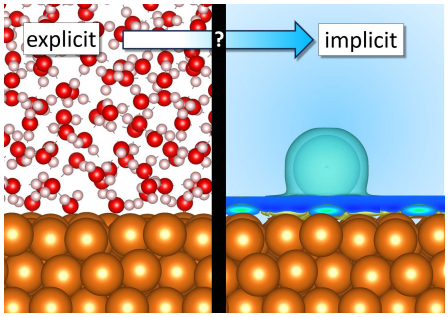
institute for pure & applied mathematics

Workshop II: Bridging Scales from Atomistic to Continuum in Electrochemical Systems

OCTOBER 6 - 10, 2025



Scientific Overview

Multi-scale approaches that link the atomistic scale to the electrode and then to the device scale are crucial for capturing the behavior of complex electrochemical systems. Coarse-graining and upscaling of models and simulations are essential in understanding and predicting observable behaviors of multiscale systems while accurately capturing phenomena at small temporal and spatial scales. There are many challenges inherent in multiscale computation. Coarse-grained models must inform the environmental conditions for atomistic simulations, while properties of the materials originating from atomic-scale interactions must be accurately accounted for in higher-length-scale models. Model validation requires predictions that can be compared to measurements.

One focus of the workshop is on the development of implicit solvation methods from interaction kernels trained upon stochastic differential equations modeling electrochemical systems. This effort seeks to incorporate temporal fluctuations crucial to electrochemical reactions into implicit solvent models. Other focuses include homogenization of electrode microstructures (including their stochasticity) to connect to the macroscale device behavior, as well as coarse-graining/up-scaling to connect atomistic properties to micro-scale/electrode-level phenomena. The ultimate goal is to obtain computationally tractable continuum-level models consistent with fundamental principles of thermodynamics. This includes derived effective boundary conditions that account for the atomic-scale phenomena such as interfacial segregation and structure. Mathematical challenges include efficient homogenization to continuum-level effective medium (e.g., implicit solvent models) and handling of stiff, nonlinear equations. Leading experts will share their insights into the theory, numerical techniques, and applications associated with interaction kernels, implicit models, and discuss their advantages and challenges.

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 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

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

David Bortz (University of Colorado Boulder)
Dimitrios Fraggedakis (Princeton University)
Juergen Fuhrmann (WIAS)
Richard Hennig (University of Florida)
Mauro Maggioni (Johns Hopkins University)
Katsuyo Thornton (University of Michigan)

Speakers

Ilenia Battiato (Stanford University)
Martin Bazant (MIT)
David Bortz (University of Colorado Boulder)
Dimitrios Fraggedakis (Princeton University)
Juergen Fuhrmann (WIAS)
Roman Grigoriev (Georgia Institute of Technology)
Richard Hennig (University of Florida)
Michael Herbst (EPFL)
Jun Huang (Forschungszentrum Jülich)
Rachel Kurchin (Carnegie Mellon University)
Manuel Landstorfer (WIAS)
Mauro Maggioni (Johns Hopkins University)
Daniel Messenger (Los Alamos National Laboratory)
Ahmad Omar (UC Berkeley)
Craig Plaisance (Louisiana State University)
Karsten Reuter (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Stefan Ringe (Korea University)
Kathleen Schwarz (National Institute of Standards and Technology)
Ravishankar Sundararaman (RPI)
Katsuyo Thornton (University of Michigan)
Salvatore Torquato (Princeton University)
Peter Voorhees (Northwestern University)
Yunan Yang (Cornell University)

NSF UCLA

For more information, visit the program webpage:
www.ipam.ucla.edu/ECHWS2