Institute for Pure and Applied Mathematics, UCLA Annual Progress Report for 2022-2023 Award # 1925919

August 7, 2023

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EXECUTIVE SUMMARY

This report covers our activities from June 11, 2022 through June 16, 2023 (which we refer to as the reporting period). This report includes the 2022 summer research programs (RIPS and GRIPS). The 2023 summer programs are underway at the time of reporting and will be included in the next annual report.

IPAM held two long programs in the reporting period:

- Computational Microscopy (September 12 December 16, 2022)
- New Mathematics for the Exascale: Applications to Materials Science (March 13 June 16, 2023)

IPAM held the following workshops in the reporting period:

- Who Counts? Sex and Gender Bias in Data (July 18-20, 2022)
- Reconstructing Network Dynamics from Data: Applications to Neuroscience and Beyond (August 29-September 2, 2022)
- Explainable AI for the Sciences: Towards Novel Insights (January 9-13, 2023)
- Learning and Emergence in Molecular Systems (January 23-27, 2023)
- Machine Assisted Proofs (February 13-17, 2023)
- Artificial Intelligence and Discrete Optimization (February 27-March 3, 2023)

IPAM held the following Thematic Schools:

- Graduate Summer School on Algorithmic Fairness (July 11-15, 2022)
- Graduate Summer School on Post-Quantum and Quantum Cryptography (July 25-29, 2022)
- Winter School on Contemporary Quantum Algorithms and Applications (February 22-24, 2023), organized in collaboration with the NSF Challenge Institute for Quantum Computation (CIQC)

Furthermore, the following public lectures were organized during this period:

- Green Family Lecture Series: Cynthia Dwork gave two talks, "Fairness, Justice, and ... Algorithms?" and "Differential Privacy and the US Census" (July 14 and 18, 2022)
- Green Family Lecture Series: Margaret Murnane gave two talks, "Building Microscopes of Tomorrow" and "Harnessing Quantum Physics for Tabletop X-Ray Lasers" (October 10-11, 2022)

During the reporting period, IPAM hosted the following special events and conferences:

• Latinx in the Mathematical Sciences (July 7-9, 2022)

IPAM typically invites participants from each of our past long programs to two reunion conferences; the first is held a year and a half after the conclusion of the long program, and the second is held one year after the first. Due to the unprecedented crisis posed by the COVID-19 pandemic, a number of reunion conferences originally scheduled during the 2019-20 and 2020-21 reporting periods were postponed. During the current reporting period, we were able to bring together several of these cohorts for an opportunity to reconnect and reflect on collaborations that followed since they attended the long programs. These conferences and culminating workshops were held at Lake Arrowhead.

- Hamilton-Jacobi PDEs Reunion Conference II (December 11-16, 2022)
- Big Data Meets Large-Scale Computing Reunion Conference II (December 11-16, 2022; postponed by 1.5 years)
- Tensor Methods and Emerging Applications for the Physical and Data Sciences Reunion Conference I (December 11-16, 2022)
- Computational Microscopy Culminating Workshop (December 11-16, 2022)
- Mathematical Challenges and Opportunities for Autonomous Vehicles Reunion Conference II (June 11-16, 2023)
- Mathematical and Computational Challenges in the Era of Gravitational Wave Astronomy Reunion Conference I (June 11-16, 2023)
- New Mathematics for Exascale: Applications to Materials Science Culminating Workshop (June 11-16, 2023)

All RIPS and GRIPS programs were held in-person in summer 2022. This report includes four 2022 student research programs:

- Research in Industrial Projects for Students at IPAM (RIPS)
- Research in Industrial Projects for Students in Singapore (RIPS-SP)
- Graduate-level RIPS (GRIPS) in Sendai
- Graduate-level RIPS (GRIPS) in Berlin

A. PARTICIPANT LIST

A list of all participants in IPAM programs will be provided to NSF in electronic form (Excel). The list will include participants for programs whose start dates fall between June 11, 2022 through June 16, 2023.

B. FINANCE SUPPORT LIST

A list of participants that received support from IPAM will be provided to NSF in electronic form (Excel). The list includes all funded participants of programs that occurred between June 1, 2022 through May 31, 2023.

C. INCOME AND EXPENDITURE REPORT

Grant # DMS 1925919:

This table shows appropriations and expenses for June 1, 2022 through May 31, 2023 for grant #1925919.

	A	В	С	D	E	F
			A-B=C		B+D=E	A-E=F
Budget Category	Appropriation	Actual Expenses	Balance	Encumbered Expenses	Total & Encumbered Expenses	Encumbered Balance
	Year 3			as of May, 2023	at May 2023	as of May, 2023
A. Operations Fund	\$2,003,333	\$2,113,190	(\$109,856)	\$223,013	\$2,336,203	(\$332,870)
B. Participant Costs	\$1,900,000	\$2,317,885	(\$417,885)	\$58,081	\$2,375,966	(\$475,966)
C. Indirect Costs	\$1,096,667	\$1,085,015	\$11,652	\$0	\$1,085,015	\$11,652
Totals	\$5,000,000	\$5,516,089	(\$516,089)	\$281,094	\$5,797,184	(\$797,184)

During Year 3, Operational Costs (e.g., salaries, benefits, equipment, supplies) were steady at \$2,336,203. Participant Support Costs (e.g., stipends, travel, housing, and subsistence for the scientists working on IPAM Programs) were at a healthy level of \$2,375,966. Indirect Costs rates are based on current facilities and administrative cost rates negotiated with the Federal government and the University of California. IPAM's work is conducted at an on-campus location which is subject to a 56% facilities and administrative cost rate. Indirect costs are not applied to equipment and participant support costs.

IPAM overspent our allocation in Year 3 for two reasons. First, our allocation is an even \$5 million per year. We typically underspend the allocation in the early grant years and overspend

in subsequent years. Also, due to the COVID-19 pandemic, several activities (reunions and summer schools) planned for the first two years of the grant to Year 3.

Registration fees for NSF-supported conferences are accounted for as program income. IPAM charges modest registration fees primarily to discourage non-serious registrations. Registration fees for workshops are \$75 for faculty and government/military participants, \$100 for industry participants, \$50 for post-doctoral scholars and \$25 for graduate students. During this reporting period, the in-person workshop registration fees collected were \$18,650 and waived for online programs. All program income collected is spent entirely on participant support expenses.

D. POSTDOCTORAL PLACEMENT LIST

IPAM appointed three postdoctoral Scholars during the reporting period. Funded by the Simons Foundation, the postdocs participated in the long programs.

Srivatsav Kunnawalkam Elayavalli

Srivatsav Kunnawalkam Elayavalli is working in operator algebras and collaborated with IPAM director Shlyakhtenko and the functional analysis group at UCLA. After completing his research at UCLA he will continue in a postdoctoral position at the UCSD Mathematics Department.

Elisa Negrini

Elisa Negrini has been an active participant in the Computational Microscopy program in Fall 2022. She has collaborated with UCLA faculty, including Stan Osher, John Miao, and Hayden Schaeffer. After completing her research at UCLA, she will continue as a postdoc in the UCLA Mathematics Department. Negrini is also serving as an academic mentor in the 2023 RIPS program.

Minh Pham

Minh Pham has been an active participant in the Computation Microscopy program in Fall 2022. He collaborated with several UCLA faculty, including Stan Osher. After completing his research at UCLA, Pham will be joining the KLA Corporation.

E. MATH INSTITUTE DIRECTORS' MEETING REPORT

MIDS Meeting 2023

April 29, 2023 Chicago, IL

Present

Brian Conrey (AIM) Michelle Manes (AIM) Akshay Venkatesh (IAS) Brendan Hassett (ICERM) Ulrica Wilson (ICERM) Kevin Corlette (IMSI) Dibyen Majumdar (IMSI) Denise Slavinski (IMSI) Selenne Bañuelos (IPAM) Christian Ratsch (IPAM) Dima Shlyakhtenko (IPAM) Hélène Barcelo (SLMath) Tatiana Toro (SLMath) David Manderscheid (NSF) Marian Bocea (NSF) Zhilan Feng (NSF) Joanna Kania-Bartoszynska (NSF) Yong Zeng (NSF)

Agenda

8:30-9:00 Refreshments

9:00-9:15 Welcome and introductions

9:15-9:35 DMS update by the Division Director, David Manderscheid

9:35-10:05 Updates from the institutes (5 minutes per institute, including questions)

10:05-10:15 Update about revisions to the MSRI solicitation

10:15-10:30 Break

10:30-10:40 PRIMES solicitation

10:40-10:50 Discussion of MSIDI proposal

10:50-11:10 Institute plans for spend out for funds left-over due to COVID

11:10-11:20 Clarification about MSPRF (NSF postdocs) possibilities for visiting institutes

11:20-11:40 Break

11:40-12:00 Clarification of what DMS needs in terms of highlights

12:00-12:15 Reminder about the request for acknowledgment of NSF support and inclusion of NSF logo

12:15-12:45 Open discussion/New business

1:00 Tour of IMSI facilities for interested NSF personnel

Minutes

DMS update by the Division Director, David Manderscheid:

DMS Division Director gave an update on recent developments at the NSF Division of Mathematical Sciences.

- The new solicitation for math institutes should be out soon.
- DMS is ramping up panels and pushing awards out the door, and hiring program officers. DMS is almost at a complete complement for next year.
- NSF is in the final stages of making an award for the National Institute for Theory and Mathematics in Biology. It's a 5-year, \$50 million grant in partnership with the Simons Foundation. 50% of funds will come from Simons, 25% from DMS, and 25% from NSF Biology. It's also renewable for another 5 years, so, basically it's \$100 million total over the next 10 years.
- The NSF Director has three basic priorities: strengthening established NSF programs, Missing Millions (now called Opportunity Everywhere), and technology, innovation, and partnerships. The new language paid off well in <u>CHIPS and Science Act</u>, which authorized the doubling of the NSF budget over a 5-year period. We're not yet on a path for this to happen, but the NSF did get a 10% increase this year. One key to this is that the 10% increase was not across the board. For most of the science directorates, increases were on the order of 2-3%. Most of the new funds (\$500 million) went to the new directorate in Technology, Innovation, and Partnerships (the TIP Directorate). \$250 million went to the directorate formerly known as EHR (now, STEM Education Directorate) to increase graduate research fellowships. The \$250 million leftover went to facilities. DMS got roughly a 2% increase (which was more than most divisions, but not keeping pace with inflation).
- There's an effort to tap into resources the other directorates get. For example: CHIPS gets increased money in EPSCOR states. This translates into a large increase in EPSCOR funds. Program officers apply for EPSCOR funds when they get relevant proposals. DMS is also partnering with other divisions and foundations like Simons to increase the budget.

Regarding the DMS going forward: Manderscheid firmly believes in supporting core programs, and not cutting funding to go after the next shiny object. However, going after new things in partnership with other divisions is worth doing. For example, Artificial Intelligence (AI) broadly defined: DMS has a partnership with Simons and the Computer Science directorate. Also, there are things like digital twins, and machine-assisted proofs. There are two other areas of interest: Mathematical Biology which is the fastest growing area. DMS put out a solicitation this year for emerging areas in mathematical biology, particularly involving AI, and got 171 proposals. Mathematical Biology is getting over 350 proposals yearly, while other areas get about 250 a year. Another area with a lot of interest is quantum computing and algorithms.

Subsequent discussion among participants touched on topics such as ways in which institutes can tap into NSF funding outside DMS and what institutes can do for DMS

Institute updates:

SLMath:

Tatiana: In 2022-2023, we changed from MSRI to SLMath; the name change will take 12-18 months. We're also turning 40, and so having a number of celebrations. We held a 40th anniversary symposium in which eight distinguished mathematicians spoke. They were people who had been involved in MSRI over the years. They talked about how their field evolved and how that evolution is related to MSRI, and big things for the future. 200 people attended Terry Tao's talk on computer-assisted proof and 130 were online. This included lots of UC Berkeley participants, including undergraduates. It was our highest number of registrants for a workshop ever.

Regarding our programs: We ran current issues in math education again. Our Organizers had a workshop for people to reflect on mentoring. We are also launching a pilot program in Atlanta called MAY-UP. It helps students to get into internships. It's for students finishing their 1st year; will be 2 weeks residential. It will bring 12 students from Morehouse, Spellman, and Clark Atlanta, and they will be working on linear algebra. We got to speak to Sen. Raphael Warnock's office. Nikema Williams will try to come by. It opens May 15.

Joanna: Are you thinking of staying in Atlanta for now?

Tatiana: We want a pilot program, and it has been difficult to find funding. Our future plan is to increase to 24 students and then have a second year for those who want to continue with activities during the academic year. We want to grow from those 3 institutions to MSIs within 200 miles of Atlanta. We want to keep it in Atlanta.

IPAM:

Dima: We create communities that are interdisciplinary and use math in all kinds of ways. Our motto is: "math changes everything". For our long programs: we did materials science with a focus on quantum one year ago. Last fall we did a program on computational microscopy with a lot of AI. Now, we're running new mathematics for the exascale, which has heavy involvement from national labs. We're seeing that new algorithms and new mathematics are required to run these huge computers effectively. Next fall, we're running a joint program with the Center for Quantum Challenge Institute located at Caltech and Berkeley. We're interested in quantum algorithms and have them talk to people in other sciences. Next spring, 2024, we're doing statistical mechanics.

In Fall 2024, we're doing a program on the mathematics of intelligence—What is intelligence? Spring 25, a program on non-commutative Optimal Transport. In Winter 2023, our machine proof workshop was well attended. Winter 2024, we're doing mathematical foundations for equity in transport systems: how can optimization be used properly, or not? How do you incentivize certain types of behaviors? What are the consequences for people?

We also have lots of summer schools: we ran two last year. Upcoming Summer 2023, we have AMIGAS, for grad students at critical transitions stages in underrepresented groups. We give them a background to where the field is going as whole and give them tools to proceed with careers. We also have student research programs. RIPS (undergrads) and G-RIPS (grad). Regarding PRIMES: we're aware of one application for this upcoming year. We heard that the deadline was a little early, but we're working our

best to make it happen. Also, our surplus update: we have some surplus due to COVID, so we're catching up on some activities. We've done additional summer schools, and we have some increased costs due to inflation (labor, travel).

David: Regarding the deadline for PRIMES: we tried to get it out as fast as possible. In the future, it will probably have 2 deadlines. We're working on revision now.

IMSI:

Kevin: We're approaching a natural "steady state" of activity. We had two long programs this year, and we're happy with both. In winter, we hosted a month-long Research Collaboration Workshop on social justice and data science. We also had some standalone workshops on Randomness in Topology, the reunion for our 1^s long program, and "Assessing the Economic and Environmental Consequences of Climate Change" with the Macro Finance Research group at UChicago. This upcoming summer:, we are hosting our 1^s edition of SUMSA, which is a mini-bridge program. There will be 27 students at IMSI for 8 weeks. In Fall 2023, we have a long program on algebraic statistics. We're anticipating 60 visitors and will expand into the south wing to accommodate them. In Spring 2024, we'll have a long program on Data-Driven Materials Informatics. Finally, in Summer 2024: we'll have a Long Program on green energy.

Ulrica: What is the target level for the summer undergrad program?

Kevin: Rising sophomore. They need to have had at least Calculus, plus something else.

David: Regarding IMSI's climate program in the fall: The NSF has a focus on the "resilient planet," and there is lots of money floating around NSF. "Climate" terms can get fraught.

ICERM:

Brendan: We have a busy summer: there's the 6-week social justice project that is continuing on from last year. We have a reunion of our Combinatorial Algebraic Geometry program that ran in the spring of 2021. We have the "Summer @ ICERM" undergraduate research program. We also have a number of large workshops. One of these is on Mathematical and Scientific Machine Learning. For that, we have partnerships with the Air Force and some private companies. We also have a workshop on Optimal Transport and Data Science, and one on Modern Applied and Computational Analysis. We think there is demand from the community to go to institutes in the summer. We have lots of people coming, and we've never been so busy. During the academic year, we're back to 2018 levels in terms of participation, and it's still rising a bit. We made changes in spending policies with a view toward the lack of spending during COVID. We've increased the volume of fellowships for teaching buyouts. We've set aside positions for visitors from non-R1 institutions. There have been lots of cost increases (rent, then airfare, and now hotels). We think we're spending 50% more per participant than we did before the pandemic. Hotel prices have gone up dramatically in the last few months. We're also doing some upcoming programs on mathematical biology.

IAS:

Akshay: Our volume of applications is back to normal. IAS as a whole has a new director. This will bring some changes and more opportunities for work in areas that haven't been represented there. The Women in Mathematics program has a program director now. The expansion of our outreach activities is happening. We have conferences and a special lecture series coming up. Our special themes this year are arithmetic combinatorics and ergodic theor and high-dimensional commutative algebra. And next year's is p-adic geometry. There is a huge demand for that topic.

David: I talked to David [Nirenberg], and I'm impressed with his openness to new ideas.

AIM:

Brian: We're moving down to Caltech on July 1. Caltech put us on the 8th floor of Caltech Hall. They'll remodel a 2^{ml} space in Kellogg a few years down the road. We have a lot in the works. Planning for 30 workshops and 100 squares between now and next fall. We had a good workshop on multiscale modeling on malaria; there was a good diversity of participants (doctors, biologists, and mathematicians). Our science board is finally meeting again this upcoming December in-person. We'll have a mini-workshop in conjunction with it on mathematics and machine learning, organized by Sergey Gukov.

Michelle: Historically, AIM has had space for hot topics workshops. We haven't had them in a while. Our new one will be on commutative algebra. A paper dropped that seemed to prove a 10-year old conjecture on a generalization of the Hilbert Syzygy Theorem to virtual resolutions of toric varieties. We wanted to bring the relevant communities together and see if they can work it out and implement. It will be in September.

Joanna: Regarding the workshops that will be in the new location in July: Is the new space conducive to AIM's style?

Brian: Yes, the new space will be the same, with a lovely view of the mountains.

Joanna: What about your format?

Brian: Yes, we're keeping the format the same. Caltech does not want any control. Once we get extra space, Squares will be in Kellogg, and the workshops in 8^{+} floor space.

Update on new MSRI solicitation:

There is a new solicitation coming up. The deadline will continue to be Pi Day. The letter of intent, if required, will be due 3 months before. There was discussion of the requirement in the previous solicitation to report citizenship of participants in institute programs to NSF, and ways to document the extent to which institute programs include members of underrepresented groups.

Currently, the DMS institute budget is 20% of the overall DMS budget — that could change depending on the proposals received. For institutes which are defunded, it is expected that wind-down funding will be available.

PRIMES

The institutes' diversity committee provided valuable input in the design of the PRIMES program. DMS expressed the hope that institutes will be open to partnerships. Part of the intention is to reach people the institutes wouldn't have reached otherwise. DMS is considering having two target dates in the year. Timing is an important issue: institutes tend to announce their programming one year in advance. Most of the funding is going to the faculty member's home institution. There is the possibility of a subaward to the math institute to cover the cost for participation. The "one co-PI" requirement is an annoyance. There is wording there that could help. It's up to institutes to decide who is "equivalent" to an Associate Director. DMS hopes this cycle will be a success and that DMS and the institutes will learn from it.

The institutes raised two concerns. One was the requirement of a Co-PI, which in some cases seems to encourage the PIs to focus on members of institute leadership as collaborators rather than on institute programming. Some institute representatives felt a letter of collaboration would be sufficient in most cases. It was pointed out that a co-PI from an institute might be needed in cases where there is a subaward to the institute. A second concern is the timing of decisions on PRIMES awards. Decisions should come in time for institutes to ensure PIs can be accommodated within programs, and should allow enough time for PIs and their home institutions to make arrangements to free the PI from teaching obligations. It was generally felt that decisions in December for programs starting in the fall of the following year, and in May or June for programs starting in the spring of the following year could work well.

There was also discussion of the criteria for selection. DMS will have reviewers and will create a panel. Proposals will be evaluated on intellectual merit, potential for broadening participation, and the solicitation-specific criteria. In this case, the latter includes the impact of the proposed project on the institutional research environment, the pertinence of the institute activity to the faculty participant's research program, and the impact on the career of the faculty participant and on the relevant department's ability to better prepare students for advanced degree programs and/or careers in science and engineering.

MSIDI:

The institutes raised a timing issue related to the current MSIDI proposal: spending on proposed activities may need to start as soon as July, and asked whether any updates on the status of the proposal were available. DMS responded that MSIDI is decoupled from institute programs. DMS is looking for diversity-enriching activities in core institute activities, but for MSIDI, institutes should talk about timing issues with people in the Infrastructure program.

On the topic of things the institutes do together, it was mentioned that the congressional briefings which AMS and MSRI have collaborated on in the past will now involve all of the institutes on a rotating basis.

COVID spend-out funds:

Each institute reported on projections of spending through the current grant cycle in light of underspending due to the COVID pandemic. The institutes generally expected to compensate for COVID underspending due to a number of factors: added activities, increased scale of activities through the remainder of the grant cycle, increases in the need for staffing, and increases costs of travel and lodging

Clarification about MSPRF (NSF postdocs) possibilities for visiting institutions

DMS offered clarification of the ways in which NSF postdocs can spend time at institutes. In the first year, an NSF postdoc can spend time at an institute, but must remain an NSF postdoc. The institute can provide funding for travel and housing. During the second or third year, the Postdoc can attend a program at an institute or they can take leave from their NSF postdoc and attend an institute as an institute postdoc. The choice can be made between the postdoc and the institute, depending on the flexibility of the postdoc's home institution. The home institution might not let the postdoc go due to teaching, so the postdoc might have to take a leave of absence. Postdocs must inform the NSF.

Highlights:

DMS asked to hear from institutes regularly. Ex: What happened this month? These updates are different from the highlights posted on the mathinstitutes.org website: the latter are things the institutes are proud of, or something big. Also of interest: anything that is interesting that is connected to AI, machine learning, quantum—all the initiatives at the NSF. Also, anything great in terms of growing participation or the workforce. Regarding frequency: make an effort to keep eye on good stuff that is going on. It might not be weekly or even monthly, but as frequently as you can. DMS will try to advertise within NSF. Want to make sure the Directorate is proud of what the institutes are doing, and inclined to give us future funding. Really spectacular things might be sent to the Office of Public Affairs (OPA). Pictures and videos are helpful.

NSF logos:

DMS encouraged the institutes to continue to display the NSF logo prominently on webpages, flyers, and announcements, and to encourage participants to acknowledge the institute's grant in publications from activities.

Open Discussion/New Business:

Next year's MIDS will be at AIM in Pasadena

--dates: April 26-27, 2024

F. PARTICIPANT SUMMARY

In this report, we are reporting on participants of programs that took place between June 11, 2022 through June 16, 2023. We have included the participants of the reunion conference. This report does not include the participants of our RIPS/G-RIPS 2023 summer programs which will be captured in the next reporting cycle.

We include registered on-line participants as well as in-person participants in all statistical computations. There have been 226 registered remote participants in IPAM events during the reporting period. For an unknown reason, all in-person "government/military" participants registered as "industry participants" in our system.

Participant Category	In-person Participants	Remote Participants	Total
Faculty	741	78	819
Government/Military	0	11	11
Graduate Student	526	61	587
Industry	138	28	166
Postdoc	290	37	327
Undergraduate Student	152	11	163
Other	142		142
Total Participants		2215	·



Participants by Category

Also note that we do not collect RSVPs or collect participants data for "Public Lectures".

When self-reporting gender, participants are asked to select one or more of the following options: "Female", "Male", "Nonbinary", "I identify as:", or to select "Prefer to not self-identify". If "I identify as:" is selected, a free-form field is available to enter gender. The codes in the table below correspond to various combinations of these possible choices. The code "D" indicates that the participant preferred to not self-identify. Otherwise, each choice made corresponds to addition (or omission) of the corresponding letter in the gender code:

- F: "Female"
- M: "Male"
- N: "Nonbinary"
- O: "I identify as..."

This results in 15 possible non-empty combinations, such as "F" (only "Female" is checked), "FM" (both "Female" and "Male" is checked), and so on. Combinations that did not occur this year are not listed.

Due sue Trune	Total	Participant Gender Code								No.
Program Type	Participants	F	FM	FN	М	MN	MO	Ν	NO	Reporting
Board Meetings	35	8			17					25
Long Programs	99	25			71					96
Reunion Conferences	84	25			52					77
Special Events and Conferences	257	90		1	150			1	2	244
Student Research Programs	227	75			109			3		187
Summer Schools	115	37			66					103
Workshops	1398	344	4	2	958	2	2		1	1313
Total	2215	604	4	3	1423	2	2	4	3	2045
Percent of No.	Reporting (%)	29.5	0.2	0.1	69.6	0.1	0.1	0.2	0.1	

Five participants selected "I identify as:" (and possibly other choices) and entered the following into the free-form field: "genderqueer", "Male" (3 entries), and "Queer".

Participants were also asked to self-identify as members of certain underrepresented ethnic groups; it was possible to select more than one option.

		Underrepresented Ethnic Groups							
Program Type	Total Participant s	Amer. Indian	Black	Hispanic	No. Reporting Ethnicity				
Board Meetings	35		2	3	24				
Long Programs	99		1	4	98				
Reunion Conferences	84		4	3	79				
Special Events and Conferences	257	1	11	141	248				
Student Research Programs	227		4	17	195				
Summer Schools	115		4	6	109				
Workshops	1398	1	30	71	1349				
Total	2215	3	56	245	2102				
Percent of No. Re	eporting (%)	0.1	2.7	11.7					
	All underrep	presented	ethnic groups:	304	14.5%				

There were 1,396 <u>unique participants</u> for this same period. (Some of the participants attended more than one program, usually multiple workshops within a long program.) Out of these, 1,279 reported gender. Out of those reporting gender, 374 (29.2%) identified as Female. A further 4 identified as both Female and Male; 3, as Female and Non-binary; 889 (69.5%) as Male; 2, as Male and Non-binary; 2, as Male and supplied another gender identity; 2, as Non-binary; and 2, as Non-binary and supplied another gender identity.

There were 1,192 unique participants who reported ethnicity. Of them, 236 (19.8%) were members of an underrepresented ethnic group.

G. POSTDOCTORAL PROGRAM SUMMARY

366 postdocs participated in IPAM's programs during the reporting period (June 11, 2022 - June 16, 2023). Seven postdocs participated in IPAM's student research programs. See tables G1 and G2 below.

Table G1: Postdo	Table G1: Postdoctoral Gender Distribution									
	Total	Participant Gender								No.
Program type	Participants	F	FM	FN	М	MN	MO	Ν	NO	Reporting
Long Programs	25	5			19					24
Reunion Conferences	18	7			11					18
Special Events and Conferences	23	4		0	17					21
Student Research Programs	7	1			3					4
Summer Schools	9	3			6					9
Workshops	245	62	1	1	170	1				235
Total	327	82	1	1	226	1	0	0	0	311
Percent of No.	Reporting (%)	26.3	0.3	0.3	72.7	0.3	0	0	0	

Table G2: Postdoctoral Ethnicity Distribution									
		Underrepresented Ethnic Groups							
Program Type	Total Participants	Amer. Indian	Black	Hispanic	No. Reporting Ethnicity				
Long Programs	25		1	2	23				
Reunion Conferences	18			1	17				
Special Events and Conferences	23			11	21				
Student Research Programs	7				4				
Summer Schools	9				8				
Workshops	245	1	8	11	216				
Total	327	1	9	25	287				
Percent of No. Reporting (%)		0.3	3.1	8.7					
All underrepresented ethnic groups: 35					12.2%				

H. GRADUATE STUDENT PROGRAM SUMMARY

As with previous years, a robust number of graduate students participated in IPAM's workshops and long programs during the reporting period, as well as in Graduate-level RIPS. A few participated in RIPS-LA as academic mentors. Graduate students often find a compelling thesis topic at an IPAM program, and also frequently make contacts that lead to their first jobs. See table H or further breakdown. A significant number participated in LatMath as well as the thematic schools.

Table H1: Gradua	Table H1: Graduate Student Gender Distribution									
	Total	Participant Gender								No.
Program Type	Participants	F	FM	FN	М	MN	MO	Ν	NO	Reporting
Long Programs	20	6			14					20
Reunion Conferences	20	9			10					19
Special Events and Conferences	110	32	1		74				1	108
Student Research Programs	21	10			8			2		20
Summer Schools	79	27			48					75
Workshops	337	100	1	1	223		1		1	326
Total	587	184	2	1	377		1	2	2	568
Percent of No.	Reporting (%)	32.3	0.4	0.2	66.4	0	0.2	0.4	0.4	

Table H2: Graduate Student Ethnicity Distribution									
		Underrepresented Ethnic Groups							
Program Type	Total Participants	Amer. Indian	Black	Hispanic	No. Reporting Ethnicity				
Long Programs	20			1	18				
Reunion Conferences	20			2	17				
Special Events and Conferences	110	1	3	54	105				
Student Research Programs	21		1		19				
Summer Schools	79		3	5	77				
Workshops	337		13	19	296				
Total	587	1	20	81	530				
Percent of No. Reporting (%)		0.2	3.8	15.3					
	All underrep	resented ethr	nic groups:	102	19.2%				

I. UNDERGRADUATE STUDENT PROGRAM SUMMARY

Typically, undergraduate students participate in RIPS-LA, RIPS-Singapore, and RIPS Projects Day. However, we saw a number of undergraduate students attend other programs at IPAM during the reporting period. We saw a smaller than expected number of undergraduate students in the LatMath program, likely due to its unusual timing (summer).

Table I1: Undergr	Table I1: Undergraduate Student Gender Distribution									
Program Type P	Total	Participant Gender								No.
	Participants	F	FM	FN	М	MN	MO	Ν	NO	Reporting
Special Events	20	12			_					10
and Conferences	20	12			/					19
Student Research Programs	113	57			51					108
Workshops	30	5	1		23					29
Total	163	74	1	0	81	0	0	0	0	156
Percent of No.	Reporting (%)	47.4	0.6	0	51.9	0	0	0	0	

Table I2: Undergraduate Student Ethnicity Distribution								
		Underrepresented Ethnic Groups						
Program Type	Total Participants	Amer. Indian	Black	Hispanic	No. Reporting Ethnicity			
Special Events and Conferences	20			2	18			
Student Research Programs	113			12	104			
Workshops	30		2		25			
Total	163	0	2	14	147			
Percent of No. Reporting (%)		0	1.4	9.5				
	All underrep	resented ethr	nic groups:	16	10.9%			

J. PROGRAM DESCRIPTION

STUDENT RESEARCH PROGRAM: Graduate Research in Industrial Projects for Students (G-RIPS) Berlin 2022 (June 20-Aug. 12, 2022).

Graduate-Level Research in Industrial Projects for Students (G-RIPS) in Berlin offers graduate students in mathematics and related disciplines the opportunity to work on industry-sponsored research problems. Students from the U.S. and Germany work on cross-cultural teams on three research problems designed by the industrial sponsor. The projects are of serious interest to the sponsor and offer a stimulating challenge to students; most involve both analytic and computational work. At the end of the program, the teams present the results of their work and prepare a final report. English is the only language required for participation.

Round-trip travel to Berlin and accommodations in Berlin are included. Students also receive a meal allowance and a stipend of \$4,300. (These terms apply to U.S. participants recruited by IPAM.)

Five U.S. students participated in G-RIPS Berlin in 2022 together with four European students. Each team consists of two US students and two European students (one US student worked separately with a research group at MODAL). The students worked on projects that were sponsored by some of the most important companies in Germany. This year, the list of industrial partners included Cray Germany GmbH, Biotronic GmbH/1000shapes GmbH, and FICO and Gurobi Optimization.

2022 SPONSORS	PROJECT TITLE
Cray Germany GmbH	High performance computing (HPC) for real-world simulations
Biotronic GmbH /	Auto-ML for bio-medical data-analysis
1000shapes GmbH	
FICO and Gurobi	Machine learning for combinatorial optimization
Optimization	

Cray Germany GmbH Project

Project Title: High performance computing (HPC) for real-world simulations

Project Description: Object stores have been recognized as one of the crucial building blocks for Exascale HPC systems since they permit novel usage of permanent data storage outside of the POSIX file system paradigm. DAOS, the Distributed Asynchronous Object Storage, is one of the most scalable examples, and using a combination of NVRAM and SSD storage offers both high metadata and block storage performance, while being resilient to failures of the storage infrastructure.

In this project we propose to investigate offload capabilities from processes to the DAOS object store. Subsequently, the technical question is, how the offloading of data actions to DAOS can be implemented. We propose to design an API so that a user process can trigger data processing on the DAOS server by shipping code to the DAOS server similar to stored procedures, or activating software container deployed on the DAOS server, or lazy objects within DAOS.

Biotronic GmbH/1000shapes GmbH Project

Project Title: Auto-ML for bio-medical data-analysis

Project Description: The amount of available bio-medical data has rapidly increased in recent years. Not only in the scientific context, but also in hospitals and in industry, more and more detailed data on a wide variety of diseases are being collected and are available in public databases. Analyzing this data has not only become the bottle-neck due to the size of the datasets, but also because designing appropriate models has become very time-consuming due to the many possible options and algorithms. Some years ago, there might have been a standard way how a particular data type (e.g. genomics data) should have been analyzed – however, these days it is very rare that a one-size-fits-all analysis approach exists for a particular data type. In fact, the contrary is the case: designing a good machine leaning model involves putting together multiple components which have tons of (hyper-)parameters and calibration steps. This often involves steps for preprocessing, feature selection, classification, interpretation and so on. As a result, designing a suited and well working machine learning model often involves a timeconsuming (cyclical) process of putting together a multi-component analysis pipeline, finetuning the parameters, evaluating the results, replacing some of the components with other algorithms, another fine-tuning, more evaluation and repeating over again. This goes on until a good combination of algorithms and parameters is found. However, whether it was the best combination for this dataset can in most cases not be determined: maybe there is this other algorithm that would have resulted in a better outcome but was not tried out?!

The main idea of Auto-ML is that machine learning algorithms take over the construction of the analysis pipeline which before has been done manually – including a smart way for hyper-parameter optimization. There are several frameworks available today that are implementing the Auto-ML toolbox and allow experiments with own data-sets (see e.g. this review by Waring et al. https://doi.org/10.1016/j.artmed.2020.101822)

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In this project we will use bio-medical data-sets from our project sponsors to evaluate the power of Auto-ML approach and compare it to the current state-of-the-art solutions. The aim is to generate new machine-learning models for disease diagnosis.

FICO and Gurobi Optimization Project

Project Title: Machine learning for combinatorial optimization

Project Description: While most combinatorial optimization solvers are presented as generalpurpose, one-size-fits-all algorithms, this project's main scientific question is the following: Is machine learning a viable option for improving traditional combinatorial optimization solvers on specific problem distributions, when historical data is available?

This general problem captures a practical scenario highly relevant to many application areas, where a practitioner repeatedly solves problem instances from a specific distribution, with redundant patterns and characteristics. For example, managing a large-scale energy distribution network requires solving very similar CO problems on a daily basis, with a fixed power grid structure while only the demand changes over time. This change of demand is hard to capture by hand-engineered expert rules, and ML-enhanced approaches offer a possible solution to detect typical patterns in the demand history. Other examples include crew scheduling problems that have to be solved daily or weekly with minor variations, or vehicle routing where the traffic conditions change over time, but the overall transportation network does not.

In the 2021 NeurIPS conference, one of the major venues for machine learning research, featured a competition on precisely this question [https://www.ecole.ai/2021/ml4co-competition/]. Researchers submitted many different approaches to solve three different challenges: Creating primal solutions, improving dual bounds, and configuring solvers by parameter tuning. The task of the G-RIPS project will be to select one of the three challenges and improve upon the existing approaches submitted to last year's competition.

The project is supervised by MODAL SynLab in collaboration with industry partners FICO [https://www.fico.com/en/products/fico-xpress-optimization] and Gurobi Optimization [https://www.gurobi.com/], both of which provide market-leading optimization solvers for mixed-integer programming.

Comments from our participant survey:

- I learned how to code in python, work in a team, collaborate with people from foreign countries, and create an excellent presentation and written report. These will all help me in the future, no matter what I do!
- [G-RIPS Berlin] has shown me that I probably would enjoy having a career in industry.
- The opportunity to work abroad in a foreign country, and engage with a completely new community of researchers and subject matter experts from such diverse backgrounds was really fantastic. Furthermore, despite the fact that my specialization is computational techniques, the materials science curriculum in my PhD program has very little attention given to computer science. I've generally had to self-teach myself these skills "on the side," as it were (which is difficult because the engineering classes I do have to take don't leave a lot of time left over for "on the side" learning). The best part about participating in this program was finally having a chunk of time carved out that allowed me to focus on a project solely on the computer science side. I'm really quite grateful to GRIPS for creating the environment that supported this.

STUDENT RESEARCH PROGRAM: Graduate Research in Industrial Projects for Students (G-RIPS) Sendai 2022 (June 20-Aug. 9, 2022).

Graduate-Level Research in Industrial Projects for Students (G-RIPS) in Japan offers graduate students in mathematics and related disciplines the opportunity to work on industry-sponsored research problems in Sendai, Japan. Students from the U.S. and Japan work on cross-cultural teams on research problems designed by industrial sponsors. The projects are of serious interest to the sponsor and offer a stimulating challenge to students; most involve both analytic and computational work. At the end of the program, the teams present the results of their work and prepare a final report. IPAM encourages the U.S. students to publish and/or present their research at conferences in the year following the program. English is the only language required for participation.

Round-trip travel to Sendai and accommodations in Sendai are included. Students also receive a meal allowance and a stipend of \$4,300, and conference support to present their research. (These terms apply to U.S. participants recruited by IPAM.)

Eight U.S. students participated in G-RIPS Sendai in 2022 together with eight Japanese students. Each team consisted of two US students and two Japanese students. The students worked on projects that were sponsored by some of the most important companies in Japan. This year, the list of industrial partners included Toyota (more precisely, F-MIRAI, that is supported by Toyota), Mitsubishi, and NEC.

2022 SPONSORS	PROJECT TITLE
F-MIRAI (Toyota)	Mathematical approaches for mobility services in suburban areas
Mitsubishi	Construction for incomplete map matching based on local and global geometries
	Multi-objective optimization for best early prediction of extreme weather events
NEC	Application of annealing machines to production planning optimization

F-MIRAI Project

Industrial Partner: F-MIRAI center at University of Tsukuba

Toyota will lead the way to the future of mobility, enriching lives worldwide with the safest and most responsible ways of moving people. In the near future, cars are expected to connect with people and communities and to perform in new roles as part of human social infrastructure. New domains of service such as AI, autonomous driving, robotics, and connected cars are becoming especially important. Toyota aims to reach the ultimate goal of sustainable mobility, creating a mobile future society full of smiles. Toyota and the University of Tsukuba have jointly established the R&D Center for Frontiers of MIRAI in Policy and Technology (F-MIRAI), which advances toward Society 5.0 through the development of infrastructure for future communities and the formation of industrial centers through long-term collaborative action.

Project Title: Mathematical approaches for mobility services in suburban areas

Project Description: In this project students will study and design Mobility-as-a-Service (MaaS) for the campus of the University of Tsukuba through analyses of person-trips and other related datasets. The model will include various modes of transportation including (autonomous) private vehicles, buses, bicycles, and walks.

Mitsubishi Projects A and B

Industrial partner: Mitsubishi Electric Corp., founded in 1921, is an electronic and electric equipment manufacturer developing products and solutions in widely diverse fields, including home appliances, industrial equipment, and space technologies. The Advanced Technology R&D Center was established to support the business of Mitsubishi Electric Group through the development of a broad scope of projects covering both basic and new advanced technologies. The main research themes include power electronics, mechatronics, satellite communications, next generation key devices, system solutions for electric power, transportation, factory automation, and automobiles.

Project A title: Construction for incomplete map matching based on local and global geometries

Project A description: In this project students will consider how to build and evaluate matching methods between incomplete maps based on local and/or global geometries. The students will

work on implementations as well as a comprehensive mathematical formulation to guide the implementations.

Project B title: Multi-objective optimization for best early prediction of extreme weather events

Project B description: In this project students will use a mathematical approach to develop an optimization strategy for the number and location of meteorological sensing instruments (such as LiDAR), to get the best early prediction of extreme weather events.

NEC Project

Industrial Partner: NEC Corporation

<u>NEC</u>, founded in 1899, is now particularly addressing the development of solutions for society that will help resolve many issues the world is facing and which will engender the creation of a brighter and more prosperous society. Through co-creation initiatives with many different stakeholders, including customers, business partners, private individuals, government agencies, and international institutions, we are actively devising new business models to create social value by harnessing our extensive information and communication technology (ICT) assets.

Project title: Application of annealing machines to production planning optimization

Project description: In this project students will work on the combinatorial optimization problem of production planning. This is also known as a job-scheduling problem. They will study how to formulate the problem and how to apply annealing to it. The students will be able to use the latest annealing machines provided by NEC.

Comments from our participant survey:

- [GRIPS-Sendai] Greatly boosted my network, and secured me a position with Tohoku University (and a tentative possibility to apply to Mitsubishi Electric)
- I am more knowledgeable about possibly being a manager or general industry research.
- I think GRIPS has given me experience in working on industrial problems and it has prepared me to work in groups with people from different cultural backgrounds and different areas of specialization.
- The program has introduced me to what industry projects would look like.

STUDENT RESEARCH PROGRAM: Research in Industrial Projects for Students (RIPS) Los Angeles 2022. JUNE 21 - AUGUST 19, 2022.

The Research in Industrial Projects for Students (RIPS) Program provides an opportunity for talented undergraduates studying math, computer science, and related disciplines to work in teams on a real-world research project proposed by sponsors from industry or the public sector. The student team, with support from their academic mentor and industry mentor, will research the problem and present their results, both orally and in writing, at the end of the program. The REU program is nine weeks. IPAM provides each undergraduate student with a stipend of

\$3,800. IPAM organizes two RIPS cohorts every year: one at the UCLA campus in Los Angeles, and another in Singapore.

Round-trip travel and accommodations costs are covered by IPAM. Students also receive a meal allowance and a stipend, and conference support to present their research. These terms apply to U.S. participants recruited by IPAM.

36 students participated in RIPS 2022 (in Los Angeles) and 4 students participated in the RIPS Singapore program.

2022 LA SPONSORS	PROJECT TITLES
Aerospace Corp.	Distributed Kalman Filter Designs and Experiments for Proliferated Low
	Earth Orbit (pLEO) Satellite Constellations
AMD	Uncertainty Quantification Methods for AI-based Surrogates of
	Scientific Applications
Google	Budget Conservation in the Training of Differentially Private Models
GumGum	Traffic Shaping for Real Time Advertising
HRL	Topological and Geometric Analysis of Adversarial Image Data
IBM	How Quantum Teleportation Can Improve Routing in Quantum Circuits
LLNL	A State-Based Parallel in-Time Multigrid Approach to Constrained
	Optimization
Meta	Measures and Standards of Fairness in AI Embeddings
Roswell	Signal Processing for Molecular-Electronic Sensor Chip Data
Biotechnologies	

Sponsors and projects: RIPS-Los Angeles

Project 1: Aerospace Corp: Distributed Kalman Filter Designs and Experiments for Proliferated Low Earth Orbit (pLEO) Satellite Constellations

Government and private entities are working on developing proliferated low Earth orbit (pLEO) satellite constellations due to their lower latency, lower replacement costs, and higher resilience to satellite outages relative to traditional satellites in geostationary or medium Earth orbit. However, the development of these constellations has raised new position, navigation, and timing challenges as pLEO constellations cannot rely exclusively on information from ground stations. In this project we tackle the timing aspect of these challenges. Specifically, we explore the performance of various distributed Kalman filters for synchronizing the satellite clocks across a constellation. Three distributed Kalman filters are examined: the Naive algorithm, the Primitive Distributed Kalman Filter (PDKF), and the Decentralized Collaborative Localization (DCL) algorithm. Performance of each is measured by "wrapping" them with a centralized Kalman filter that provides us with an estimate of the clock uncertainties accounting for all cross-covariance information between satellites. We show that the clocks converge quickly to low error using the DCL algorithm when we introduce an appropriately chosen update order and tune the filter's parameters.

Project 2: AMD: Uncertainty Quantification Methods for AI-based Surrogates of Scientific Applications

In recent years, there has been growing interest in using machine learning algorithms rather than traditional numerical simulations for scientific computations, as this data-driven approach greatly reduces computational cost. To enhance the extrapolation capacity of models, physics-informed neural networks are developed to enforce physical constraints. When tuned to approximate known functions, physics-informed neural networks render accurate approximations; however, without prior knowledge of the target function, the untraceable nature of neural networks translates to uncertainty in the model output. We aim to quantify the uncertainty of predictions through the application of Bayesian and ensemble methods. We apply these methods to approximate a paraboloid and then the solution to the wave equation with both standard neural networks and physics-informed neural networks. We demonstrate that the embedding of physics information in neural networks reduces the model uncertainty while improving the accuracy. Between the two uncertainty quantification methods, our results show that the Bayesian neural networks render over-confident results while model outputs from a well-constructed ensemble are appropriately conservative.

Project 3: Google LLC: Budget Conservation in the Training of Differentially Private Models

Google aims to develop practical methods for differentially private model selection so that Google Ads clients can build machine learning models on marketing data without compromising the sensitive information of Google users. Currently, clients can only train and test a prohibitively small number of models before exceeding their privacy budget. This project investigates two approaches for increasing the number of privatized model-building iterations a client may perform. The first approach attempts to minimize the privacy cost of each model-training iteration by using the subsample and aggregate framework to release a differentially private estimate of test metrics. We show that our algorithm produces high quality predictions of classification accuracy for a variety of datasets and machine learning models, indicating that this class of algorithms presents a promising direction for future research. Our second approach explores techniques for generating differentially private synthetic datasets which can be used to train models with zero marginal privacy cost. We generate comprehensive benchmarks to characterize the utility of various synthetic data generation techniques, namely methods based on covariance and marginal estimates, clustering, and GANs. We compared performance across a wide range of datasets and machine learning models, allowing us to identify applicable use cases for these algorithms.

Project 4: GumGum: Traffic Shaping for Real Time Advertising

Functioning as an ad exchange service, GumGum exchanges millions of advertisements a day with online publishers. When an ad space becomes available on a publisher's website, GumGum alerts their Demand Side Platforms (DSPs) and sends them a bid request, at which point the DSPs choose to either place a bid for the ad space or ignore the bid request completely. Each time a bid request is sent out, GumGum and the respective DSP incur a certain infrastructure cost. As there is a large amount of digital publishers, there is often

more supply of ad space than demand for it from the DSPs; however, only an estimated 5% of bid requests get auctioned on and accepted by the publisher involved. In order to reduce infrastructure costs, this project aimed to develop an algorithm that utilizes ad space information to decide whether or not GumGum should send a bid request to each individual DSP. The goal of this project was to lower the amount of bid requests sent to each DSP while not significantly decreasing GumGum's revenue. Once a preliminary model was created, we implemented various feature selection methods, tuned the hyperparameters, and explored the effects of seasonality and recency in order to improve the model's accuracy. These improvements allowed the model to reduce traffic by 25% while maintaining a revenue loss notably below 1%. In this report, we will discuss the data which we used, the random forest classification algorithm, the methods used to improve the model, the results for our classification method, as well as future directions that can be pursued to improve our model.

Project 5: HRL Laboratories: Topological and Geometric Analysis of Adversarial Image Data

Recent advances in computing have allowed neural networks to reach new levels of sophistication and classify data with unprecedented accuracy. Nevertheless, these models remain susceptible to adversarial attacks and can be fooled by small perturbations of the input data. Training models to be robust against adversarial attacks is important as neural networks are being used in more applications. In this project, we use techniques from topology and geometry to understand the space of adversarial examples and to detect its structural differences from the space of natural data. In particular, we focus on using Topological Data Analysis (TDA) to study this structure. We begin by generating adversarial attacks on the MNIST and ImageNette datasets using the Fast Gradient Sign Method (FGSM) and Projected Gradient Descent (PGD). We then use dimensionality reduction techniques, such as Principal Component Analysis (PCA) and Variational Autoencoders (VAEs), both to make TDA more computationally feasible and to try to capture structure within the high-dimensional image data. Not finding any significant structural differences between the natural and adversarial datasets, and moreover, little structure in the natural dataset which cannot be attributed to noise, we call into question the validity of the manifold hypothesis for natural image data.

Project 6: IBM: How Quantum Teleportation Can Improve Routing in Quantum Circuits

Hardware constraints in modern quantum architecture post a major obstacle to large-scale quantum computing. Due to the restrictions of qubit connectivity, most quantum algorithms cannot be directly performed on current quantum systems. To execute the two-qubit gates in these algorithms, additional logic must be inserted to move the qubits being acted next to each other. Traditional protocols for solving the quantum routing problem use SWAP gates, which swap the states of any two connected qubits. Ideally, the routing solution aims to minimize the number of gates or the depth of gates, but finding an optimal solution is an NP-hard task.

New developments in quantum hardware technology may allow for better solutions. The

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latest generation of quantum computers has mid-circuit measurement and feed-forward capability. With this technology, quantum circuits can use quantum teleportation to efficiently swap qubits that are not directly connected. In our project, we implemented two transpiler passes that use teleportation for routing. One improves upon an existing algorithm for small and intermediate scale quantum circuits. The other uses a completely novel approach to maintain the strict guarantee that every CNOT gate can be implemented in constant depth.

Project 7: Lawrence Livermore National Laboratory: A State-Based Parallel in-Time Multigrid Approach to Constrained Optimization

Many computer simulations, such as weather forecasting and airfoil modeling, are time dependent. Unfortunately, the traditional simulation approach of sequential time marching is becoming a bottleneck as computer architectures must increasingly rely on higher concurrency to provide greater peak performance. The multigrid reduction in time (MGRIT) method and open source software XBraid were developed to take advantage of existing simulation codes and technologies as much as possible, allowing scientists to migrate to a parallel-in-time simulation paradigm more easily than would otherwise be possible. This project will build upon a new extension of the MGRIT solver idea called TriMGRIT that can be applied to time-dependent constrained optimization algorithms, which require the solution of a (nonlinear) system that is fully coupled in time. For some application problems, the current algorithm, which employs the adjoint-based Schur complement, can break down. One major goal of this project is to examine TriMGRIT using the state-based Schur complement approach, which provides a potential solution to problems that could not previously be solved through TriMGRIT. The new TriMGRIT ideas will be compared to existing sequential and parallel optimization solvers.

Project 8: Meta: Measures and Standards of Fairness in AI Embeddings

In the field of machine learning, the advancement of deep learning methodologies has resulted in a greater demand for computational resources. The low computational "cost" of embeddings make them an attractive choice, as they act as an intermediary representation of data that can be used by multiple downstream models. However, potential bias in embeddings may result in unfairness in the downstream tasks themselves. In this report, we evaluate several past metrics of fairness on word embeddings, and propose our own metrics for embeddings, including a generalization of the established Word Embeddings Association Test (WEAT) metric for word embeddings. We also introduce two new mitigation methods that successfully reduce bias in embeddings while maintaining performance in classification tasks on real world data sets; the first is inspired by factor analysis, while the second is a generalization of an existing mitigation approach for word embeddings. Lastly, we run our mitigation methods on generated data sets to examine the trade-offs between fairness and performance under various fairness conditions.

Project 9: Roswell Biotechnologies: Signal Processing for Molecular-Electronic Sensor Chip Data

Roswell Biotechnologies[™] has developed a microchip based on a molecular electronics design

that can sense biological interactions at the molecular level. Each chip has 16,000 sensors and has the ability to record data in parallel. While interaction data is greatly useful, the recorded signals often contain noise, and complex applications including DNA sequencing involve sensing, interpreting, and resolving four different types of interactions, one for each base. The goal of this RIPS project is to develop tools for time-series analysis of such sensor data. Specifically, we design a simulator to generate realistic, synthetic signals, and we develop tools for peak finding, noise modeling, signal-state estimation using hidden Markov models, signal alignment using dynamic time warping, and denoising using Kalman filtering and total variation. By integrating these tasks and results, we can process raw time series into clean, labeled signals that will enable biological discoveries from the data collected by the innovative Roswell sensor chips.

Sponsors and projects: RIPS-Singapore

2022 SP SPONSORS	PROJECT TITLES
Google	Constructing User Financial Profiles from SMS Messages
Grab	TCGConv: Edge Representation Learning in Temporal Graphs
MOHT	Schizophrenia Behavior Modeling through Digital Phenotyping – a
	HOPE-S project
P&G	Data mining on Skin Care Stability

Project SP-1: Google: Constructing User Financial Profiles from SMS Messages

Short Message Service (SMS) messages are a rich form of data for user financial modeling. This study built models for classifying and extracting financial information from SMS messages. We created a synthetic dataset that was suitable for this task by combining template-generated messages and messages from public datasets. Then we implemented multiple models for message classification. Our experiments show that Support Vector Machine achieves the highest accuracy of 98% for detecting financial messages, while fine-tuning the pretrained BERT model gives the best accuracy (79%). Moreover, we experimented with a publicly available tool for information extraction and achieved 91% F1-score. Finally, we gave recommendations on using our results to build a production-level system that can construct user financial profile from SMS.

Project SP-2: Grab: TCGConv: Edge Representation Learning in Temporal Graphs

Graph Neural Networks (GNNs) have been very successful in generalizing deep learning methods to relational data such as social networks. However, current GNNs primarily focus on learning node representations while edges are only used as auxiliary information. Despite the importance of edge representation learning and edge-level downstream tasks such as edge classification, little attention has been paid to them. Furthermore, existing edge embedding methods predominantly apply to static graphs. To bridge these gaps, we present a novel framework, Temporal Conjugate Graph Convolution (TCGConv), to learn edge representations in temporal graphs. TCGConv consists of Conjugate Graph Transformation (CGT), which reverses the role of nodes and edges, and Long Short-Term Memory (LSTM) aggregator, which

captures temporal information during the aggregation process. We then conduct extensive experiments on a public transaction dataset to validate our framework. These experiments show that our proposed model significantly outperforms the baseline models, which are impractical in real-time applications as they disregard the temporal constraints by peeking into the future, and its variants, demonstrating the effectiveness of our model to incorporate temporal information.

Project SP-3: MOHT: Schizophrenia Behavior Modeling through Digital Phenotyping – a HOPE-S project

To build a holistic care system for patients with schizophrenia, the Ministry of Healthcare Office for Healthcare Transformation conducted the Health Outcomes through Positive Engagement and Self-empowerment clinical trial. Digital phenotyping (DP), a form of mobile device data collection, was used within the study. It has been investigated in other studies as a tool that could aid in the prediction of relapses in patients with schizophrenia. Our survival analysis supported this conclusion by demonstrating that the proportion of REM sleep a patient experiences is a significant factor determining their likelihood of relapsing and that time dependency of the DP data is important for accurately predicting patient behavior during periods where patients are unobserved. In our regression objective to predict patient scales for schizophrenia, our deep learning models and autoregressive models outperformed time-naive linear models. In our anomaly detection task, our results show that multivariate models showed no significant improvement in performance.

Project SP-4: Procter & Gamble: Data mining on Skin Care Stability

Stability tests are essential to ensure cosmetic products are compliant with specific physical, chemical, and microbiological standards. At Procter & Gamble, there are many types of stability tests associated with skin care products. The standard confirmatory stability test requires monitoring products over 3 years at normal temperature. Accelerated stability and degradation tests at one or more higher temperature and stress levels are measured at a shorter time to inference the confirmatory stability and enable fast decision making.

Following the practices in the degradation modelling and machine learning domain, our project titled 'Data Mining on Skin Care Stability' aims to implement data mining and statistical machine learning methods to assess the quality of current ADT data from Procter & Gamble and check whether we can use them to make good inference of confirmatory stability test results. Meanwhile, the project aims to assess the opportunity to remove certain measuring time steps from accelerated test by analysing information loss and model performances.

Participant Survey Results.

IPAM surveys RIPS participants (both LA and Singapore) both pre- and post-participation. They surveys are designed to elicit feedback from participants as well as to gauge the effect of the program.




























The surveys rated the Los Angeles program very highly. Both Los Angeles and Singapore programs have shown significant positive impact on student attitudes towards viewing mathematics as a viable career path (in and out of academia), and their desire to obtain an

advanced degree. We are working with our Singapore partners to address student feedback related to ensuring a supportive an inclusive environment, as well as providing good academic mentorship. Part of the reason had to do with the program restarting after a COVID-related hiatus. Several members of IPAM leadership visited Singapore (including coming for the 2023 opening day) to discuss these issues.

Some selected students comments include:

• A great experience overall, but Midterms can be shorter

• I believe there should be more consideration of what people's skills are when selecting project groups [for Singapore]. My group programmed the entire time which I have no knowledge of how to do. My team was not helpful in ensuring I understood what was going on. I felt some of the other projects had more mathematics where I could have used my skills. The program structure was not well planned out. The academic mentors were also given very vague instructions so the result was my academic mentor never showing up until food was provided, or the midterm/final presentation practice. Because he was never there he wasn't very helpful with his feedback. Finally, I voiced my concerns several times..., not feeling very confident with my project, and not feeling respected in my team. Each time I was either not responded to or told a generic answer such as "it's okay to not know about what's going on with your project." The concept of the program is good but it lacks execution

• I wish Singapore RIPS had a bit more structure. Perhaps workshops on some essential technologies like github, python to bring everyone to the similar baseline. Pre-existing knowledge had a huge impact on the quality of the project as well as team morale. Someone with a pure math background might feel discouraged when they have to learn many new skills that other teammates are already familiar with.

• It was wonderful. The support from our industry mentor and [RIPS Director] was essential for the project. I gained confidence on presenting and doing research and I feel tremendously grateful.

• Overall, I really liked this program and I'm glad I chose it over other, pure REU programs. It helped me decide that I want to work in industry.

• Thank you for an amazing experience. This program helped me grow as a leader, teammate, researcher, and professional.

• Thank you for this program. It's been the best of my life. Thanks for the support in preparing presentations and report. I learned a lot with that and from my industry mentor.

• The organization of each of the activities from the beginning, with midterms to the finals, helped me to better understand the project and to feel that I have contributed. Thank you very much for all the help and support in the preparation of our finals. This summer was my best learning experience.

• The RIPS is very diverse programme. It provided me with a lot of career paths I was not known of. Additionally, I met people from around the world and [got] to know about their culture.

• This program was amazing and I'm super thankful for this experience and the friends I made along the way. I'm excited to go to JMM to present our results and have a reunion! My feedback would be to give more details about what to bring to the dorms further in advance. I also think the first couple days should require everyone to set up SSH and Github. [IT Director

Jim] was incredibly helpful with tech issues but we never figured out how to SSH through VS code on a macbook.

LATINX in the Mathematical Sciences Conference (July 7-9, 2022)

ORGANIZING COMMITTEE:

Selenne Bañuelos (California State University, Channel Islands) Rodrigo Bañuelos (Purdue University) Pamela E. Harris (Williams College) Anthony Várilly-Alvarado, Chair (Rice University) Mariel Vázquez (University of California, Davis)

This was the third in a series of LatMath conferences showcasing the achievements of Latinx in the mathematical sciences. 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. Initially scheduled for 2021, the conference was postponed to 2022 due to the pandemic.

LatMath was principally funded through a separate grant funding the Mathematical Sciences Institutes Diversity Initiative (MSIDI). However, a small amount of funds from the present proposal were used to support the conference.

- I had a great time. Ginger and team made us feel very welcome. Thank you for the wonderful experience!
- Kudos to all involved in making this an exceptional experience!
- Great first conference, was paired up with amazing mentors and had many opportunities to network and meet new people! The constantly changing event date and webpage could have been more informative and better communicated. And many of the talks could have been better, I know it is an academic conference but many people seemed as though they had not practiced or timed their presentation. Overall amazing event planning, organization and execution.
- Fantastic conference. The connections I made were you excellent. Seeing a group of strong, successful Latinx mathematicians has been very inspiring to me.
- The scientific quality of the conference was very high, and I was happy to be a part of it. That said, I am a vegan, and I found that there were essentially no vegan options during the meals. I realize that vegan is a very specific diet, but I felt that there could have at least been a vegetarian main dish at the banquet. Instead, the vegetarians wound up eating mainly salad and hummus with bread.
- My only very negative score was for the website, which was missing key information until very close to the conference dates (it made it hard for me to decide on when to schedule my flights and lodging). Also the long PDF with the meeting info had several big typos and other issues.

- This was an excellent conference from the safety protocols for COVID to the research that was presented. Thanks to the organizers for the work that went into it.
- I loved coming to this conference to catch up with my fellow Latinx mathematicians, network,
- and meet the next generation. It is hard to balance how to fill the schedule, but I think that there are enough Latinx mathematicians to have more Scientific sessions.
- I loved each speaker's intro about their journeys to where they are now.
- Running the conference at the Luskin center made a huge difference in the quality of the event. Having the talks where people eat/sleep facilitated having constant and ongoing conversations.
- The way the academic career panel was described in the conference flyer, it wasn't clear that it was focused on mid-career people rather than grad students. Overall I really liked th food, banquet, etc but there weren't enough good options for vegetarians
- I attended as a recruiter representing LANL. It would have been nice to give a 15-minute presentation about opportunities at LANL on the first day of the conference in addition to having a booth
- The details on the website were added very late and would have been nice to know some things beforehand but in general, it was great
- I would have liked having a better organized list of presenters at the scientific talks before the conference. This would have allowed me to plan some of my student meetings around the ones of most interest to me. I also thought that 2 hours for the small number of student posters was too long. Maybe inviting undergraduate local students would have helped have more of these (CSU Long Beach, CSU Los Ángeles, CSU Fullerton, UCI, CSU Channel Islands, etc.) The only reason I am saying this was that I don't recall seeing students from any of these institutions and some of these have great records of student research.
- The venue is very expensive--\$13 for a glass of wine at the banquet is extortionate. Grad students and junior faculty should not be subjected to such prices.
- The conference provided an incredibly supportive environment for mentoring and it was inspiring in terms of both mathematics and giving back to the mathematics community.
- Thank you!
- Thank you so much! I'll be at the next one

SUMMER SCHOOL: Algorithmic Fairness (July 11-15, 2022)

ORGANIZING COMMITTEE: Noa Dagan (Harvard Medical School) Cynthia Dwork (Harvard University) Guy Rothblum (Apple Inc.)

As algorithmic decisions and likelihood predictions reach ever more deeply, and with increasing consequence, into our lives, there is an increasing mandate that they be "fair". This program comprises a short course on the theory of algorithmic fairness taught by Dwork and Rothblum, as well as research talks by leading researchers in some application areas.

After an investigation of an array of "first wave" fairness definitions and their behaviors under composition, the course will highlight a class of desiderata that aim to bridge the gap between statistical and individual fairness notions and examine the meaning of likelihood predictions through the lens of complexity theory. Attention will be paid to open fairness questions surrounding the choice of data by which individuals are represented to the algorithm, and the proxies used for outcomes, the fairness desiderata, and the pressing problem of moving from algorithms that reproduce the world as it is to algorithms that lead us to a more ideal world. The course will end with a deeper look into 1-2 application areas.

Comments from our participant survey:

- I would appreciate water to be available in the lecture room. I was unsure why water was never provided, but coffee / tea / lemonade was always there... Regardless, a fantastic summer school. Thank you to the organizers!
- I feel like in the FAccT community, there's very theoretical work on the mathematical side and very theoretical work on the philosophical side and then some work in between that tries to bring the two sides together. I feel like the summer school too focused on the mathematical side for the first days and I would have appreciated a higher level overview and more discussions about, for example, how individual fairness can be used in practice. How do we find this "magic metric"? What does similarity mean? What does difference mean? To what degree are we all similar / different? What are relevant differences in different contexts? How can / should we include sensitive attributes in the metric to compensate for differentially expressive features? Obviously, these are difficult questions, so I wasn't expecting to get answers to them, but I was hoping for interesting discussions about them. I did have them, but during the breaks - I was hoping we'd have more of a guided discussion about them and get input from different speakers. I also had the feeling that the limitations of individual fairness were barely considered while the limitations of group fairness kept coming up - many of which also apply to individual fairness. A discussion of Reuben Binns's paper "On the apparent conflict between individual and group fairness" would've been interesting to discuss in this context.
- Thank you for organising this summer school. I'm glad I attended in-person and would recommend to others.
- Luskin conférence center was amazing.
- It was a fantastic summer school, and I am very grateful to all of the staff for making it possible! I learnt so much and I met a lot of wonderful students working on similar research topics.
- Great summer school and organization! Truly enjoyed it! In particular, the support provided by the IPAM staff and Breanna especially was really really outstanding!

WORKHOP: Who Counts? Sex and Gender Bias in Data (July 18-20, 2022)

ORGANIZING COMMITTEE

Ruha Benjamin (Princeton University) Cynthia Dwork (Harvard University) Patricia Williams (Northeastern University) As algorithmic decisions and likelihood predictions reach ever more deeply, and with increasing consequence, into our lives, there is an increasing mandate that they be "fair".

Who counts? Machine learning algorithms learn from training data; when these are biased so are the algorithms they produce. The workshop will examine sources of sex and gender bias in data, with emphases on impoverished women; women of color; trans and non-binary persons; and older women.

Comments from our participant survey:

- It would be good if students can also participate in the summer school online if they can not make it.
- Hybrid worked well enough. I accept the trade-off between in-person networking and someone's ability to only participate from afar. But I'm glad I was in-person as remote attendance would have been nowhere near the experience I enjoyed by travelling to UCLA.
- Too many talks squeezed into the three days. A four day event would have been more appropriate in my opinion.

GREEN FAMILY LECTURE SERIES: Lectures by C. Dwork "Fairness, Justice, and ... Algorithms?" and "Differential Privacy and the US Census" (July 14 and 18, 2022)

IPAM does not keep track of public lecture participants.

SUMMER SCHOOL: Post-quantum and Quantum Cryptography (July 25-29, 2022)

ORGANIZING COMMITTEE Gorjan Alagic (University of Maryland) Anne Broadbent (University of Ottawa) Dana Dachman-Soled (University of Maryland) Jonathan Katz (University of Maryland) Thomas Vidick (California Institute of Technology) Mark Zhandry (NTT Research and Princeton University)

After decades of theoretical work demonstrating the power of quantum computation, steady experimental progress has led us to the point where practical realizations of quantum computers are on the horizon. It has long been recognized that the advent of quantum computers poses a serious threat to most cryptosystems currently in use. On the flip side, ever since Wiesner's discovery of conjugate coding in the 1970s and the Bennett-Brassard protocol for quantum key distribution it has been known that quantum information can be leveraged to achieve security guarantees with no classical analogue.

The goal of this summer school is to present an in-depth introduction to post-quantum and quantum cryptography for advanced undergraduate and graduate students, as well as young researchers, in mathematics, computer science, and physics. Lecturers in the school will discuss both topics hand in hand: post-quantum cryptography, or the art of analyzing security of classical cryptosystems against attacks, and quantum cryptography, or the art of leveraging quantum effects to develop new cryptographic schemes that are made possible by quantum information.

The school will combine tutorial-style lectures with more advanced research talks by leading researchers in the area. The tutorials will be aimed at establishing a common language between all participants, including the formalism of quantum computation (qubits, quantum circuits, information measures, etc.) and basics of cryptography (security definitions, public- and private-key primitives, etc.). Research talks will cover topics of current interest in post-quantum cryptography, such as quantum attacks on classical cryptosystems, cryptography based on lattices and other post-quantum assumptions, security in the quantum random oracle model and quantum cryptography, such as quantum key distribution, delegation of quantum computation, quantum homomorphic encryption, and more.

This summer school will include a poster session; a request for posters will be sent to registered participants in advance of the summer school.

Comments from our participant survey:

- In light of the need to mask indoors I wish that there had been an agreement not to provide food or drinks besides water in the conference room. I felt it had the effect of encouraging people to drink coffee, tea, and soda unnecessarily during the talks and making it less safe for everyone.
- I appreciate the support since I know that IPAM did their best to help me make the most of this school even when childcare support is in general not available. Thank you a lot!
- This was my first IPAM workshop, and I was extremely impressed. It was a fantastic workshop overall. I also appreciated the COVID safety measures.
- Thank you for the incredible conference! It was the best one I have attended.
- I would like some days to have longer blocks to discuss/work with colleagues but I understand this was a summer school and maybe that is to the main aim. The Staff was great, thank you!

WORKSHOP: Reconstructing Network Dynamics from Data: Applications to Neuroscience and Beyond (Aug. 29-Sept. 2, 2022)

ORGANIZING COMMITTEE Erik Bollt (Clarkson University) Tiago Pereira (University of São Paulo (USP)) Aneta Stefanovska (Lancaster University) Sebastian van Strien (Imperial College) This workshop will explore a unique combination of data- and model-driven approach by inviting mathematicians and scientists focusing on neurosciences and beyond. We will have an in-depth discussion of data-driven modeling techniques, dynamics reconstruction and characterization over multiple scales treating the underlying systems as structures in space as well as structures in time. Problems to be discussed include: predicting critical transitions from multivariate time series; extracting interactions between brain areas and the effects of anaesthetics; understanding the effects pathologies in the network connectivity and modeling ways to alleviate them; introducing and studying models that depart from functional connectivity.

Comments from our participant survey:

- I was very impressed with the wide range of topics in both the neuroscience and the mathematical applications used to study it.
- Its hard to satisfy everyone, topics were broad as expected; I'm more applied these days so I didn't appreciate the math as much, found the hypotheses made some of the more math parts (not all) less relevant for me personally
- I am used to attending workshops on a particular topic in my field. This workshop reached across different ways of looking at Neuroscience which was great, but then some topics were not so relevant anymore. Also, some speakers felt that they had something to share so they did, rather than sharing what was relevant to the theme of the workshop, so for the longest time i was waiting for them to move out of the theory and close to loop to how it applies to neuroscience
- Most of the non mathematicians where able to clearly describe their collaborators data and theories.
- It was a very interesting interaction between mathematics and other disciplines like neurosciences, physics, biology.
- some were spot on, my favorite ones were the first one each morning that seemed the most focused and relevant.
- Most participants were physically there and there was plenty of time for discussions
- Little difficulty during talk, but virtual speakers did not engage after their talk had concluded.
- The interaction nature was very good, probably the best part of the workshop
- I really enjoyed the fact that the schedule is not fully packed. Some participants were able to establish collaborations during the workshop thanks to the ample discussion time.

LONG PROGRAM: Computational Microscopy (Sept. 12-Dec. 16, 2022)

ORGANIZING COMMITTEE

Peter Binev (University of South Carolina) Angus Kirkland (University of Oxford) Gitta Kutyniok (Ludwig-Maximilians-Universität München) Jianwei (John) Miao (University of California, Los Angeles (UCLA)) Margaret Murnane (University of Colorado Boulder) Deanna Needell (University of California, Los Angeles (UCLA)) Stanley Osher (University of California, Los Angeles (UCLA)) Zineb Saghi (Commissariat à l'Énergie Atomique (CEA)) Amit Singer (Princeton University) Paul Voyles (University of Wisconsin-Madison) Laura Waller (University of California, Berkeley (UC Berkeley))

Microscopy is critical for discovery and innovation in science and technology, accelerating advances in physics, chemistry, biology, materials science, nanoscience and energy sciences. Recent years have witnessed at least three revolutions in microscopy. First, the 2014 Nobel Prize in chemistry recognized super-resolved fluorescence microscopy, which brings optical microscopy into the nanoscale. Second, the 2017 Nobel Prize in chemistry was awarded to cryoelectron microscopy (cryo-EM) for the high-resolution structure determination of biomolecules in solution. Third, coherent diffractive imaging (CDI) has been developed to transform our conventional view of microscopy by replacing the physical lens with computational algorithms, allowing lensless imaging with a resolution only limited by the diffraction signal. All these groundbreaking developments require the use of advanced computational algorithms and mathematical tools.

The goal of this long program proposal is to bring together senior and junior applied mathematicians, physicists, chemists, materials scientists, engineers and biologists to discuss and debate on the current status and future perspectives of modern microscopy using computation, mathematics and modeling. Cryo-EM has revolutionized biology and life science (including very recently solving the 3D atomic structure of COVID-19, which has been greatly facilitating the development of the vaccines) and aberration-corrected electron optics and high brightness X-ray sources have transformed physical science imaging. The next steps in these fields will advance by orders of magnitude the temporal resolution and energy resolution, while maintaining atomic spatial resolution, in a variety of sample environments from near zero Kelvin in vacuum to temperatures of a thousand degrees in a highly corrosive atmosphere. These advances will transform research in macromolecules, materials, energy technologies, quantum devices, and other fields. However, they all result in multidimensional, multimodal, big and extremely noisy data. Therefore, sophisticated mathematical and computational methods to derive the maximum possible useful scientific information from the minimum possible quanta of radiation are urgently needed. The four workshops will bring together leading applied mathematicians, physicists, data scientists and computational scientiststo discuss strategies to tackle these major scientific challenges through a combination of advanced algorithms, mathematical modeling, computational tools, big data processing and deep learning.

The long program had four component workshops, and a culminating workshop, which are described in separate sections below.

Comments from our Participant Surveys:

- really enjoyed the program and the people participating it. very friendly staff and great organization!
- YouTube recording is posted very timely and in great quality.
- The computing support IPAM was great, but there were a lot of issues with wifi during the program (my understanding is that this was a campus wide issue at UCLA)
- For reimbursement: I have not received it yet, but I hope there will be no problems with my additional costs due to the visa problems. The processing so far was very smooth. Thanks.
- You all are great, thanks for an amazing semester! Thank you again for the generous support to enable my family to travel with me this semester. It has made a huge difference in my ability to participate in the program. We are very grateful! I hope you can continue to support participants with spouses and/or children.
- The program was having a very wide audience and range of topics. Maybe the participants could be encouraged to include more background material in their presentations. Possibly, there could be some formulation of expectation that the participants organize better. Ultimately, I think it worked out, but I also think that a lot of initial time was not used a 100% effectively. Of course, it depends what is meant by effective. Maybe, given the diversity of the participants, there is no better way then letting things settle. I enjoyed the program very much. Thanks!

TUTORIALS WORKSHOP, Computational Microscopy Long Program (Sept. 13-15, 2022)

The workshop had the same organizing committee as the long program; the vast majority of participants were from the long program core. The goal is to build a foundation for the participants of this program who have diverse scientific backgrounds.

- Remote speakers are unavailable for informal discussion, which is a significant loss. It's still probably better to have them speak remotely than not at all, but its not as good as in person.
- If technically possible, you may use a second microphone that can be handed to the person asking a question in the audience. This would make the discussions much more

accessible to the remote participant. Alternatively, the speaker could repeat the question before answering it.

- I really enjoyed listening to the talks, the topics were very interesting! However, I felt like the order in which the talks were scheduled seemed a little arbitrary and some of the more mathematical talks were very difficult if not impossible to follow for someone with a non- mathematical background and vice versa.
- The top-most question is due to limited interaction possibility using remote participation in a setting targeted primarily at physical attendance. I would have chosen to attend, but was prevented from doing so. I think this is ok and I am happy that I could have access at all. It's also great, you're putting up the videos. This helps with the time zone shifts.
- Travel and housing were both quite expensive. My flight exceeded the IPAM maximum by a small amount [...], but I could not find housing even close to the IPAM maximum.

[Note: a room block at the maximal IPAM rate was arranged for IPAM participants, but expired two weeks before the workshop]

WORKSHOP I, Diffractive Imaging with Phase Retrieval, Computational Microscopy Long Program (Oct. 10-14, 2022)

ORGANIZING COMMITTEE

Tetsuya Ishikawa (RIKEN SPring-8 Center) Jianwei (John) Miao (University of California, Los Angeles (UCLA)) Margaret Murnane (University of Colorado Boulder) Stanley Osher (University of California, Los Angeles (UCLA)) Ian Robinson (Brookhaven National Laboratory) Laura Waller (University of California, Berkeley (UC Berkeley))

For centuries, lens-based microscopy has played an important role in the evolution of modern science and technology. In 1999, a new form of microscopy, termed coherent diffractive imaging (CDI) or lensless imaging, was demonstrated and transformed our traditional view of microscopy, in which the diffraction patterns of a non-crystalline specimen or a nanocrystal were measured and then directly phased to obtain high-resolution images. The well-known phase problem (that is, how to recover a function from the magnitude of its Fourier transform) was solved by combining redundant measurements with iterative algorithms. For the past twenty years, various CDI methods such as plane-wave CDI, Bragg CDI and ptychography have been broadly implemented using synchrotron radiation, X-ray free electron lasers, high harmonic generation, light and electron microscopy. The goal of this workshop is to bring together leading CDI experts, applied mathematicians, physicists, materials scientists, engineers and biologists to disseminate results, exchange ideas and debate future perspectives of this rapidly growing cross-disciplinary field. Topics to be covered, but not limited to, include: How to improve the spatial resolution of CDI to atomic and the temporal resolution to attosecond? How to achieve single-

particle imaging of protein complexes at high resolution? What are the outstanding problems in phase retrieval for applied mathematicians? What research areas will benefit most from quantitative X-ray, electron and Fourier ptychography? How to push the frontier of strain imaging of materials? What new research directions are enabled by magnetic imaging using CDI methods? How to deal with big data and incorporate machine learning into CDI methods?

