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Institute for Pure and Applied Mathematics
a National Science Foundation Math Institute
at the University of California, Los Angeles

NEWSLETTER

LEADER IN NOVEL MATERIALS DISCOVERY ENJOYS INTERDISCIPLINARY SUPPORT AT IPAM

The importance of advanced new materials was recognized by the Obama administration in 2011 when it launched the Materials Genome Initiative – a multi-agency endeavor aiming to accelerate the discovery and deployment of advanced materials systems. Matthias Scheffler, a director of the Fritz Haber Institute in Berlin and professor at UC Santa Barbara, is among the leaders of the basic science effort to use computational materials science to solve equations that could lead to novel materials discovery. Through his involvement with the Institute for Pure and Applied Mathematics (IPAM), Scheffler is building momentum for the endeavor by bringing together colleagues from around the world.

Density Functional Theory (DFT) dates back more than a half-century to work by Walter Kohn, together with Pierre Hohenberg and Lu Sham, that would later earn him a Nobel Prize (shared with John Pople). A computational method widely employed for decades in solid-state physics, DFT has been refined in recent years to the extent that it is now considered an accurate and computationally tractable method for calculating essentially all properties of matter. The method is increasingly used in industry, such as in research and development of pharmaceuticals, chemicals and catalysts, and diverse engineering industries. "We can not only calculate existing materials, but also make predictions about completely unknown materials, their stability and their properties, which may become experimentally and even commercially useful," Scheffler says. "The number of so far unexplored materials is practically infinite. Thus, there is no doubt that in the next years scientists will identify new materials with novel property profiles that could open new opportunities in fields such as energy, mobility, safety, information, and health."

Scheffler has been at the center of these advances: His research group in Berlin (together with the group of Volker Blum, who is now professor at Duke University), contributed what is currently the most

Matthias Scheffler
Fritz Haber Institute

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INGRID DAUBECHIES GIVES GREEN FAMILY LECTURES

Ingrid Daubechies
Duke University

Photo by David von Becker

IPAM's 2016 Green Family Lecture Series, held in May, featured Ingrid Daubechies, James B. Duke Professor of Mathematics and Electrical and Computer Engineering at Duke University. Daubechies was the president of the International Mathematical Union from 2011-2014. She has received many awards for her pioneering work on wavelets, digital signal processing, and time-frequency analysis. Applications of her work range from fMRI and geophysics to paleontology and fine art painting.

Her first talk, entitled "The Master's Hand: Can Image Analysis Detect the Hand of the Master?" described image processing tools used to determine whether a painting is an original, or whether or not two parts of a painting were painted by the same artist. Her second talk, "Bones, Teeth, and Animation," described how distances between pairs of two-dimensional surfaces (such as teeth) allow biological morphologists to compare different phenotypical structures and to study relationships of living or extinct animals with their surroundings and each other. She also gave a research talk to the participants of the Culture Analytics program. You can watch videos of her talks on IPAM's YouTube channel or at **www.ipam.ucla.edu/videos**. ■

FEATURES

REGULARS

OTHER

NOTE FROM DIRECTOR RUSSEL CAFLISCH

Over the last year, IPAM brought together mathematical scientists, engineers, social scientists, humanists and artists for two long programs on Culture Analytics and Traffic Flow Management. These programs put IPAM at the center of the rapidly expanding application of mathematics to the humanities, social sciences and civil systems, by addressing issues such as the formation and influence of online social networks, the representation and analysis of data, and the future of self-driving cars, as well as the routes to collaboration among such a diverse group. The programs were preceded by workshops on Networks for the Humanities in 2010 and 2011, Mathematics of Traffic Flow in 2011, and Social Learning in 2014, which helped IPAM get started in these fields.

