

Kadison–Singer Problem Solved

By Dana Mackenzie

What is the best kind of mathematical problem? Does it resemble a distant mountaintop, beckoning people from far and wide to attack the summit, simply “because it’s there”? Or is it like a vast subterranean river, connecting different realms of mathematics, mysteriously disappearing below the surface and reappearing where you least expect it?

Proponents of either kind of problem have a good case. But this year, it was the turn of one of the great subterranean rivers of mathematics to emerge into the limelight. In June, a three-member team of mathematicians and computer scientists posted a proof online for the Kadison–Singer conjecture (sometimes called, more accurately, the Kadison–Singer problem). It’s a problem whose source lies in the forbidding uplands of C^* -algebras and quantum physics. But through the 1990s and 2000s, it kept surfacing in other places. It meandered through operator theory, complex analysis, graph theory, and signal processing, before finding a formulation as a seemingly simple problem in finite-dimensional geometry.

As Dan Spielman of Yale University explains it, he got interested in the Kadison–Singer problem partly by accident. In 2009, he published a paper with two former students, Nikhil Srivastava and Joshua Batson,

on sparsification of graphs. Graphs, in this context, are networks, most likely very large and somewhat random. A good example is the Internet or Facebook. To understand networks, graph theorists ask questions like: What are the cliques? If the edges have distances or weights on them, what is the shortest path that visits every node (the traveling salesman problem)? These are very difficult questions to answer for a typical dense network, with a large number N of nodes and an even larger number (proportional to N^2) of links. It would be very useful for certain applications to replace a dense network with a simpler approximation—a network whose total number of links is proportional to N but that would nevertheless have a similar overall structure.

A widely used tool for measuring the similarity of graphs is the spectrum of the Laplacian operator of the graph. This is a discrete analogue of the differential Laplacian operator that mathematicians and physicists have used for two centuries to describe objects in the plane, in space, and in higher dimensions. The classical problem of “hearing the shape of a drum” asks what the eigenvalues (or spectrum) of the Laplacian reveal about the shape of a space. Analogously, the goal of sparsification is to create a network that “sounds” like another one but is much simpler.

Sparse approximations of the “complete graph,” a network of N vertices in which every vertex is connected to every other, had been known for some time. These approximations have proved incredibly useful in computer science and engineering; for example, they have been used to construct error-correcting codes, hash functions for cryptography, and pseudo-random number generators. Spielman, Srivastava, and Batson had generalized this result to show the existence of approximations for any graph. Their usefulness, however, was limited by the fact that the researchers could not control the weights on the edges.

When Spielman told him about the work, Gil Kalai of the Hebrew University of Jerusalem remarked that their theorem sounded a lot like one version of the Kadison–Singer problem. In fact, the Kadison–Singer conjecture, if true, would give Spielman’s group the control over the edge weights that had been missing.

A couple months later, Adam Marcus arrived at the Yale mathematics department; a newly minted PhD, he was looking for a new project to work on. Spielman suggested the Kadison–Singer problem, which, he says, got Marcus “very excited.” The two of them started collaborating with Srivastava, who now works at Microsoft Research in India. Little did they suspect that it would take five years of hard work to get an answer. “But they were rewarding years,” Spielman says. “We kept feeling as if we were making progress. It was like a computer video game, giving you just enough information to keep you working on it.”

The original version of the Kadison–Singer problem looks about as unrelated to graph theory as a problem could possibly be. What Richard Kadison and Isadore Singer asked in 1959 is whether “pure states” on abelian von Neumann algebras could be extended uniquely to pure states on non-abelian algebras.

The question almost defies translation into simple English, but let’s give it a shot. We can think of the elements of a von Neumann algebra as infinitely large matrices. In quantum physics, they would be observable quantities, such as position, momentum, or spin. A state is a function of

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2013 SIAM Elections

Meet the 2014 SIAM Leadership

As of January 1, L. Pamela Cook of the University of Delaware is SIAM’s president-elect. Cook served as SIAM vice president for publications in 2012 and 2013 (an appointed position left vacant by her election). A SIAM Fellow, class of 2009, she will begin a two-year term as SIAM president on January 1, 2015, succeeding Irene Fonseca.

The membership also chose several other new officers and board and council members, all taking office on January 1.

Daniel Szyld, a professor in the Department of Mathematics at Temple University, was elected vice president at large, succeeding Nicholas Higham, who had held the position since 2010. Simon Tavener of Colorado State University was elected to a second term as SIAM secretary.

Randall LeVeque of the University of Washington was elected to the Board of Trustees. C.T. (Tim) Kelley of North Carolina State University and Robert Kohn of the Courant Institute, New York University, were elected to the board for second terms; as in 2012, Kelley was elected board chair at the group’s December 2013 meeting.

Liliana Borcea of the University of Michigan and Felix Otto of the Max Planck Institute for Mathematics in the Sciences were newly elected to the SIAM Council, while Angelika Bunse-Gerstner of Universität Bremen and Oscar Bruno of the California Institute of Technology were re-elected to their seats on the council.

Cynthia Phillips of Sandia National Laboratories, recently appointed vice president for programs, succeeded Sven Leyffer on January 1.