Comments from our Participant Surveys:

- Hybrid format is more inclusive to marginalized groups who cannot attend in person for various reasons. Thank you for leading this inclusivity.
- A little too high for mathematical talks sometimes, I guess it was difficult to follow for a majority of the audience. But interesting nonetheless
- Oftentimes, the time for discussion after the talks was too short (and thus extended well beyond the scheduled time for the talk into the break)
- The workshop might have been one day too long. There was a fair amount of repetition in the topics covered by speakers and it would have been ok to reduce the program to four days.
- I enjoyed the chance to participate in the workshop! It brought together people who would normally not be at the same workshop (such as experimentalists in x-ray imaging, and mathematicians working on relevant image reconstruction problems). Participation was stronger the first three days than it was the last two days. Perhaps a 3 day workshop is a better match to the time people can take out from their normal schedules with full concentration? Having ample time for discussion after each talk was great! But if one did a 3 day workshop, one could perhaps eliminate some of the 10 minute gaps after the conclusion of Q&A from one talk and before the start of the follow-on talk, and squeeze one more talk in per day while shortening the workshop from 5 days to 3. Thanks again for a great workshop, with ample time for discussion between a varied set of participants!
- really enjoyed this workshop! great work for organizing this!
- The quality of the projector was not sufficient for many of the images shown during the talks
- Excellent workshop!

GREEN FAMILY LECTURE SERIES: Lectures by M. Murnane "Building Microscopes of Tomorrow" and "Harnessing Quantum Physics for Tabletop X-Ray Lasers" (October 10-11, 2022)

IPAM does not keep track of public lecture participants.

WORKSHOP II, Mathematical Advances for Multi-Dimensional Microscopy, Computational Microscopy Long Program (Oct. 24-28, 2022)

ORGANIZING COMMITTEE

Peter Ercius (Lawrence Berkeley National Laboratory) Angus Kirkland (University of Oxford) Andy Minor (University of California, Berkeley (UC Berkeley)) Deanna Needell (University of California, Los Angeles (UCLA)) Paul Voyles (University of Wisconsin-Madison) Yimei Zhu (Brookhaven National Laboratory)

In 1959, Richard Feynman challenged the electron microscopy community to build a better microscope that could identify all the atoms in a chemical structure. As Feynman's challenge has now been addressed in several systems, a bigger challenge going beyond Feynman's 1959 vision is to develop multi-dimensional (D) electron microscopy (with D > 3) to locate and identify all atomic species in complex systems, with additional dimensions such as time, energy, temperature and external bias. Such a powerful tool would have transformative impact in physics, chemistry, materials science, nanoscience and other fields. Addressing this major challenge requires the advancement and integration of state-of-the-art electron microscopy methods such as atomic electron tomography, ptychography, 4D scanning transmission electron microscopy and spectroscopic techniques as well as powerful computational algorithms and mathematical modeling. The goal of this workshop is to connect mathematicians with experts in imaging, physics, materials science, and computer science to advance modeling, simulation and analysis by incorporating state-of-the-art mathematical and computational tools and methods into multi-dimensional electron microscopy. It will be instrumental to build foundations for interdisciplinary research by engaging all these research areas. This workshop will provide the opportunity to present and exchange ideas, share data, and introduce new tools and develop new imaging paradigms needed in a variety of fields.

- [Regarding remote participation] There may be less discusson, but being able to watch the videos on demand is great and definitely makes up for the missing discussions.
- The discussions during coffee breaks, etc. are invaluable. At least one remote speaker had a very bad connection.
- [Regarding remote participation] In the main, excellent only a couple of frozen moments during a couple of the zoom talks
- Some remote speakers have slow internet that resulted in several interruptions of their talks. In such cases, it would be better to prerecord the talk and have a discussion with the speaker after watching it.

- Make sure the remote people are reminded each time to hit "raise hand." It seems like people kept entering things in the chat that we couldn't see.
- I think the in person party was strongest. I would also have liked to see the long term mathematician topics on Monday rather than Friday.
- The math talks were *really* interesting. We are already trying to implement some of the ideas we learned about.
- Some of these lectures were amazing! I learned a lot of new approaches.
- Electron microscopy in materials is not a very large community, so I had seen many of the other speakers give talks recently which were quite similar to what they discussed at IPAM.
- Personally I would sometimes like to hear more about the algorithms people used, and what are their strengths and weaknesses.
- It was hard to engage with the remote speakers. The ones in person were all very accessible
- The WiFi was very unreliable all week (not IPAM's fault, but still frustrating)
- As a core participant, I found that with most talks overrunning and everyone being so keen to talk to the speakers, in the end there is not a lot of time to interact with them. Moreover, despite having 2 hour lunch breaks every day, the speakers are taken away (or they just go on their own?), so the first two workshops felt more like events for the speakers rather than for the benefit of the long program participants. As neither workshop was within my area of research I didn't mind, but it would be disappointing if that will be the case for the next two workshops. I noticed that many people skip breakfast (or have it during the break after the first talk), so maybe providing lunch at IPAM for everyone instead of breakfast would be more beneficial in terms of opportunities to interact with the speakers?
- Having a better quality coffee would have been wonderful

[Notes: Due to some software incompatibility, Apple Silicon computers had difficulty connecting to the WiFi network in early Fall 2022. This issue was eventually addressed campus-wide. UCLA was aware of the issue and working on it during the first several weeks of our long program. Several workarounds were available to enable the WiFi connection].

WORKSHOP III, Cryo-Electron Microscopy and Beyond, Computational Microscopy Long Program (Nov. 14-18, 2022)

ORGANIZING COMMITTEE Bridget Carragher (New York Structural Biology Center (NYSBC)) Wah Chiu (Stanford University) Amit Singer (Princeton University) Sriram Subramaniam (University of British Columbia) Hong Zhou (University of California, Los Angeles (UCLA)) Cryogenic electron microscopy (cryo-EM) has revolutionized biology and life science as a powerful alternative to X-ray crystallography or NMR spectroscopy for macromolecular structure determination. Advances in algorithms for data and image processing and in hardware for image acquisition have made cryo-EM a routine method to determine the 3D structure of suitable macromolecules with identical or similar conformations at near-atomic resolution.

The implementation of these advanced algorithms with user-friendly software packages has also made the method straightforward in practice. Despite these exciting advances, major challenges still remain, such as higher throughput, mapping continuous deformations, reconstruction of small macromolecules, and in sample preparation. For pleomorphic structures, cryo-electron tomography (cryo-ET) is the method of choice, but it is typically limited to lower resolution compared to cryo-EM, and it remains a daunting challenge to determine macromolecular structures in situ at high resolution. Overcoming these major challenges in cryo-EM and cryo-ET requires significant advances in sample preparation, hardware development and computational algorithms. The goal of this workshop is to bring together leading experts in cryo-EM, biologists, applied mathematicians and physicists to discuss and debate the current challenges and future perspectives of this very exciting cross-disciplinary field.

- Recording the lectures and including remote speakers and participants significantly expanded the potential audience, even if remote participants lost the opportunity for in person interactions.
- My supervisor was able to attend from remote and answer questions when my talk was given.
- The discussions in and after the talks were unusually good. Very nice to have so much time for in depth discussion of each talk.
- The audio during Q&A (both asking a questions and hearing the speaker) was very good for remote speakers.
- Make some breaks longer in the morning (the middle break?)
- May need to better explain to remote participants how to ask questions, etc. The session chairs seemed to have marginal understanding of the system.
- As a life scientist, I would appreciate if more structural biology talks (experimental work) are incorporated into the main program at the next year's workshop.
- The quality of the recorded YouTube presentations is excellent. Few sites make efforts to cut between the different feeds. The editing was handled very professionally, and I have already pointed several colleagues at the recordings of the sessions.
- If you plan to continue to make this workshop interdisciplinary, it would be helpful if they can try to emphasize the relevance to biology more in detail. Some presenters did a great job whereas others didn't do it sufficiently.

- All but one of the mathematical talks was quite good and on-topic.
- Excellent selection of talks by top figures in the field
- It would have been nice if the speakers would focus more on the problems they have rather than the quick fixes they used to get to the result
- All the topics are interesting but are not clear that all are relevant to mathematical treatments.
- I got the sense that the audience had a very large breadth of expertise in both mathematics and experimental science (physics, chemistry, biology), and this was probably a limiting factor at some moments, but as someone from the latter category I think I had a decent handle on most of the mathematics that was presented. At times it was a bit overwhelming, but that seems appropriate given by relatively low familiarity with the subject matter in those cases. I didn't mind it in those cases.
- As a non-mathematician, I had trouble understanding the content of mathematical talks at times.
- It was mixed, but several of the mathematical lectures likely went over the heads of most non-mathematicians in the audience. I felt I could reasonably follow most of them, but several could do a better job in defining their variables and avoiding highly discipline-specific notation. Including examples and practical graphs would help make the mathematical talks more accessible to a non-mathematician audience.
- In my opinion, some talks by non-mathematicians were too low. I've read their papers and didn't get any extra insights.
- Fantastic workshop! I really liked the style in which there were 10 min Q&A sessions built in after each talk in addition to 15 min breaks. This allowed time for both group discussion and one-on-one discussions after, in favor of just cramming a maximum number of talks into the allotted time. I found this much more valuable than back-to-back talks like I have experienced at similar events in the past.
- This was one of the best meetings I've ever been to even though I could not understand the math enough at times. Great overview of cryoEM and ET field from various angles.
- Another poster session or something similar to facilitate discussion among all participants would be nice.
- Some more time for interaction (writing things on the white board) would have been better. There was lots of time for chit chat, but some time in a sort of work session together would have been nice. I did this a bit at lunch time and after the session, but people were pretty tired...
- I really liked the breadth of interests of the program's attendees and the attempt on the part of the organizers to include a variety of perspectives and expertise. This made the workshop very refreshing and educational. For me, it was a unique opportunity to ask a room of mathematicians for expert advice regarding some of my research directions. I also learned a great deal about what the mathematical/computational sides of the field are thinking about these days and what progress has been made.

- I would like to come back next year. The only comment I have is that it would be helpful if you can have the schedule/agenda for the workshop little earlier next year. It was hard to plan my trip not knowing when the last talk would be. (e.g., originally I was told that it would end at 5 pm on Fri so I booked a flight for Saturday, but it actually ended around noon so I could have flown out on Fri.) I look forward to next year's workshop!
- Overall an excellent and worthwhile week! My impression was that both mathematicians and others got a lot out of the meeting. I certainly feel like I learned enough and made enough contacts to justify the week of travel.
- The worst thing about the coffee breaks was the coffee. Have not had such a bad coffee for years.
- Have some structured activities like white paper writing/drafting (I attended a workshop at The Fields Institute for Research in Mathematical Sciences and we did this) http://www.fields.utoronto.ca/ - speed mentoring - career panel
- Thank you for organizing such an awesome workshop!

[Notes: it is not clear to what "next year's workshop" is mentioned in several of the comments, since IPAM is not running any programs on topics related to microscopy in 2023-24. As part of the workshop introduction, the IPAM director routinely explains that we always look for new workshop and program ideas, so it is possible that this is related to some possible future application for a workshop at IPAM, although such an application would not have produced a workshop in 2023-24 anyways].

WORKSHOP IV, Multi-Modal Imaging with Deep Learning and Modeling, Computational Microscopy Long Program (Nov. 28-Dec. 2, 2022)

ORGANIZING COMMITTEE

Peter Binev (University of South Carolina) Sergei Kalinin (Oak Ridge National Laboratory) Gitta Kutyniok (Ludwig-Maximilians-Universität München) Deanna Needell (University of California, Los Angeles (UCLA)) Paul Weiss (University of California, Los Angeles (UCLA))

Multimodal microscopy that combines complementary nano- and atomic-scale imaging techniques is critical for extracting comprehensive chemical, structural, magnetic, and functional information. Experiments from correlative electron, X-ray, optical and scanning probe microscopes have generated very large data sets, and the scientific community desperately needs more efficient methods. Methodologies such as compressed sensing and deep learning developed for natural images come without any performance guarantee for the microscopy problem. Furthermore, when multimodal data is collected, the data processing of each modality usually is separate, and the combined results are checked for consistency. Simultaneous processing has the advantage to require less data for extracting the same amount of information. To achieve this, however, one must have consistent imaging modalities for each detector and stable mathematical learning procedures to fuse the data in reliable and reproducible ways. The goal of the workshop is to bridge the gap between mathematicians, physicists, materials scientists, and engineers to advance data acquisition, modeling, simulation, and analysis in multimodal microscopy. It will be instrumental to build foundations for interdisciplinary research by engaging all these subject areas. This workshop will provide the opportunity to present and exchange ideas, share data, and introduce new mathematical techniques needed in this cross-disciplinary field.

- I think [hybrid format is] less effective since engagement and discussions are for the most part between the people who are actually present at the workshop.
- It is definitely preferable to attend workshops in person. Hybrid is good too because it gives the option of both in case of travel or sickness issue.
- The only instruction to clarify is the location of IPAM since the address provided when punched into google maps does not correspond to the building. A labeled map would help!
- They responded to my emails in a timely manner.
- Due to the hybrid format some people were not present, so one could not interact with those.
- The only technical issue for me was that I had trouble finding the zoom link for lectures that I could not attend in person, and that some of the online presenters had internet issues.
- Many presentations were disconnected from the main theme of the IPAM long program 'computational microscopy'.
- AS ALWAYS at conferences, most made no effort to introduce their subject to nonexperts. Extra bad as we were given ample time to do so. As a result little cross disciplinary interaction began to my knowledge.
- I am an experimentalist and hardly understood the lectures.
- A lot of the lectures were very advanced, and I had trouble understanding their topics. That is mostly on my part, because I am not as familiar with advanced math. Their lectures were applicable to our field, but I still struggled.
- the MRI talks were very interesting for the microscopists!
- after decades of experience i think we are dealing with human nature. We are terrible at interacting effectively. It takes a long time for experimentalists and theorist to click. Always.
- [Lectures by non-mathematicians] were relevant to our field of research.
- the maths were often disconnected from 'computational microscopy'. 2

- i think a format needs to be imposed. Even something silly sounding like: you MUST devote 10 minutes of your talk to an explanation a lay audience can comprehend. And maybe have 3 (good) students sit through all talks and give scores
- [The lectures] were appropriate, but again were difficult for me to understand.
- Mixed in both cases, but that is part of the deal. The discussions were particularly valuable this week.
- Discussion times during the week would have been appreciated.
- a little less than average. there was no significant effort to embrace the multidisciplinary intent of the meeting.
- I found this workshop to be very helpful, especially for networking and understanding the industry.
- Very well organized, very helpful staff!
- There was only one interaction where a colleague was trying to speak with one of the staff members, but the staff member seemed preoccupied with something else. It would have been great to see them chat a bit more.
- Loved the workshops, many thanks to all the organizers!
- a strong, visible chair required. someone believing in and actively promoting the networking aspect. a little thing: many speakers never bothered to upload talk title or abstracts. someone (the strong overall chair i mentioned) needs to really cajole people early on to get in the spirit of the meeting. nothing says "i don't really have time for this" like not sending in your talk title.
- The coffee could be much better
- Thank you for hosting, and we're looking forward to the next one!
- Perhaps organizing talks in subtopics on a daily basis and leaving more space for questions and discussions would be a good idea. Especially speakers could be invited to bring up to the audience the types of problems they are hoping to address in a more formal way. There may be more on portunities for collaborations we may have missed. Amazing conference overall

[Notes: for a period of time, Apple Maps have misidentified the IPAM building as well as several other UCLA buildings. This issue was reported and corrected.]

CULMINATING WORKSHOP, Computational Microscopy Long Program (Dec 11-16, 2022)

IPAM long programs end with a culminating workshop for long-term ("core") participants. The workshop is held at the UCLA Lake Arrowhead Conference Center. The organizing committee is the same as for the long program itself. The purpose of the workshop is to summarize what is learned during the program. Working groups that formed during the long program give reports about their progress. Additionally, all participants collaborate to produce a White Paper, which

serves to both capture developments discussed during the program itself and to map out potential future developments. The white paper is available at the IPAM web site, <u>https://www.ipam.ucla.edu/news/white-paper-computational-microscopy/</u>

Comments from our Participant Surveys: No comments were submitted.

Participants from past IPAM long programs are usually invited to two reunion conferences, which take place 1.5 and 2.5 years following the completion of the long program. Thus, normally, there are three groups at the IPAM Lake Arrowhead event: the core from the program that just finished (attending the culminating workshop), and first and second reunions of two past long programs. Due to the COVID-19 pandemic, it was not possible to hold these reunion conferences (which are by nature in-person events) for several past IPAM programs. We offered some long programs from that time to have their reunions on a shifted schedule. As a result, we had three reunion conferences in December 2022.

REUNION: Hamilton-Jacobi PDEs Reunion Conference II (December 11-16, 2022) ORGANIZERS Wilfrid Gangbo (UCLA) Adam Oberman (McGill) Shanley Osher (UCLA)

This reunion occurred on-time, 2.5 years after the completion of the program. However, the program itself started in March 2020 and was severely disrupted by COVID. Its first reunion, organized in January 2022, was disrupted by the Omicron wave. For many participants, this is was the first opportunity to come together since March 2020.

An alumni survey of the program was performed, since this was the last activity associated with the long program.

The long program alumni survey, conducted 2.5 years after the program, gathered 9 responses. One of participants self-identified as a graduate student during the long program, three were postdocs, and five were faculty. All participants indicated that they are currently employed or will start a job shortly in a field related to the subject of the IPAM long program they attended. A majority of the participants indicated that their involvement in the long program at IPAM had a positive impact on their research, collaborations, and career. Participants were asked to indicate their agreement by checking the corresponding boxes for the statements that applied to them.

ANSWER CHOICES	RESPONS	SES
The IPAM Long Program influenced my research interests.	88.89%	8
The IPAM Long Program influenced my career goals.	33.33%	3
The IPAM Long Program was useful preparation for my career.	55.56%	5
The IPAM Long Program introduced me to people who later became my PhD advisor, postdoc advisor, or collaborators in research.	55.56%	5
I continue to collaborate with people I met at the IPAM Long Program.	100.00%	9
In the next year or two, I expect to publish an article that was inspired by or started during this IPAM Long Program.	88.89%	8
The IPAM Long Program led me to collaborate outside of my discipline.	77.78%	7
I have recommended IPAM or one of its programs to a colleague or student.	77.78%	7
Total Respondents: 9		

One participant wrote, "motivated by the program, I have a sketch for a new research program." Another stated, "I did not work before with Hamilton Jacobi equations. I am really happy to see there are a lot of connections to imaging and optimization."

At the completion of the program, we also performed several bibliographic analyses of the program. The results can be found in section L.

REUNION: Big Data Meets Large-Scale Computing Reunion Conference II (December 11-16, 2022)

ORGANIZERS Joachim Buhmann (ETH Zürich) Hans-Joachim Bungartz (Technical University Munich (TUM)) Claudia Draxl (Humboldt-Universität) Jeffrey Hittinger (Lawrence Livermore National Laboratory) Frank Jenko (Max Planck Institute for Plasma Physics and UCLA)

This reunion was delayed by 1.5 years, taking place 4 year after the completion of the program, instead of the normal 2.5 years. The first reunion was also delayed, taking place in December 2021, 3 years after the end of the program. However, program organizers made a compelling case that a reunion event was useful even at this stage. Indeed, a number of topics discussed during the original program – such as applications to Plasma Physics – have become increasingly relevant with the news from the National Ignition Facility where controlled fusion has for the first time produced more energy that was put in.

An alumni survey of the program was performed, since this was the last activity associated with the long program. The long program exit survey gathered 27 responses. About 44% of those who responded self-identified as recent PhDs (5 years or less from PhD), and 56% identified as having received a PhD more than 5 years before the program. About one third of those

responding identified as a mathematician or a statistician (30%), followed by computer scientists (22%), Engineers (22%) and Physicists (18%).

