introduction of orthogonal polynomials on the sphere for a family of wright functions invariant under a finite reflection group, called the *h*-harmonics, in the work of Dunkl, highlighted by the introduction of the Dunkl operators [11, 1989], a family of commuting first order

differential-difference operators that play the role of differential operators in the ordinary harmonic analysis on the sphere. The study of harmonic analysis in terms of h-harmonic expansions on the sphere was started in [15], but picked up pace only in the past a few years. By now, all results in [1, 14] have been extended to the case of weighted space [5, 6, 7].

- 2. The second one is the realization that *h*-harmonic expansions in the weighted  $L^p$  spaces are closely related orthogonal expansions on the unit ball and on the simplex [16], which lead to significant progress in these two compact domains, of which little quantitative works were known previously. This realization further opens up the possibility of quantitative studies of analysis on the weighted spaces on the sphere for doubling weights [3, 4, 16].
- 3. The modulus of smoothness defined via spherical means have the drawback of difficult, or impossible, to compute, making the results impractical. Ditzian [10, 1997] introduced a new class of moduli of smoothness that has interesting features but does not solve the problem of computability. Only last year, two of the organizers introduced a new modulus of smoothness that essentially reduced many problems in approximation theory on the sphere to the circle, and provides a most satisfactory solution for the problem [8, 9].

All three participants of the Research in Team have been actively involved in the recent developments of these directions.

### **Scientific Progress Made**

The recent development and new results have changed the landscape of approximation theory and (weighted) harmonics analysis. The two participants, Dai and Xu, have been working on a research monograph entitled "Approximation theory and Harmonic Analysis on Unit Sphere", which will be the first research monograph dedicated entirely to this subject. One of the main objectives of the program is for the two authors to discuss the organization and details of the book. Besides the book, the participants in the research team also discussed in depth several research problems, which are listed below.

1. Intertwining operator. This operator, usually denoted by  $V_{\kappa}$ , intertwines between Dunkl operators  $\mathcal{D}_i$ and the differential operator  $\partial_i$  in the sense that  $\mathcal{D}_i V_{\kappa} = V_{\kappa} \partial_i$ . It is known to be a positive linear operator that encodes essential information on the *h*-harmonics. For example, the reproducing kernel  $P_n^h(\cdot, \cdot)$  of the space of *h*-harmonics of degree *n* is given by

$$P_n^h(x,y) = \frac{n+\lambda_\kappa}{\lambda_\kappa} V_\kappa \left[ C_n^{\lambda_\kappa}(\langle \cdot, y \rangle) \right](x), \qquad \lambda_\kappa := \sum \kappa_v + \frac{d-2}{2},$$

which becomes the well-known formula of zonal harmonics for ordinary harmonics when all parameters  $\kappa_v = 0$  and, hence,  $V_{\kappa} = id$ . In the case of the weight function  $w_{\kappa}(x) = \prod_{i=1}^d |x_i|^{2\kappa_i}$ ,  $\kappa_i \ge 0$ , associated with the reflection group  $\mathbb{Z}_2^d$ , the intertwining operator is an integral operator given by

$$V_{\kappa}(x) = c_{\kappa} \int_{[-1,1]^d} f(t_1 x_1, \dots, t_d x_d) \prod_{i=1}^d (1+t_i)(1-t_i^2)^{\kappa_i-1} dt.$$

Currently many deeper results are established only for the case of  $\mathbb{Z}_2$ , such as the critical index of the Cesàro means, because of the availability of this explicit formula of  $V_{\kappa}$ .

The participants discussed in depth how to deduce information of  $V_{\kappa}$ , for reflection groups other than  $\mathbb{Z}_2$ , without knowing explicitly an explicit formula. After applying appropriate cut-off functions, some of the problems reduces to a sharp upper bound of  $V_{\kappa}\chi_{c(x,r)}$ , where c(x,a) denotes a spherical cap

centered at x with radius r > 0 and  $\chi_E$  denotes the characteristic function of E. They also discussed the case of  $V_{\kappa}$  for the group of  $D_3$ , the simplest case beyond  $\mathbb{Z}_2^d$ .