Last year was also notable for outstanding public lectures, including the 2016 Green Family Lectures by Ingrid Daubechies on mathematics for art and for biological morphology, a public lecture by Takashi Tokieda on the mathematics and art of paper folding, and a talk by Sadasivan Shankar on innovation. This diversity of topics was mirrored in IPAM's one-week workshops on Algebraic Geometry for Coding Theory and Cryptography, Shape Analysis and Learning, Partial Order, Uncertainty Quantification, and Energy Economics.

This has also been a banner year for IPAM's fundraising. To support child-care for participants, renovation of our building and other costs that our main NSF grant cannot cover, to increase our program offerings, and to diversify our financial support, IPAM seeks funding from individuals, corporations, foundations and other government agencies. Our 15th Anniversary Campaign exceeded its goal of $100,000, much of which came through donations to "name a seat" in our seminar room. About thirty seats were named, leaving sixty remaining seats for anyone who missed out on this opportunity! IPAM also received a new grant from the Simons Foundation for almost $1,000,000 over the next 5 years to support our video facility and senior program participants. For support of individual workshops, IPAM received grants from the AFOSR, ARO, ONR and the NSF's Office of International Science and Engineering. In addition, two IPAM workshops were supported by the DOE and NIH. We are most grateful to the individuals and institutions who have contributed to this fundraising success.

I hope that you enjoy this Newsletter and that you will stay involved with IPAM. Participating in a program or workshop, attending a public lecture, joining our Frontiers Society or naming a seat in our seminar room are just a few of the ways that you can further engage with IPAM. ■

Russel Caflisch
IPAM Director

APPLIED MATHEMATICIAN LEADS IPAM PROGRAM PROVIDING UNDERGRADUATES WITH REAL-WORLD RESEARCH EXPERIENCE

Susana Serna (pictured in center)
Autonomous U. of Barcelona

Susana Serna first boarded the long flight to Los Angeles for a meeting at UCLA's Institute for Pure and Applied Mathematics in 2005, fresh from having defended her PhD dissertation. Serna participated in Grand Challenge Problems in Computational Astrophysics – the first IPAM program to bring numericists and applied mathematicians together with physicists to gain a better understanding of astrophysical phenomena. By the time she left, she knew she would be returning regularly. "IPAM has had a huge impact on my career," says Serna, an associate professor at Universitat Autònoma de Barcelona in Barcelona, Spain. "I have met so many interesting people I never would have met at the typical meetings I attend, and it's made such a difference in my work."

An applied mathematician who specializes in numerical analysis, Serna is particularly interested in physics and engineering applications. "My goal is to provide accurate and effective simulations of physical processes to contribute to a better understanding of the phenomena behind them," she explains.

To get there, Serna focuses on developing reliable numerical approximations for physical models represented by nonlinear partial differential equations. She has made important contributions to the fields of computational fluid dynamics and plasma physics through the analysis and development of high-order, accurate and non-oscillatory numerical methods for hyperbolic conservation laws and Hamilton-Jacobi equations, the characterization and numerical approximation of the complex wave structure arising in magnetohydrodynamics (a model describing the dynamics of fluids in the presence of a magnetic field), granular flows, and special relativistic flows under non-standard equations of state.

Since visiting IPAM for the first time more than a decade ago, Serna has returned seven times to participate in a variety of programs,

(*continued on next page*)

UCLA POSTDOC LEADS STUDENTS ACROSS THE IPAM BRIDGE

Stephen DeSalvo is a Program in Computing (PIC) instructor in the math department at UCLA

IPAM is a bridge connecting mathematicians and specialists in other fields. I crossed it myself numerous times in various stages of my career, first as a participant in Research in Industrial Projects for Students (RIPS). This spring, I had the opportunity to lead my computing students across the bridge, with a remarkable outcome.

As a participant in the spring 2016 program on Culture Analytics, I saw the potential for innovation. The goal of the program was for mathematicians, computer scientists, social scientists and humanists to find ways to challenge each other and benefit from the diversity of thought and expertise. As a programming enthusiast and instructor of a yearlong sequence in programming at UCLA, I recognized an opportunity to show my students how to apply their computing skills in an unexpected way.

