

KIERON BURKE PERSONIFIES IPAM'S INTERDISCIPLINARITY

When Kieron Burke was working on his PhD at the University of California, Santa Barbara, in the late 1980s, he remembers density functional theory (DFT) being “a slightly obscure thing.”

In the 1960s, Burke's doctoral adviser, Walter Kohn, had developed the fundamental elements of DFT — a method for setting up and solving quantum mechanics equations for the electrons in any substance. But long after Burke completed his doctoral studies, DFT became a mainstay in many branches of science, particularly chemistry and materials science — thanks in no small measure to research by many people, including Burke. Today, Burke notes, as many as

50,000 scientific papers each year reference the use of DFT in their calculations. “In my lifetime it's gone from a theorist's game in trying to catch up with the experiments, to something that's driving a huge amount of science,” he marvels.

Given the quantum mechanics, solving the equations for electrons in everyday matter becomes exponentially more costly as their number increases — to the point that even the most powerful supercomputer at the Department of Energy (DoE) can't abide standard methods beyond 20-30 atoms. Through a simple approximation, DFT allows for quick solutions to quantum chemical calculations for molecules



Kieron Burke
UCI

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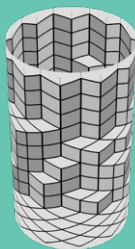
GEOMETRY, STATISTICAL MECHANICS, AND INTEGRABILITY

(MARCH 11 – JUNE 14, 2024)

In the last 20-30 years probability theory and statistical mechanics have been revitalized with the introduction of tools from geometry, notably conformal geometry and discrete analyticity, but also algebraic geometry and integrable systems.

Recent connections between classical and discrete geometric structures on surfaces,

and combinatorial models such as the dimer model, Ising model and the Tutte polynomial reveal a significant connection with geometry, notably hyperbolic geometry and polyhedra.



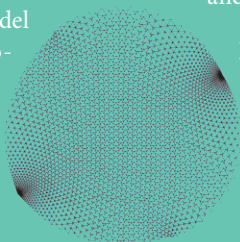
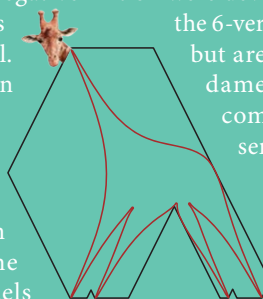
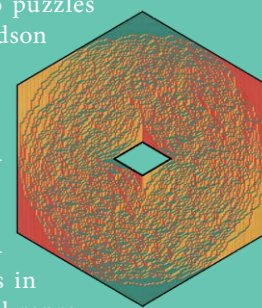
Other recent work on the dimer model has led to connections with knot theory, Lorentzian geometry, and symplectic geometry. From another direction, the combinatorics of the totally nonnegative Grassmannian has connections with the dimer model. Likewise, the isotropic Grassmannian and orthogonal Grassmannian have connections with spanning trees and the Ising model.

Finally, there are well-known connections between some statistical mechanics models and representation theory, such as Young diagrams, Gelfand-Tsetlin

patterns, Knutson-Tao puzzles and Littlewood-Richardson coefficients and their generalizations. The Bethe Ansatz and the Yang-Baxter equation were developed for the 6-vertex model

but are now fundamental tools in combinatorial representation theory.

This program will bring together researchers in this somewhat disparate realm of ideas, united by the underlying themes of geometry and statistical mechanics. ■



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NOTE FROM DIRECTOR DIMA SHLYAKHTENKO



Dima Shlyakhtenko
IPAM Director

With the effects of the COVID-19 pandemic subsiding, IPAM was able to fully resume its operations last year. We have run two impactful long programs, on Computational Microscopy and Mathematics for Exascale

Computing, both bustling with activity. The latter program featured a first for IPAM—a week-long hackathon that brought together theoreticians and practitioners writing code for numerical simulations. Our workshop on Machine Assisted Proofs last February set a post-pandemic record for attendance of over 100 participants. And this August we held a celebration of 23 years of the Research in Industrial Projects for Students (RIPS) program, bringing back alumni enjoying mathematics careers in academia as well as in industry.

