

IPAM Discussions Lead to Exciting New Direction for Materials Science Research

As a core participant in IPAM's "Navigating Chemical Compound Space" program (CCS) in the spring of 2011, Klaus-Robert Müller found himself far from home – both physically and metaphorically. For Müller, a professor of machine learning at Technische Universität Berlin, being away from the daily responsibilities of running a large lab for an extended period of time and bringing his machine learning expertise to a meeting of chemists and quantum physicists proved to be a fruitful combination: The collaborations Müller initiated at CCS on the use of machine learning techniques for materials science have led to a novel and exciting research

direction with the potential to make a huge impact in fields ranging from energy to drug discovery.

Machine learning – teaching machines to learn from data – has become a key to everything from search technology employed by the likes of Google to social network analysis. It has also become standard technology for transforming huge amounts of data into insights and knowledge. In the mid-1990s, Müller began applying his machine learning expertise to the field of neuroscience, and ended up making a major contribution to advancing a thennew field known as brain-computer interfacing.

Neuroscientists use electroencephalography (EEG) to evaluate experimental data involving the brain's reaction to stimuli. Given that the signal from the brain is complex and "noisy," the typical technique for researchers was to take the average from hundreds of measurements of reactions to the same event. Müller's group first established a "single trial analysis" technique that enabled researchers to bypass the need to conduct multiple measurements and subsequently developed a brain-computer interface approach to decoding the EEG signals in real time. "Previously, a patient needed to spend 100-300 hours on a learning experiment to change the brain signals such that they could be decoded through feedback," Müller explains. "When we came into this we thought, why not have the subjects think whatever they want to think, and have the machine do the decoding." In 2003, Müller's group published the first paper showing that this was possible -

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Klaus-Robert Müller Professor of Computer Science, Technische Universität Berlin Director, Bernstein Focus on Neurotechnology Berlin

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Emily Carter to Give Simons Lecture at IPAM

More than a hundred scientific societies, universities, research institutes, and organizations around the world have dedicated 2013 to showcasing the role of mathematics in understanding and addressing the world's environmental challenges. IPAM is among the participating organizations of this initiative, called "Math of Planet Earth." IPAM's fall long program, Materials for a Sustainable Energy Future, is one of the featured activities.

IPAM will also host one of the nine "Math of Planet Earth" public lectures sponsored by the Simons Foundation. The speaker will be Dr. Emily Carter, Founding Director of the Andlinger Center for Energy and the Environment at Princeton University. Dr. Carter's lecture will be held on November 4, 2013, in the Korn Convocation Hall at UCLA.

The title of her talk is "Quantum Mechanics and the Future of the Planet." She will describe her research on energy systems ranging from fuel cells to fusion reactors, and the essential role of quantum mechanics in the quest for sustainable energy. For more information, go to http://www.ipam.ucla.edu/programs/msews3/lecture.aspx. A video of her talk will be available online.





Note from the Director

Russel Caflisch

This spring marked the end of my fifth year, and of my first term, as director of IPAM. I'm staying on for a second term because I strongly believe in IPAM's goal of bringing mathematics to bear on the important challenges of our time. We address this goal mainly through our programs. The past year included long programs on Materials Defects representing applied mathematics and physical science, and for the pure mathematicians, Interactions Between Analysis and Geometry. The winter workshops included Multi-modal Neuroimaging on a physiology topic, as well as three workshops on Structure and Randomness in System Identification, Adaptive Data Analysis, and Convex Relaxation Methods, which were loose-connected through their emphasis on sparse representation.

Moreover, during the last year we've started a number of initiatives that I want to see through. These include renovation of IPAM's seminar room, efforts to increase the number of industrial participants in IPAM programs, revamping IPAM's website and brand, and preparing the renewal proposal for IPAM's main NSF grant. The first step in our branding process was adopting the slogan "Math Changes Everything" which succinctly expresses our view of the central role of mathematics in science and other disciplines. A new logo and website will be released soon.

Another part of IPAM's mission is engagement with the community, for example through our public lecture series. Last year IPAM's public lectures included Klaus-Robert Müller's talk on the Brain Computer Interface, and the Green Family Lectures by Wendelin Werner on Geometry and Randomness. In the coming year IPAM will present Emily Carter speaking on sustainable energy and quantum mechanics, a talk by Jon Kleinberg on social network analysis, and in the spring, the Green Family Lectures featuring Avi Wigderson.

This newsletter is aimed at engaging with you, our reader. I encourage you to deepen your engagement by attending an IPAM event and by joining IPAM's Frontiers Society. Support from IPAM enthusiasts through the Frontiers Society is enabling many of the current initiatives, such as video recording and renovation of the lecture room.

IPAM: Where Math Creates Connections

Roja Bandari graduated from UCLA in 2013 with a Ph.D. in Electrical Engineering

As a participant in the 2010 IPAM program "Networks and Network Analysis for the Humanities," I formed an appreciation for IPAM's ability to connect scholars of diverse fields. Organized by Dr. Timothy Tangherlini, the program led to research collaborations between mathematicians, computer scientists, and humanities scholars that continue today. At Professor Tangherlini's suggestion, I joined IPAM's RIPS program as an academic mentor for a data science project. Subsequently, IPAM's director invited me to work on a special project: mapping the connections between IPAM programs. The graph on the right is the result of this work. A detailed version of the graph is available at http://www.ipam.ucla.edu/research.aspx.

The graph represents the connections between IPAM programs (workshops and long programs) from 2000 to 2013. It also demonstrates the breadth of topics that are discussed at IPAM. Each node in the graph represents an IPAM program, and its size corresponds to the number of participants in the program. Clusters of programs, depicted in different colors, emerge naturally as a result of a graph-theoretic community detection algorithm. This is similar to the analysis of other networks, such as co-authorship networks in scientific publications.



The thickness of an edge connecting two nodes reflects the proportion of participants who took part in both programs. More specifically, the weight of an edge between two programs is equal to the number of their mutual participants divided by the number of unique total participants in the two programs (i.e., the Jaccard Index). Letting A and B be sets of participants in each program, the edge weight is $(n(A \cap B))/(n(A \cup B))$, where n represents set cardinality. A community detection algorithm then clusters programs such that the links between programs in the same cluster are more likely than those in different clusters. Each cluster, represented by a different color,



Bridging Mathematical Disciplines Helps IPAM Organizer Make Sense of Incomplete Data

With her focus on breaking down traditional disciplinary barriers, collaborating with researchers outside of her expertise and applying knowledge from one scientific arena to another, Maryam Fazel epitomizes many of the characteristics of IPAM. And so it's no surprise that in recent years, she has become an active participant and program organizer.

Fazel, an assistant professor of electrical engineering at the University of Washington, has been at the center of new developments at the intersection of optimization, data analysis and systems science. "These are three very different areas," she notes. "But all involve related mathematical problems, and it's typical that techniques from one area can also be used in another."

For the past several years, Fazel's main focus has been on the problem of estimating low-rank matrices amid incomplete or "noisy" information. A low-rank matrix is one in which the rows and columns of the matrix form a low dimensional space. For example, if a group of individuals rank their preferences on a few items, the challenge becomes how to use that limited information to make inferences about unknown rankings.

"If we assume individuals tend to share certain tastes and preferences, then we can use the rank estimation to infer missing entries," Fazel explains. That ability to capture order and complexity from unknown or "noisy" information is of great interest in the "big data" era. "We have so much data, but also so much that is missing," Fazel says.

One of the most popular applications started in 2006 when the company Netflix launched a three-year competition for the best algorithm to improve its recommender system – extrapolating from customers' expressed preferences on movies to predict other movies they would like. Other applications include making predictions about people's political positions using data gathered for other purposes. The issue of estimating low-rank matrices is also of great interest in very different venues, including control engineering – for example, in the building of robots or aircraft.

Fazel's interest in this problem began a decade ago, when she was

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New Direction for Materials Science Research

effectively reducing the experimental time from hundreds of hours to 10 minutes. The finding led to an explosion in the brain-computer interface field, with applications that are both clinical and non-clinical. At the time Müller started, there were approximately a dozen research groups in the world; today, there are about 400.

In 2011, Müller was invited to bring his machine-learning perspective to CCS. Although his focus had been far afield from those of the other program participants, because Müller had been trained as a theoretical physicist their language didn't sound foreign. "After a couple of hours of listening to the talks, I realized I should know these topics," Müller says, laughing. "And I also realized that these were people I could help."

In informal conversations with colleagues at the IPAM program, Müller suggested an out-of-the-box strategy – using machine learning rather than the far more arduous density-functional theory to predict the outcome of a complex mathematical equation for assessing new molecules. The strategy proved viable, reducing the computing time for solving the difficult problem from roughly five hours to milliseconds, with the same accuracy.

That has led to what Müller calls "high dreams." He established several collaborations with other CCS attendees that are ongoing and have produced a number of papers – the first of which was submitted before CCS had even ended.

While the early work has focused on molecules, Müller and his collaborators hope to apply the new approach to materials science. Although far more challenging, it's a direction with substantial rewards. "If you want to know the properties of a superconductor or of some material that can serve as a solar cell or battery, that can take 3-4 months of computing time per material," Müller notes. "Imagine having the technology to go through millions of possible compound materials candidates to find the most promising ones for nextgeneration superconductors, which you would then analyze using the physics techniques. It's too early to say that we will be able to do this, but we have high hopes and so far we have not seen any limits to the potential for our methods."

Müller, who returned to IPAM at the beginning of 2013 as the main organizer of "Multimodel Neuroimaging" (delivering a public lecture entitled "Toward Brain Computer Interfacing") and will return for a visit during this fall's program "Materials for a Sustainable Energy Future," says the IPAM setting and format played a key role in sparking the new direction. "The great thing about IPAM is you have a lot of senior people who are away from their daily responsibilities and distractions," Müller says. "Everyone is in a different state of mind, has time to think, and is more open to new ideas. Added to that, you are spending long periods of time getting to know people in relaxed settings. That helps to develop a level of trust that you need when you are proposing a collaboration involving something radically different."



News and Notes

Wendelin Werner Addresses IPAM Audience



Wendelin Werner visited IPAM on June 6-7, 2013 to give the 2013 Green Family Lectures, an annual series made possible through an endowment by former IPAM Director Mark Green and his family. Werner is a French mathematician working at the interface of probability theory with complex analysis and mathematical physics. In 2006, Werner received the Fields Medal for his work on stochastic Loewner evolution

and the geometry of two-dimensional Brownian motion. He became a member of the French Academy of Sciences in 2008. His two talks, entitled "Drawing Pictures at Random" and "Random Mountains," attracted large and enthusiastic crowds.

IPAM To Host Blackwell-Tapia and Latinos in Mathematics Conferences

IPAM is proud to host and support two upcoming meetings that promote diversity in the mathematical sciences. In November 2014, IPAM will host the Blackwell-Tapia Conference for the second time. This biennial conference honors David Blackwell and Richard Tapia, two seminal figures who inspired a generation of African-American, Native American and Latino/a students to pursue careers in mathematics. In April 2015, IPAM will hold the first "Latinos in Mathematics" (LAT@MATH) conference, the inspiration of IPAM Trustee Tatiana Toro, professor of mathematics at the University of Washington, and Alejandro Adem, director of Pacific Institute for the Mathematical Sciences (PIMS).

Hales Begins Second Term as Chair of Trustees

Dr. Alfred W. Hales has agreed to serve another three years as Chair



of IPAM's Board of Trustees. Since his appointment in 2010, he has provided IPAM with exceptional leadership, especially in initiating IPAM's fundraising efforts. Dr. Hales is best known for his service as Chair of UCLA's mathematics department and Director of the Center for Communications Research (CCR) - La Jolla and for the Hales-Jewett Theorem, which he formulated and proved with Robert Jewett. He is a Fellow of the AAAS and the American Mathematical Society. IPAM is thrilled that he will continue to serve for another term.

IPAM Talks Now Available on Video

In 2012, with support from donors, IPAM purchased highdefinition video equipment and hired a professional videographer to record many of our workshops, summer schools and public lectures. The demand is especially high for our tutorial lectures that begin each long program, and the talks offered during our graduate summer schools. You can stream the videos from our website, http://www.ipam.ucla.edu/videos.aspx. The videos are available in different formats and resolutions.

Skip Garibaldi Joins IPAM

IPAM is pleased to introduce its new Associate Director, Skip Garibaldi, Professor of Mathematics at Emory University. He replaces Jinqiao Duan, who returned to IIT this summer. Dr. Garibaldi studied at Purdue (BS) and UCSD (Ph.D.), held postdoctoral positions at the Swiss Federal Institute of Technology in Zurich and at UCLA, and held visiting positions at Université d'Artois, Université Paris-Nord, and IHES. His research in algebra has been funded by the National Science



Foundation and the National Security Agency. He is featured in the museum exhibit "MathAlive!" that is currently touring the country.

IPAM Hosts Women's Collaboration Conference

Research Collaboration Conferences seek to build communities of female researchers in different areas of mathematics and representing the entire career spectrum. A series of these meetings, held at Banff over several years, focused on the field of number theory. In July 2013, IPAM hosted one on shape modeling, entitled "Modeling Boundaries of Objects in 2- and 3-Dimensions." Organizers Kathryn Leonard (CSU Channel Islands) and Luminita Vese (UCLA) recruited team leaders and assigned the participants into one of four working groups presented with an open question in shape modeling. Each group is expecting to present their results at conferences and publish. Microsoft Research and the National Geospatial-Intelligence Agency provided financial support. We expect to host more of these conferences at IPAM in the future.

IPAM To Offer Graduate "RIPS" in Berlin

In 2014, IPAM will offer Graduate RIPS-Berlin (G/RIPS) for the first time. Similar to our undergraduate program Research in Industrial Projects for Students (RIPS), it will offer graduate students in mathematics and related disciplines the opportunity to work on industry-sponsored research problems. IPAM's partner is the Research Campus MODAL in Berlin, Germany. MODAL's existing industrial partners will provide the student teams with interesting and challenging research problems. The sponsors in 2014 will include a biotech company, a rail network, and a gas utility. More information will be available online this fall, and applications are due February 12, 2014.

IPAM News: www.ipam.ucla.edu/news.aspx.

Videos of IPAM Lectures: www.ipam.ucla.edu/videos.aspx.

RECOGNITION

Bin Yu Begins Term as IMS President

IPAM's Science Advisory Board member Bin Yu is currently serving as the President of the Institute of Mathematical Statistics (IMS). The IMS is a leading international professional and scholarly society devoted to the development, dissemination, and application of statistics and probability. Bin Yu is Professor of Statistics and Electrical Engineering & Computer Science at University of California Berkeley.

Cheney and Osher Honored at SIAM Meeting

At the 2013 National Meeting of the Society for Industrial and Applied Mathematics (SIAM), held in July, Stan Osher, professor of mathematics at UCLA and IPAM's Director of Special Projects, gave the John Von Neumann Lecture, the highest honor awarded by SIAM. In addition, Margaret Cheney, professor of mathematics at Colorado State University, gave the prestigious Sonia Kovalevsky Lecture. Dr. Cheney participated in IPAM's 2003 long program on Inverse Problems, and was an organizer of the 2012 Synthetic Aperture Radar workshop.



American Academy of Arts & Sciences Elects 2013 Fellows

The Fellows and Foreign Honorary Members of The American Academy of Arts and Sciences for 2013 include several individuals affiliated with IPAM. Bin Yu (UC Berkeley) serves on IPAM's Science Advisory Board and has given talks at several workshops. Richard Tapia (Rice University) served on IPAM's Board of Trustees from 2000-2004. Henri Berestycki (Ecoles des Hautes Études en Sciences Sociales) has spoken at IPAM workshops, and Nicholas Read (Yale University) helped organize the Random Shapes long progam.

RIPS 2012 Students Present Research at JMM

Twenty-two RIPS-LA and RIPS-Hong Kong students, representing twelve industry sponsors, presented their research at the 2013 Joint Math Meetings. At the MAA Undergraduate Poster Session, two teams from each program won Outstanding Presentation awards: Austin Alleman and Arturo Fernandez (LAPD); Juan Ramirez (IBM); Elizabeth Cangialosi and Aashish Gadani (BGI); and Skyler Seto and Karen Larson (Huawei). Additionally, two teams were selected to give oral presentations of their research at the AMS Session on Undergraduate Research in Applied Mathematics: Imanol Arrieta Ibarra, Christie Quaranta, Eric Schwartz, and Elena Sizikova (Shoah Foundation), and Louis Bohorquez and Jason Xu (Aerospace Corporation).

MARK YOUR CALENDARS

November 4, 2013. Dr. Emily Carter, Founding Director of the Andlinger Center for Energy and the Environment at Princeton University, will give the public lecture "Quantum Mechanics and the Future of the Planet." The lecture will begin at 4:30 pm in the Korn Convocation Hall, UCLA.

January 8, 2014. Jon Kleinberg, Tisch University Professor of Computer Science at Cornell University, will give a public lecture about the analysis of social networks. Time and location to be announced.

February 12, 2014. Application deadline for IPAM's Research in Industrial Projects for Students (RIPS) Program in Los Angeles and Hong Kong, and G/RIPS in Berlin.

May 19-23, 2014. The 2014 Green Family Lecture Series will feature Avi Wigderson, Professor of Mathematics at the Institute for Advanced Study, Princeton. The details will be announced in the spring. ■



We seek the support of those who share our commitment to mathematical innovation. Join or renew your membership in IPAM's Frontiers Society at the Champion (\$1000), Visionary (\$500), or Innovator (\$100) levels to support IPAM's efforts to foster the interaction of mathematics with a broad range of science and technology, build new interdisciplinary research communities, and engage and transform the world through mathematics.

Your donation will help IPAM provide child care grants for program participants with young children, support the redesign of our website, and contribute to the upcoming renovation of our lecture hall. To read more about the membership benefits and IPAM's fundraising priorities, and to make a contribution to IPAM at any level, go to ipam.ucla. edu/donate/.

FRONTIERS SOCIETY MEMBERS 2012-2013

IPAM wishes to thank the following individuals who joined or renewed their memembership in the past year, and all others who donated to IPAM:

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- Dr. Tatiana Toro and Mr. Daniel Pollack

Missing Data

doing her Ph.D. research. "We had fewer tools and fewer motivating problems to work on back then, but it was still mathematically very interesting," she says. Her group proposed algorithms to address the problem, but could not prove that they would always succeed. But over the next few years, a new area within the field of signal

UPCOMING PROGRAMS

2013-2014 Long Programs

Materials for a Sustainable Energy Future September 9 - December 13, 2013

Algebraic Techniques for Combinatorial and Computational Geometry March 10 - June 13, 2014

2013-2014 Workshops

Mathematics of Social Learning January 6 - 10, 2014

Mathematical Challenges in Ophthalmology January 16 - 18, 2014

Rough Paths: Theory and Applications January 27 - 31, 2014

Translating Cancer Data and Models to Clinical Practice February 10 - 14, 2014

Stochastic Gradient Methods February 24 - 28, 2014

2014 Summer Programs

Research in Industrial Projects for Students: Hong Kong June 8 - August 8, 2014

Research in Industrial Projects for Students June 22 - August 22, 2014

Graduate Level Research in Industrial Projects for Students: Berlin June 29 - August 22, 2014

Graduate Summer School: Electronic Structure Theory for Materials and (Bio)molecules July 21 - August 1, 2014

2014-2015 Long Programs

Mathematics of Turbulence September 8 - December 12, 2014

Broad Perspectives and New Directions in Financial Mathematics March 9 - June 12, 2015 processing gained momentum. Known as compressed sensing, it had a major impact on magnetic resonance imaging. In 2010, Fazel and her colleagues published a paper that was the first to make a connection between this compressed sensing approach to signal processing and low-rank matrix estimation. "Even though this was a completely different field, it turns out the mathematics is very similar," she explains. The paper paved the way for a new research direction,

both for Fazel's group and for others, and set the stage for significant progress in the field of low-rank matrix estimation in the three years sin



While at the 2010 IPAM program on optimization, Fazel met Lieven Vandenberghe, professor of electrical engineering and mathematics at UCLA and a member of the organizing committee. They identified two research areas, machine learning and system identification, that were tackling similar mathematical problems – both with the goal of constructing models from limited or noisy observations – but had little opportunity for interaction. After a subsequent discussion with IPAM director Russel Caflisch, Fazel and Vandenberghe organized a IPAM workshop held in January 2013, "Structure and Randomness in System Identification and Learning," that brought the two research communities together.

