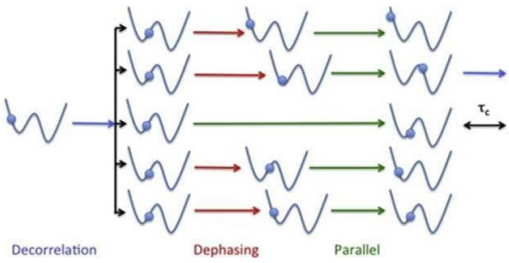
institute for pure & applied mathematics

Workshop I: Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing



MARCH 27 - 31, 2023

Scientific Overview

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.

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

Long Program Schedule

This workshop is part of the long program on “New Mathematics for the Exascale”.

- 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 MaterialsModeling Using ExascaleComputing: 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

Participation

Additional information about this workshop including links to register and to apply for funding, can be found on the webpage listed below. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM’s mission, and we welcome their applications.

Organizers

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

Invited Speakers

Manuel Athenes (Commissariat à l'Énergie Atomique)
David Bolwer (University College London)
Vasily V. Bulatov (Lawrence Livermore Nat Lab)
Eric Cances (École Nat. des Ponts-et-Chaussées)
Virginie Ehrlacher (École Nat. des Ponts-et-Chaussées)
Jaafar El-Awady (Johns Hopkins University)
Giulia Galli (University of Chicago)
VikramGavini (University of Michigan)
Laura Grigori (Sorbonne Université)
Markos Katsoulakis (Uni of Mass Amherst)
PaulKent (Oak Ridge National Laboratory)
TzanioKolev (Lawrence Livermore National Lab)
Heather Kulik (MIT)
Tony Lelièvre (École Nationale des Ponts-et-Chaussées)
Lin Lin (UC Berkeley)
Anders Nikklasson (Los Alamos National Lab)
DannyPerez (Los Alamos National Laboratory)
Reinhold Schneider (Technische Universität Berlin)
Daniel Schwen (Idaho National Laboratory)
Aidan Thompson (Sandia National Laboratories)

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For more information, visit the program web page:
www.ipam.ucla.edu/NMEWS1