ESI Erwin Schrödinger International Institute for Mathematical Physics

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DVR 0065528

CECAM Workshop on

"From trajectories to reaction coordinates: making sense of molecular simulation data"

September 16 – 18, 2015

organized by

Peter G. Bolhuis (U Amsterdam), