ipam institute for pure & applied mathematics

New Mathematics for the Exascale: Applications to Materials Science

## March 13 - June 16, 2023

Scientific Overview

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.

Long Program Schedule

- New Mathematics for the Exascale Opening Day: March 13, 2023
- New Mathematics for the Exascale Tutorials: March 14-17, 2023
- Workshop I: Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing: March 27-31, 2023
- Workshop II: Scale-Bridging Materials Modeling at Extreme Computational Scales: April 17-21, 2023
- Workshop III: Complex Scientific Workflows at Extreme Computational Scales: May 1-5, 2023
- Workshop IV: Co-design for the Exascale and IPAM Hackathon: May 22-26, 2023
- Culminating Workshop at Lake Arrowhead: June 11-16, 2023
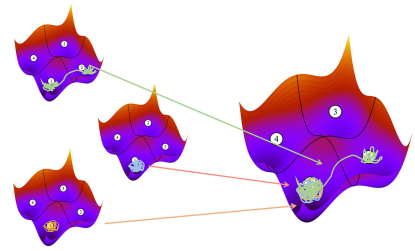
Organizers

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

Participation

This long program will involve senior and junior researchers from several communities relevant to this program. You may apply for financial support to participate in the entire fourteen-week program, or a portion of it. We prefer participants who stay for the entire program. Applications will be accepted through October 13, 2022 but offers may be made up to one year before the start date. We urge you to apply early. Mathematicians and scientists at all levels who are interested in this area of research are encouraged to apply for funding. Supporting the careers of women and minority researchers is an important component of IPAM's mission and we welcome their applications. More information and an application is available online.