

## Workshop II: Collective Variables in Classical Mechanics

### Monday October 24, 2016

- 8:00–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:50–9:00 *Welcome and Opening Remarks*
- 9:00–9:50 **Michele Parrinello** (University of Lugano)  
*Fluctuations, collective variables, and rare events*
- 10:00–10:15 *Break*
- 10:15–11:05 **Maria Emelianenko** (George Mason University)  
*Coarse-graining approaches in materials systems undergoing coarsening*
- 11:15–11:30 *Break*
- 11:30–12:20 **Graeme Henkelman** (University of Texas at Austin)  
*Machine learning of chemical reactions*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Frank Noe** (Freie Universität Berlin)  
*Finding slow modes and accessing very long timescales in molecular dynamics*
- 3:30–4:00 *Break*
- 4:00–4:50 **Gabriel Stoltz** (École Nationale des Ponts-et-Chaussées (ENPC))  
*Parametrizing coarse-grained molecular systems from ab-initio computations: some elements*
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

### Tuesday October 25, 2016

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Susan Sinnott** (Pennsylvania State University)  
*Design and Discovery using Material Modeling Methods*
- 10:00–10:15 *Break*
- 10:15–11:05 **Peter Kroll** (University of Texas at Arlington)  
*Modeling and Simulation of Amorphous Ceramics: From Graphs and Networks to Predictive Simulations*
- 11:15–11:30 *Break*

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- 11:30–12:20 **Jörg Neugebauer** (Max-Planck-Institut für Eisenforschung GmbH)  
*Collective variable description of crystal anharmonicity*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Aleksandr Chernatynskiy** (Missouri University of Science and Technology)  
*Thermal conductivity as a function of chemical composition and structure of materials*
- 3:00–3:15 *Break*
- 3:15–4:05 **Simon Phillpot** (University of Florida)  
*Charge Optimized Many-Body (COMB) Potentials for Simulation of Complex Materials Structures: Applications and Rational Design*
- 4:15–4:30 *Break*
- 4:30–5:20 **Yara Yingling** (North Carolina State University)  
*Identifying relevant parameters for modeling stimuli-responsive biopolymeric morphologies*

### Wednesday October 26, 2016

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Christof Schütte** (Freie Universität Berlin)  
*Finding Reaction Coordinates in Molecular Dynamics*
- 10:00–10:15 *Break*
- 10:15–11:05 **Yannis Kevrekidis** (Princeton University)  
*Data and the computational modeling of complex/multiscale systems: The science of crystal balls*
- 11:15–11:30 *Break*
- 11:30–12:20 **Mark Tuckerman** (New York University)  
*Exploration and learning of free energy landscapes of molecular crystals and oligopeptides*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Eric Vanden-Eijnden** (Courant Institute of Mathematical Sciences)  
*Modeling reactive events in molecular systems*
- 3:00–3:15 *Break*
- 3:15–4:05 **Mauro Maggioni** (Duke University)  
*TBA*
- 4:15–4:30 *Break*
- 4:30–5:20 **Cecilia Clementi** (Rice University)  
*TBA*

## Thursday October 27, 2016

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Ben Leimkuhler** (University of Edinburgh)  
*Bayesian inference and model reduction with observation data*
- 10:00–10:15 *Break*
- 10:15–11:05 **Jonathan Weare** (University of Chicago)  
*Trajectory stratification for rare event simulation*
- 11:15–11:30 *Break*
- 11:30–12:20 **J. Nathan Kutz** (University of Washington)  
*Data-driven methods for discovery of observables and Koopman embeddings in dynamical systems*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Dimitrios Giannakis** (Courant Institute of Mathematical Sciences)  
*Extraction and Prediction Of Coherent Patterns in Incompressible Flows through Space-Time Koopman Analysis*
- 3:30–4:00 *Break*
- 4:00–4:50 **Gregory Beylkin** (University of Colorado Boulder)  
*On numerical calculus of probability density functions*

## Friday October 28, 2016

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Leslie Greengard** (New York University)  
*Fast, hierarchical algorithms in computational science*
- 10:00–10:15 *Break*
- 10:15–11:05 **Steve Stuart** (Clemson University)  
*Thermodynamically Motivated Approaches to Collective Variables*
- 11:15–11:30 *Break*
- 11:30–12:20 **Blas Uberuaga** (Los Alamos National Laboratory)  
*Applications of accelerated molecular dynamics in materials science: Insights into kinetic processes in complex materials*
- 12:30–2:00 *Lunch (on your own)*

