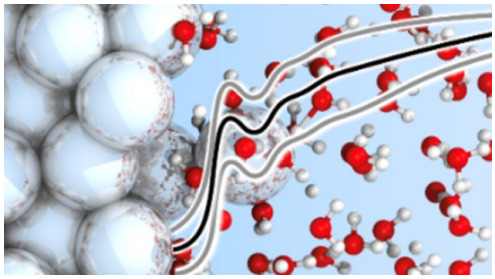
institute for pure & applied mathematics

Workshop IV: Electrochemistry Hackathon: Bridging the Gap Between Implicit and Explicit Methods



November 17-21, 2025

Scientific Overview

This collaborative hackathon will bring together long-term participants of the IPAM program, with their strong backgrounds in mathematics, electrochemistry, and computational science, to bridge the gap between implicit (deterministic) and explicit (stochastic) methods, as well as deterministic and stochastic methods, in electrochemistry. Participants will work in small interdisciplinary teams to implement and optimize the developed approaches from the previous workshops. The hackathon will foster creative problem-solving, encouraging the integration of both deterministic and stochastic aspects to simulate electrochemical systems more accurately. This interactive event will culminate in the presentation of novel solutions and an open-source platform for fruitful discussions on the future of electrochemical modeling

Topics include:

- Implementation and test of interaction kernels and implicit solvent approaches developed in the program in existing DFT codes
- Development and analysis of electrochemical model systems to benchmark the developed algorithms
- Implement and analysis of various potentiostats and electrostatic boundary conditions to define standards for the modeling community
- Benchmark the accuracy and performance of implicit solvent approaches against interaction kernel and fully explicit approaches and/or of coarse-grained models against explicit microscale models

Long Program Schedule

This workshop is part of the long program Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry

- Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry Opening Day : September 3, 2025
- Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry Tutorials : September 4-9, 2025
- Workshop I: Embracing Stochasticity in Electrochemical Modeling : September 15-19, 2025
- Workshop II: Bridging Scales from Atomistic to Continuum in Electrochemical Systems: October 6-10, 2025
- Workshop III: Boundary Conditions for Atomistic Simulations in Macroscopic Electrochemical Cells : October 27-31, 2025
- **Workshop IV: Electrochemistry Hackathon: Bridging the Gap Between Implicit and Explicit Methods: November 17-21, 2025**
- Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry Culminating Workshop at Lake Arrowhead : December 7-12, 2025

Participation

Additional information about this workshop including links to register and to apply for funding, can be found on the web page 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

Richard Hennig (University of Florida), Fei Lu (Johns Hopkins University), Jörg Neugebauer (Max-Planck-Institut für Eisenforschung), Keith Promislow (Michigan State University), Ravishankar Sundararaman (Rensselaer Polytechnic Institute), Ping Yang (Los Alamos National Laboratory)

Speakers

TBA

NSF UCLA

For more information, visit the program webpage:

www.ipam.ucla.edu/ECHWS4