For the advanced programming class, the students typically create their own game over a 6-week period. This time, however, I invited the students to meet the IPAM visiting researchers and gave them the option to work on the researchers' projects.

One of the IPAM researchers, Mila Oiva of the University of Turku, had reached an impasse in her work involving optical character recognition of Polish newspapers. After experimenting with their own custom algorithms and obtaining a deeper understanding of the challenges, the students eventually found a black box package that outperformed all others and created an easy-to-use interface. This project thus provided an invaluable learning experience, as well as a concrete deliverable that will help facilitate further research.

A second project was to visualize various connections between Soviet writers in the 1950s, led by Ekaterina Lapina-Kratasyuk of the National Research University Higher School of Economics in Moscow. It involved a relatively small amount of data, which was generally drawn by hand using global intuition. There were two groups working independently on this project, one starting from the ground up, and another using black box tools like R. Each project provided a unique glimpse into this fascinating data set.

These projects introduced the students to cross-disciplinary research, and also enabled the students to explore careers in data science. With IPAM's recently renewed funding from the NSF, I look forward to crossing that bridge again in the years to come. ■

Stephen DeSalvo
UCLA

Real-World Research Experience

(continued from page 2)

particularly those involving transport and convection. Serna says she is particularly drawn to the depth and interdisciplinary nature of the IPAM programs. "With other conferences that I attend, I'm there for no more than a week and it's to present my work," she explains. "Here, you stay a few weeks or longer. The presentations aren't 20 minutes; they are more like an hour. And you attend different workshops and seminars that give you lots of opportunities to interact with the other attendees. You learn so much and open yourself up to new problems that you might choose to pursue after you leave. It is just a completely different dynamic."

Moreover, Serna explains, IPAM is different in that she meets and interacts with experts from outside of her field. "At a typical professional meeting you see a lot of people you already know, and they are from your specific field," she says. "IPAM brings people in from different backgrounds and disciplines, which helps you understand things from other points of view. I have collaborated with physicians and plasma physicists whom I never would have otherwise gotten to interact with. IPAM is always introducing new, challenging state-of-the-art problems. In every program I attend, there is always so much to learn."

Before assuming, beginning this summer, the role of director of IPAM's Research in Industrial Projects for Students (RIPS) program – a nine-week opportunity for talented undergraduates to work in teams on research projects proposed by sponsors from industry or the public sector – Serna had served as a RIPS academic mentor every summer since 2008, when she was a postdoctoral fellow in the UCLA Department of Mathematics. She has since overseen student projects for multiple sponsors, most recently the Lawrence Livermore National Laboratory. The RIPS teams (there are currently nine, each consisting of four students), with support from their academic mentor and industry mentor, study their problem and present their results, both orally and in writing, at the end of the program. As a mentor and now director, Serna supervises and provides guidance to students as they use mathematical tools to tackle real-world research projects.

The teaching in RIPS works both ways. With her extensive research experience, Serna is able to provide insightful advice and guidance to the students in the RIPS program. But Serna is quick to point out that she is also energized by the students, who are chosen from hundreds of applicants. "It's a very rewarding experience to work with students who are so talented and motivated," Serna says. "They come in with a great deal of energy, and within two weeks they already have results and an idea, along with mastery of the project and the tools they need to be successful. It's an amazing adventure that has helped to make summer one of my favorite times of the year." ■

NEWS AND RECOGNITION

NSF DIRECTOR CÓRDOVA VISITS RIPS - HONG KONG

On June 20, 2016, NSF Director France Córdova and Nancy Sung, Head of the NSF's Beijing office, visited Hong Kong University of Science and Technology (HKUST) and met with the participants of the RIPS-Hong Kong program. Tony Chan, President of HKUST, and Brian Bedell, the U.S. Consul in Hong Kong, also participated in the meeting. The eight American and eight local students described their RIPS projects and their educational and career plans to Córdova and Sung. RIPS, or Research in Industrial Projects for Students, is IPAM's summer research program for students featuring industry-sponsored projects; this is the sixth year of RIPS-Hong Kong, in partnership with HKUST.