I am very happy to announce that IPAM has met and surpassed its fundraising goal of \$300,000 (which was doubled to \$600,000 by the Dean of Physical Sciences)

to establish an endowment in support of IPAM's work on Equity, Diversity and Inclusion. The money is being put to a good use. This past July, IPAM ran the inaugural AMIGAs program, focusing on critical skills for applied mathematics graduate students from traditionally underrepresented groups. A collaborative workshop "Women in Data Science and Mathematics" ran in August; and this coming October we will run a second Practicum for Undergraduates in Number Theory (PUNDiT).

Looking at the year ahead, we are happy to be offering a variety of exciting programs in several areas of pure and applied mathematics, living up to our slogan: Math Changes Everything! ■

SAMITHA SMARANAYAKE SPEARHEADS IPAM'S EFFORT TO ENSURE EQUITY IN TRANSPORTATION SYSTEMS

As cities strive to become more livable through transportation and other infrastructure development, planning decisions increasingly rely on algorithms and artificial intelligence. But Cornell University's Samitha Samaranayake, whose interests include modeling and understanding questions around large-scale transportation networks, points out that if these algorithms are developed without attention to where needs are greatest, they have the potential to perpetuate societal inequities.

"In transit planning, there can be a ridership-versus-coverage tradeoff — if you want to move as many people as possible, you run the buses on the high-density corridors, which is typically where property values are higher; but if you want to serve people living in the low-income communities, you might need to compromise on how many people you move," explains Samaranayake, an assistant professor in Cornell's School of Civil and Environmental Engineering and a graduate field faculty member in the School of Operations Research and Information Engineering, the Center for Applied Math, and the Systems Engineering Program at Cornell.

"Historically, transportation is an area that has been highly discriminatory in terms of

having adverse effects on low-income communities," Samaranayake adds, "and if we aren't purposeful with these algorithms, that is what will continue to occur."



Samitha Samaranayake
Cornell University

With that in mind, Samaranayake is organizing a workshop on Mathematical Foundations for Equity in Transportation Systems, to be held at IPAM next January. The workshop will bring together a diverse group of participants — including computer scientists, social scientists, transportation experts, and mathematicians — to exchange ideas on the desired objectives of these systems, improve

the understanding of how equity should be considered in the plans, and determine how math can help to meet those objectives.

Samaranayake studied computer science at MIT as an undergraduate, during which he spent a significant portion of his time conducting his thesis research at Synopsys, a Silicon Valley tech company. He then worked as a software engineer at Oracle before returning to school for his PhD in transportation networks at the University of California, Berkeley, followed by a postdoctoral fellowship at MIT.

In his PhD studies he focused on problems related to optimizing traffic flow, and on the then-emerging technology of ridesharing. But Samaranayake quickly became convinced that the concept of ridesharing — a misnomer, he notes, since people aren't typically sharing rides with others, but rather using the apps for the equivalent of potentially safer and more efficient taxi use — fails to improve the ratio of passenger miles traveled to vehicle miles traveled. "If we want to use transportation technology to improve societal impacts in cities, it has to include a well-integrated component of moving masses of people together, rather than individuals one at a time," he says.

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Ensuring Equity in Transportation Systems

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Today, Samaranayake's primary research interest is in mathematical modeling and algorithm design for large-scale transportation network problems — particularly, those at the intersection of mass transit and emerging transportation technologies. Through algorithm engineering — gaining theoretical insights from successful data-driven and heuristic approaches, and vice versa — he has focused on developing hybrid transit systems: services designed to fully integrate traditional fixed-line mass transit and agile, demand-responsive transportation modes. Samaranayake works closely with public transit agencies and private shuttle operators to gain practical insights, calibrate models, and ensure the real-world relevance of his algorithms.

Samaranayake's first IPAM experience came in 2015, when he attended a long program, New Directions in Mathematical Approaches for Traffic Flow Management, as a postdoctoral fellow. "It was a great experience, mixing with so many important people in transportation as well as the more junior people like myself," he says. "Unlike typical conferences, you're with the same people all day, with plenty of time outside of the talks to get to know about their work. It helped me not only to interact with people in my area, but also

to understand the bigger picture, both upstream and downstream of the area I work in." Samaranayake returned to participate in an IPAM workshop on autonomous vehicles in 2019, and then was part of the long program, Mathematical Challenges and Opportunities for Autonomous Vehicles, in 2020.

While the AI community has devoted considerable effort to addressing prediction bias in sectors such as health care, both the implications and the math are different when it comes to using algorithms to build long-term infrastructure and services — and much less attention has been paid to that area, Samaranayake says. He hopes that bringing a diverse group of experts together for the Mathematical Foundations for Equity in Transportation Systems workshop in January 2024 will mark an important step toward expanding the number of academics working across disciplinary boundaries to address transportation issues through the lens of equity.

"There's a lot of heavy math lifting to be done in infrastructure systems, and that work has the potential to produce substantial societal benefits," Samaranayake says. "IPAM, which brings mathematicians together with experts from other disciplines to think about solutions to impactful problems, is the ideal setting for doing this." ■

IPAM BROADENS ELISA NEGRINI'S SCIENTIFIC PERSPECTIVE

Thanks to her year at IPAM, Elisa Negrini entered her postdoctoral position in the UCLA Mathematics Department uniquely prepared — having already gotten to know the people in the department, as well as having forged collaborations both with fellow department members and with individuals in fields to which Negrini previously had little exposure.

Negrini began her PhD program at Worcester Polytechnic Institute in Massachusetts focusing on pure math, but as she progressed toward her doctorate she gravitated toward applied math — in particular, applications of machine learning to physical systems. The opportunities afforded by IPAM to collaborate across disciplines prompted her to apply to the institute as a Simons Postdoctoral Fellow. "I wanted a postdoc that would allow me to work with real data and explore applications," Negrini explains. "IPAM, which had scheduled a long program on computational microscopy, was an ideal way to develop my knowledge on deep learning and AI."

Negrini was an active participant in Computational Microscopy, held in the fall of 2022, which brought together applied mathematicians and domain experts to discuss strategies for tackling current challenges in the field through a combination

of advanced algorithms, mathematical modeling, computational tools, big-data processing, and deep learning.

"Typically, at conferences, it's just the people in your field, and the discussions are restricted to the language you all speak," Negrini says. "At



Elisa Negrini
IPAM

IPAM, I got to meet people from all of these disciplines, and instead of going out and trying to network, they were coming into my office. Because my expertise has applications in so many areas, I got to collaborate with chemists and physicists on projects involving

topics I hadn't known anything about, meet people outside my field whom I wouldn't have met otherwise, and produce original research." One such paper, on reconstructing images of biological cells from diffraction patterns using an iterative algorithm, written with physicist Jianwei (John) Miao and mathematician Stanley Osher — Negrini's mentor during her IPAM postdoctoral experience — was recently submitted; a paper from a second collaboration used AI for computational microscopy in the low-dose regime.

For her upcoming UCLA postdoc, Negrini is focusing on physics-informed machine learning for plasma physics; she will also be teaching. In summer 2023, she served as a mentor for IPAM's Research in Industrial Projects for Students (RIPS) program, in which undergraduates studying math, computer science, and related disciplines work in teams on applied research projects proposed by industry sponsors, with support from academic and industry mentors. "The RIPS students make it easy for me because they come in with such excitement," says Negrini. "I help them without solving the problems for them, and it's wonderful to observe them overcoming obstacles and then feeling that sense of accomplishment." ■

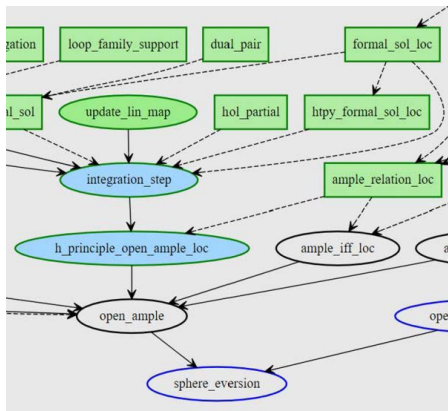
NEWS STORIES

MACHINE ASSISTED PROOFS

Credit: Jordan Ellenberg

In February of 2023, IPAM hosted a workshop on Machine-Assisted Proofs. This program had been in the works for more than a year, but ended up being held at a timely moment, when unexpectedly rapid development in large language models (LLMs) in late 2022 had brought focused national attention to the question of how machines could assist or even replace human ingenuity.

As the title of the workshop suggests, the speakers at the conference focused on the former outlook, in which novel techniques in machine learning are potential boosters of human creativity and effort. Our workshop was the first to bring together three groups that have largely worked separately: machine learning developers, often from industry; pure mathematicians at the forefront of using machine learning as a tool in their own work; and formalizers, researchers leading the project of encoding contemporary research mathematics in a



form that can be interpreted and checked by machines. The dominant mood at the workshop was one of excitement and synergy. We saw Georgie Williamson (“What Can The Working Mathematician Expect From Deep Learning?”) talk about his collaboration with DeepMind, in which machine learning was used to identify a potential conjecture in representation theory which

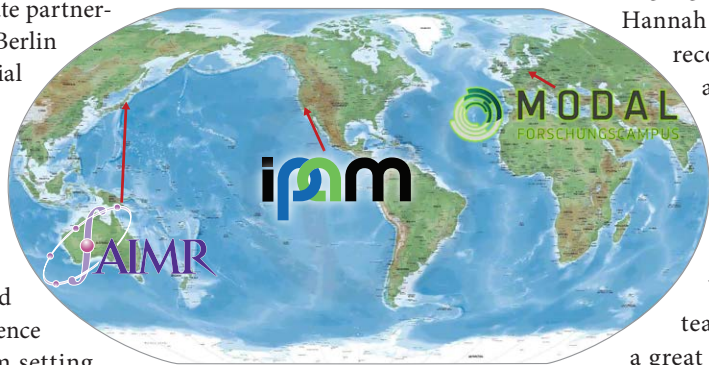
human mathematicians are hard at work on proving; Heather Macbeth (“Algorithm and Abstraction in Formal Mathematics”) talked about the ways our value system as mathematicians will have to change as more mathematics is formalized; and Tony Wu, from Google (“Autoformalization with Large Language Models”) talked about a grand project that synthesized many of the themes of the workshop, namely: using LLMs to generate short formal proofs of desired mathematical statements, which — being formal — can then be automatically checked by the proof verifiers build by the formalization community. In formal mathematics, by contrast with so many other domains where LLMs are being applied, there are robust barriers against “hallucination”!

Participants left the workshop with a feeling of wide-open potential and a clear sense of avenues for future work at the interface between machine learning and pure mathematics. ■

GRADUATE LEVEL SUMMER RESEARCH PROGRAM G-RIPS

The Graduate-Level Research in Industrial Projects for Students (G-RIPS) program offers graduate students in mathematics and related disciplines the opportunity to work on industry-sponsored research problems. In 2014 IPAM started G-RIPS Berlin in partnership with the Research Campus MODAL, which is a public-private partnership between the Zuse Institute Berlin (ZIB), the FU Berlin, and industrial partners. The inaugural G-RIPS partners were SAP Germany, Deutsche Bahn, and Open Grip Europe. Since 2014, many more of the over 30 industrial partners of MODAL have participated in G-RIPS, and offered students an opportunity to experience cutting-edge research in a team setting. Inspired by the success of G-RIPS Berlin, IPAM added a second G-RIPS program in 2018 in Sendai, Japan. It is in partnership with the Tohoku Forum for Creativity (TFC) and the Advanced Institute for Materials Research (AIMR) at Tohoku University. The participating industrial sponsors of the last 5 years have included Toyota, NEC, Fujitsu, Mitsubishi, and IHI. Former G-RIPS

Sendai student Jeffrey Yeh commented: “I will definitely recommend G-RIPS to other graduate students. It is often difficult for me to see the real applications of mathematics while studying it, and this program really helped me to see the connection between math and industry problems.”