Members of the board and council for 2014,

including elected and appointed officers who serve ex officio (*), are:

Board: Kathryn Brenan (Aerospace Corp.), Lisa Fauci (Tulane University), Irene Fonseca* (Carnegie Mellon University), Samuel Gubins* (Annual Reviews), Mary Ann Horn (Vanderbilt University), Tim Kelley, Tamara Kolda (Sandia), Robert Kohn, Randall LeVeque, George Papanicolaou (Stanford University), Jeffrey Saltzman (AstraZeneca), Fadil Santosa (University of Minnesota), and Robert Schreiber (Hewlett Packard Laboratories).

Council: Michele Benzi (Emory University), Liliana Borcea, Oscar Bruno, Angelika Bunse-Gerstner, Pam Cook*, Timothy Davis (University of Florida),

Lawrence Craig Evans (University of California, Berkeley), Irene Fonseca*, Thomas Grandine* (The Boeing Company), Andreas Griewank (Humboldt Universität Berlin), Samuel Gubins*, Bruce Hendrickson (Sandia), Thomas Hou (Caltech), Rachel Kuske (University of British Columbia), C. David Levermore* (University of Maryland), Felix Otto, Cynthia Phillips*, Simon Tavener*, Daniel Szyld*, Peter Turner* (Clarkson University), and Carol Woodward (Lawrence Livermore National Laboratory).



Felix Otto



Liliana Borcea

SIAM thanks those whose terms ended in 2013: board member Stephen Wright; past president Nick Trefethen and vice presidents Nick Higham and Sven Leyffer; and council members Margot Gerritsen and Mary Silber.

The Evolution of SDM, a Premier Data Mining Conference

By Chandrika Kamath

Now in its 14th year, the SIAM International Data Mining Conference has evolved into a well-established and highly regarded meeting. A recent ranking of data mining conferences* lists SDM as second only to the longer running, and much larger, Knowledge Discovery and Data Mining (ACM KDD) conference, in terms of the average number of citations per paper. KDD, which has accepted 1212 papers since its start in 1995, has 18.8 citations per paper, while SDM, which held its inaugural meeting in 2001, has 611 papers, with an average of 11.0 citations per paper.

This is indeed good news for both SDM and SIAM. The credit goes largely to the authors and the tireless efforts of the program chairs and program committee members, who each year carefully review the nearly 400 submissions and select the best for presentation at the meeting. As the conference papers are available online (<http://www.siam.org/proceedings/>), they are widely accessible through search engines, making the latest research in the field accessible at one’s fingertips.

SDM is unique among data mining conferences in focusing on the mathematical and statistical aspects of the field. Held in cooperation with the American Statistical Association, it is smaller than other data

mining conferences, typically attracting 250–300 participants from universities, industry, and national laboratories, in a multitude of countries. Student-oriented activities, such as the doctoral forum, have enabled many students to attend their first conference, where they have the opportunity to present their work and receive feedback from a friendly audience. The size of the meeting is conducive to informal interactions among participants; an evening reception, held in conjunction with the poster session, provides a venue for networking, as many participants prefer posters to talks as a medium for exchanging ideas. Travel support from the National Science Foundation, SIAM Student Travel Awards, IBM Research, and Google have been invaluable in making SDM accessible to students.

From a technical viewpoint, SDM has evolved over the years, keeping current with a rapidly changing field. The focus in the early years was on techniques like association rules and on applications in science and business. This evolved into an emphasis on the mining of text documents, prompted by the need to search web pages, and bio-informatics, motivated by the sequencing of the human genome. More recently, algorithms for analyzing complex networks have become popular, and certain application domains, such as health care and cybersecurity, are providing a rich set of problems that cannot be solved without sophisticated data mining techniques.

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*See <http://www.kdnuggets.com/2013/11/top-conferences-data-mining-data-science.html>.

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Oxford Student Chapter Hosts Sixth Annual Conference

SIAM student chapters continued to proliferate around the world in 2013. The new chapter in Magdeburg, Germany’s third, held its opening workshop in June, with invited speakers representing a wide range of application areas. Also in 2013, the well-established Oxford University chapter hosted the sixth in its series of UK-wide conferences with, as reported by Dominic Yeo, an unofficial theme: “Questions worth asking are sometimes found in unusual places.”

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Quo Vadis, Scientific Software?

“Few in our community can forge a career on scientific software, even if their results affect and enable the work of hundreds of other scientists,” Wolfgang Bangerth and Timo Heister write. After building a good case for the unsustainability of the situation, they recommend steps that the community can take to remedy it. The underlying challenge, they say, “is to change the habits of our community.”

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these matrices; in physics, we can think of it as the probability of measuring a certain value of the observable in question. When the algebra is “abelian” (i.e., the product of two matrices A and B is the same in either order), the matrices correspond to observables that can be measured simultaneously. But by Heisenberg’s uncertainty principle, some observables, such as position and velocity, cannot be measured simultaneously. These correspond to matrices that do not commute. Kadison and Singer asked whether a certain kind of state defined on a commuting set of matrices can be extended in a unique way to a larger non-commuting set. To put it in physical terms: Can a series of measurements of one observable uniquely constrain the other observables that can’t be measured at the same time?