The table below summarizes responses to the question on the value of program activities. Generally, participants rated all program components highly. One participant commented "*Hats off to IPAM for organizing a program on Big Data and Extreme Computing, a timely subject as data becomes truly "big" in the sense that algorithmic complexity and storage per core become limiting, rather than in the traditional sense that data is "big" enough for quality learning alone.*"

	1-POOR	2	3	4-EXCELLENT	N/A	TOTAL
Value of opening day activity at Temescal Park.	0.00%	0.00%	14.81%	55.56%	29.63%	
	0	0	4	15	8	27
Quality or usefulness of the series of workshops.	0.00%	0.00%	11.11%	88.89%	0.00%	
	0	0	3	24	0	27
Quality or usefulness of the activities between workshops.	0.00%	0.00%	44.44%	44.44%	11.11%	
	0	0	12	12	3	27
Value of the culminating workshop at Lake Arrowhead.	0.00%	0.00%	7.41%	59.26%	33.33%	
	0	0	2	16	9	27
Overall merit or quality of the long program.	0.00%	0.00%	7.41%	92.59%	0.00%	
	0	0	2	25	0	27

Overall, most participants were very satisfied with IPAM resources. The table below summarizes responses:

	1 - VERY DISSATISFIED		2	3	4 - VERY SATISFIED	N/A	TOTAL
Facilities (your office, the lecture hall, etc.)		0.00%	0.00%	11.11%	85.19%	3.70%	
		0	0	3	23	1	27
Program staff support		0.00%	3.70%	0.00%	96.30%	0.00%	
		0	1	0	26	0	27
Computing resources and support		0.00%	0.00%	18.52%	62.96%	18.52%	
		0	0	5	17	5	27
Housing resources and support		0.00%	0.00%	7.41%	70.37%	22.22%	
		0	0	2	19	6	27
Financial support and reimbursement		0.00%	3.70%	22.22%	59.26%	14.81%	
process		0	1	6	16	4	27
Online resources		0.00%	0.00%	0.00%	88.46%	11.54%	
		0	0	0	23	3	26

Comments included positive comments such as "IPAM programs are honed by experience and make use of time very efficient for participants", as well as some critical comments, such as "The air-conditioning was too cold for many participants, and a window would have been nice in the office, but overall the institute was great!".

The majority of participants liked collaborative opportunities they had at IPAM. The table below summarizes their responses:

	NONE	LOW	MEDIUM	HIGH	TOTAL
Collaboration within your discipline or sub-discipline.	0.00% 0	11.11% 3	33.33% 9	55.56% 15	27
Collaboration outside your discipline or sub-discipline.	3.70% 1	3.70% 1	7.41% 2	85.19% 23	27
Collaboration between junior and senior participants.	0.00%	3.85% 1	30.77% 8	65.38% 17	26

More than 80% rated the possibility to collaborate outside one's discipline or sub-discipline as "high", which illustrates the highly interdisciplinary nature of this program. Two-thirds of participants responded that the possibility of collaboration between a junior and senior participant was "high". One person responded that "*I especially enjoyed meeting younger*

entrants. I like meetings when I don't know a significant number of the participants and am pleasantly surprised"

Most participants agreed when presented with statements about the program meeting their expectations and being of help with furthering their career and research goals. The table below summarizes these responses:

	1 - STRONGLY DISAGREE	2	3	4 - STRONGLY AGREE	TOTAL
The IPAM long program met my expectations.	0.00% 0	0.00% 0	14.81% 4	85.19% 23	27
The long program will have a positive impact on my research and career.	0.00% 0	3.70% 1	11.11% 3	85.19% 23	27
The long program was a valuable mentoring opportunity for the "junior" participants.	0.00% 0	7.69% 2	15.38% 4	76.92% 20	26
I formed new collaborations that will lead to publications or other outcomes.	3.70% 1	14.81% 4	37.04% 10	44.44% 12	27
I would participate in another IPAM long program.	0.00% 0	0.00% 0	11.11% 3	88.89% 24	27

One of the respondents commented that "*The IPAM long program didn't meet my expectations*. It far succeeded them. ©".

At the completion of the program, we also performed several bibliographic analyses of the program. The results can be found in section L.

REUNION: Tensor Methods and Emerging Applications for the Physical and Data Sciences Reunion Conference I (December 11-16, 2022)

ORGANIZERS

Thomas Barthel (Duke University) Gero Friesecke (Technische Universtitat München)

This reunion took place on-time, 1.5 years after the completion of the long program. The long program itself was fully on-line, and this is the first time that many of the participants had a chance to meet face-to-face. The reunion was on the smaller side, with 14 participants. Nonetheless, the program featured a high level of activity, featuring interaction between algebraic geometers and quantum physicists using low-rank tensor approximations. The alumni survey of the program will be performed at the time of the second reunion.

WORKSHOP: Explainable AI for the Sciences: Towards Novel Insights (Jan. 9-13, 2023)

ORGANIZING COMMITTEE

Tülay Adali (University of Maryland Baltimore County) Jaesik Choi (Korea Advanced Institute of Science and Technology (KAIST)) Pamela Douglas (UCLA Medical School) Oliver Eberle (Technische Universität Berlin) Klaus-Robert Müller (Technische Universität Berlin) Wojciech Samek (Fraunhofer Institute for Telecommunications, Heinrich Hertz Institute, HHI)

Explainable AI (XAI) has become an active subfield of machine learning. XAI aims to increase the transparency of Machine Learning (ML) models such that a model's prediction can be better understood, evaluated, and actioned. Explanation techniques are now available for many standard machine learning models and applications – typically in the form of heatmaps that visualize which features have been most importantly influencing a model prediction for a given data point. In ML solutions based on matrix and tensor decompositions, explainability might be more direct when there is a good model match. Explainability is critical not only for the simple reason that one would like to have confidence over the solutions, but also because one would like to obtain further insights about the problem from the learned models. XAI has become essential for a variety of disciplines e.g. the Sciences, Medicine and the Humanities where ML has become an indispensable tool for data analysis and modeling. Recently, XAI has even helped to yield genuine novel scientific insights in disciplines like medicine and chemistry. Previous workshops have mainly focused on XAI tailored to specific domains. The purpose of this workshop is to explore whether there are common patterns of XAI challenges across disciplines.

- I prefer hybrid over excluding high-quality remote talks, but I think in-person interaction can not be replaced. I felt it did not matter much for the talks themselves if the person was remote or present in-person.
- Quite a few speakers were only present for the day of their/session of their talk, which unfortunately made it difficult to interact with them.
- Long lunch break makes it difficult for some timezones.
- I think the workshop format could benefit from encouraging speakers to bring along one additional member of their group. This could increase the likelihood of interacting with different perspectives or in general the motivation of speakers to stay over several days or at least have someone represent them/their work that was presented.
- Suggestions for lunch would have been helpful. The presence of IPAM scholars/speakers during the entire workshop would have been interesting. More informal echange around the workshop would have helped the disclosing possible synergies.
- Maybe encouraging more local participation from UCLA / LA students/staff to allow for more possible talks on collaboration etc.
- I think talks are somewhat overlapped, mostly focused on computer vision/image classification related work.
- There was no social contact besides the Q&A time after the talks
- due to [the respondent's] remote participation, opportunities to engage in discussion was very limited.

• Fantastic organization and technical support - special thanks to Rich and Breana!

WORKSHOP: Learning and Emergence in Molecular Systems (Jan. 23-27, 2023) ORGANIZING COMMITTEE

Xavier Bresson (National University of Singapore) Cecilia Clementi (Freie Universität Berlin) Klaus-Robert Müller (Technische Universität Berlin) Patrick Riley (Relay Therapeutics) Max Welling (Microsoft Research)

For molecular systems we know the laws of physics to extreme precision. Yet, our ability to compute properties of these systems to numerical precision is very limited. This is mainly due to two sources of computational intractability: quantum mechanics and chaos. On one side, the accurate solution of the Schrödinger equation for large molecular systems is computationally prohibited. One the other side, even if we knew the forces exactly, the dynamical equations for the atoms would exhibit chaotic behaviour, which implies that, just as the weather, we have limited capacity to predict future trajectories. Some aspects of these systems remain predictable at a macroscopic scale, but they require completely different variables, such as pressure, temperature and entropy. We call this emergent theory thermodynamics.

In the completely different discipline of machine learning, a fairly similar phenomenon takes place. The microscopic variables of an image are given by its constituent pixel values. When we analyse the image with a deep neural network (DNN), we will detect edges in the first layer, corners in the next layer, then the object parts and finally, at the top of the neural network, entire objects. We understand the world at the "emergent" level of objects and their relations, not at the level of pixels and edges. In deep learning (DL) emergence happens automatically through learning and some inductive biases such as symmetries.

A major question we want to address in this workshop is whether we can apply the same learning paradigm to the field of molecular science to learn the correct emergent variables and dynamics.

- [Hybrid format is fine] as long as the number of online talks is limited
- good format for meeting with people, but the schedule is a bit mentally demanding, which takes away some energy from conversations
- This was another great workshop at IPAM, it's a great programme!
- Concerning the food, I would have appreciate (even) more vegetarian/vegan options. Also, would have been great to have some non-alcoholic beers at the reception.
- \$600 is not enough for flight and ground transportation from the East coast.

- This was (again) excellent workshop and I enjoyed it very much. It is always a great pleasure to visit IPAM, the programmes are really great, and I hope I will have the opportunity to participate in again in the future.
- This was a truly fantastic workshop. Maybe the best I have ever attended

WORKSHOP: Machine Assisted Proofs (Feb. 13-17, 2023)

ORGANIZING COMMITTEE Erika Abraham (RWTH Aachen University) Jeremy Avigad (Carnegie Mellon University) Kevin Buzzard (Imperial College London) Jordan Ellenberg (University of Wisconsin-Madison) Tim Gowers (College de France) Marijn Heule (Carnegie Mellon University) Terence Tao (University of California, Los Angeles (UCLA))

A number of core technologies in computer science are based on formal methods, that is, a body of methods and algorithms that are designed to act on formal languages and formal representations of knowledge. Such methods include interactive proof assistants, automated reasoning systems (including first-order theorem provers and satisfiability solvers), computer algebra systems, and knowledge representation and database systems. Methods based on machine learning have also led to the discovery of new mathematical results.

The goal of this workshop is to bring mathematicians and computer scientists together to explore potential applications of these technologies to the domain of pure mathematics, building upon the exciting recent developments in this subject.

The workshop aims to have equal representation from both the computer science and pure mathematics communities and to encourage constructive dialogue. On the computer science side, we intend to attract experts who have developed the technologies enumerated above and who have shown an interest in mathematical applications. On the mathematical side, we hope to attract researchers from a diversity of fields who are intrigued by the possibility of using the new technologies in their work and are open to exploration. The meeting will promote an exchange of ideas, and we hope to leave ample time for open-ended conversation and collaborative discussion.

Comments from our Participant Surveys:

Related to the hybrid part of the workshop:

• I had to teach that week, so the hybrid format allowed me to participate as much as I could

- There are generally fewer opportunities to chat with participants who are not present in person.
- The online talks were a bit more difficult to engage with. That said, some of the best speakers were virtual. I think that it is better to have an excellent virtual speaker than replace them with a mediocre live speaker.
- For me, and for this time, this was truly effective. Perhaps some other time I would prefer to be physically present.
- I would say [remote participation was] "half as effective", specially in terms about the interaction possibilities, but hybrid events allow for much more participation (in particular, I'm from a developing country with scarce access to travel grants).
- It is hard to see what is written on the board. It would be nice if there were a special camera that brings out what is written on the board. Given that speakers did this infrequently, it was not of any consequence.
- It was a very popular workshop, with lots of questions. I wish I could have been there to engage in more profound conversations.
- I only had one question to ask directly, which I was able to ask. Other questions I asked via email to the speakers, who responded promptly.
- I noted that most speakers were (friendly and on-spot) interrupted with questions. This would be a bit more awkward to do while using Zoom, but I think that this is a mainly unavoidable issue of virtual participation.
- I missed the first day's talks, but this was my fault. I didn't realize the times were in PST at first. The time converter sent in the e-mail was really helpful.
- Pacific time is 10 hours away from Eastern European time (Finland). I was unable to
- watch the second half of the program for each day. But you posted it quickly on your streaming channel. Of course, you are not able to ask questions then. I guess there is nothing that can really be done about this. Such is life.
- I was 5hrs later here: tiresome, but mostly manageable
- The frequent and relatively long breaks were great. Much preferable to more talks with short breaks.
- Schedule is very good as is. Shorter breaks would make it harder to take time after talks to digest what we just heard. In my past experiences, workshops that try to cram lots of talks in with minimal breaks cause me to forgot a lot of what I heard by the time I leave and are also exhausting.
- Any changes to suit remote participants like me would not be good for those physically
- present. So I guess the schedule was quite adequate. The important thing is, you fortunately did not have too many talks after the lunch break. Also, these almost one hour talks are more informative than shorter talks. I liked it as it was.
- In an online conference I helped organize we had a Gather Town poster session that was very useful for younger participants. I know this would be extra work for IPAM, but it might make the online part a bit more engaging, more participatory.

- I thought the digital aspects of the workshop were managed perfectly: as a speaker, presenting was easy and the recordings were uploaded very quickly. The remote presenters and attendees were easy to communicate with during the sessions. It is unfortunate that the remote participants were not available for more informal discussions during the breaks, but I have not seen any good way of making that work as well as inperson events.
- Maybe mute the zoom during the small breaks between speakers. This isn't a real big issue. When the small breaks started though the microphone being used for the zoom input must switch or something because the volume got louder and would hurt my ears if I didn't remember to turn it down once the speaker was finished.
- I was present in person and did not use online conferencing software. I enjoyed the Zoom
- hand-raising robot which was effective
- I think that this was one of the better balanced hybrid events I have attended. There were
- clearly great advantages to being there in person, but it seemed that remote participants could still gain significant value.
- I was able to participate easily via Zoom and most talks were followed by very interesting question and answer sessions. Since I was teaching this week I had to miss some talks and watched them on YouTube. Unfortunately the questions and answers are not part of these recordings and I'm wondering if this could be changed if speakers agree to have them included.
- It would be useful to have a short round of introductions similar to the junior participants for the people who are participating remotely. This would largely help people there in person to be aware of people that they might want to talk to who they may not be aware of. Having contact information for the participants would also be useful since we can't just walk up to someone during a tea/coffee break when we're remote, it would be nice if we could easily find out how to contact people to potentially have a quick one-on-one zoom call with or something during the workshop.
- It would have been nice if slides and other material were easily available to remote participants AT the time of the talk or before. As it is, the slides or papers I have I have had to request from the speakers.
- Fantastic line up of speakers. It could have used some tempering on the ethical and sociological impacts that these advances will have on our Mathematical communities, in the rich (developed) world and in the 'underfunded' countries. Perhaps something to consider for a followup!
- Great workshop, wonderfully organized and expertly ran.
- I really appreciate you broadcasting this workshop online, since I cannot attend international workshops in person for financial and health problems.
- I think it was a very good conference. As we say, "if it ain't broken, don't fix it". Thanks!!
- I warmly thank for this opportunity, and I was very surprised by the quickness in making the video material available and its excellent edition.

Regarding other aspects of the workshop:

- Topics were from a large spectrum, and not always easy to follow. However it gave me an idea of what the other end of the spectrum is expecting, and how we could better contribute to help them.
- Some were too technical for the computer scientists in the audience I believe.
- this conference was electric, basically every presentation was fascinating
- Overall the level of the talks was excellent.
- I loved ALL of the talks! I thought that there was a good breadth of applications and ideas, and they offered explanations that I could understand, regardless of my (lack of) expertise.
- I liked the diverse and very interesting choice of the speakers!
- Really excellent mix of talks.
- Overall, the lectures were among the best and most interesting I have seen at a workshop.
- The lectures were AMAZING.
- Some talks were highly specialized and that made them hard to follow for non-experts in the area
- Not all pieces of maths were relevant as such, but the formalisation issues generally were
- The lectures by non-mathematicians were somewhat broadly distributed and not all overlapped with my specific research area. Still it was very good to have an overview of some exciting work in the other related fields.
- great cross-discipline reach in these presentations
- [non-mathematician lectures] were also really great, and introduced topics so that Mathematicians could follow along
- Some talks were a bit too technical but this is understandable in such a specific field.
- Even the topics that were far from my expertise were interesting and engaging because of the excellent preparation of the speakers.
- [Lectures by non-mathematicians] were AMAZING too!
- Not all systems etc. were relevant, but the general points were.
- presentations were well aimed to include non specialists
- There were obviously talks at all levels, and many managed to reach the whole audience. But some speakers clearly didn't realize that that a sizable portion of the audience either had no mathematics or no ITP/ATP background at all. It would have been great if the presentations had more introductory content, and/or if they were scheduled so that the more technical talks come later in the week.
- A few speakers assumed too much background about computing but most did an admirable job.
- Some talks by computer scientists were too heavy dependent on the plafform they were talking about.
- Overall, the speakers did a great job of making the talks accessible but still technically

interesting.

- The lectures about automated theorem provers were a bit to specialized.
- I cannot give a meaningful response here, because there was high variance in the level of Talks
- This event was incredible and meant a lot to me; the balance of participants was quite good, as well as the opportunities for interacting and the breaks between talks.
- Some talks were only peripherally related to my own interests, but I enjoyed them nonetheless.
- This meeting was really wonderful. It brought together different communities in interesting and fruitful ways.
- Everything I was hoping for!
- Great mix of people
- Although I participated remotely, I have made contact with at least three researchers. And through one of those contacts I am able to start new and interesting work.
- It was disappointing that I had to change travel plans and participate remotely instead of in person as originally planned. I would have liked at least some opportunities to interact with the speakers and other participants, but that didn't appear to be possible.
- It's been somewhat of a hassle to declare my expenses for reimbursement, partly because I am unable to cash US checks and partly because the webform crops invoices to portrait format so I had to resubmit all my details. I would have also appreciated a clearly marked vegan/vegetarian option at the breakfast buffet. I could usually find something suitable but again it was a bit of a hassle.
- I was expecting to see more representation of minorities, in particular I expected to meet more latino students.
- Thank you so much for enabling me to attend this wonderful conference! The staff at the Luskin was also really incredible; they made my stay enjoyable. The nearby food amenities and proximity to the Mathematical Sciences building was also great. I just had a wonderful time!
- Would have preferred more healthy food options at breakfasts and breaks.
- I'd like travel support! Or maybe provided lunches or something so it's not eating out every meal.
- Thanks a lot for the invitation and providing such a nice environment!
- Thanks!
- it was my first conference at IPAM, and I came away very impressed
- Even though the workshop presented an excellent opportunity to discuss with other participants, I felt that there could have been more opportunities like the reception to have longer engagements, since the breaks were a bit short (if frequent) and lunch was too free form. Perhaps a workshop dinner one day would help.