2. The participants also discussed the differential operators  $D_{i,j} := x_i \partial_j - x_j \partial_i$ , which can also be written as partial derivative in terms of the  $\theta_{i,j}$  angle of the polar coordinates in  $(x_i, x_j)$ -plane. These operators are also the infinitesimal operator of the group representation of SO(d). The Laplace-Beltrami operator  $\Delta_0$  on the sphere satisfy a decomposition

$$\Delta_0 = \sum_{1 \leqslant i < j \leqslant d} D_{i,j}^2,$$

which indicates that  $D_{i,j}$  are more primitive than  $\Delta_0$  and, as a result, should encode more information. Their essential presence in the recent work of characterization best approximation on the sphere [8] suggests that they deserve a more through look. As results of the discussions, several new identities are derived and the boundedness of the Riesz transforms defined via  $D_{i,j}$  is established.

3. Another problem being discussed is the proof of the equal area partitions of the sphere, which states that, for each given integer N, the sphere  $S^{d-1}$  can be partitioned into N connected pieces with all pieces having the same area. This is a useful concept that has potential applications in cubature rules and play a role in the recent announced proof on optimal spherical design [2], which states that for each positive integer n there is a cubature rule of equal weight on the sphere  $S^{d-1}$  that uses  $O(1)n^{d-1}$  many points on the sphere. This announced proof is scrutinized but the participants were not able to verify the entire proof.

### **Outcome of the Meeting**

- 1. For the book project, the discussion settled a number of issues, including the treatment of homogeneous spaces, details on multiplier theorems, on operators defined by cut-off functions, on approximation on the sphere, as well as on technical details of *h*-harmonics. As a result of the discussion, the first four chapters of the book are more or less in shape and substantial progresses are made on Chapters 5 and 6.
- 2. The Riesz transforms on the sphere can be defined by  $R_{i,j}f := D_{i,j}(-\Delta_0)^{-\frac{1}{2}}f$ . Making use of an operator defined by a smooth cut-off function, this operator is shown to be weak type (1,1) and, hence, bounded in  $L^p(S^{d-1})$  for 1 .
- 3. Based on the discussions on the intertwining operators, Wang has established a theorem on Cesàro means on the sphere for the weight function w<sub>κ</sub>(x) associated with the group G := G × {e}, where G is any finite reflection group and w<sub>κ</sub> is invariant under G. Let S<sup>δ</sup><sub>n</sub>(w<sub>κ</sub>; f) denote the Cesàro means of the h-harmonic expansions associated with w<sub>κ</sub>. The new result states that

(1) For all 
$$1 \leq p \leq \infty$$
,

$$\sup_{n \in \mathbb{N}} \|S_n^{\delta}(w_{\kappa}; f)\|_{\kappa, p} \leq c \|f\|_{\kappa, p} \text{ for all } f \in L^p(w_{\kappa}; S^{d-1})$$
  
if and only if  $\delta > \lambda_{\kappa} := \frac{d-1}{2} + \sum_{v} \kappa_{v}.$   
(2) Let  $1 satisfy  $|\frac{1}{p} - \frac{1}{2}| \ge \frac{1}{2\lambda_{\kappa} + 2}$ . If$ 

$$\sup_{n \in \mathbb{N}} \|S_n^{\delta}(w_{\kappa}; f)\|_{\kappa, p} \leqslant c \|f\|_{\kappa, p} \text{ for all } f \in L^p(w_{\kappa}; S^{d-1}),$$

then

$$\delta > \lambda_{\kappa} := \max\left\{ \left(2\lambda_{\kappa} + 1\right) \left| \frac{1}{p} - \frac{1}{2} \right| - \frac{1}{2}, 0 \right\}.$$

# **List of Participants**

Dai, Feng (Department of Mathematical and Statistical Sciences, University of Alberta)Wang, Heping (Capital Normal University ( Beijing China))Xu, Yuan (University of Oregon)

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# Chapter 57

# **Probabilistic and Statistical Properties** of Stochastic Volatility Models (11rit160)

# Sep 04 - Sep 11, 2011

Organizer(s): Rafal Kulik (University of Ottawa) Philippe Soulier (Université Paris Ouest)

## **Overview of the Field**

One of the standardized features of financial data is that log-returns of stock prices are uncorrelated and possibly heavy tailed, but their squares, or absolute values, are (highly) correlated. Furthermore, data exhibit heteroskedasticity and leverage. In the financial time series context, leverage is understood to mean negative dependence between previous returns and future volatility (i.e. a large negative return will be followed by a high volatility).

