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

NEWSLETTER

BOARD MEMBER CYNTHIA DWORK ORGANIZES SUMMER SCHOOL, WORKSHOP ON ALGORITHMIC FAIRNESS AND SEX/GENDER BIAS

Cynthia Dwork will never forget the first meeting she attended as a member of the IPAM Science Advisory Board — even if, by necessity, she had to remain quiet.

"I had severe laryngitis," recalls Dwork, the Gordon McKay Professor of Computer Science at the Harvard Paulson School of Engineering. "But I experienced a stellar collection of people — knowledgeable, thoughtful, and inclusive — that it's been an honor to work with." At the end of that first meeting, Dwork conveyed her thoughts in writing for the group: "Best board ever."

For Dwork, IPAM's appeal starts with its tagline: math changes everything. "It's true," she says. "And what I love about IPAM is the breadth of what 'everything' means. It's not just that math gives more theorems, but that math changes our world. IPAM's broad appreciation for the many benefits to studying math really attracts me."

Dwork has contributed to changes in our world through her own work, which uses theoretical computer science to place societal problems on a firm mathematical foundation. She started her career in distributed computing before moving to cryptography — specifically, the subfield that seeks remedies for the failure of cryptographic protocols to compose securely. Dwork co-invented non-malleable cryptography, which takes into


Cynthia Dwork
Harvard University

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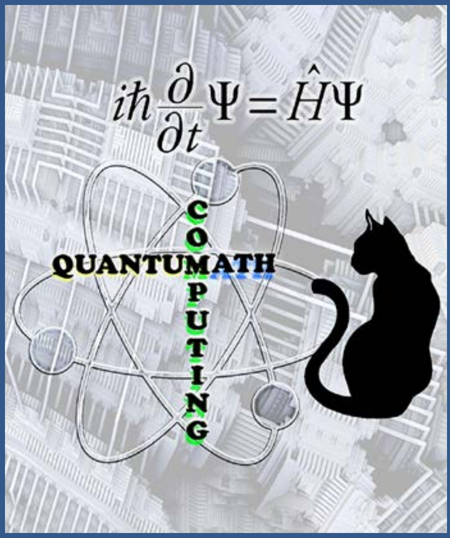
MATHEMATICAL AND COMPUTATIONAL CHALLENGES IN QUANTUM COMPUTING (SEPTEMBER 11 – DECEMBER 15, 2023)



The aim of this program is to empower mathematics to change quantum information science, and to explore the rich overlap between pure and applied mathematics and quantum information science. The program will convene many sub-communities of mathematics together with many sub-communities within quantum science (both theoretical and experimental) so as to encourage cross fertilization of ideas and the creative emergence of discoveries and new communities.

Among the important challenges addressed in this program is the effort to understand fully what are the new capabilities that quantum models for computation offer beyond classical models. Another important challenge is that of describing the structure and dynamics of complex quantum systems. Descriptions of few-body quantum systems are relatively well at hand and understood, even though surprises continue to arise. For larger systems, scientific progress has relied on various effective mathematical treatments. The drive to control large-scale quantum systems and use them to realize quantum computation challenges us to extend our treatments and obtain a deeper understanding of their structure and limitations. A third challenge is understanding where quantum information science can address current limitations in applied mathematics, data science, and numerical simulation. This program will bring together mathematicians, physicists, computer scientists, and others interested in pushing the boundaries of quantum computing. ■

FEATURES

HIGHLIGHTS

INFORMATION

NOTE FROM DIRECTOR DIMA SHLYAKHTENKO

The past year saw continued impact of the COVID-19 epidemic on every aspect of our lives. Since summer 2021, almost all IPAM programs were held in person, often with a substantial hybrid component. Despite difficulties involving travel (especially from outside the US), the 2021 fall program on gravitational waves attracted a very dynamic core group of scientists who discussed the many mathematical challenges – from signal processing to inverse problems, to machine learning, to numerical general relativity – that arise in modern multi-messenger astrophysics. A special highlight of the program was a Green Family Lecture by UCLA's Nobel Laureate Andrea Ghez.

IPAM's infrastructure investments made it possible for our events to be held in hybrid format. These included upgrades to our main lecture room making two-way communication between in-person and remote participants seamless. We have even created a robotic device that embodies remote participants in the lecture room – raising a "hand" when a remote participant asks a question and showing their face on a speaker-facing monitor. This technology was put to a good use starting with fall long program workshops.