- Overall the workshop was an amazing experience. However, I do have some comments: 1. As a junior participant, I never received a confirmation that I was actually going to present. It was only because I asked in the morning of the first day (which turned out to be the day I was presenting) that I found out this was actually happening. There were two days on the schedule this could have happened and I received no email prior to arriving saying which one I would be a part of. Additionally, there was supposed to be a 10 min break between the talk before the junior presentations and the junior presentation. This did not happen and was rather disorienting making it harder to give my presentation. 2. For some reason, the portal that I used to book the Lutskin hotel only allowed me to stay for 5 nights (two months before the workshop), when the instructions in the email specified I should be able to stay for 6 nights. When I called the hotel, they were able to book me a 6th day, so perhaps there is some bug in the previously mentioned portal. 3. I believe I did not receive any email mentioning anything about dietary restrictions regarding the food offered in the workshop. I am vegan, and there weren't always options available to accommodate me. Specifically, there was exactly one breakfast for which the only thing I could eat was fruit. Additionally, there was nothing I could have in all or most of the snack periods in the afternoons. Perhaps I should have emailed ahead of time, but it would probably be helpful if a survey would be sent about this before a future workshop. I might have been hungry every once in a while, but that's not that big of a deal. But other people might have allergies that might make things more complicated. 4. There were way too many emails being sent to everybody before the workshop. Specifically, I was receiving emails that were not relevant to me at all such as forms I didn't have to fill out. I was even told that I hadn't registered properly when I in fact had (and had received confirmation of said facts). None of this lead to anything bad happening, but it was rather confusing and made me worry about the organization of the workshop previous to me coming.
- As a current PhD student, this workshop had an incredibly deep, lasting effect on me; I've been struggling for years on where I fit as a student, in terms of my community, and this conference seems to be exactly the group of individuals with whom I have the most in common! Everyone was exceptionally friendly, I didn't experience any elitism and I felt so supported, like everyone was investing in my success. I am super grateful to the staff and organizers for all of their hard work, for the opportunity to attend, and for putting on such an impactful workshop. When the word "interdisciplinary" is mentioned, I am typically skeptical, but this was an incredibly interdisciplinary workshop. It resonated so much with me and the space was just such a positive experience for me that I felt a bit sad the night before the last day; I didn't want the workshop to end! Thank you so much for everything; I hope that in the future I will have an opportunity to participate again!
- Thanks for a wonderful workshop.
- Overall, this was a fantastic workshop. Many thanks to IPAM and the organizers.

It would be nice to have a workshop-internal wiki for collecting documents, slides, etc. and exchanging information needed to share transport from and to the airport. Before the workshop, each participant could also upload in this wiki a slide with contact information, photo and topics of interest; this would ease identify potential later collaborations.

- Many thanks to all the staff, everything was amazing.
- I was able to participate easily via Zoom and most talks were followed by very interesting question and answer sessions. Since I was teaching this week I had to miss some talks and watched them on YouTube. Unfortunately the questions and answers are not part of these recordings and I'm wondering if this could be changed if speakers agree to have them included.
- Thank you for hosting this workshop as hybrid. I attended online, but the physical participants' voice was a bit unclear to me.
 I felt that everyone at IPAM did a great job. It was a very welcoming environment that really encouraged interaction. PS. I loved the breakfasts!
- You should patent, or open-source, the Zoom robot! Seriously, I would like my University to have one.
- I think it has been a really good conference. Don't change what is working well.
- Very happy that this workshop took place, and very happy that the virtual option was available since external circumstances disrupted my plans to be there in person. I think virtual participation is extremely important to broaden the reach of workshops like this beyond those who have the resources and time to physically attend (especially people with limited funding). I'd like to see more ways to engage remote participants so we can benefit not just from the talks but from the networking and interactions between people. I know everyone has COVID/Zoom fatigue, but remote is here to stay and it would be great to make it better integrated into programs to improve inclusivity/accessibility.
- If there was a nsf official on the panel that would have been nice. I don't think having only highly regarded mathematicians there was sufficient to address the questions.
- You guys are great!

WINTER SCHOOL on Contemporary Quantum Algorithms and Applications (Feb. 22-24, 2023)

ORGANIZING COMMITTEE Bill Fefferman (University of Chicago) Jarrod McClean (Google) Jens Palsberg (University of California, Los Angeles (UCLA)) Richard Ross (University of California, Los Angeles (UCLA)) The Challenge Institute for Quantum Computation (CIQC),Center for Quantum Science and Engineering, and IPAM are pleased to present the third annual Winter School in Quantum Information Science; this is the first time the school meets in person.

This year's school will turn its focus to Contemporary Quantum Algorithms and Applications and will provide both an in-depth primer of the building blocks of quantum algorithms and survey of recent advances for both near-term (NISQ) and far-term (Fault Tolerant) quantum platforms. Topics that will be included in this winter school include:

- Introduction and basic algorithms
- Algorithms for NISQ: an honest assessment
- Quantum machine learning
- Quantum simulation
- Quantum complexity theory

The school is aimed at experimentalists and new theory students working in quantum information science and related fields. We aim to convene a multidisciplinary group of students and researchers who will disseminate and accelerate developments in the field, and to draw on their own research to help inspire new approaches and application domains. Applications are now being accepted. Financial support will be offered to young researchers subject to demonstrated need and availability.

Participants and speakers for this school were supported by CIQC, with IPAM supplying some of the logistics. CIQC used its own evaluation methods for this event.

WORKSHOP: Artificial Intelligence and Discrete Optimization (Feb. 27-March 3, 2023)

ORGANIZING COMMITTEE

Xavier Bresson (National University of Singapore) Bistra Dilkina (University of Southern California (USC)) Andrea Lodi (Cornell University) Pascal Van Hentenryck (Georgia Institute of Technology)

In recent years, the use of Machine Learning techniques to Operations Research (OR) problems, especially in the Discrete Optimization (DO) a.k.a. Combinatorial Optimization context, opens very interesting scenarios because DO is the "home" of an endless list of decision-making problems that are of fundamental importance in multitude applications.

The workshop will bring together experts in mathematics (optimization, graph theory, sparsity, combinatorics, statistics), operations research (assignment problems, routing, planning, Bayesian search, automation, scheduling), machine learning (deep learning,

supervised, self-supervised and reinforcement learning) and artificial intelligence at large (including multi-agent systems, interpretability, fairness, etc.). In addition, the focus will be on

- Algorithmic challenges and potential of the interaction between AI and OR;
- Data requirements in which such an interaction can be profitable; and
- Application areas that are likely to lead to game-changing results (e.g., transportation, supply chain, public policy, energy).

Comments from our Participant Surveys:

- The workshop was great in the sense that the remote component was seamless for physical participants and most presentations were on site. However, I believe it was not as effective for remote participants
- I think nothing goes beyond in-person interactions, but a hybrid backup option helps people who have a last minute conflict.
- I miss discussing with the remote speakers.
- The only difficulty was that the virtual speakers do not have the opportunity of chats over coffee breaks.
- I think remote lectures are simply less effective.
- I was incredibly happy with the quality of the talks. I found the speakers also very open to questions afterwards, and think the large breaks with the nice lobby encourage this.
- Great workshop and selection of talks
- It was a fantastic workshop
- Great workshop and selection of talks!
- I appreciated how the hotel was payed for in advance. The facilities were a great fit for the amount of participants. Breakfast was done very well, especially the muesli and decaf. The staff were very supportive in responding to all emails and in how they handled a participant getting corona.
- The fact that lunches were not organized was a missed opportunity for great collaboration. These were two hours each day that, if held as organized lunches, would have greatly increased the networking and discussion opportunities.
- It has been a fantastic experience, thanks IPAM!
- On the hybrid format: The hand robot was funny, and the few online questions were handled perfectly.

Long program: New Mathematics for the Exascale: Applications to Materials Science (March 13-June 16, 2023)

ORGANIZING COMMITTEE

Irene Beyerlein (University of California, Santa Barbara (UCSB)) Jack Deslippe (Lawrence Berkeley Laboratory) Virginie Ehrlacher (École Nationale des Ponts-et-Chaussées) Vikram Gavini (University of Michigan) Tim Germann (Los Alamos National Laboratory) Tzanio Kolev (Lawrence Livermore National Laboratory) Amedeo Perazzo (Stanford University) Danny Perez (Los Alamos National Laboratory) Anna Vainchtein (University of Pittsburgh)

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 10¹⁸ 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.

The long program had four component workshops, and a reunion conference, which are described in separate sections below.

- This long-term program was truly great! I learned lots of new stuffs from this program.
- Very much enjoyed the program and found it very useful.
- Thank you so much to all the IPAM staff for the support they provided us during the long program.
- The staff members are all nice and very helpful.

- The IPAM staff is excellent. They were always extremely helpful and contributed to the overall great experience I had during my participation in the NME2023 program.
- The support staff were absolutely excellent. Couldn't have asked for any more support from each of them.
- The reimbursement process is very slow: I still have not received funds to cover my second month (and we are now at the end of the programme). I know this is not IPAM's fault, but please apply pressure to the UCLA finance department to try to improve things! The slowness of reimbursement is particularly challenging for junior participants, and can have a serious impact on creditworthiness of your participants.
- I was slightly disappointed to see that many of the more senior participants did not actively participate in the working groups and were not present outside of the workshop weeks.
- Excellent program!
- I think the culminating retreat played an important role in consolidating the results of the long program. Without that final focus, things might have fizzled out.
- The program was truly a life-changing experience both from a career point of view and from a personal point of view. I am very grateful that I was able to attend. My only criticism is small but I would say that the reimbursement of funds was relatively slow and left some people (mostly the junior attendees) struggling to get by with rent payment back at their home location alongside their air-bnb payments. I suggest a strategy which reimburses the junior attendees first since these are the people most likely to struggle with cash flow.
- Thank you again for organising a wonderful programme! As mentioned above, any improvement to the speed at which reimbursements are processed would make IPAM a more accessible place for all researchers.

TUTORIALS WORKSHOP, New Mathematics for the Exascale: Applications to Materials Science Long Program (March 14-17, 2023)

The workshop had the same organizing committee as the long program; the vast majority of participants were from the long program core. The goal is to build a foundation for the participants of this program who have diverse scientific backgrounds.

- This was a unique opportunity to share technical insights on a range of multidisciplinary topics that are not treated in conventional academic meetings. My understanding of the future challenges and opportunities facing the field has increased significantly.
- Not many (any?) lectures by mathematicians, but all involved math to various extents
• The relevance and quality of the lectures was very high.

WORKSHOP I: Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing, New Mathematics for the Exascale: Applications to Materials Science Long Program (March 27-31, 2023)

ORGANIZING COMMITTEE

Virginie Ehrlacher (École Nationale des Ponts-et-Chaussées) Vikram Gavini (University of Michigan) Danny Perez (Los Alamos National Laboratory) Steve Plimpton (Sandia National Laboratories)

The vast majority of the computing power available to the materials science community is consumed by a relatively small number of workhorse methods, such as molecular dynamics and density functional theory. These methods have been adapted to run on parallel platforms for decades, but the focus has firmly been on weak-scaling, i.e., on scaling the problem size with the number of processors. While high-performance weak-scaling implementations of these methods are extremely valuable, the focus on increasing length-scales limits opportunities for scientific discovery. Transformative impact requires the capability to leverage computing resources to simultaneously and flexibly increase length scales, time scales, and accuracy.

Increasing simulation timescales requires a deep understanding of the mathematics of rare in order to inform novel methods that are specially tailored from the start, as well as strong-scaling computational engines that can leverage large computational resources on problems of relatively small sizes. This requires a dramatic rethinking of how basic algorithms in materials science are derived and implemented. Similarly, the exponential increase in computer resources now enables very high accuracy simulations with methods such as coupled clusters or quantum Monte Carlo. These methods are extremely powerful, but they tend to scale poorly with the number of electrons. The development of new flexible methods where accuracy can be systematically adjusted in order to modify the tradeoff between size and time scales would therefore be extremely beneficial.

This workshop will focus on recent development of new mathematical approaches to intensive calculations at massive scale with a focus on new ways to improve scalability (both weak and strong) and extend simulations along the size, time, and accuracy axes simultaneously.

Comments from our Participant Surveys:

We received 12 responses to the post-workshop questionnaire, and no comments were submitted. Of the 12 respondents, 11 rated the overall quality of the workshop as "Excellent", and 1 rated it

as "Average". All respondents stated that they were "Satisfied" or "Very Satisfied" with various aspects of the workshop and its organization.

WORKSHOP II: Scale-Bridging Materials Modeling at Extreme Computational Scales, New Mathematics for the Exascale: Applications to Materials Science Long Program (Apr 17-21, 2023)

ORGANIZING COMMITTEE

Irene Beyerlein (University of California, Santa Barbara (UCSB)) Thomas Hudson (University of Warwick) Thomas Swinburne (Centre National de la Recherche Scientifique (CNRS)) Anna Vainchtein (University of Pittsburgh)

Quantitatively predicting the properties of "real" structural materials is an extremely challenging endeavor, as macroscale properties depend on characteristics of the material at every scale, from nanometers (short range order, point defects, etc.), to micrometers (grain size, extended defects, etc.), to centimeters (texture, etc.). Similarly, relevant timescales range from atomic vibrations (picoseconds) to microstructural evolution times (hours to years). This extreme breadth of size and time scales makes the accurate simulations with fully-resolved atomic-scale tools (e.g., molecular dynamics) hopeless. Practical solutions must therefore rely on scale-bridging approaches that systematically upscale the lower scale physics into computationally tractable higher-scale constructs. The premise of this workshop is that extreme-scale computing can breathe new life into the field of multiscale modeling by addressing the problems identified above with brute force computing. This workshop will focus on new mathematical approaches to multiscale/multiphysics modeling, with a particular emphasis on the many theoretical and numerical challenges faced at the exascale. The goal is to bring together specialists in a range of massively parallel algorithms and researchers interested in improving the scalability of current techniques.

Topics that will be covered in this workshop include:

- Scalable mathematical formulations for concurrent multi-scale simulations at massive scales.
- Automated derivation of coarse-grained model from massive-scale simulations.
- Uncertainty-quantification-driven parameterization of multiscale models.
- Design of scalable multiscale solvers.
- Implementation of concurrent multiscale models at massive scales.

Comments from our Participant Surveys:

- very much appreciated the zoom streaming.
- There should be a better balance between talks of mathematicians and nonmathematicians. The majority of the talks at this workshop were by non-mathematicians
- Lectures by mathematicians are appropriate level in general but a little bit high for me
- IPAM should provide allergen information for the food that it serves (some people have dietary restrictions or/and are allergic to some ingredients)
- It would great to increase the quality of the tea bags.
- 15 minute coffee breaks were too short.
- I particularly liked having short breaks between the talks. This really helps to relax, recharge and have a quick chat with speakers before continuing. Please keep this format!
- I particularly liked having short breaks between the talks. This really helps to relax, recharge and have a quick chat with speakers before continuing. Please keep this format!
- Great Workshop, great organization and venue, wonderful environment to foster discussion and collaboration.

WORKSHOP III: Complex Scientific Workflows at Extreme Computational Scales, New Mathematics for the Exascale: Applications to Materials Science Long Program (May 1-5, 2023)

ORGANIZING COMMITTEE

Jörg Neugebauer (Max-Planck-Institut für Eisenforschung GmbH) Amedeo Perazzo (Stanford University) Joshua Schrier (Fordham University) Ping Yang (Los Alamos National Laboratory)

One of the key changes in the landscape of high-performance computing in materials science in the last decade is the explosion of high-throughput applications where massive amounts of relatively small quantum calculations fuel the rapid exploration of the chemical space of materials. Such high throughput workflows are prime candidates for the efficient exploitation of exascale resources. This workshop proposes to build on these early successes and to take the next logical step by exploring the challenges and opportunities associated with integrating massive-scale compute-intensive simulations into a wider range of complex scientific workflows. The underlying goal is to identify and explore opportunities to maximize the impact of large-scale computing by improving its integration with various aspects of the scientific enterprise. This workshop will aim at developing new mathematical and computational approaches that enable the inclusion of massive-scale computing into complex scientific workflows.

Topics that will be covered in this workshop include:

- Integration of direct simulations, online data analysis, and experimental data.
- Mathematical methods for data assimilation.
- Large-scale inverse problems.
- Computation-aided online experimental design at massive scales.
- Active exploration of chemical space using massive quantum calculations.
- Workflow infrastructure.
- Integration of numerically-intensive calculations with ML/data-science at scale.

Comments from our Participant Surveys:

- Appreciated the open time between talks, but would have appreciated a more structured discussion earlier in the workshop, and smaller group discussions.
- I learned what is happening in the latest topics of computational chemistry and physics.
- I really loved the workshop format, with long talks and lots of opportunity to ask questions and engage with speakers between talks.
- Great workshop. Showed different perspectives. Very interesting discussions.
- A very stimulating workshop!
- Very relevant in terms of applications at physical l/chemical phenomena
- Very nice collection of topics, and the right speakers
- The interpretation of what a workflow is varies hugely from person to person. So some of the talks were perfectly in line with my interests, others were pretty far away.
- Computer science talks were more out of my domain and harder to follow, but there was enough at the right level to keep it interesting and relevant.
- I think the discussion portion could have been a bit better. I think the question(s) being asked weren't well defined, so the conversation was a bit open ended. [An organizer] was doing a good job trying to focus the conversation, but he may have steered the conversation a bit too much, rather than letting it organically develop
- You could have kept the coffee out longer
- Reimbursement is not immediate.
- The staff and the IPAM professors made me feel like part of their group and the UCLA community.
- Kudos to Ms. Banjo and her administrative staff for a smooth daily momentum, courtesy, and professionalism.
- A great workshop! IPAM is the best.

WORKSHOP IV: Co-design for the Exascale and IPAM Hackathon, New Mathematics for the Exascale: Applications to Materials Science Long Program (March 27-31, 2023)

ORGANIZING COMMITTEE

Jack Deslippe (Lawrence Berkeley Laboratory) Tim Germann (Los Alamos National Laboratory) Rebecca Hartman-Baker (Lawrence Berkeley Laboratory) Tzanio Kolev (Lawrence Livermore National Laboratory) Elaine Raybourn (Sandia National Laboratories)

The final workshop of this program will be an event designed to promote the generation of tangible products from the long program and to explore the best practices in setting up a computational co-design process that ranges from derivation of the key formalisms, to the design of the computational approach, and finally to its implementation. The vision of the program is that the long-term participants will self-organize into working groups designed to identify, analyze, and solve key problems that impede the effective use of extremescale computing in materials science. In order to ensure that these advances make their way into the hands of the community at large, this IPAM "hackathon" will gather code developers, mathematicians, method developers, and computer scientists and engineers from the computer vendors for a week of discussion, hands-on development, and implementation of the new ideas generated during the program. A key objective will be to ensure the transition from "research" codes into "production" codes that can be used and further improved by the community. As such, significant parts of the workshop will involve participants organizing into working groups in order to solve (or take the first steps in solving) practical issues that will have been raised throughout the program. The workshop will include a short series of talks where lead developers of various projects will share their experience and processes when attacking new problems related to evolving architectures, either in terms of new mathematical formalism, increasing computational scales, and architectural details.

Comments from our Participant Surveys:

- Thank you to IPAM and its staff for organizing, hosting, and supporting this enjoyable and very productive workshop!
- Ginger and her team are wonderful to work with. The environment of IPAM is inclusive and welcoming. The IPAM faculty and staff inspire others. Rich (video) is also great to work with.

CULMINATING WORKSHOP, New Mathematics for the Exascale: Applications to Materials Science Long Program (June 11-16, 2023)

IPAM long programs end with a culminating workshop for long-term ("core") participants. The workshop is held at the UCLA Lake Arrowhead Conference Center. The organizing committee is the same as for the long program itself. The purpose of the workshop is to summarize what is learned during the program. Working groups that formed during the long program give reports about their progress. Additionally, all participants collaborate to produce a White Paper, which serves to both capture developments discussed during the program itself and to map out potential future developments. The white paper is available at the IPAM web site, https://www.ipam.ucla.edu/news/white-paper-new-mathematics-for-the-exascale-applications-to-materials-science/

Comments from our Participant Surveys:

• I think the culminating retreat played an important role in consolidating the results of the NME2023 long program. Without that final focus, things might have fizzled out.

Participants from past IPAM long programs are usually invited to two reunion conferences, which take place 1.5 and 2.5 years following the completion of the long program. In June 2023, we organized reunion conferences for the Fall 2020 Autonomous Vehicles program, and the Fall 2021 Gravitational Waves program.