Of course, technical details need to be worked out. “You’re talking about non-normal pure states, non-physical states, which only exist by the axiom of choice,” says Nik Weaver, a functional analyst at Washington University in St. Louis. (The axiom of choice is a well-known assumption that often leads to very non-intuitive results, but is also indispensable for reasoning about infinite-dimensional spaces.) For so-called “normal” states, which might actually be observed in a physics experiment, the answer to the Kadison–Singer question is yes, as Kadison and Singer proved. They suspected, however, that the answer for the non-normal states was no. With admirable foresight, they did not actually state this as a conjecture. As it turned out, their guess would have been wrong.

In its original formulation, the problem was of great interest to specialists in operator algebras, but rather inaccessible to anyone else. Beginning around 1979, however, the underground river began to well up in different places and under different names: the Paving conjecture, the Bourgain–Tzafriri conjecture, the Feichtinger conjecture. The mathematicians who posed these problems were not always aware of each other, and it wasn’t until 2006 that Peter Casazza of the University of Missouri (with three other mathematicians) put them all together. “We

didn’t start out looking for equivalent versions of Kadison–Singer,” Casazza says. “We were actually trying to solve the problem, and kept moving to different areas of research, hoping that one of them had deep enough results to handle the problem. It was a fluke that each time we entered a new area of research, this was equivalent to their most famous unsolved problem.”

Almost imperceptibly, however, the river was approaching its destination—the conjecture was becoming simpler to state, if not to prove. A major step forward was the discovery of finite-dimensional versions of the problem. One of Casazza’s favorite versions involves finite sets of vectors called “frames.”

Linear algebra students learn in college that an “orthonormal frame” of vectors ($\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$) can be used to reconstruct any vector \mathbf{x} from an N -dimensional space, as follows:

$$\mathbf{x} = (\mathbf{x} \cdot \mathbf{v}_1) \mathbf{v}_1 + (\mathbf{x} \cdot \mathbf{v}_2) \mathbf{v}_2 + \dots + (\mathbf{x} \cdot \mathbf{v}_N) \mathbf{v}_N.$$

In fact, many other collections of vectors—with far more than N elements—also enable the reconstruction of \mathbf{x} via the same formula: in some cases exactly, in others approximately.

If the vector \mathbf{x} is thought of as a signal, frames make it possible to reconstruct \mathbf{x} from a redundant set of measurements. The question that arises then is: What if data are lost in transmission? Can \mathbf{x} be recovered from subsets of the frame? The Kadison–Singer conjecture says yes. Any frame can be partitioned into smaller frames, with uniform bounds both on the number of smaller frames and on the loss of fidelity.

In 2013, Spielman, Marcus, and Srivastava finally proved a closely related conjecture of Weaver, which involves partitioning a set of vectors into just two “balanced” subsets. The balancing condition amounts to saying that the largest root of a certain polynomial will be less than 0.9 (or some fixed constant less than 1). In fact, Spielman’s team proved that the largest root of the *average* polynomial over all possible partitions is less than 0.9.

“It’s like saying that the average family has 2.5 children,” Spielman says. “If the average family has 2.5 children, you know that some families have two or fewer.” Similarly, one might think that if all the roots

of the average polynomial for all partitions are less than 0.9, then there must be at least one specific polynomial with that property.

In fact, that was what Spielman’s group thought at first. But, he says, “It was a mistake.” There are no general relationships between the roots of an average of a set of polynomials and the roots of the individual polynomials. But the group discovered one case in which they are related—namely, when the roots of the polynomials “interlace.” The researchers had to build up the theory of interlacing polynomials essentially from scratch, but ultimately it allowed them, as Spielman says, “to use the average to reason about individuals.”

Their highly innovative result applies immediately to graph theory. For example, as Nick Harvey of the University of British Columbia points out, one promising approach to the traveling salesman problem is to find “optimal thin trees” for a given graph. These are sparse subgraphs with no loops. The Kadison–Singer theorem proves that optimal trees exist that *look* like good approximations from the perspective of the Laplacian spectrum. If the “optimal spectrally thin trees” could be converted to optimal thin trees (admittedly a big if), it would be a major breakthrough on the traveling salesman problem.

The result could also have applications to signal processing. If your cell phone works better 20 years from now, you might have Kadison and Singer (and Spielman, Marcus, and Srivastava) to thank. But one major hurdle needs to be overcome between now and then. The proof is non-constructive, which means that it does not give a recipe for computing balanced partitions, or any of the other equivalent objects whose existence it promises. “If you want to turn the proof into an algorithm, it would take exponential time,” Spielman says. In other words, as a practical search method the proof is not much better than trial and error. In future years, it will be a major project for computer scientists to translate the theoretical existence theorem into a practical tool for engineers. Says Casazza, “It’s the engineers, in the end, who will decide whether this is really valuable.”

Dana Mackenzie writes from Santa Cruz, California.

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Interestingly, classical algorithms, including classification and clustering techniques, remain popular research areas, perhaps reflecting their timelessness and utility in practical problems.

Of course, in this age of Big Data, scalable techniques are an active area of research, and the success of IBM’s Watson has prompted the coupling of data analysis with decision support, while placing the conclusions drawn from data on a sound mathematical footing. To help the community keep up with this constantly changing field, SDM provides tutorials on the latest techniques and application areas, as well as workshops, where participants interested

in focused topics can present their ongoing work for discussion.