With the Omicron surge in the winter, most of the activity associated with the special Hamilton-Jacobi long program reunion was moved on-line. Although our workshop on Quantum Numerical Linear Algebra was forced to be fully virtual, the remaining winter workshops (Calculus of Variations in Probability and Geometry, and Mathematics of Intelligence) featured in-house audiences.

In contrast, the IPAM building was quite full during the spring 2022 Quantum Mechanics program, even by pre-pandemic standards. The program paved the way towards practical and error-controlled quantum-mechanical calculations with tens of thousands (or even millions) of quantum particles. The core group attracted some of the foremost researchers from quantum mechanics and quantum chemistry. Besides the four workshops normally associated to the long program, the participants self-organized to form two more mini-workshops.

Last summer saw a very successful IPAM RIPS program in Los Angeles – with nine excellent projects and one of the strongest (and most diverse) international student researcher groups in our history. We were able to resume RIPS-Singapore, as well as G-RIPS Berlin and G-RIPS Sendai (both aimed at graduate students), in person. We also ran two graduate summer schools and a workshop. One school focused on Post-Quantum and Quantum Cryptography: the art of analyzing security of classical cryptosystems against attacks, and the art of leveraging quantum effects to develop new cryptographic schemes made possible by quantum information. The other school focused on mathematical formulations and approaches to Algorithmic Fairness – a topic of increasing importance due to the omnipresence of decision-making algorithms

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PREPARATION FOR NEW ERA OF SUPERCOMPUTERS

High-performance computing is entering the era of the exascale: supercomputers capable of 10^{18} — or a billion-billion — calculations per second. That's a 1,000-fold jump from the first petascale computers that came online in 2008, when Danny Perez was a postdoctoral fellow at Los Alamos National Laboratory (LANL).

As a computational physicist who is now a technical staff member at LANL, Perez is part of a group that develops novel methods to simulate materials, including those used for nuclear energy, particle accelerators, and other applications. And for that research, which involves atomic-scale simulations known as molecular dynamics, the quantum leap in computing power poses formidable challenges.

"If you have an engineering application involving a material in a nuclear reactor, you want to understand how it will survive the radiation environment and evolve with time, so it's critical to be able to make predictions over long timescales," Perez says. "When a new computer comes out, you can often simulate a larger system in the same amount of time without having to rearrange

Danny Perez
LANL

the way you do the simulation. But for long timescales, a sticking point has been that these shiny, big machines often don't help unless you come up with new methods or algorithms to rearrange the way you do the simulation, because you are typically bound by the need for communication and synchronization between the processors, and not by the raw computing power."

The reason, Perez explains, has to do with the growing complexity of the massively parallel architectures of the newer machines. "It's not like you have a super desktop with only one giant CPU that does everything," he says. "Instead, you have millions of distinct cores spread out over many different nodes. To learn to efficiently use these computers is by no means trivial. If you just take your code that you developed 10 years ago and try to run it on the new machine, you'll get awful performance."

The monumental nature of the effort in the U.S. Department of Energy and beyond to develop efficient codes and methods for the new era of supercomputers, along with the great interest among applied mathematicians in the problem, led Perez to become involved in organizing a long program

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Preparation for New Era of Supercomputers

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for IPAM. "New Mathematics for the Exascale: Applications to Materials Science," scheduled for March 13 through June 16, 2023, will bring together applied mathematicians, materials scientists, computer scientists, and method developers interested in unlocking the potential of the upcoming exascale architectures through novel mathematical approaches. "A big part of my own research for the last 6-7 years has been to start planning and developing codes and methods for these exascale machines," Perez says. "Thinking about this challenge for my set of problems, I realized that many materials scientists working at different scales are facing the same issues. I thought it would be great to bring this extended community together with mathematicians to share challenges and see if we can bring in new insights."

Perez's first exposure to IPAM came shortly after he joined LANL as a postdoctoral fellow. His mentor, Arthur Voter, had attended multiple IPAM programs and suggested to Perez that he attend a workshop. Perez subsequently was invited to attend an IPAM long program, and then a second one — this time as a workshop organizer. "The connections with IPAM came from the fact that our physics-based methods are interesting for mathematicians to understand and analyze," he says. "With people I met at IPAM over the years, we developed a rigorous mathematical understanding of how these methods work and of how their errors can be controlled and quantified, so that we now know exactly what it is we're doing once we do applications. It's been fruitful to build this community of people who are interested in the same problems from both the formal side of things and the application side."