REUNION: Mathematical Challenges and Opportunities for Autonomous Vehicles Reunion Conference II (June 11-16, 2023)

ORGANIZERS Hani Mahmassani (Northwestern University) Benjamin Seibold (Temple University) Jonathan Sprinkle (University of Arizona) Daniel Work (Vanderbilt University)

This reunion occurred on-time, 2.5 years after the completion of the program. However, the program was fully virtual, and the first time the participants had a chance to meet face-to-face was in June 2021, at their first reunion.

An alumni survey of the program was performed, since this was the last activity associated with the long program.

Because the Autonomous Vehicles program was virtual, there was no culminating workshop, and a white paper was not written in 2021. However, participants decided to write a white paper at

their 2023 retreat. At this time, the white paper is still being edited; IPAM will post it on our web site once it is completed.

The long program exit survey gathered 22 responses. About 55% of those who responded selfidentified as recent PhDs (5 years or less from PhD), and 45% identified as having received a PhD more than 5 years before the program. The majority of those responding identified as engineers (63%), followed by mathematician or a statistician (23%), and computer scientists (14%).

The table below summarizes responses to the question on the value of program activities. Generally, participants rated all program components highly. This is remarkable, given the online nature of the program:

	1-POOR	2	3	4-EXCELLENT	N/A	TOTAL
Value of Opening Day activities.	0.00%	4.55%	13.64%	72.73%	9.09%	
	0	1	3	16	2	22
Quality or usefulness of the series of workshops.	0.00%	0.00%	18.18%	81.82%	0.00%	
	0	0	4	18	0	22
Quality or usefulness of the activities between workshops.	4.55%	13.64%	36.36%	40.91%	4.55%	
	1	3	8	9	1	22
Value of the Culminating Workshop.	4.55%	9.09%	13.64%	59.09%	13.64%	
	1	2	3	13	3	22
Overall merit or quality of the long program.	0.00%	4.55%	13.64%	81.82%	0.00%	
	0	1	3	18	0	22

The majority of participants liked collaborative opportunities they had during the program, despite the fact that all interactions were online, and not in-person. The table below summarizes their responses:

	NONE	LOW	MEDIUM	HIGH	TOTAL
Collaboration within your discipline or sub-discipline.	4.55% 1	9.09% 2	45.45% 10	40.91% 9	22
Collaboration outside your discipline or sub-discipline.	4.55% 1	4.55% 1	45.45% 10	45.45% 10	22
Collaboration between junior and senior participants.	4.55% 1	4.55% 1	40.91% 9	50.00% 11	22

This was also a result of the fact that the organizers and senior participants worked hard to make the online format a success. One participant commented: "Senior participants are very dedicated for collaboration."

Most participants agreed when presented with statements about the program meeting their expectations and being of help with furthering their career and research goals. The table below summarizes these responses:

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	1 - STRONGLY DISAGREE	2	3	4 - STRONGLY AGREE	TOTAL
The IPAM long program met my expectations.	0.00% 0	9.09% 2	31.82% 7	59.09% 13	22
The long program will have a positive impact on my research and career.	0.00% 0	4.55% 1	31.82% 7	63.64% 14	22
The long program was a valuable mentoring opportunity for the "junior" participants.	0.00% 0	9.09% 2	36.36% 8	54.55% 12	22
I formed new collaborations that will lead to publications or other outcomes.	9.09% 2	18.18% 4	27.27% 6	45.45% 10	22
I would participate in another IPAM long program.	0.00% 0	4.55% 1	13.64% 3	81.82% 18	22

In addition, a bibliographical analysis of the program was performed. The results are presented in Section L.

REUNION: Mathematical and Computational Challenges in the Era of Gravitational Wave Astronomy Reunion Conference I (June 11-16, 2023)

ORGANIZERS

Manuela Campanelli (Rochester Institute of Technology) Marco Cavaglia (Missouri University of Science and Technology) Jose Antonio Font (University of Valencia) Igor Rodnianski (Princeton University) Gunther Uhlmann (University of Washington)

This reunion took place on-time, 1.5 years after the completion of the long program. The reunion was average size, with 19 participants. Participants from theoretical and experimental sides of gravitational waves reported on novel approaches and discussed future collaborations. The alumni survey of the program will be performed at the time of the second reunion.

K. PROGRAM CONSULTANT LIST

IPAM consulted a variety of scholars and practitioners in the scientific planning of its programs. The list below includes program organizers for the programs that took place during this reporting period or upcoming programs for which organizing committees have begun meeting. The list excludes IPAM's scientific staff (directors) and members of IPAM's Science Advisory Board and Board of Trustees, who are listed in "Section O, Committee Membership". On occasion, IPAM scientific staff and Board Members are organizers of workshops and long programs, in which case they are included in the list below.

First Name	Last Name	Institution Name	
Erika	Abraham	RWTH Aachen University	
Tülay	Adali	University of Maryland Baltimore County	
Gorjan	Alagic	University of Maryland	
Jeremy	Avigad	Carnegie Mellon University	
Rodrigo	Bañuelos	Purdue University	
Selenne	Bañuelos	California State University, Channel Islands	
Ruha	Benjamin	Princeton University	
Irene	Beyerlein	University of California, Santa Barbara (UCSB)	
Thomas	Barthel	Duke University	
Peter	Binev	University of South Carolina	
Erik	Bollt	Clarkson University	
Xavier	Bresson	National University of Singapore	
Anne	Broadbent	University of Ottawa	
Joachim	Buhmann	ETH Zürich	
Hans-Joachim	Bungartz	Technical University Munich (TUM)	
Kevin	Buzzard	Imperial College London	
Manuela	Campanelli	Rochester Institute of Technology	
Bridget	Carragher	New York Structural Biology Center (NYSBC)	
Marco	Cavaglia	Missouri University of Science and Technology	
Wah	Chiu	Stanford University	
Jaesik	Choi	Korea Advanced Institute of Science and Technology	
		(KAIST)	
Cecilia	Clementi	Freie Universität Berlin	
Dana	Dachman-Soled	University of Maryland	
Noa	Dagan	Harvard Medical School	
Jack	Deslippe	Lawrence Berkeley Laboratory	
Bistra	Dilkina	University of Southern California (USC)	
Pamela	Douglas	UCLA Medical School	
Claudia	Draxl	Humboldt-Universität	
Cynthia	Dwork	Harvard University	

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Oliver	Eberle	Technische Universität Berlin
Virginie	Ehrlacher	École Nationale des Ponts-et-Chaussées
Jordan	Ellenberg	University of Wisconsin-Madison
Peter	Ercius	Lawrence Berkeley National Laboratory
Bill	Fefferman	University of Chicago
Jose Antonio	Font	University of Valencia
Gero	Friesecke	Technische Universtitat München
Wilfrid	Gangbo	University of California, Los Angeles (UCLA)
Vikram	Gavini	University of Michigan
Tim	Germann	Los Alamos National Laboratory
Tim	Gowers	College de France
Pamela E.	Harris	Williams College
Rebecca	Hartman-Baker	Lawrence Berkeley National Laboratory
Marijn	Heule	Carnegie Mellon University
Jeffrey	Hittinger	Lawrence Livermore National Laboratory
Thomas	Hudson	University of Warwick
Tetsuya	Ishikawa	RIKEN SPring-8 Center
Frank	Jenko	Max Planck Institute for Plasma Physics
Sergei	Kalinin	University of Tennessee
Jonathan	Katz	University of Maryland
Angus	Kirkland	University of Oxford
Tzanio	Kolev	Lawrence Livermore National Laboratory
Gitta	Kutyniok	Ludwig-Maximilians-Universität München
Andrea	Lodi	Cornell University
Hani	Mahmassani	Northwestern University
Jarrod	McClean	Google
Jianwei (John)	Miao	University of California, Los Angeles (UCLA)
Andy	Minor	University of California, Berkeley (UC Berkeley)
Klaus-Robert	Müller	Technische Universität Berlin
Margaret	Murnane	University of Colorado Boulder
Deanna	Needell	University of California, Los Angeles (UCLA)
Jörg	Neugebauer	Max-Planck-Institut für Eisenforschung GmbH
Adam	Oberman	McGill University
Stanley	Osher	University of California, Los Angeles (UCLA)
Jens	Palsberg	University of California, Los Angeles (UCLA)
Amedeo	Perazzo	Stanford University
Tiago	Pereira	University of São Paulo (USP)
Danny	Perez	Los Alamos National Laboratory
Steve	Plimpton	Sandia National Laboratories
Elaine	Raybourn	Sandia National Laboratories

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Patrick	Riley	Relay Therapeutics	
Ian	Robinson	Brookhaven National Laboratory	
Igor	Rodnianski	Princeton University	
Richard	Ross	University of California, Los Angeles (UCLA)	
Guy	Rothblum	Apple Inc.	
Zineb	Saghi	Commissariat à l'Énergie Atomique (CEA)	
Wojciech	Samek	Fraunhofer Institute for Telecommunications,	
		Heinrich Hertz Institute, HHI	
Joshua	Schrier	Fordham University	
Benjamin	Seibold	Temple University	
Amit	Singer	Princeton University	
Jonathan	Sprinkle	University of Arizona	
Aneta	Stefanovska	Lancaster University	
Sriram	Subramaniam	University of British Columbia	
Thomas	Swinburne	Centre National de la Recherche Scientifique (CNRS)	
Terence	Тао	University of California, Los Angeles (UCLA)	
Gunther	Uhlmann	University of Washington	
Anna	Vainchtein	University of Pittsburgh	
Pascal	Van Hentenryck	Georgia Institute of Technology	
Sebastian	van Strien	Imperial College	
Anthony	Várilly-Alvarado	Rice University	
Mariel	Vázquez	University of California, Davis	
Thomas	Vidick	California Institute of Technology	
Paul	Voyles	University of Wisconsin-Madison	
Laura	Waller	University of California, Berkeley (UC Berkeley)	
Paul	Weiss	University of California, Los Angeles (UCLA)	
Max	Welling	University of Amsterdam	
Patricia	Williams	Northeastern University	
Daniel	Work	Vanderbilt University	
Ping	Yang	Los Alamos National Laboratory	
Mark	Zhandry	NTT Research and Princeton University	
Hong	Zhou	University of California, Los Angeles (UCLA)	
Yimei	Zhu	Brookhaven National Laboratory	

L. PUBLICATIONS LIST

The following is a summary of bibliographic analysis of the 2018 program Big Data Meets High Performance Computing, whose last activity was in December 2022.

We asked program participants to tell us about published papers that they consider to be influenced by the program. These surveys are administered before the second reunion of the program, which is normally 2.5 years after the completion of the main part of the program. Due to the COVID-19 pandemic, the second reunion of the program was delayed by 1.5 years, and thus the survey was administered 4 years after the completion of the program. This resulted in the following list:

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- 4. Anderson C.R., et al., *High order discretization techniques for real-space ab initio simulations*, Journal of Chemical Physics **148** 2018-03-21. **Paper link:**<u>SCOPUS ID:85044258533</u>
- 5. Anderson C.R., et al., *High-precision real-space simulation of electrostatically confined few-electron states*, AIP Advances **12** 2022-06-01. **Paper link:**<u>SCOPUS</u> <u>ID:85133679310</u>
- 6. Araki S.J., et al., *A grid-based nonlinear approach to noise reduction and deconvolution for coupled systems*, Physica D: Nonlinear Phenomena **417** 2021-03-01. **Paper link:** <u>SCOPUS</u> <u>ID:85098596817</u>
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- 15. Buhmann J.M., et al., *Robust optimization in the presence of uncertainty: A generic approach*, Journal of Computer and System Sciences **94** 2018-06-01, 135-166. **Paper link:** <u>SCOPUS ID:85033777923</u>
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Collaboration network analysis

In addition, we have performed an automated collaboration analysis, seeking to identify pairs of collaborators that have not worked with each other prior to the program. In the graph below, such pairs are marked with red edges, while authors that collaborated prior to the year of the program are joined with blue edges.



The program had some success in forming new collaborations, bringing several new researchers to existing collaboration clusters.

The following is a summary of bibliographic analysis of the 2020 program High Dimensional Hamilton Jacobi PDEs, whose last activity was in December 2022.

We performed several bibliographic analyses of the program. A survey was administered asking participants to report on the papers that were stimulated by the program. As a result, 102 participants reported the following 317 papers.

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In addition, we have performed an automated collaboration analysis, seeking to identify pairs of collaborators that have not worked with each other prior to the program. In the graph below, such pairs are marked with red edges, while authors that collaborated prior to the year of the program are joined with blue edges.



The program was successful in both bringing several new researchers to existing collaboration clusters, as well as forming collaborations that join clusters of previously collaborating authors. In addition, seven authors collaborated for the first time.

The following is a summary of bibliographic analysis of the 2020 Long Program Mathematical Challenges and Opportunities for Autonomous Vehicles, whose last activity was in June 2023.

We asked program participants to tell us about published papers that they consider to be influenced by the program. This resulted in the following list:

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In addition, we have performed an automated collaboration analysis, seeking to identify pairs of collaborators that have not worked with each other prior to the program. In the graph below, such pairs are marked with red edges, while authors that collaborated prior to the year of the program are joined with blue edges.



The program was successful in forming new collaborations, bringing several new researchers to existing collaboration clusters.

M. INDUSTRIAL AND GOVERNMENTAL INVOLVEMENT

We have significant involvement of industry and government labs in our summer program, Research in Industrial Projects for Students (RIPS)-Los Angeles. Companies and other organizations sponsor research projects and one or more representatives of the organization interact with the student team. Many of them are listed as participants of RIPS and RIPS Projects Day. Additionally, significant numbers of industry and government participants took part in our long programs and workshops; the table below lists workshops with 4 or more industry participants.

Workshop Name	Industry Participants
Machine Assisted Proofs	20
Artificial Intelligence and Discrete Optimization	7
Workshop IV: Multi-Modal Imaging with Deep Learning	7
and Modeling	
Mathematics for the Exascale: Applications to Materials Science Tutorials	5
Learning and Emergence in Molecular Systems	5
Latinx in the Mathematical Sciences Conference 2022	5
Workshop IV: Co-design for the Exascale and IPAM Hackathon	4

We seek the advice of government and industry by recruiting corporate and government leaders to serve on our Science Advisory Board and Board of Trustees. See section O for a complete list of members and their affiliations.

There were 228 participants that identified as being from Government or Industry; of these 162 came to IPAM in person. There were 78 unique Government or Industry participants.

Of these, 14 unique participants came from government or military institutions, including: Air Force Research Laboratory, Argonne National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, National Security Agency, National Science Foundation, Oak Ridge National Laboratory. Of these, 8 were speakers or organizers at various programs.

There were 20 unique participants from companies such as Amazon, Artificial Intelligence Center, DeepMind, Facebook/Meta, Genentech, Google, Google AI, Google Brain, IBM, Lizora Technlogies, Microsoft Research, Navigate BioPharma, Netflix, Nvidia, Relay Therapeutics, RIKEN SPring-8 center, SCM, SLAC, RAND, and Toyota Research Institute who served as speakers or organizers.

N. EXTERNAL SUPPORT

In addition to the funding listed in Table N below, IPAM receives substantial in-kind financial support from UCLA. The Director's entire salary/benefits and administrative stipend are paid directly by UCLA. The Director of Special Projects is released from two courses at the cost of replacing him by a junior person academic. IPAM is not charged for the use of its centrally located building, maintenance, or custodial care. Also, UCLA offers IPAM centralized administrative support, technology, recreational facilities, and access to renown libraries, though it is difficult to quantify such support monetarily.

IPAM received gifts towards its endowment and current use funds from several donors, including Advanced Micro Devices, Aerospace, Meta, IBM, Lawrence Livermore National Laboratory, AVCO Charitable Foundation, and Theodore H. Gamelin. As of March 31, 2023 (the last date for which figures are available), IPAM's total endowment stood at \$3,268,743. The endowment is designed to generate approximately 4% per year in income.

The table shows other funding received by IPAM from April 1, 2022 through March 31, 2023.

Table N: Other Funding Support	2022-23
Simons Postdoctoral Grant	\$357,408
Sub-total	\$357,408
UCLA Funding	
Dean Physical Sciences	\$97,211
Vice Chancellor for Research	\$153,142
Sub-total	\$250,353
Endowments and Current Gifts	
Endowments – New Gifts & Investment Income	\$527,810
New Current Use Gift Funds	\$65,535
Sub-total	\$593,345
TOTAL	\$1,201,106

O. COMMITTEE MEMBERSHIP

IPAM's committees include the Board of Trustees and Science Advisory Board. The members during the reporting period are listed below. The IPAM directors are ex officio members.

Board of Trustees, 2022-23 Membership

Name	Institution	Department or Title
Katy Borner	Indiana	Distinguished Professor of Engineering and
	Bloomington	Information Science
Russel Caflisch	New York	Director Courant Institute
	University	
Brenda Dietrich	Cornell University	Professor, Operations Research
Katherine Ensor	Rice University	Noah G. Harding Professor of Statistics
Diana Farrell	Independent	Director and Trustee
Edray Goins	Pomona College	Professor of Mathematics
Louis J. Gross	University of	Professor of Ecology and Evolutionary
	Tennessee, Knoxville	Biology
Overtoun Jenda	Auburn University	Professor of Mathematics
Tyler Kleykamp	Georgetown University	Fellow, State Chief Data Officer Network
Wen Masters	Georgia Tech Research Institute	Vice President, Cyber Technologies at MITRE
Nancy Potok	NAPx	CEO
	Consulting	
C. Matthew Snipp	Stanford	Professor, School of Humanities and
Time Come	Driversity	Vie Duridant Endand Enconting
Tina Sung	University	Networks
Costis Toregas	George	Director, Cyber Security and Privacy
	Washington University	Research Institute
Mariel Vasquez	UC Davis	Director, Center for the Advancement of Multicultural Perspectives in Science

Science Advisory Board, 2022-2023

The list below includes new members whose terms started in January 2023.

Name	Institution	Discipline or Department
Michael Brenner	Harvard College	Professor of Applied Mathematics and Applied Physics
Emery Brown	MIT/ Harvard	Professor of Medical Engineering and
	Medical School	Computational Neuroscience
Kieron Burke	UC Irvine	Professor of Chemistry and Physics
Emmanuel Candes	Stanford University	Professor of Mathematics and Statistics
Cecilia Clementi	FU Berlin	Professor of Physics
Cynthia Dwork	Harvard University	Professor of Computer Science
Jordan Ellenberg	University of Wisconsin - Madison	Professor of Mathematics
Jeffrey Hittinger	Lawrence Livermore Nat. Lab	Director, Center for Applied Scientific Computing
Kiran Kedlaya	UC San Diego	Professor of Mathematics
Richard Kenyon	Yale University	Professor of Mathematics
Xihong Lin	Harvard University	Chair of Department of Biostatistics
Svitlana Mayboroda	University of Minnesota	Professor of Mathematics
Marina Meila	University of Washington	Professor of Statistics
Lauren Ancel Meyers	University of Texas at Austin	Professor of Biology and Statistics
Klaus-Robert Muller	Technische Universitat Berlin	Chair of Machine Learning Group
Jelani Nelson	UC Berkeley	Professor of Electrical Engineering and Computer Science
Pablo Parrilo	MIT	Professor of Electrical Engineering and Computer Science
Terence Tao	UCLA	Professor of Mathematics
Eric Tchetgen Tchetgen	Wharton School, U Pennsylvania	Professor of Statistics

Jean-Luc Thiffeault	University of Wisconsin - Madison	Professor of Mathematics
Ryan Tibshirani	UC Berkeley	Professor in the Departments of Statistics and Machine Learning
Luca Trevisan	UC Berkeley	Professor of Computer Science
Rachel Ward	University of Texas - Austin	Professor of Mathematics
Amie Wilkinson	University of Chicago	Professor of Mathematics
Daniela Witten	University of Washington	Professor of Statistics and Biostatistics