To model such phenomena, Robert Engle introduced the ARCH (AutoRegressive Conditionally Heteroscedastic) family, further extended to G(eneralized)ARCH. His work was rewarded with the Nobel Prize in Economics (2003). This model is now well understood but fails to capture the long memory property of squares. However, recent applications are focused on models with long memory in squared log-returns. Therefore we deal in our project with models of the form

$$Y_i = \sigma(X_i) Z_i , \qquad i \ge 1 ,$$

where  $Z_i$  are independent, identically distributed random variables, and  $X_i$  is a long memory process with a memory parameter (Hurst parameter) H. If  $X_i$ ,  $i \ge 1$ , and  $Z_i$ ,  $i \ge 1$ , are independent, then the model is called the Long Memory in Stochastic Volatility (LMSV) process. In general, there is no independence assumption and the models are referred to as the Stochastic Volatility with Leverage process.

In order to model the high variability of financial data, it is assumed that  $Z_i$  are in the domain of attraction of the Fréchet law, i.e. as  $x \to \infty$ ,

$$P(|Z| > x) = x^{-\alpha}L(x),$$

where  $L(\cdot)$  is a function that is slowly varying at infinity.

Although models such as the LMSV process introduced above, and also EGARCH, LARCH, FIGARCH processes, are widely used in practice, there is little understanding of their probabilistic structure, especially if

heavy tails are involved, whereas, in contrast, there is a wealth of results on partial sums, sample covariances or parameter estimation for linear processes with finite or infinite moments, with short or long memory. There is also a number of publications on ARCH-type models, which exclude long memory.

# **Recent Developments and Open Problems**

Tools used in this area involve the deep theory of dependent sequences, point process techniques and time series analysis. Davis and Mikosch (2001) established point process convergence for the stochastic volatility process without long memory. This convergence yields the convergence of partial sums and sample covariances. Surgailis and Viano (2002), using specific techniques of strongly dependent time series, dealt with partial sums in a special case of stochastic volatility model with leverage and finite variance. Surgailis (2008) studied partial sums of LARCH( $\infty$ ) processes with heavy tails.

As for statistical inference, Hurvich et al. (2005) studied estimation of the memory parameter, whereas Kulik and Soulier (2011) established limit theorems for the tail empirical process based on heavy tailed LMSV models. As a consequence, they obtained the asymptotic normality of the Hill estimator of the tail index of the marginal distribution.

However, to the best of our knowledge, there are no results for sample covariances, in the case of stochastic volatility models with both long memory and heavy tails, and possible leverage. The only available result on partial sums is the one established in Surgailis (2008).

### **Scientific Progress Made**

During the meeting we focused on two topics, finishing the paper entitled *Limit theorems for long memory* stochastic volatility models with infinite variance: Partial Sums and Sample Covariances.

We established limit theorems for partial sums and sample covariances for stochastic volatility models with long memory, heavy tails and possible leverage. The basic idea is to decompose these statistics into a martingale part and a long memory part. Convergence of the first part is treated using the point process methodology. As for the long memory part, we apply existing tools available for subordinated long memory processes. In due course, however, one has to establish many new technical results, which are of independent interest.

Interestingly, although the leverage does not have any effect on the asymptotic behaviour of partial sums, it may have a significant effect on the sample covariances. The rates of convergence and limiting distributions may differ in a non trivial way between the models with or without leverage.

# **Outcome of the Meeting**

Based on the scientific progress described in the previous section, we were able to finish our paper on sample covariances for stochastic volatility models, see Kulik and Soulier (2011b). The paper has been submitted to *Advances in Applied Probability* and posted on arxiv, arXiv:1109.5298.

As mentioned above, the presence of leverage is a significant property of the data. From a theoretical point of view, it has an effect on the asymptotic behaviour of certain statistics. Hence, during the meeting, we started to investigate tests for leverage effects based on sample covariances-type statistics.

# Note

The participants would like to thank BIRS for hospitality. It was for both of us a great opportunity to focus on research for the entire week.

# **List of Participants**

Kulik, Rafal (University of Ottawa) Soulier, Philippe (Université Paris Ouest)

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# Summer School Reports

Summer School Reports

# Chapter 58

# **Advanced Mathematical Methods to Study Atmospheric Dynamical Processes and Predictability (11ss065)**

# Jul 10 - Jul 15, 2011

**Organizer(s):** Craig Bishop (Navy Research Laboratory Monterey) Sarah Jones (University of Karlsruhe, Institute for Meteorology and Climatology) Thomas Jung (European Centre for Medium-Range Weather Forecasts) Istvan Szunyogh (Texas A & M University) Olivier Talagrand (Laboratoire de Meteorologie Dynamique / Ecole Normale Suprieure) Heini Wernli (ETH Zurich)

# Introduction

The summer school was organized by the Dynamical Processes and Predictability Working Group (PDP WG) of THORPEX<sup>1</sup>. THORPEX is a 10-year international research and development program to accelerate improvements in the accuracy of one-day to two-week high impact weather forecasts for the benefit of society, the economy and the environment. The PDP WG provides the connection between the operational weather prediction and the academic communities in THORPEX. The summer school was organized for early career scientists working on mathematically challenging problems of weather prediction or mathematical problems which are highly relevant for weather forecasting.

