

Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces

Monday October 16, 2017

- 8:00–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:50–9:00 *Welcome and Opening Remarks*
- 9:00–9:40 **Arthur Voter** (Los Alamos National Laboratory)
Local Hyperdynamics
- 10:00–10:15 *Break*
- 10:15–10:55 **Thomas Swinburne** (Los Alamos National Laboratory)
Temperature accelerated rate matrix construction in the ParSplice framework
- 11:15–11:30 *Break*
- 11:30–12:10 **Tony Lelièvre** (Ecole des Ponts ParisTech)
Metastability: a journey from stochastic processes to semiclassical analysis
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Wei Cai** (Stanford University)
Atomistic Modeling of Thermally Activated Processes for Crystal Dislocations
- 3:30–3:45 *Break*
- 3:45–4:25 **Gideon Simpson** (Drexel University)
Mathematical Underpinnings of Diffusive Molecular Dynamics
- 4:45–5:15 *Lightning Poster Presentations*
- 5:15–6:45 *Poster Session & Reception (Hosted by IPAM)*

Tuesday October 17, 2017

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:40 **Zhiyao Duan** (University of Texas at Austin)
Long-Time Dynamics Simulations of Surface Segregation in Pd-Au Nanoparticles
- 10:00–10:15 *Break*
- 10:15–10:55 **Jutta Rogal** (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS))
Finding reaction coordinates during phase transformations in metals
- 11:15–11:30 *Break*

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- 11:30–12:10 **Benjamin Jourdain** (Ecole Nationale Des Ponts et Chaussees (LAMI))
Convergence and efficiency of adaptive importance sampling techniques with partial biasing (joint work with G. Fort, T. Lelièvre and G. Stoltz)
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Peter Bolhuis** (Universiteit van Amsterdam)
Twenty years of path sampling: origins and recent developments
- 3:30–4:00 *Break*
- 4:00–4:40 **Ron Elber** (University of Texas at Austin)
Milestoning

Wednesday October 18, 2017

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:40 **Werner Krauth** (École Normale Supérieure)
Fast stochastic sampling with irreversible, totally asymmetric, Markov chains
- 10:00–10:15 *Break*
- 10:15–10:55 **David Aristoff** (Colorado State University)
ANALYSIS AND OPTIMIZATION OF WEIGHTED ENSEMBLE SAMPLING
- 11:15–11:30 *Break*
- 11:30–12:10 **Kristen Fichthorn** (Pennsylvania State University)
Kinetics of Fivefold-Twinned Nanowire Growth in Colloidal Syntheses
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Charles Edouard Bréhier** (Université Claude-Bernard (Lyon I))
Mathematical analysis of an Adaptive Biasing Potential method for diffusions
- 3:30–4:00 *Break*
- 4:00–4:40 **Mira Todorova** (Max-Planck-Institut für Eisenforschung GmbH)
Free energy sampling for electrochemical systems

Thursday October 19, 2017

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:40 **Gerhard Hummer** (Max Planck Institute of Biophysics)
Extracting free energies and rates from simulation trajectories on biased potentials
- 10:00–10:15 *Break*

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- 10:15–10:55 **Eric Vanden-Eijnden** (Courant Institute of Mathematical Sciences)
Accelerated Sampling Methods and Path Finding Algorithms Based on Transition Path Theory
- 11:15–11:30 *Break*
- 11:30–12:10 **Brian Van Koten** (University of Chicago)
STABILITY AND CONVERGENCE OF THE STRING METHOD
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Jianfeng Lu** (Duke University)
Path integral molecular dynamics with surface hopping
- 3:30–4:00 *Break*
- 4:00–4:40 **Hélène Zapolsky** (Université de Rouen (Haute-Normandie))
Quasiparticle Atomistic Approach to model a Self-Assembly Kinetics of Complex Structures and Structural Defects.

Friday October 20, 2017

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:40 **Jonathan Weare** (University of Chicago)
Ensemble preconditioning for Markov chain Monte Carlo
- 10:00–10:15 *Break*
- 10:15–10:55 **Daniel Packwood** (Kyoto University)
Machine learning and dissimilarity analysis for surface-assisted molecular self-assembly
- 11:15–11:30 *Break*
- 11:30–12:10 **Livia Bartok-Partay** (University of Reading)
Nested sampling for computational thermodynamics
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:10 **Zhipan Liu** (Fudan University)
Stochastic Surface Walking Method for Reaction Sampling and the Combination with Machine Learning
- 3:30–4:00 *Break*
- 4:00–4:40 **Jörg Neugebauer** (Max-Planck-Institut für Eisenforschung GmbH)
Free energy sampling strategies for structurally complex materials