France Córdova & **Tony Chan** (pictured front center) with RIPS - Hong Kong Participants

STAN OSHER AWARDED 2016 WILLIAM BENTER PRIZE

In May, IPAM Director of Special Projects, Stan Osher (UCLA), was awarded the 2016 City University of Hong Kong's William Benter Prize in Applied Mathematics "for his significant contributions to applying mathematics to solving real world problems." Adding to an already impressive and noteworthy list of achievements, this prize recognizes his life's work in areas such as high-resolution numerical schemes for shock capturing which has been highly influential in computational mechanics. Osher has also created pioneering algorithms for image processing, and his work on capturing moving interfaces using implicit representation has brought about breakthroughs in movie animation. Coincidentally, William Benter visited IPAM in spring 2015 to talk about his development of quantitative methods for the horse-racing market.

STACEY BEGGS WINS UCLA GREEN GALA AWARD

Stacey Beggs, IPAM's Assistant Director, was presented with UCLA's Green Gala Award for her work on sustainability at UCLA's Inaugural Green Gala on May 23, 2016. Stacey has worked with UCLA to make IPAM the first zero waste facility at UCLA, and as such, is a leader in the campus effort to achieve zero waste by 2020. The award is a testament to what Stacey and IPAM have accomplished.

Stacey Beggs
IPAM Assistant Director

IPAM PARTICIPANTS ELECTED TO NATIONAL ACADEMIES

Earlier this year, four IPAM speakers were elected into the National Academy of Sciences for their "distinguished and continuing achievements in original research." Yuval Peres (Microsoft Research) was a workshop speaker on three occasions, and will speak at one of the workshops in the upcoming Understanding Many-Particle Systems with Machine Learning program. Roberto Car (Princeton), Steven Evans (UC Berkeley), and Larry Wasserman (Carnegie Mellon) were also recognized. In addition, three IPAM speakers were elected into the National Academy of Engineering. Geoff Hinton (U Toronto and Google) was an organizer and speaker in IPAM's Deep Learning summer school. Also elected were Emily Carter (Princeton) and Chris Van de Walle (UC Santa Barbara).

IPAM WELCOMES NEW BOARD MEMBERS

In the past year, nine individuals have joined IPAM's Science Advisory Board and Board of Trustees. Last fall, Monique Miller (Wilshire Funds Management) and Steven Koonin (NYU) accepted the invitation to join the Board of Trustees. In June, Jeannette Wing (Microsoft Research) also joined the Board. IPAM welcomed six new members of the Science Advisory Board this year: Pablo Parrilo (MIT), Cecilia Clementi (Rice), Michael Kearns (Univ. of Pennsylvania), and Michael Brenner (Harvard) became members last fall, and we recently recruited Jordan Ellenberg (Wisconsin) and Emery Brown (Harvard and MIT) to join. They will help guide IPAM's activities and scientific direction.

IPAM MODERNIZES ITS ENTRANCE

Participants will be greeted this year by IPAM staff at our custom-built reception desk recently installed in IPAM's lobby! This beautiful piece of furniture was made possible by gifts from our Frontiers Society members, including former IPAM director Mark L. Green and his wife, Kathryn Kert Green, whose $15,000 gift was presented to IPAM at the 15th anniversary event last fall.

Mark Green
IPAM's New Reception Area

RONALD STERN TO SERVE AS CHAIR OF BOARD OF TRUSTEES

Starting in January 2017, Ronald Stern will begin a three-year term as chair of IPAM's Board of Trustees. Ronald Stern is a Professor Emeritus at UC Irvine, where he was Chair of the Department of Mathematics and Dean of the School of Physical Sciences. He currently serves on the boards of the Pacific Journal of Mathematics and the Friends of the International Mathematic Union, and has served on many others throughout his career. Stern received his PhD from UCLA in 1973. His research focuses on low dimensional topology. He has been an active and influential member of IPAM's Board of Trustees since 2010.

