

Workshop III: Complex Scientific Workflows at Extreme Computational Scales

MAY 1 - 5, 2023

Scientific Overview

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.

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

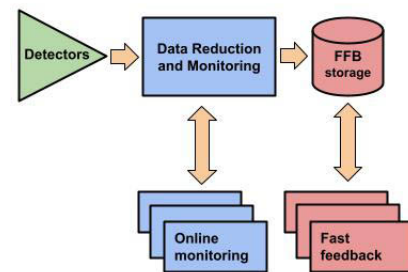
Long Program Schedule

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 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

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

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

Invited Speakers

Ben Blaiszick (ANL/U Chicago); Jamie Sethian (LBL/Berkeley); Linda Hung (Toyota Research Institute); Kristin Persson (Materials Project, LBL); Claudia Draxl (Humboldt Universität Berlin); Carla Gomes (Cornell); Maxim Ziatdinov (ORNL); Alán Aspuru-Guzik (University of Toronto); Michele Ceriotti (EPFL Switzerland); Johannes Köster (Duisburg/Essen); Ralf Drautz (ICAMS, Bochum); Jan Janssen (LANL); Jeff Donatelli (LBL); Jana Thayer (SLAC); Arianna Gleason (Stanford); Frederic Poitevin (SLAC); Ariana Peck (SLAC); Johannes Blaschke (LBL/NERSC); and Deborah Bard (LBL/NERSC).



For more information, visit the program web page:

www.ipam.ucla.edu/NNEWS3