Next spring's long program will seek to foster the development of new mathematical tools that facilitate ultra-scalable algorithms for a broad range of applications in computational materials science. "IPAM is the perfect venue to rethink from the ground up how we express the algorithms, what equations we're going to solve and how we're going to solve them, which requires mathematicians, computer scientists, and materials scientists working together and learning from one another," Perez says. "I don't know of any equivalent to IPAM in pure materials science, where you can gather a bunch of people for three months to work together. It's a very stimulating environment where you can meet hardcore mathematicians, people who are more on the application side, and then those in between, like myself. IPAM is great at grouping all of these disciplines together in a way that allows people to make connections, using mathematics as the glue. Although I am not a mathematician myself, I always feel welcome and at home at IPAM." ■

KEVIN STUBBS MAKES MOST OF HIS YEAR AT IPAM

Kevin Stubbs had originally planned to pursue graduate education in engineering — but, as he explains it, "I got more and more pure as time went on." He moved from computer engineering to mathematics for his PhD at Duke University, completing his dissertation on the use of Wannier functions to effectively reduce the size of impossibly large systems and facilitate the mathematical modeling of the electrical properties of materials.

But, for whatever purity is associated with Stubbs' academic pursuits, his goals skew more toward the pragmatic — using math to solve complex problems. That problem-solving orientation is what led Stubbs to accept a one-year position in August 2021 as a Simons Postdoctoral Fellow at IPAM, where he has collaborated with mathematicians and other scholars to advance his research in developing fast algorithms for high-dimensional problems, with a particular focus on quantum chemistry and materials science.

Stubbs has taken full advantage of the opportunity. Among other things, he brought both enthusiasm and new ideas to "Advancing Quantum Mechanics with Mathematics and Statistics," IPAM's long program last spring. The program featured what Stubbs refers

Kevin Stubbs
UC Berkeley

to as a "who's who of quantum chemistry," including researchers interested in using quantum mechanics to study the chemical properties of twisted bilayer. One of the long program's co-organizers, UC Berkeley associate professor Lin Lin, heads a group that Stubbs has joined after completing his postdoctoral fellowship. While at IPAM, Stubbs has worked with Lin's team on its research into twisted bilayer.

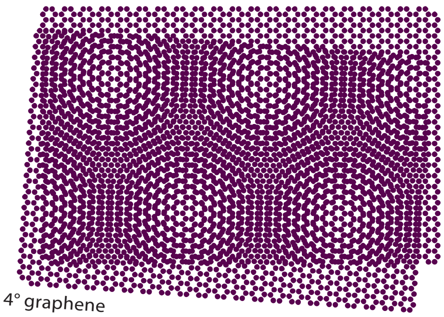
Stubbs' interest in quantum computing led him to become involved in IPAM's Research in Industrial Projects for Students (RIPS) program, mentoring a team working on quantum computing problems. RIPS provides an opportunity for talented undergraduates studying math, computer science, and related disciplines to work in teams on real-world research projects proposed by industry sponsors. "It was really fun to see the clever ideas these students are able to come up with," Stubbs says. "I often found myself surprised."

He has also consulted with Stanley Osher, IPAM's director of special projects, on their overlapping interests. Beyond the specifics of the research, Stubbs views Osher as a model for the type of high-impact work he is interested in pursuing. That impact hit home for Stubbs during a recent conversation with his mother, a physician. "She told me about how MRI scans became much faster about 10 years ago," Stubbs says. "That was because of the algorithms that Stan had developed." ■

NEWS STORIES

$5M SIMONS GRANT AWARDED TO IPAM PARTICIPANTS

Interest in two-dimensional (2D) materials was sparked by the exfoliation of graphene by Geim and Novoselov in 2004, that led to a Noble Prize in 2010. Graphene is a material with a single layer of carbon atoms that have a hexagonal structure. Subsequently, a number of other 2D materials have also been investigated. The unique electronic, optical, and mechanical properties of 2D materials have started an extraordinary level of experimental, theoretical, and computational activity in the materials science and physics communities. Interest in the mathematics community has recently emerged to develop rigorous foundations, improved models, and computational methods. IPAM sponsored a workshop on "Theory and Computation for 2D Materials" during January 13-17, 2020 that facilitated exchanges between the mathematics community and the physics communities working on 2D materials.



Moiré Pattern in Graphene*

Placing a 2D lattice on another with a small rotation gives rise to periodic "moiré" patterns on a superlattice scale much larger than the original lattice-analogous to the beating of two waves with slightly different wavelengths (see the image of two twisted hexagonal lattices. This effective large-scale fundamental domain has opened the possibility of discovering new phenomena at the moiré scale that were previously inaccessible at the atomistic scale.