The physical model of the atmosphere is a high-Reynolds-number, stratified fluid, which can be treated as an ideal fluid except for a narrow boundary layer at the surface of the Earth. Mathematical models of the atmosphere are typically based on the Eulerian equations of fluid dynamics. Since the independent variables in these differential equations are the spatial location and the time, the equations are partial differential equations. Analytical solutions to these equations exist only for very special initial and boundary conditions [35]; thus, the solution of the equations requires a numerical solution strategy for any realistic initial and boundary conditions.

The computer code implementation of a particular numerical solution strategy is called a (numerical)

<sup>&</sup>lt;sup>1</sup>http://www.wmo.int/pages/prog/arep/wwrp/new/thorpex\_new.html

model. In addition to weather prediction, atmospheric models are also employed to simulate and predict changes in the climate, and to monitor and predict changes in the chemical composition of the atmosphere. As the skill of the models is continuously tested by operational forecast applications, *numerical weather prediction models provide the consistently most accurate solutions of the atmospheric governing equations for realistic initial conditions*. Hence, forecast models provide a unique opportunity to study the behavior of a truly complex physical system.

# **Overview of the Field**

The atmosphere is one of the most intensely studied complex physical system, which is, in large part, motivated by the never-ending quest for improved numerical weather prediction techniques. The development of such techniques has greatly benefitted from advances of applied mathematics. In return, the search for improved weather prediction techniques stimulated new research in dynamical system theory. Perhaps the best known example for atmospheric research that led to important developments in mathematics is the work by the late meteorologist Edward Lorenz<sup>2</sup>, who was the first to use computer-aided simulations to explore the qualitative behavior of a dynamical system. His work played an important role in the emergence of the discipline of dynamical systems theory. A more recent example for a development in dynamical systems theory that was motivated by a practical problem of numerical weather prediction is the emergence of efficient computational algorithms for the estimation of Lyapunov vectors [19, 46]. While the development of these algorithms was motivated by practical challenges in operational ensemble weather forecasting, they are expected to play an important role in the investigation of such fundamental issues as the hyperbolicity of dynamical systems. Another recent example for atmospheric research leading to mathematical results of broader interest is the emergence of techniques to quantify the spatio-temporal propagation of information in complex physical systems. [28, 34].

Due to the time constraint imposed by the 5-day length of the summer school, the organizers had to be selective when choosing the particular topics covered by the summer school. Thus the present summary should be viewed as a collection of some of the most important and mathematically challenging research problems in weather forecasting rather than a comprehensive review of recent mathematical developments with some significance for the atmospheric sciences. In addition to lectures that were designed to provide an overview of the mathematical foundation of atmospheric modeling, covering such basic topics, as the derivation of the partial differential equations that govern atmospheric motions<sup>3</sup> and the relevant basics of dynamical systems theory,<sup>4</sup> the emphases were placed on such rapidly developing subjects, as the assimilation of observed information into the model initial conditions and the quantitative prediction of the spatio-temporal evolution of influences in the model forecasts.

# **Presentation Highlights**

#### Heini Wernli: Potential Vorticity

Potential vorticity (PV) is a fundamental quantity of balanced flow dynamics. In essence, PV is defined as the scalar product between the absolute vorticity vector and the gradient of the potential temperature field. For adiabatic and frictionless motions (e.g., in cloud-free areas in the tropopause region) the PV is materially conserved. Moreover, according to the so-called invertibility principle, the distribution of PV anomalies in the interior of the atmosphere together with suitable boundary conditions (e.g., the surface potential temperature field) can be inverted in to obtain the balanced flow associated with the anomalies. The

<sup>&</sup>lt;sup>2</sup>1917-2008

<sup>&</sup>lt;sup>3</sup>John Methven: 'Atmospheric Dynamics: Equations and Wave Phenomena' 'Atmospheric Dynamics: Effects of Moisture'

<sup>&</sup>lt;sup>4</sup>Eward Ott: 'Introduction to Chaotic Dynamics'.

third essential aspect of PV is related to its diabatic production or destruction. PV thereby provides a unique framework to investigate the mutual relationship between diabatic processes (e.g., cloud condensation) and the large-scale atmospheric flow.