FRONTIERS SOCIETY

Thank you for making our fifteen anniversary campaign an enormous success! You helped us raise over $100,000 in one year. We are humbled by the demonstration of support for IPAM. 67 individuals and couples contributed to the campaign, 24 of whom donated $1,500 or more to "name a seat" (or two) in the IPAM lecture hall.

While the anniversary campaign is over, IPAM's still needs your support for its innovative programs and improvement projects. Please renew your membership or join IPAM's Frontiers Society, or make a gift at any level, online or by mail. We will continue to offer the opportunity to name a seat in the lecture hall as long as seats last! Go to www.ipam.ucla.edu/donate for more information. Thank you!

THANK YOU!

CONTRIBUTIONS 2015 - 2016

IPAM wishes to thank the following individuals who joined or renewed their membership in the Frontiers Society in the past year:

15TH ANNIVERSARY SEAT NAMING CAMPAIGN ($1500+)

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Tanya Beder and Joseph H. Bretton
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CORPORATE GIVING

IPAM received gifts of $10,000 or more from the following companies in the past year:

Amgen
Arete
The Aerospace Corporation
CSX
Google
GumGum
HRL Laboratories
Microsoft
Twitter

Other companies that donated to IPAM include American Century, AstraZeneca, IBM, and MathWorks. For more information on corporate giving, go to www.ipam.ucla.edu/donate/corporate-giving.

FOUNDATION AND GOVERNMENT SUPPORT

Additional support for IPAM programs came from the following foundations and governmental organizations:

Air Force Office of Scientific Research
Army Research Office
Department of Energy
J.B. Berland Foundation
LAPD Foundation
Los Alamos National Laboratory
National Institute of Health
Office of Naval Research
NSF Office of International Science and Engineering
Simons Foundation

UPCOMING PROGRAMS

LONG PROGRAMS

Understanding Many-Particle Systems with Machine Learning
September 12 - December 16, 2016

Computational Issues in Oil Field Applications
March 20 - June 9, 2017

Complex High-Dimensional Energy Landscapes
September 11 - December 15, 2017

Quantitative Linear Algebra
March 19 - June 15, 2018

WORKSHOPS

Turbulent Dissipation, Mixing and Predictability
January 9 - 13, 2017

Beam Dynamics
January 23 - 27, 2017

Big Data Meets Computation
January 30 - February 3, 2017

Emerging Wireless Networks
February 6 - 10, 2017

Regulatory and Epigenetic Stochasticity in Development and Disease
February 27 - March 2, 2017

Gauge Theory and Categorification
March 6 - 10, 2017

OTHER PROGRAMS

Modern Math Workshop
October 12 - 13, 2016

Research in Industrial Projects for Students
- *Los Angeles, June 19 - August 18, 2017*
- *Hong Kong, June 12 - August 11, 2017*
- *Berlin, June 19 - August 11, 2017*

Computational Genomics Summer Institute
July 10 - 14, 2017

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

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 2018 at the upcoming meeting.

SUMMER SCHOOLS

Summer schools are one to 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.

LONG PROGRAMS

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 three or 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 2018-2019 will be reviewed at the next SAB meeting.

EXPLORATORY WORKSHOPS

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.

Mark Your Calendars

February 1, 2017. Application deadline for Computational Genomics Summer Institute, an NIH-funded program cosponsored by IPAM.

February 14, 2017. Application deadline for IPAM's Research in Industrial Projects for Students (RIPS) Program in Los Angeles and Hong Kong, and Graduate-level RIPS in Berlin.

March 6 - 8, 2017. The 2016 Green Family Lecture Series will feature Edward Witten, Fields Medalist and professor of mathematical physics at the Institute for Advanced Study. The details will be announced in January.

