Rare Events in High-Dimensional Systems

Monday February 23, 2009

8:00–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*

8:50–9:00 *Welcome and Opening Remarks*

9:00–9:50 **Christof Schuette** (Freie Universität Berlin)
Transition Network Approaches to Protein Folding

10:00–10:15 *Break*

10:15–11:05 **Cecilia Clementi** (Rice University)

11:15–11:30 *Break*

11:30–12:20 **John Chodera** (University of California, Berkeley (UC Berkeley))
Bridging timescales between atomistic simulation and experiments with master equation models of protein folding and dynamics

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Frank Noe** (Freie Universität Berlin)
Markov state models and folding pathways for macromolecules

3:30–4:00 *Break*

4:00–4:50 **Vijay Pande** (Stanford University)
Simulating long time scale phenomena with Markov State Models

5:00–7:00 *Poster Session & Reception (Hosted by IPAM)*

Tuesday February 24, 2009

8:00–9:00 *Continental Breakfast*

9:00–9:50 **David Chandler** (University of California, Berkeley (UC Berkeley))
Sampling large deviation functions and order-disorder in trajectory space

10:00–10:15 *Break*

10:15–11:05 **Bernhardt Trout** (Massachusetts Institute of Technology)
Investigating Complex Molecular Processes Via Likelihood Maximization and the Finite Temperature String Method

11:15–11:30 *Break*

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11:30–12:20 **Peter Bolhuis** (Universiteit van Amsterdam)
Efficient sampling of trajectories connecting arbitrary states

12:30–2:00 *Lunch (on your own)*

2:00–2:50 **Jorge Kurchan** (École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris (ESPCI))
Mapping out of equilibrium into equilibrium

3:00–3:15 *Break*

3:15–4:05 **Baron Peters** (University of California, Santa Barbara (UC Santa Barbara))
Accurate reaction coordinates and transition state ensembles from simulation: applications to nucleation

4:15–4:30 *Break*

4:30–5:20 **Ioannis Kevrekidis** (Princeton University)
Some computational examples of rare events in complex systems

Wednesday February 25, 2009

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Ron Elber** (University of Texas at Austin)
Computing rates on rough energy landscapes with Milestoning

10:00–10:15 *Break*

10:15–11:05 **Arthur Voter** (Los Alamos National Laboratory)
Recent advances and ongoing challenges in accelerated molecular dynamics methods

11:15–11:30 *Break*

11:30–12:20 **Kristen Fichthorn** (Pennsylvania State University)
Accelerated Molecular Dynamics with the Bond Boost Method

12:30–2:00 *Lunch (on your own)*

2:00–2:50 **Graeme Henkelman** (University of Texas at Austin)
Adaptive kinetic Monte Carlo for simulating dynamics in atomic systems

3:00–3:15 *Break*

3:15–4:05 **Normand Mousseau** (University of Montreal)
Kinetic activation-relaxation technique: An off-lattice self-learning kinetic Monte Carlo algorithm

4:15–4:30 *Break*

4:30–5:20 **Weiqing Ren** (New York University)
The string method for computing transition pathways in complex systems

Thursday February 26, 2009

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Benoit Roux** (University of Chicago)
Mapping large conformation transitions in biomolecular systems

10:00–10:15 *Break*

10:15–11:05 **Gérard Ben Arous** (New York University)
Universal phenomena for slow relaxation in random media

11:15–11:30 *Break*

11:30–12:20 **Mark Tuckerman** (New York University)
Enhanced conformational sampling and free energies via novel spatial-warping transformations and adiabatic dynamics.

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Giovanni Bussi** (Università di Modena)
Optimal Langevin modeling of out-of-equilibrium molecular dynamics simulations

3:30–4:00 *Break*

4:00–4:50 **Gerard Barkema** (Utrecht University)
Simulation and theory of nucleation

Friday February 27, 2009

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Eric Vanden-Eijnden** (New York University)
Transition Path Theory or how to explain the mechanism of reactive events in complex systems.

10:00–10:15 *Break*

10:15–11:05 **Maddalena Venturoli** (New York University)
Markovian milestoning with Voronoi tessellations

11:15–11:30 *Break*

11:30–12:20 **Giovanni Ciccotti** (Università di Roma “La Sapienza”)
Minimum Free Energy paths and the Kinetics of phase transitions in two dimensional Ising models

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Sara Bonella** (Università di Roma “La Sapienza”)
Free energy barriers for local hydrogen diffusion in sodium alanates

3:30–4:00 *Break*

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4:00–4:50 **Thomas Miller** (California Institute of Technology)
Understanding the dynamics of hydrophobic assembly