The lecture first introduced the definition of PV, its typical atmospheric values and the climatological mean structure of atmospheric PV. The main characteristics (material conservation, invertibility and diabatic effects) have been discussed and illustrated with examples from the literature and a case study of a North Atlantic cyclone. In the final part of the lecture, a series of classical papers on the theory and application of PV has been briefly reviewed starting with the historical paper [29] and seminal paper [23] that led into the decades of "PV thinking" and provided a novel concept for understanding extratropical cyclogenesis. Also discussed was the paper [8], which pointed out the conceptual analogy between PV thinking and classical electrostatics, underlining the fundamental physical significance of the PV concept. Finally, the papers [21, 22, 41], which discuss the PV concept from a flux-form perspective, were mentioned.

# Peter Lynch: The Emergence of Numerical Weather Prediction: from Richardson to the ENIAC

The development of computer models for numerical simulation of the atmosphere and oceans is one of the great scientific triumphs of the past fifty years. These models have added enormously to our understanding of the complex processes in the atmosphere and oceans. The consequences for humankind of ongoing climate change will be far-reaching. Earth system models are the best means we have of predicting the future of our climate.

The basic ideas of numerical forecasting and climate modeling were developed about a century ago, long before the first electronic computer was constructed. However, advances on several fronts were necessary before numerical prediction could be put into practice. A fuller understanding of atmospheric dynamics allowed the development of simplified systems of equations; regular observations of the free atmosphere provided the initial conditions; stable finite difference schemes were developed; and powerful electronic computers provided a practical means of carrying out the calculations required to predict the changes in the weather.

In his lecture, P. Lynch traced the history of computer forecasting from Richardsons prodigious manual computation [32], through the ENIAC (Electronic Numerical Integrator and Computer) integrations [33] to the early days of operational numerical weather prediction and climate modeling [20]. The useful range of deterministic prediction is increasing by about one day each decade. This talk had set the scene for the story of the remarkable progress in weather forecasting and in climate modeling over the past fifty years, which was treated in subsequent lectures.

### Dale Durran: Strengths and Weaknesses of Common Numerical Methods for Simulating Atmospheric Flows

This presentation focused on key properties of broad categories of numerical schemes as they relate to modeling atmospheric flows. These categories included spatially discrete (finite difference and finite volume) methods, truncated series expansions (spectral, pseudo-spectral and finite elements), hybrid methods (spectral element and discontinuous Galerkin) and the fluid dynamical viewpoint used to formulate the governing equations (Eulerian, Lagrangian and semi-Lagrangian). Specific topics addressed in this general context included: (i) the utility of high order methods, (ii) when it is necessary to avoid overshoots and undershoots in scalar conservation laws (and strategies to achieve this), (iii) the sense in which discontinuous Galerkin methods are high-order finite volume schemes and the potential advantages of this approach on MPI computer architectures, and (iv) the relation between large time steps and the CFL condition in semi-Lagrangian methods. An up-to-date comprehensive treatment of the topic can be found in the recent edition of the standard textbook [17] by the lecturer.

#### Peter Lynch: Balance in the Atmosphere: Implications for NWP

Earth's atmosphere is in a constant state of near balance. There are many instances where large forces nearly cancel each other: the vertical attraction due to gravity is almost exactly balanced by the vertical gradient of pressure; the horizontal pressure force is approximately equal and opposite to the effective force due to the Earth's rotation; and so on. When the equilibrium is disturbed, extreme weather may result on a short time scale, or substantial changes in climate regime over longer periods. The lecture looked at some of the close balances in the atmosphere and considered what happens when they are disturbed.

The spectrum of atmospheric motions is vast, encompassing phenomena having periods ranging from seconds to millennia. The motions of interest to the forecaster typically have timescales of a day or longer, but the mathematical models used for numerical prediction describe a broader span of dynamical features than those of direct concern. For many purposes these higher frequency components can be regarded as noise contaminating the motions of meteorological interest. The elimination of this noise is achieved by adjustment of the initial fields, a process called initialization. The lecture reviewed the principal methods of initialization and considered their relative merits. An up-to-date description of these methods can be found in [32].