Stay Connected

Novel Materials Discovery

(*continued from page 1*)

accurate and efficient computer code for DFT, FHI-aims, to calculate the electron structure, chemical binding, and stability of materials with high-performance computers. Scheffler and his colleagues have also led the way in combining the code with statistical mechanics and multi-scale methodology to enable longer time scales and larger space scales. Now, Scheffler's group is seizing on developments over the last decade that are introducing quantum chemistry methodology into the DFT field. "By drawing from these parallel movements, we can go beyond DFT, getting even more accurate than what we have today," Scheffler says.

Scheffler first became involved with IPAM in 2005 as an organizer of the three-month program Bridging Time and Length Scales in Materials Science and Bio-Physics, and since then he has engaged in activities that have made IPAM an important center for math applied to DFT and statistical mechanics. He was a key organizer of the 2013 program Materials for a Sustainable Energy Future, which brought together researchers from mathematics, physics, materials science, engineering, chemistry, biology, and computer science with the goal of better understanding the mathematical structure of continuum models governing material properties, as well as the electronic, atomic, and molecular structure of such new materials. "Our energy consumption is problematic in that we are putting too many harmful gases in the atmosphere. However, we may well find ways to transform CO_2 into useful chemicals, including fuels," Scheffler says. "We know thermoelectric materials that transform wasted heat into electricity but these, too, are inefficient. Much of the energy we consume is not used economically. We need to find novel materials that exhibit significantly improved performance and help in the energy and environmental sectors."

In the last few years, researchers have begun to use machine learning in materials science and DFT, and some of that effort has originated or been further developed at IPAM. This includes the materials science applications of compressed sensing for identifying the "needles in the haystack" – the few important new materials from the countless possibilities. "We are still at the basic level of advancing the methodology, but we are convinced that this type of science will help us to solve the mentioned energy and environmental challenges," Scheffler says. "It might bring us better superconductors, new types of solar cells, more fuel-efficient jet turbines. IPAM will surely contribute through the development of better methodologies to analyze the big data we are presently creating in computational materials science."

One of Scheffler's current scientific priorities is the development of the Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence in which top European groups in computational materials science, in collaboration with four high-performance computing centers, are developing a materials encyclopedia, big-data analytics and advanced graphics tools for materials science and engineering. The effort grew out of the Scheffler-led NoMaD Repository, an ambitious project to host, organize, and share materials data. The repository is unique in that it accepts all codes used in computational materials science. The NOMAD Laboratory is currently using big-data analytics that were developed in part at IPAM to cull materials of interest from the repository.

"When you work at the forefront of these research communities – physics, chemistry, materials science – you realize that everything new you would like to do is highly interdisciplinary, yet we don't always interact as much or as efficiently as we should," Scheffler says. "IPAM's great strength is its ability to bring these communities together so that we can learn from each other and advance the field." ■

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IPAM WORKSHOP: BIG DATA MEETS COMPUTATION

This workshop, to be held at IPAM in early 2017, will examine the interface of high performance computing (HPC) and big data. In HPC, one of the key challenges toward exascale computing is to overcome the communication bottleneck. Data motion tends to clearly limit the overall performance and determine the (enormous) energy consumption of future supercomputers; some even say "flops are for free." Therefore, it is crucial to develop novel ways of efficiently representing, reducing, reconstructing, and transferring huge amounts of data. At the same time, the analysis of large sets of (simulation) data requires sophisticated data analytics, which, in return, becomes more and more computationally intensive and thus contributes increasingly to HPC. Hence, computing technology and Big Data technology are intrinsically linked and further insights, methods, and algorithms have to be considered jointly within that context. The fusion of HPC and Big Data is a young field with an endless number of applications and huge potential. This workshop seeks to be a catalyst at this frontier and will bring together leading innovators and pioneers from applied mathematics, computer science, and various applications areas. ■