The new year marks several changes for SDM: A new steering committee, with Srinivasan Parthasarathy (Ohio State University) as chair, will oversee the selection and management of the organizing committee for the conference each year. Joining him will be the newly elected officers of the SIAG on Data Mining and Analytics—Zoran Obradovic, Jeremy Kepner, Kirk Borne, and Takashi Washio. They will help ensure that SDM remains a well-regarded, smoothly running conference and continues to meet the technical needs of the more mathematically inclined members of the data mining



Srinivasan Parthasarathy

community. SIAM was prescient in starting the SDM conference in 2001, long before “data mining” became a household term. Its strong support of the conference ensures a bright future indeed for SDM. We welcome you to join us at SDM14, in Philadelphia, April 24–26, to learn about the latest in the field from highly cited authors.

Chandrika Kamath is a researcher at Lawrence Livermore National Laboratory, where she is involved in the analysis of data from scientific simulations, observations, and experiments. She chaired the SDM steering committee from 2007 to 2014 and from 2011 to 2013 was chair of SIAG/DMA.

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Summer 2014 Research Opportunities for Undergraduates

Undergraduates who are looking for summer research opportunities are encouraged to visit the National Science Foundation’s “Search for an REU Site” web page at http://www.nsf.gov/crssprgm/reu/reu_search.cfm and click on the “Mathematical Sciences” link. Students can also find links to research opportunities in the mathematical sciences that have been identified by *SIAM News* press time, funded both by NSF and by other institutions, on the SIAM website at <http://connect.siam.org/summer-2014-research-opportunities-for-undergraduates/> and <http://www.siam.org/students/resources/fellowship.php>.

IMA To Host Workshop on Careers in Industry

By Thomas Grandine, William Kolata, and Richard Braun

The Institute for Mathematics and its Applications will hold a workshop for faculty and students interested in exploring careers and opportunities for mathematical scientists in industry. The workshop will be held on the campus of the University of Minnesota in Minneapolis, April 7–9, 2014.

The IMA workshop will emphasize both opportunities for mathematical scientists in industry and implications for graduate programs in the discipline. The agenda draws on two SIAM reports, from 1996 and 2012, as briefly described below.

SIAM's First MII Report

In 1996, with funding from the National Science Foundation and the National Security Agency, SIAM published the first *SIAM Report on Mathematics in Industry* (<http://www.siam.org/reports/mii/1996/report.php>). SIAM undertook the project primarily to address the issue of demand for mathematicians in industry and government and to investigate, from the perspective of the employers of those who held such jobs, how well their employees had been trained.

In summary, we found that from the perspective of nonacademic employers, the value of mathematicians, as in academic careers, resides in their habit of mind, rigorous thinking, and confidence in careful reasoning. The managers interviewed also mentioned several areas in which graduate education needed to be improved: experience in real-world problem solving, communication skills, and effective use of computer software and systems.

Following publication of the 1996 report, six regional NSF-funded workshops were held to communicate the conclusions of the report.

The 1996 report and the follow-up workshops resulted in greater awareness of the nature and extent of mathematics in industry among faculty and students. The efforts also encouraged the development of non-academic workforce programs by government agencies and private foundations. The Sloan Foundation, for example, funded efforts to develop Professional Science Master's Degree programs, and NSF created the GOALI (Grant Opportunities for Liaison with Industry) program.

The 2012 Update

In 2008, with funding from NSF, SIAM began to examine the evolution of non-academic opportunities for the mathematical sciences, this time with the focus solely on industrial careers. The results of this project

were published in the 2012 *SIAM Report on Mathematics in Industry*.^{*} The insights from the first report remained largely valid, but the second report documented significant changes in the mathematical and computational sciences in industry. Most noticeably, organizations now collect orders of magnitude more data than they used to, and face the challenge of extracting business-enhancing information from the data. Computing technology has continued to advance rapidly, and companies make more and more aggressive use of high-performance parallel computing. Scientific and technical services and finance together have become as important to U.S. GDP as manufacturing once was.

A highlight of the 2012 report is the section on case studies that illustrate emerging applications of the mathematical and computational sciences in industry. Along with big data and predictive analytics, themes highlighted in this section include the developing sophistication of mathematical modeling and advanced computation in industry, and the emergence of companies that use mathematical and computational modeling to extract complex interactions and predict emergent properties of biological systems.

The 2012 report documents the technical knowledge and skills needed to succeed in industry. Requirements include mastery of the core areas of the mathematical sciences, with depth in one area and enough breadth that it is possible to quickly come up to speed in another. Also important are a sufficient grasp of an application discipline relevant to the prospective employer and proficiency in a programming language. As to the required soft skills, communication and teamwork were mentioned in the first report; the new report also cites the need for enthusiasm, self-direction, the ability to complete projects, and a sense of the business. It is clear that no academic program can, by itself, provide all of these requirements.

The challenge for educators and students is to find the right mix of formal academic courses, education in soft skills, and real-world experience in industry. The challenge to government agencies is to develop workforce programs that foster the transition of graduates in the mathematical and computational sciences into productive careers in industry. Work remains to be done. For example, NSF's MPS directorate made 51 awards in the GOALI program; however, none of these were from the Division of Mathematical Sciences.

^{*}The report is available at <http://www.siam.org/reports/mii/2012/index.php>.