The Simons Foundation has awarded a $5M Target Grant for the project "Moiré Materials Magic" to Alan MacDonald, Eric Cances, Svetlana Jitomirskaya, Efthimios Kaxiras, Lin Lin, Mitchell Luskin, Angel Rubio, and Maciej Zworski. According to Mitch Luskin, the project was hatched at lunch during the IPAM Workshop in January 2020. Several of the PIs of the grant participated in that workshop, and many have participated in multiple recent IPAM events.

LATINX IN THE MATHEMATICAL SCIENCES CONFERENCE 2022

On July 7-9, 2022, IPAM hosted a conference showcasing the achievements of Latinx in the mathematical sciences. The third in the series, the goal of the conference was to encourage Latinx to pursue careers in the mathematical sciences, to promote the advancement of Latinx currently in the discipline, to showcase research being conducted by Latinx at the forefront of their fields, and, finally, to build a community around shared academic interests. This conference was sponsored by the Mathematical Sciences Institutes Diversity Initiative, with funding from the National Science Foundation Division of Mathematical Sciences, Los Alamos National Laboratory, and UCLA.

This conference included several career panels, plenary talks, scientific sessions, a special public event with Dr. Richard A. Tapia, pre-conference activities for undergraduate and graduate students, mentoring and networking activities, reading of testimonios (stories of Latinx and Hispanic mathematicians), participation of high school students, a banquet, and more.

The Latinx in Math Conference 2022 aimed to offer a rewarding, enlightening, supportive, and fun experience to every participant. The conference was hugely successful in its goals as participants reported finding the conference to be "an incredibly supportive environment for mentoring and it was inspiring in terms of both mathematics and giving back to the mathematics community."

Seeing a group of strong, successful Latinx mathematicians was reportedly "incredibly inspiring" for most participants. The conference overall was an "open and welcoming atmosphere" which allowed for a tremendous amount of networking to occur over three days.

We are looking forward to hosting the next Latinx in the Mathematical Sciences Conference in 2025!

NOTE FROM DIRECTOR DIMA SHLYAKHTENKO *(continued from page 2)*

in our daily lives. It was followed by a workshop Who Counts? Sex and Gender Bias in Data, featuring interdisciplinary discussions that examined sources of sex and gender bias in data, with emphases on impoverished women; women of color; trans and non-binary persons; and older women. Cynthia Dwork's (Harvard) Green Family Lecture Series was a special highlight during these activities.

IPAM also held two very special events aimed at improving equity, diversity, and inclusion in mathematical sciences. The LatMath conference – the third in a series – celebrated achievements of Latinx mathematicians. And PUNDiT – a series of mini-courses aimed at undergraduates interested in number theory – was one of our first in-person events last fall. The success of these events led to the establishment of a special IPAM EDI endowment – aiming to raise $300K by next summer, to be matched 1:1 by the Dean of Physical Sciences. We are happy to report that 2/3 of the goal has already been reached!

As we look ahead to next year, IPAM anticipates increased return to in-person scientific research and collaboration true to its slogan: math changes everything! ■

DONOR RECOGNITION

CORPORATE GIVING

IPAM offers opportunities for corporations to participate in our scientific programs, propose topics for programs, and support activities that promote diversity in math and science. IPAM received gifts from the following companies in the past year:

- **Advanced Micro Devices Inc.**
- **The Aerospace Corporation**
- **AFRL**
- **Aquatic**
- **Google**
- **GumGum, Inc.**
- **HRL Laboratories, LLC**
- **IBM**
- **Lawrence Livermore National Laboratory**
- **Los Alamos National Laboratory**
- **Meta**

In addition to support from our main NSF grant, IPAM also received grant funding from the **Simons Foundation Institute Grant, and the NSF Mathematical Sciences Institutes Diversity Initiative.**

For more information on corporate giving, please visit our donor page at **www.ipam.ucla.edu/donate/corporate-giving**.

IPAM'S FUNDRAISING PRIORITIES

Facilities Improvement. Upkeep and enhancement of IPAM's space is essential in ensuring a healthy and safe workplace. Your gift will help create and maintain a welcoming place for our participants and the math community.

Child Care Fund. Help IPAM support participants whose attendance in programs is dependent on securing reliable care for their children.

Equity, Diversity, and Inclusion. Help IPAM improve EDI in all of its activities.