The research projects in each program cover a wide range of topics that include optimization, biomedical applications, image processing, quantum computing, and more. In both G-RIPS programs, the emphasis on strong research projects is enhanced by a cultural experience for the students. The research teams always consist of 2 US students together with 2 Japanese students

(Sendai) or 2 European students (Berlin). In addition to the research program that includes seminars, visits to the participating industrial sponsors, and formal written and oral presentations, each program is complemented by cultural activities and language classes. Former G-RIPS student Hannah Horner wrote: “I would definitely recommend G-RIPS to other graduate students, especially if they have any interest in traveling abroad. G-RIPS is a great program for students to get applied research experience and the opportunity to live in a foreign country. Working with an international team on an industrial problem is a great experience to help prepare for a career in research after graduate school.”

IPAM is grateful to Hiroshi Suito in Sendai and Tim Conrad in Berlin for all the work they are putting into this fruitful collaboration that has enabled many students to spend an unforgettable summer abroad. We are looking forward to continuing and expanding both programs in the future. ■

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 and government agencies in the past year:

- **Advanced Micro Devices Inc.**
- **The Aerospace Corporation**
- **Air Force Research Laboratory**
- **Toyota**
- **Relay Therapeutics**
- **IBM**
- **Lawrence Livermore National Laboratory**
- **Los Alamos National Laboratory**
- **SAP**

In addition to support from our main NSF grant, IPAM also received grant funding from the **Simons Foundation**, and the **NSF Infrastructure Program through 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 EQUITY, DIVERSITY, AND INCLUSION ENDOWMENT

Many thanks to everyone who donated. We have surpassed our goal of the \$600,000 endowment to support EDI activities. The fund will be used to increase diversity and inclusion in our programs.

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.

IPAM’S FRONTIER SOCIETY

Please consider joining IPAM’s Frontier Society. Your contribution will help us continue to run high quality programs attracting both internationally renowned experts as well as promising young scholars. Depending on the level of your membership, benefits include an IPAM gift (T-shirt or other), preferred seating at all IPAM public lectures, free parking, invitations to exclusive IPAM events, and free registration to all IPAM workshops and conferences. See the IPAM webpage for details of the membership levels.

All Frontier Society members will be listed in the annual newsletter. With a gift of \$2,000, you may name a seat in IPAM’s lecture hall. Donors giving \$7,500 or more will be recognized on IPAM’s donor wall.

DONATE HERE

For more information and to donate, check here:

www.ipam.ucla.edu/donate



FRONTIERS SOCIETY MEMBERS 2023-2024

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+)

Robert S. Baker

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UPCOMING PROGRAMS

LONG PROGRAMS

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

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

Mathematics of Intelligences
September 9 – December 13, 2024

Non-commutative Optimal Transport
March 10 – June 13, 2025

WORKSHOPS

Symmetric Tensor Categories and Representation Theory
January 8 – 12, 2024

Mathematical Foundations for Equity in Transportation Systems
January 22 – 26, 2024

Tensor Networks
February 5 – 9, 2024

Mathematical Approaches for Connectome Analysis
February 12 – 16, 2024

Challenge Institute for Quantum Computation Winter School:
February 20 – 23, 2024

EnCORE Workshop on Computational vs Statistical Gaps in Learning and Optimization
February 26 – March 1, 2024

SUMMER RESEARCH PROGRAMS

RIPS Los Angeles 2024
June 24 – August 23, 2024

RIPS Singapore 2024
May 20 – July 19, 2024

G–RIPS Berlin 2024
June 18 – August 8, 2024

G–RIPS Sendai 2024
June 24 – August 16, 2024

CALL FOR PROPOSALS

IPAM seeks proposals from the mathematical, statistical, and scientific communities for its long programs, winter workshops, summer schools, and exploratory workshops. Programs are selected on the basis of their scientific impact and contribution to IPAM’s goals of improving equity, diversity and inclusion in mathematics and other sciences. Submitted proposals are reviewed by IPAM’s Science Advisory Board (SAB) at its annual meeting in early November. To receive fullest consideration, please send your proposals by September 30 to the IPAM Director at director@ipam.ucla.edu.

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 2025 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 2025–2026 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.