"So often, you find people in different areas of engineering and the sciences who are working on the same foundational mathematical problems but using different terminology and techniques," Fazel observes. "Making connections through shared mathematical problems and building bridges between these different scientific areas has been a theme in my own research, and it's one of the great strengths of IPAM."

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Professor of Electrical Engineering

University of Washington

Call for Proposals

IPAM seeks proposals from the mathematical, statistical, and scientific communities for long programs, winter workshops, summer programs, and exploratory workshops. Proposals are reviewed by IPAM's Science Advisory Board (SAB) at its annual meeting in November. To receive full consideration, please send your program idea to the IPAM Director at director@ipam.ucla.edu by October 1.

Winter Workshops are typically five days in length, with 20-25 presentations. The proposal should include a short description of the mathematical and scientific content, names of individuals to serve on the organizing committee, and names of individuals that you would like to invite as speakers or participants. The SAB will consider proposals for winter 2015 at the upcoming meeting.

Summer Schools are generally two or three weeks in length and incorporate both tutorials (a series of 3-4 talks) and research talks illustrating applications. They are directed toward graduate students and postdocs. The requirements for summer school proposals are comparable to those for winter workshops. The SAB will consider proposals for summer 2015 in November.

Long Programs generally have two complementary streams: one mathematical and one (or more) from other related scientific disciplines where there is the potential for a fruitful and exciting interaction. Alternatively, this might be an interaction between two disparate branches of mathematics. A long program opens with tutorials, followed by four one-week workshops and a culminating workshop.

The proposal should include a brief description of the topic, names of individuals to serve on the organizing committee, and a preliminary list of faculty, postdocs, graduate students, and representatives of industry and government you would like to invite. A Long Program Proposal Template is available online. Proposals for academic year 2015-2016 will be reviewed at the next SAB meeting.

Exploratory Workshops address urgent problems that mathematics may help solve. They are two or three days long, and can be organized in less than a year. The proposal should follow the guidelines for Winter Workshops, above, and will be considered at any time.

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Creating Connections

reflects the interests of participants as demonstrated by the programs they attend. As a hierarchical representation, this graph describes IPAM's programs at



various levels. At the coarsest level of clusters, it shows the range of application areas and of mathematical fields. At the level of programs, the graph shows that there are strong relations between programs, and at the finest level, these connections are seen to consist of interactions between individual participants across multiple programs.

IPAM is the bridge that links my education as an electrical engineer to my interest in mathematics and computational social science, and in particular, the ways humans interact with one another and

Roja Bandari Ph.D. in Electrical Engineering University of California, Los Angeles

with information. I am glad that I was able to demonstrate how IPAM has been that bridge for many other scholars throughout the years.

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IPAM Hosts Interdisciplinary Program on Mathematics of Turbulence

Turbulence is one of the main examples of complex nonlinear multiscale dynamics. It is ubiquitous in fluid flows and plays a major role in problems ranging from the determination of drag coefficients and heat and mass transfer rates in engineering applications, to important dynamical processes in environmental science, ocean and atmosphere

dynamics, geophysics, and astrophysics. Understanding turbulent mixing and transport of heat, mass, and momentum remains an important open challenge for 21st century physics and mathematics.

To help achieve this understanding, IPAM will host a long program on Turbulence in the fall of 2014. The participants will examine fundamental issues in mathematical fluid dynamics, scientific computation, and applications. Partial differential equations (PDEs) accurately model the essential physical phenomena in many situations. This program will include rigorous and reliable mathematical estimates of physically important quantities for solutions of these PDEs. Physicists, engineers, analysts, and applied mathematicians will share problems, insights, results and solutions. Improving communication across disciplinary boundaries is a central goal of the program.