GIVING OPPORTUNITIES

You can donate online or by mail. See **www.ipam.ucla.edu/donate** for details. Giving opportunities include:

IPAM's Equity, Diversity, and Inclusion Endowment. Help IPAM reach its goal of raising a $600,000 endowment to support EDI activities. Gifts to this fund received until June 30, 2023 will be matched 1:1 by the Dean of Physical Sciences! Over $400,000 is raised already.

Director's Endowment Fund. Your support will help fulfill high priority needs that cannot be supported by federal grants, such as family expenses for participants and other special needs.

IPAM's Frontiers Society. The 3 levels of membership: Innovator ($150), Visionary ($800), and Champion ($1,500), will help us continue to run high-quality programs attracting both renowned experts and promising young scholars.

Donor Wall. Donors giving $5,000 or more will be recognized on IPAM's donor wall.

Name a Seat. With a gift of $2,000, you may name a seat in IPAM's lecture hall.

Contact Sharon Chang with any questions at **schang@support.ucla.edu.** ■

FRONTIERS SOCIETY MEMBERS 2021-2022

IPAM thanks everyone who joined the Frontiers Society, gave to the Director's Endowment Fund, and all others who donated to IPAM in the past year. Special thanks to those who made multi-year pledges!

CHAMPIONS ($1,500+)

E.S. Tae and Betty C. Tse

John B. Garnett and Dolores Garnett

Stanley J. Osher and Suzanne C. Lauver

Virginia D. Hales and Alfred W. Hales

VISIONARIES ($800-$1,499)

Dimitri Shlyakhtenko

INNOVATORS ($150-$799)

Christopher Acklen

Allen Clement and Joanie Clement

Yun Jiang

Tatiana Toro and Daniel Pollack

Michael P. Chohen

Terry J. McKiernan and Claudine C. Tazartes

Vijay Pedapudi

Jun Zhang and Qingping Tao

Judy J. Wu

UPCOMING PROGRAMS

LONG PROGRAMS

New Mathematics for the Exascale: Applications to Materials Science
March 12 – June 16, 2023

Mathematical and Computational Challenges in Quantum Computing
September 11 – December 15, 2023

Geometry, Statistical Mechanics, and Integrability
March 11 – June 14, 2024

WORKSHOPS

Explainable AI for the Sciences: Towards Novel Insights
January 9 – 13, 2023

Learning and Emergence in Molecular Systems
January 23 - 27, 2023

PUNDiT-2: Practicum for Undergraduates in Number Theory
February 4 - 5, 2023

Machine Assisted Proofs
February 13 - 17, 2023

Winter School on Contemporary Quantum Algorithms and Applications,
February 22 – February 24, 2023

Artificial Intelligence and Discrete Optimization
February 27 - March 3, 2023

Women in Data Science and Mathematics
August 7 – 11, 2023

Chiral-induced Spin Selectivity Through a Quantum Lens
August 30 - 31, 2023

SUMMER RESEARCH PROGRAMS

RIPS Los Angeles 2023
June 20 – August 18, 2023

RIPS Singapore 2023
May 22 – July 21, 2023

G-RIPS Berlin 2023
June 19 – August 11, 2023

G-RIPS Sendai 2023
June 19 – August 8, 2023

CALL FOR PROPOSALS

IPAM seeks proposals from the mathematical, statistical, and scientific communities for its long programs, winter workshops, summer schools, and exploratory workshops. Proposals must include a plan for recruitment and involvement of members of underrepresented groups. Submitted proposals are reviewed by IPAM's Science Advisory Board (SAB) at its annual meeting in November. To receive fullest consideration, please send your proposals by September 30 to the IPAM Director at director@ipam.ucla.edu. A brief extension to this deadline is possible; please email the Director for consideration.

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 2024 at its upcoming meeting. Proposals for workshops on multiscale physics will be considered for inclusion in a series of workshops made possible by an endowment from the Julian Schwinger Foundation for Physics Research.

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, described above, and will be considered at any time.

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. 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 senior researchers and representatives of industry and government you would like to invite. In addition, the proposal should delineate how it will contribute to the goals of improving equity, diversity and inclusion in mathematics and other sciences. A long program proposal template is available online. Proposals for academic year 2024–2025 will be reviewed at the next SAB 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.

Mark Your Calendars

October 10 & 11, 2022. Margaret Murnane (UC Boulder) will give two public lectures as part of the Green Family Lecture Series.

February 13, 2023. Application deadline for IPAM's Research in Industrial Projects for Students Programs in Singapore and Los Angeles.