As the program for the IMA workshop described in the accompanying article was taking shape, SIAM met in Amsterdam with leaders of European mathematics-in-industry efforts. Shown here are, clockwise from left: Wil Schilders (representing the European Consortium for Mathematics in Industry), Maria Esteban (SMI), Volker Mehrmann (GAMM), Mario Primicerio (SIMA), and, from SIAM: vice presidents for industry Thomas Grandine (current) and Kirk Jordan (former), vice president for programs Sven Leyffer, president Irene Fonseca, and executive director James Crowley. Topics discussed were drawn in part from publications shown in the foreground, including *Mathematics and Industry* and *European Success Stories in Industrial Mathematics* (European Science Foundation/European Mathematical Society) and SIAM's updated (2012) *Mathematics in Industry* report.

The IMA Workshop

The workshop will bring together faculty, postdocs, graduate students, and industry representatives. Faculty who attend the IMA workshop will learn about the advantages of engaging in collaborations with industry, for both their departments and their students. Students and postdocs will learn about internships, collaborations, and careers in industry. For industrial mathematicians and scientists, the workshop will be a setting in which they can promote careers in their companies and highlight opportunities for collaborations and internships. The industrial participants will also have a chance to

influence the design of academic programs.

The format of the IMA workshop, instructions for applying to participate in it, and information about the availability of financial support can be found at http://www.ima.umn.edu/2013-2014/SW4.7-9.14/?event_id=SW4.7-9.14.

Thomas Grandine is a senior technical fellow at The Boeing Company. William Kolata is SIAM's technical director. Richard Braun is a professor of mathematical sciences at the University of Delaware and an associate director and visiting professor at the IMA.

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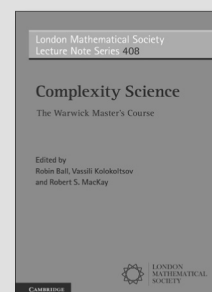
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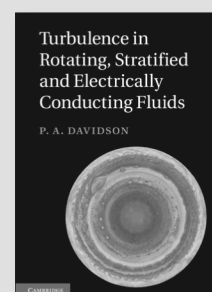
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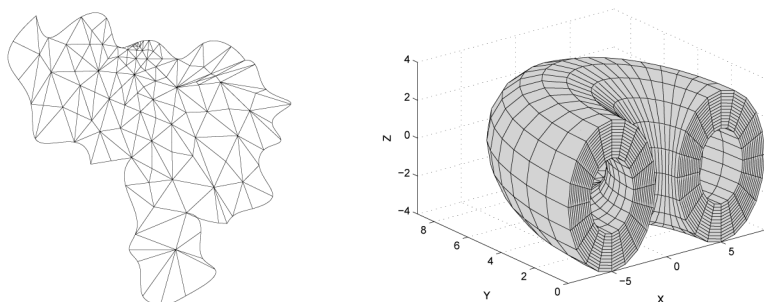
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Problems Across the Applied Sciences and Engineering Engage New Student Chapter in Magdeburg

Germany’s third SIAM student chapter held its opening workshop in Magdeburg on June 19, 2013. The chapter is a collaboration of two institutions in the city of Magdeburg: the Otto von Guericke University (OVGU) and the Max Planck Institute for Dynamics of Complex Technical Systems (MPI DCTS). At the time of the workshop, the newly formed chapter already had 20 members from a variety of areas in applied mathematics and engineering.

As the chapter aims to foster the use of mathematics across the applied sciences, we invited speakers from different scientific backgrounds. Peter Benner, managing director of MPI DCTS, opened the workshop, after which we heard from our principal guest: Edda Klipp of Humboldt University, Berlin, who spoke about yeast cell cycles and the related mathematical modeling.

We had also invited Matthias Stein

(MPI DCTS), who discussed relativistic effects for electrons in magnetic fields, and Sebastian Sager (OVGU), who described the optimization of time-dependent processes. Members of the student chapter rounded out the program with presentations of their current PhD research.

The workshop was well received by students and faculty from both MPI DCTS and OVGU, despite record high temperatures for the date. The variety of topics covered by the speakers was matched by the interests of the audience, which included the mathematical and biological sciences and engineering.

We believe that this workshop is just the first of many valuable activities of the SIAM student chapter in Magdeburg.—*Peter Benner, MPI DCTS, and Martin Hess, President, Otto von Guericke University Magdeburg Chapter of SIAM.*



The inaugural slate of officers for the SIAM chapter in Magdeburg, from left: Heiko Weichelt, Martin Hess, Norman Lang, Jessica Bosch, Matthias Voigt, Kristin Held, and Constantin Kwiatkowski.

Oxford Student Chapter Hosts Sixth Annual Conference

The sixth Oxford University SIAM Student Chapter Conference had an unofficial theme: Questions worth asking are sometimes found in unusual places. SIAM past president Nick Trefethen (Oxford) welcomed delegates with an account of events that followed his casual observation that the measure given by the body mass index (BMI) resulted in counterintuitive predictions about the healthiness of some of his friends and colleagues. Following everyone’s favourite statistical mantra—the plural of “anecdote” is not “data”—he described some preliminary research into the history of the metric, and the media circus that followed his informal suggestion of an alternative index that would apply the exponent -2.5 rather than -2 to the subject’s height. Delegates worried about justifying research to funding bodies agreed that this was nothing compared to Trefethen’s efforts to explain his reasoning to the popular press!