#### **Olivier Talagrand: Introduction to Data Assimilation**

Data Assimilation, which originated from the need of defining initial conditions for Numerical Weather Prediction, is the process by which observations of the atmosphere or the ocean are combined together with a numerical model of the dynamics of the flow in order to determine as accurately as possible the state of that flow.

All the information that is used in assimilation (observations and model) will always be affected with some uncertainty, which will propagate to the final estimate. From a theoretical point of view, it is convenient to consider assimilation as a problem in Bayesian estimation, viz., determine the conditional probability distribution for the state of the flow, conditioned by the available information [27, e.g.]. Because of the very large numerical size of the problem, and of the poor knowledge of the uncertainty affecting a large part of the available information, Bayesian estimation is impossible in practice. The notion of Bayesian estimation is nevertheless very useful in that it provides guidelines for continuous research and development.

In most algorithms used at present for assimilation, a background estimate coming from the past is updated with new observations. Most algorithms are heuristic extensions to mildly nonlinear situations of statistical linear estimation, which achieves Bayesian estimation in the circumstances when the link between the data and the unknowns is linear, and the errors affecting the data are additive and gaussian. Two large classes of algorithms exist at present. In sequential assimilation, the optimal form of which is Kalman Filter, the background produced by the assimilating model is constantly updated with new observations. In variational assimilation, the model is globally adjusted to the background and to the observations available over a period time. Both those classes of algorithms were described in later lectures.

A third class of algorithms, the particle filters, are independent of any linear or gaussian hypothesis. Particle filters evolve an ensemble of points in state space that are meant to sample the current conditional probability distribution for the state of the flow. The ensemble is updated with new observations according to Bayes rule on conditional probabilities. Particle filters for atmospheric and oceanic applications are actively studied [45]. One major difficulty is at present their high numerical cost [42]. Data assimilation, from its origin in Numerical Weather Prediction, has progressively extended to many diverse applications in geophysical sciences, and is related to many aspects of, among others, probability theory, dynamical systems and stability theory, and algorithmics.

#### Pierre Gauthier: 3D and 4D variational data assimilation

All major operational weather prediction centers use variational schemes for data assimilation. Most of the operational systems are based on the 4D formulation: the first 4D system was introduced by the European Centre for Medium Range Weather Forecasts (1997) and was followed by Meteo-France (2000), UK Met Office (2004), Japan Meteorological Agency (2005), Meteorological Service of Canada (2005) and the Fleet Numerical Meteorological and Oceanography Center (2009). The 4D-Var approach allows for an inclusion of a digital filter initialization procedure in the data assimilation process [18], an online observation quality control procedure [25, 1, 26] and an online observation bias correction procedure for satellite radiances [16, 14, 2]. Current implementations of 4D-Var do not include an explicit representation of the effects of model errors on the background.

The most intense ongoing research and development efforts focus on introducing an online estimation of the model errors into the data assimilation algorithms. Since these algorithms do not use the model as a strong constraints, that is, they do not assume that the model provides a perfect representation of the dynamics, they are called weak-constraint 4D-Var schemes. While the general idea of weak-constraint 4D-Var is not new [40], the search for specific schemes that could be applied in practice started only very recently[44, 43]. Another interesting development is the growing interest in ensemble-based variational schemes [9, 10].

#### Istvan Szunyogh: Ensemble-based Kalman Filters

The first correct formulations of Ensemble-based Kalman Filter (EnKF) schemes were published in 1998 [24, 11]. EnKF schemes rapidly became the most popular class of data assimilation schemes in academic research, as the development of a high-quality EnKF-based data assimilation system is a more feasible than the development of a 4D-Var scheme for a small academic research group. The relative simplicity of an EnKF-based system is due to the general features of EnKF scheme that (i) they provide a straightforward, computationally efficient approach to obtain spatio-temporally varying estimates of the background error covariance and (ii) do not require the availability of a code of the tangent-linear dynamics and its adjoint and a code of the linearized observation operator and its adjoint.

EnKF schemes restrict all calculations to the linear space spanned by the ensemble perturbations, which are defined by the difference between the members of a background ensemble and the ensemble mean of the background. The key assumption made by all practical implementations of EnKF schemes is that a sufficiently accurate correction to the background state estimate can be made in the low-dimensional linear space spanned by a small ensemble of forecasts. (Without making this assumption, the computation cost of an EnKF scheme would be unaffordable in practice.) The results of a large number of independent numerical experiments suggest that the background error covariance, or at least its flow-dependent part, can be efficiently estimated by a small, operationally affordable, ensemble. These results has generated a growing interest in ensemble-based schemes at the operational centers. At the time of the summer school, all major operational schemes. These schemes employ an ensemble to estimate the flow-dependent part of the background error and use a variational approach to find the minimizer of the cost function.