February 24, 2023. Application deadline for IPAM's Graduate-level Research in Industrial Projects for Students (G-RIPS) Programs in Berlin and Sendai.

For more information, go to **www.ipam.ucla.edu.**

Stay Connected

Cynthia Dwork Organizes Program on Algorithmic Fairness

(continued from page 1)

account security risks when intentionally misbehaving — or simply erroneously programmed — agents are active participants in cryptographic protocols, rather than just passive eavesdroppers.

In the early 2000s, after conversations with Helen Nissenbaum, a philosopher who specializes in addressing societal problems arising from new technologies, and who was in the process of formulating Contextual Integrity as a concept of privacy, Dwork began to focus on the issue of privacy-preserving data analysis — ensuring that large databases containing detailed and sensitive information can be used to unlock insights while maintaining the privacy of the individuals in the dataset. She spearheaded the invention, together with McSherry, Nissim, and Smith, of differential privacy, which is now the subject of intense activity across many disciplines.

The first time she attended an IPAM meeting, Dwork struck up a conversation with Mark Green, IPAM co-founder and director emeritus, and was taken with Green's vision for the institute. After organizing a pair of workshops, she accepted an invitation to join the Science Advisory Board. Dwork has brought her expertise in theoretical computer science to the Board, and has been instrumental in bringing in other experts from her field. "Mark was always nudging me to do a workshop or a summer school," Dwork says, smiling. "And this summer, I did both."

Dwork co-organized the graduate summer school on Algorithmic Fairness, which was held at IPAM July 11-15, followed by the thematically connected workshop "Who Counts? Sex and Gender Bias in Data," July 18-20. The issue of algorithmic fairness — concerns that machine-learning models, increasingly consequential throughout society, could perpetuate and exacerbate existing biases and historical injustices — has roots in some of Dwork's own work starting a little more than a decade ago. "At that time, most companies weren't yet worried about whether or not their artificial intelligence techniques were embodying the biases of society, but to us it was clear they would," Dwork notes. "And there was no theory — even defining the goal of 'algorithmic fairness' had to be thought out, so that was where we started. In the last several years, the technical work has gotten very exciting. To keep the research grounded in the problems of the real world, it was, and still is, an opportune time for wide, interdisciplinary, discussion. And this is what we had at IPAM."

The summer school program included a short course on the theory of algorithmic fairness taught by Dwork and computer scientist Guy Rothblum, as well as talks by leading researchers in various application areas. The ensuing workshop examined sources of sex and gender bias in data, with special emphasis on women of color, trans women, and non-binary persons. Many of the summer school students applied to and were admitted to stay for the workshop.

"From the summer school, we ended up with a cohort of people who were aware of the technical questions and progress, which allowed them to attend the less-mathematical, interdisciplinary discussion armed with that knowledge," Dwork explains. "The workshop then helped to raise awareness among the data science practitioners and theoreticians that things they may have done automatically could well be wrong if they missed social and historical factors. Our goal is to create bilingual citizens — to help the non-math people understand what the math can and cannot do, and for the math people to understand the context in which they're working and help to articulate the problems in a way that captures real-world issues.

"IPAM welcomed and provided crucial infrastructure for this complex, compound operation that had two distinct parts — a school and a workshop — but needed to work together. That validated the importance of what we see as a very important use of math. There are few places where this could have been done so successfully." ■

Institute for Pure and Applied Mathematics

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NEW MATHEMATICS FOR THE EXASCALE: APPLICATIONS TO MATERIALS SCIENCE (MARCH 13 - JUNE 16, 2023)

The explosive increase in computing power delivered by modern supercomputers promises unprecedented simulations scale and fidelity. Their massively-parallel architectures however pose formidable challenges to algorithm and software development. For example, fully harnessing exascale computers, which will deliver in excess of 10^{18} operation per second, will require simultaneously executing on the order of a billion operations without being limited by communication and synchronization overhead. This severely constrains the types of simulations that are expected to make efficient use of upcoming exascale architectures, and hence risks limiting their scientific impact in the computational sciences.

The aim of this program is to foster the development of new mathematical tools and formalisms that will enable a new generation of ultra-scalable algorithms for a broad range of applications in computational materials science. Topics of interest will include strategies for scalable single-scale simulations, novel massively-parallel scale-bridging algorithms, and integration of extreme-scale computing into experimental and data science workflows. The program will bring together applied mathematicians, materials scientists, computer scientists, and method developers interested in unlocking the potential of upcoming exascale architectures through novel mathematical approaches. ■