Chris Budd (Bath) selflessly gave up time on his birthday to give the first plenary talk. Reinforced by the cake presented by the chapter, he took the audience on an engaging tour through a series of problems he had been asked to solve over the course of his career by Bristol Zoo. Along with interesting insights from fluid and thermodynamical theory, the take-home message was that there is no limit to the places where great mathematical problems can be found, and where the answers are of real immediate importance to the people involved. (Not least were the fish dying at an alarming rate until Budd’s application of some numerical analysis to a model of the aquarium’s heating system.) I’m sure no one expected quite so much discussion of penguin eggs during the excellent St. Antony’s lunch and the poster session; students from 12 universities presented 21

posters, which resulted in lots of interest and conversations across disciplines.

The trend continued through five excellent student presentations exploring a diverse range of topics in applied mathematics, from light scattering to jumps in stochastic models for finance. All speakers coped admirably with the tight time constraints. Most impressive, the audience went away at the very least with a clear idea of why the questions asked are important.

David Mortimer (BNP Paribas) had an even tougher assignment: arguing that there are still good questions to be answered in the field of financial modelling. In the event, he gave an excellent explanation of how the global economic crisis has increased the complexity of the necessary underlying assumptions. The existence of arbitrary risk-free resources is no longer valid, and he gave a compelling argument that applied mathematicians have plenty of fresh material in this area to sink their teeth into. Prizes were awarded for the best student talk (Eric Hall, University of Edinburgh) and poster (Dominic Yeo, University of Oxford).

Finishing the day in style, Sam Howison (Oxford) described models for games in which agents trade finite amounts of some commodity. The combination of competition and exhaustion of the resources leads to highly nonlinear ODEs and PDEs whose numerical solutions present many challenges. As discussed earlier by Mortimer, additional constraints produce interesting price dynamics, and Howison introduced several examples, notably oil, of these effects in the real post-recession world. Delegates thus had plenty to discuss as the conference ended on a highly sociable note over a three-course dinner with wine at a local restaurant, providing a chance to make contacts, unwind, and



Plenary speaker Chris Budd toured the applied mathematical problems he has been asked to solve for Bristol Zoo.

talk mathematics in equal measure. The chapter is particularly grateful to

St. Antony’s College for its hospitality, and to BNP Paribas as the principal sponsor of this event. The 80 student delegates (from 20 universities in the UK, with one visitor from Germany) also appreciated the chance to chat with Mortimer and the company’s other representatives over coffee, and learn that there is much more to a mathematical career in finance than simulating stochastic PDEs. The chapter is also grateful to Winton Capital for generous sponsorship throughout the year. The next Oxford University SIAM Student Chapter Conference is scheduled for May 2014.—*Dominic Yeo, University of Oxford.*



Dominic Yeo (left), recipient of the prize for best poster (and author of the accompanying article), discussed fine points of the award-winning poster with Philippe Charmoy, treasurer of the Oxford student chapter. Photos by Sara Kerens.

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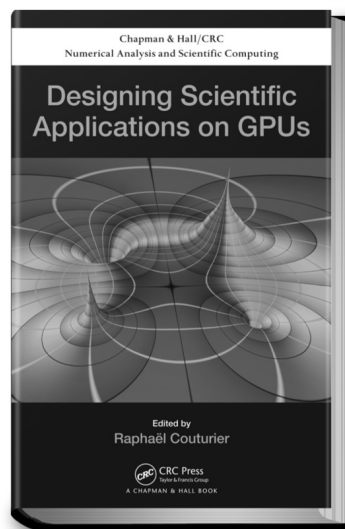
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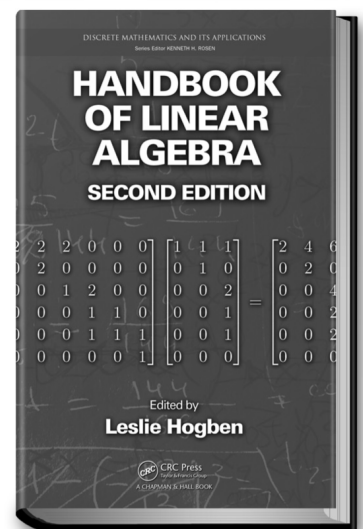
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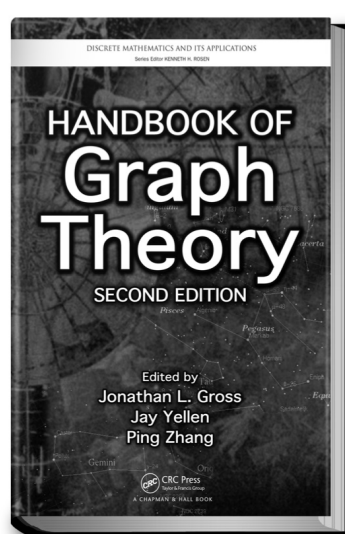
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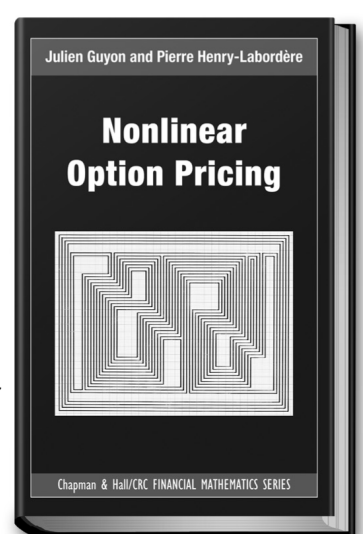
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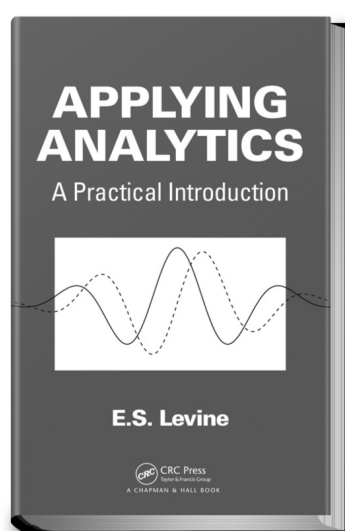
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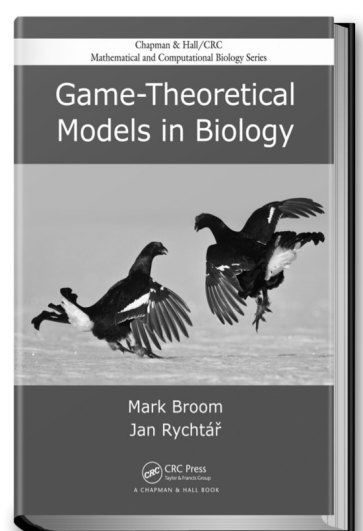
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Idea submissions or additional information needed?