Similar to the situation with variational schemes, finding efficient mathematical algorithms for the estimation and representation of errors in the model dynamics in ensemble-based schemes is a major theoretical and practical challenge [6, 5, 15]. In addition, while efficient algorithms for the estimation of observation bias, whose availability is essential for the gainful assimilation of satellite radiances, exist for the variational schemes [16, 14], observation bias correction schemes for the EnKF schemes are in their infancy[37, 4].

### Edward Ott: Using a limited area model to enhance global analyses

E. Ott proposed a data assimilation scheme that produces the analyses for a global and a nested limited area model simultaneously, considering forecast information from both model. The proposed scheme minimizes a cost function in which the control variable is the joint state of the global and the limited area model. The initial results obtained with idealized models are very encouraging: the scheme led to an improvement of both the global and the limited area analyses compared to the case where the state of the two models were analyzed independently [47].

### Craig Bishop: Observational network design and the forecast error variance reduction due to observations

In this talk, Craig Bishop began by describing how, in principle, the Kalman filter could be used to quantitatively predict the reduction in analysis and forecast error variance due to supplemental targeted observations. Noting that the computational costs of the Kalman filter are prohibitive in atmospheric and oceanic applications, he went on to describe how an approach known as the Ensemble Transform Kalman Filter (ETKF) [7, 36] provides predictions of the reduction in analysis and forecast error variance due to supplemental targeted observations in the same way as the Kalman filter but at a much lower computational cost. The cost saving is obtained via the assumption that the forecast error covariance can be perfectly described by the perturbations of a K-member ensemble forecast - where K is much smaller than both the number of observations and the number of state variables. Another assumption of the ETKF theory is that the square root of forecast error covariances conditioned on the assimilation of targeted observations can be represented in terms of an ensemble that is a linear transformation of the original or raw ensemble. The cost saving enabled by these assumptions and associated mathematical analysis enables the ETKF to compute the forecast error variance associated with a very large number of specific deployments of observational resources in a short amount of time. The technique has been used over the last decade at the National Centers Environmental Prediction Center Winter Storms Reconnaissance program to direct aircraft to locations where observations are likely to reduce the error in 2 to 4 day forecasts of high impact winter weather over the contiguous United States and Alaska. It has also been used to direct Underwater Autonomous observation Vehicles (UAVs) in oceanographic experiments. Methods to quantify the accuracy of ETKF predictions of the reduction in forecast error variance were discussed and shown to have been qualitatively correct in the Winter Storms Reconnaissance program. Craig concluded by noting that much work was still needed in order to achieve the ultimate aim of making such predictions of forecast error variance reduction due to supplemental observations quantitatively accurate.

#### Craig Bishop: Uncertainty quantification in geophysical systems

In this talk, Craig Bishop began by noting that although some aspects of the uncertainty in forecasts for geophysical systems, such as observation error variance, could be empirically quantified, chaos rendered flow-dependent forecast error variance formally unobservable. To better understand the distribution of true error covariances given a single imperfect ensemble covariance, he considered an idealized univariate model in which Bayes' theorem could be used to derive the distribution of true error variances given an imperfect ensemble variance. He went on to note that advanced regression techniques could be used to derived all of the parameters defining this model from a large number of realizations of (innovation, ensemble-variance) pairs. Consequently, the analysis provides a new (1st) method for estimating (a) the climatological pdf of true error variances, (b) the pdf of ensemble variances given a true error variance, and (c) The Posterior pdf of true error Variances Mean (PVM). The equation for this PVM of this distribution showed that a Hybrid error variance formulation that linearly combines a climatological estimate of the error variance with a flow-dependent ensemble based estimate was more accurate than estimates based solely on ensemble variances or estimates

based solely on static climatological variances. The approach assumed that the climatological distribution of true error variances was an inverse-gamma distribution and that the distribution of ensemble variances given a single true error variance was a gamma distribution. To help explain and justify this approach a "replicate Earth" paradigm was realized with the help of an application of the Ensemble Transform Kalman filter applied to Lorenz's (2005) simple model 1. The theoretically derived weights were then applied to the newly built Navy-Hybrid-4DVAR scheme. The forecast performance using the theoretical weights was found to be as good as that from weights obtained from a much more computationally expensive brute force tuning method. Thus, the new theory provided a justification for the Hybrid plus tools to facilitate its implementation.