Kieron Burke Personifies IPAM’s Interdisciplinarity

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with as many as 500 atoms — and these larger numbers, Burke explains, make all the difference. For example, DFT calculations enabled chemists to identify a better catalyst for the Haber Bosch Process, which converts hydrogen and nitrogen to ammonia, producing the fertilizer used for agricultural yields all over the world. DFT calculations predicted that hydrogen sulfide would have a high superconducting temperature under pressure, leading to the highest-temperature superconductor ever made. In fact, Burke notes, a substantial portion of supercomputer use at DoE is for DFT calculations involving materials design.

Burke, who is currently a distinguished professor in both the chemistry and physics departments at the University of California, Irvine, played a major role in fueling DFT’s growth. As a postdoctoral fellow, he was part of a team that created an approximate density functional that became far more popular than any preceding it — leading to what remains, by far, the most-cited Physical Review Letters paper ever published. Burke has spent much of his career developing new approximations and simplifications within DFT, as well as applying the approximations to broader cases.

As a trained physicist who has been part of chemistry departments throughout his

academic career, Burke feels right at home when he attends programs of the Institute for Pure & Applied Mathematics (IPAM), where fostering conversations and collaborations across disciplines is a core part of the mission. His first IPAM experience came in 2012, when Burke was invited to give a tutorial on DFT at a long program on machine learning in electronic structure calculations. “It was a meeting that was well ahead of its time, and it led to a vast amount of work that has become ever more important,” Burke says.

In the decade-plus since, Burke has returned for many programs, as well as reunion conferences at Lake Arrowhead, where he has developed and renewed collaborations. “Because the electronic structure world is now huge, there are a number of different communities running these calculations and many are using some of my formulas,” he says. “Because I’m only an hour’s drive away, I try to be there whenever there is something of interest.”

The rapid increase in computational power is driving progress in a variety of scientific realms, but Burke worries that as more people entering the field focus on the sophisticated computational tools, traditional mathematical training and analytic expertise are becoming scarce. “The people running these algorithms

will often come up against equations that require this type of math background to solve, and in that sense, IPAM’s ability to bring together mathematicians and domain scientists is very fruitful,” he explains.

Burke recently joined IPAM’s Science Advisory Board, which he hopes to use as a platform to get more physicists involved in the institute’s programming. “In between the pure math and running the computer is old-fashioned physical intuition — telling you what makes sense and what doesn’t,” he says. “Physicists, as experts in how nature works and what effects need to be captured, can help to bridge that gap.”

For Burke, the value of IPAM is in its ability to bring together experts from different backgrounds, with mathematics serving as a universal language that allows participants to communicate across the cultural barriers that have traditionally kept them siloed. “IPAM draws different kinds of mathematicians who are interested in applying their expertise to scientific problems, along with chemists, physicists, materials scientists, and others who may be computational people but can use some math help,” Burke says. “Lots of good can come from these interactions, and IPAM is probably the best place in the world for fostering that.” ■

Mark Your Calendars

November 27 & 28, 2023. Peter Shor (MIT) will give two public lectures as part of the Green Family Lecture Series.

February 5, 2024. Application deadline for IPAM’s Research in Industrial Projects for Students (RIPS) Programs in Singapore and Los Angeles.

February 25, 2024. Application deadline for IPAM’s Graduate-level Research in Industrial Projects for Students (G-RIPS) Programs in Berlin and Sendai.

May 20 & 21, 2024. Hugo Duminil-Copin will give two public lectures as part of the Green Family Lecture Series.

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

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math changes everything.

MATHEMATICS OF INTELLIGENCES (SEPTEMBER 9 - DECEMBER 13, 2024)

The quest to understand intelligence is one of the great scientific endeavors—on par with quests to understand the origins of life or the foundations of the physical world. Several scientific communities have made significant progress in fields like animal cognition, cognitive science, collective intelligence, and artificial intelligence, as well as the social and behavioral sciences. Yet these communities remain largely disconnected. Now is the time to bring them together with mathematicians to develop the mathematical foundations necessary for transformational advances in understanding natural and artificial intelligences.

This long program seeks to develop those foundations. It will build community and collaboration between participants from the domain sciences and participants from relevant mathematical fields, including dynamical systems, statistical physics, theoretical machine learning, probability and (Bayesian) statistics, information theory, high-dimensional geometry, functional analysis, the theory of programming languages, game theory, and category theory. ■