Contact:
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A Solution to the $3x + 1$ Problem?

I believe I might have solved this very difficult problem. I will welcome reader comments. See “A Solution to the $3x + 1$ Problem,” on occampress.com.

Contact: Peter Schorer, peteschorer@gmail.com.

Scientific Software

continued from page 8

Of course it is difficult for outsiders to evaluate and quantify someone’s contributions to a project, especially if the project has been the work of dozens of contributors over many years. But surely, as a community we can come up with ways to give credit where credit is due, devising a system that is at least as good as citation counts and impact factors. Some projects—PETSc is a good example—provide bibtex entries for their web pages or user manuals that list all significant contributors over the years.

Solutions?

If we accept the premise that our current system of writing software is at least not optimal, then steps toward improvement must include defining better metrics and ensuring that incentives are aligned. Some often heard suggestions along these lines are the following:

■ We need better ways to credit those who write software. If you use a particular open-source project in a publication, you should say so, and reference the most relevant publications describing it.

■ Hiring committees and grant proposal panels need to recognize the role of software. Writing successful software is a creative process; it is also—if the authors provide user support—a lot of continuing work. Yet most departments consider it less valuable than proving theorems. This rules out academic careers for many of the best authors of scientific software. Even worse, it deprives our students of the opportunity to learn to write software, something almost all of them will need to do in their professional lives.

■ We need to find better ways to credit people who contribute significant amounts of code to existing projects. Few options are now available, and creative solutions will be necessary.

■ Publication of code used to obtain the results presented in a paper needs to be made the default. There has been a recent push toward *reproducibility*, as laid out recently in these pages [10]. Full reproducibility is a high hurdle, but it will already be a step forward if

the code that accompanies a paper solves one of the problems shown in it.

Ultimately, as a community we need to come to grips with these issues. Otherwise, we will never move beyond solving toy problems, detached from what our applied colleagues need to see if they are to adopt the methods we are so good at developing!

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Wolfgang Bangerth is a professor in the Department of Mathematics at Texas A&M University. Timo Heister is an assistant professor in the Department of Mathematics at Clemson University.

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Quo Vadis, Scientific Software?

By Wolfgang Bangerth
and Timo Heister

A large majority of the papers published in SIAM journals, and elsewhere in our community, show a computational result of some kind—either as the main point (e.g., in *SIAM Journal on Scientific Computing*), for backing up theoretical claims about numerical methods (e.g., in *SIAM Journal on Numerical Analysis*), or in modeling experimental observations. Indeed, the discipline that brings us these computations—computational science—is accepted today as the third leg of science, next to theory and experimentation. Yet, although we talk a lot about the underlying methods and algorithms, we almost never talk about their incarnation in real life: software.

Alas, this is an important omission, as much remains to be improved in this area.

First, whereas science prides itself on building on the shoulders of giants, this is not the case with software. Having moved past the Bourbaki movement, we readily accept a reference to a previously proven theorem rather than proving it anew.

By contrast, many of our graduate students write the codes that illustrate their algorithms essentially from scratch. These codes themselves are rarely published. This is the equivalent of publishing a theorem and claiming that a proof exists, but not including it in the paper. Grad students in pure math can't get away with that, and ours should not either!

Secondly, as a community we hold the authors of papers and books in high esteem, but rarely give credit to those who make software available or contribute to open-source projects. Few in our community can forge a career on scientific software, even if their results affect and enable the work of hundreds of other scientists. This is remarkable—writing widely usable software is a rare skill (a claim easily verified by looking at the average graduate student's programs), a skill belittled as “just coding” only by those who don't possess it.

In other words, as a community we ought to have a conversation on how to move forward with regard both to the software that underlies our work and to those who write it. This article is an attempt to start that conversation.

