

Complex High-Dimensional Energy Landscapes Tutorials

Tuesday September 12, 2017

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00–10:00 **Christof Schuette** (Freie Universität Berlin)
Optimization problems associated with complex energy landscapes: Challenges and paradigms
- 10:15–10:30 *Break*
- 10:30–11:30 **Tony Lelièvre** (Ecole des Ponts ParisTech)
Sampling efficiently metastable dynamics: algorithms and mathematical analysis - Part 1
- 11:45–12:15 *Core Orientation with IPAM Staff*
- 12:15–2:00 *Lunch (on your own)*
- 2:00–3:00 **Graeme Henkelman** (University of Texas at Austin)
Physical Sampling I: Equilibrium
- 3:15–3:30 *Break*
- 3:30–4:30 **Houman Owhadi** (California Institute of Technology)
Principles and methods of Uncertainty Quantification, a mini-tutorial I

Wednesday September 13, 2017

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–10:00 **Tony Lelièvre** (Ecole des Ponts ParisTech)
Sampling efficiently metastable dynamics: algorithms and mathematical analysis - Part 2
- 10:15–10:30 *Break*
- 10:30–11:30 **Houman Owhadi** (California Institute of Technology)
Principles and methods of Uncertainty Quantification, a mini-tutorial II
- 11:45–2:00 *Lunch (on your own)*
- 2:00–3:00 **Kieron Burke** (University of California, Irvine (UCI))
Introduction to DFT calculations of electronic structure: Some do's and don'ts



Thursday September 14, 2017

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–10:00 **Graeme Henkelman** (University of Texas at Austin)
Physical Sampling II: Kinetics
- 10:15–10:30 *Break*
- 10:30–11:30 **Feliks Nüske** (Rice University)
Coarse-graining in conformational space
- 11:45–2:00 *Lunch (on your own)*
- 2:00–3:00 **Noa Marom** (Carnegie-Mellon University)
The complex high-dimensional energy landscapes of molecular crystals
- 3:15–3:30 *Break*
- 3:30–4:30 **Richard Hennig** (University of Florida)
Development and Optimization of Empirical Potentials as Surrogate Models for Energy Landscapes

Friday September 15, 2017

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–10:00 **Christof Schuette** (Freie Universität Berlin)
Optimal control problems associated with complex energy landscapes: Challenges and paradigms
- 10:15–10:30 *Break*
- 10:30–11:30 **Frank Noe** (Freie Universität Berlin)
Machine learning methods for physics and chemistry 1: Regression and Kernel methods
- 11:45–2:00 *Lunch (on your own)*
- 2:00–3:00 **Lorenzo Boninsegna** (Rice University)
Coarse-graining in physical space
- 3:15–3:30 *Break*
- 3:30–4:30 **Frank Noe** (Freie Universität Berlin)
Machine learning methods for physics and chemistry 2: Deep learning