#### **Olivier Talagrand: Verification of Probabilistic Forecasts**

Accepting that the purpose of probabilistic prediction is to describe our uncertainty on the future state of the atmosphere, an obvious question is the following. How is it possible to objectively (and, if possible, quantitatively) evaluate the degree to which that purpose has been achieved ? In particular, how is it possible to objectively compare the performance of two different methods for probabilistic prediction ? Except in rather extreme situations, it is not possible to say anything as to the quality of a particular probabilistic forecast, and objective validation of probabilistic forecasts can only be statistical. The point of view taken here is that is the quality of a probabilistic prediction system lies in the conjonction of two different properties. The first property is reliability, i. e., statistical consistency between the a priori predicted probabilities and the a posteriori observed frequencies of occurrence (it rains with frequency 40% in the circumstances when rain has been predicted to occur with probability 40%). In general terms, reliability is the property that, for any predicted probability distribution F, F(F) = F. where F(F) is the observed frequency distribution in the circumstances when F has been predicted. The second quality, which can be called resolution (it is also called sharpness) is that the reliably predicted probability distributions are mutually distinctly different (in the case of a binary event, the reliably predicted probabilities of occurrence are close to either 0 or 1). Both reliability and resolution can be objectively evaluated, provided a large enough number of realizations of the prediction system is available. A number of (non mutually equivalent) diagnostic tools and scores are commonly used for that purpose : as concerns reliability, reliability diagrams (for events), rank histograms and Reduced Centred Random Variable (for variables) ; as concerns resolution, Relative Operating Characteristics curve (for events). The Brier score (defined for events), and its generalization the Ranked Probability Score (defined for variables), decompose into a reliability and a resolution components. These various scores and diagnostic tools show over the years a slow but steady improvement of the quality of operational Ensemble Prediction Systems. The various scores saturate for ensemble sizes on the order of a few tens of units. The speed of saturation does not depend on the values of the scores, but on the dispersion of the predicted probabilities. The larger the dispersion, the faster the saturation (this can be shown analytically on the Brier score). The reason for the rapid saturation is that, because of the unavoidably limited size of the validation sample, only probabilistic forecasts for the occurrence of events or for values of one- or two-dimensional variables can be reliably validated. This suggests that using larger-size ensembles would be useless.

#### **Dale Durran: Mesoscale Predictability**

The classic Lorenz [31, 39] and the Anthes [3] viewpoints about mesoscale predictability were discussed and contrasted. More recent results involving the influence of the conditions imposed at the lateral boundaries of a mesoscale domain and the upscale influence of convection were reviewed. The focus then shifted to the question of whether the flow is more predictable over complex terrain.

Despite earlier research suggesting complex terrain might improve predictability, and that downslope windstorms in particular might be predictable well in advance, the recent evidence presented by the author and collaborators suggests otherwise [38]. In particular, ensemble simulations for two cases from the TREX experiment show that the development of strong downslope winds in the lee of the Sierra Nevada can be very

sensitive to small perturbations in the initial conditions at forecast lead times of less than 6 to 12 hours.

Ensemble simulations of lowland snow in the Puget Sound region of the Pacific Northwest also showed high sensitivity to initial conditions at lead times as short as 36 hours. Uncertainties associated with micro-physical and boundary-layer parameterizations were side-stepped in this analysis by linking the snow forecast to the 850-hPa temperature during times of precipitation.

#### Peter Lynch: Laplace Transform Integration of the Shallow Water Equations

P. Lynch described a filtering integration scheme, which used a modification of the contour used to invert the Laplace transform (LT). It was shown to eliminate components with frequencies higher than a specified cut-off value. Thus it is valuable for integrations of the equations governing atmospheric flow. The scheme was implemented in a shallow water model with an Eulerian treatment of advection [12]. It was compared to a reference model using the semi-implicit (SI) scheme. The LT scheme was shown to treat dynamically important Kelvin waves more accurately than the SI scheme.

A model that combined the Laplace transform (LT) scheme with a semi- Lagrangian advection scheme in a shallow water model was also considered [13]. It was compared to a reference model using the semiimplicit (SI) scheme, with both Eulerian and Lagrangian advection. It was shown that the LT scheme was accurate and computationally competitive with these reference schemes. It was also shown, both analytically and numerically, that the LT scheme was free from the problem of orographic resonance that is found with semi-implicit schemes.

## **List of Participants**

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