Software: Where We Are and Where We Are Going

The software we use today is vastly more complex than its antecedents. Papers discuss algebraic multigrid methods on thousands of processors, discretizations of the magnetohydrodynamics equations on adaptively refined unstructured meshes, and simulations of processes in geology and astronomy that require billions of unknowns. None of this is possible without a significant investment in software.

Even papers limited to one small computational aspect of a larger problem can require thousands of lines of code. Yet most of the time, authors do not make these codes available. We could think of this as merely regrettable, something that prevents others from learning from and building on these codes.

But this habit also causes serious problems for our community: If every graduate student writes the code for a new discretization from scratch, we will be stuck forever solving “toy problems” (like the proverbial “Laplace equation on the unit square”), because that's what's possible in three years of work. Unfortunately, this is no longer sufficient to convince our colleagues

in the applied sciences (who moved past this stage a long time ago) that the new algorithm is also applicable to their vastly more complex problems. The risk is that we will isolate applied mathematics and numerical analysis: If we can't convince our friends in the sciences and engineering that what we do is worthwhile, using examples they can relate to, then all we really do is dabble in esoteric corners.

Although we talk a lot about the underlying methods and algorithms in computational science, we almost never talk about their incarnation in real life: software.

There are solutions to this problem. Over the past 15 years, we have seen the development of large libraries (e.g., PETSc [1,2] and Trilinos [5,6] in linear algebra; deal.II [3,4] and FEniCS [8,9] for finite elements; Clawpack [7] for hyperbolic conservation laws) that already cover many of the standard techniques. These libraries typically come with extensive tutorials that graduate students can take as the basis for their own work. To take the example of deal.II, our own contribution: It is realistic for a gradu-

ate student to develop a new discretization and demonstrate its qualities on a nonlinear problem, using parallel algebraic multigrid solvers on adaptively refined unstructured meshes for complex geometries. The student can do this in three years of research, because all the building blocks are already there, often combined in an existing and available program in which only the discretization has to be changed.

The challenge is to change the habits of our community. We should no longer encourage or even allow our graduate students to write their programs from scratch; rather, they should build on what's already there. And they in turn should make their own codes available so that others can build on them—just as we expect students to use others' theorems and make their own proofs available.

Motivations

Part of the problem is our reward structure: Making code available to others is typically seen as a waste of time, given that it requires at least a modest amount of documentation and code cleanup. We have impact factors and citation counts

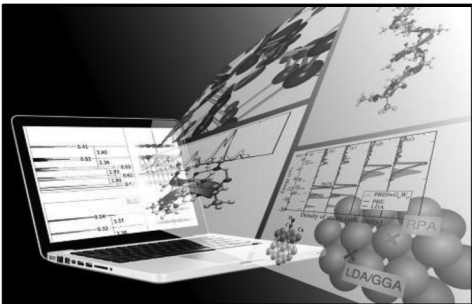
for papers, but no established way to give credit for software or means for evaluating the relevance of software. Consequently, it is often overlooked in decisions of hiring, tenure, and promotion.

While this may be something of an obstacle for the leaders of widely used open-source software packages, it is a real problem for younger contributors of, say, a few thousand lines of often good code for one of these packages. This code represents a significant investment of their time, and they benefit the community by making their results available to everyone. Yet, with the exception of the principals of a project, few late-comers will generate name recognition or other tangible benefits by contributing their work. It is not that the principals want all the credit for themselves (all the projects mentioned earlier have pages that give credit to contributors, listing, in the case of deal.II, around 70 people who have made substantial contributions). The problem is that we currently have no way for others to claim this credit, beyond providing a link to a web page. Given this lack of widely accepted recognition, it is difficult to motivate the best people to put their time into making software available to everyone; in fact, they may jeopardize their careers by doing so.

See **Scientific Software** on page 7

INSTITUTE FOR PURE AND APPLIED MATHEMATICS

Los Angeles, California



Hands-on Summer School: ELECTRONIC STRUCTURE THEORY FOR MATERIALS AND (BIO)MOLECULES

July 21 - August 1, 2014

ORGANIZING COMMITTEE: Volker Blum (Duke University), Christian Carbogno (Fritz-Haber-Institut der Max-Planck-Gesellschaft), and Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft)

Scientific Overview

Electronic structure theory (for total energies, forces, neutral and charged excitations, dynamics and transport, etc.) has reached a level where quantitative analyses and predictions of hitherto unknown properties and functions of materials - including bulk materials, isolated molecules, surfaces, nanostructures, clusters, liquids, (bio)molecules in their environment, and more - are possible. Finding better or even novel functional materials is critical for nearly every aspect of our society. Key issues include the “energy challenge” and “managing the environment”.

This ten-day Hands-on Summer School introduces the basics of electronic-structure theory and teaches how actual calculations are performed. Morning lectures on the most important topics will be given by internationally renowned experts. In the afternoon (and evening) the participants will put this knowledge into practice. We will also discuss recent developments towards the “Materials Genome”, and how to treat large amounts of data.

Participation

This summer school will provide a rare opportunity for researchers in mathematics, physics, chemistry, engineering, and related sciences to learn about recent research directions and future challenges in this area. Funding is available to support graduate students, postdocs, and other researchers in the early stages of their career, as well as more senior researchers interested in undertaking new research in this area. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission and we welcome their applications. The application is available online, and is due March 31, 2014.

www.ipam.ucla.edu/programs/gss2014

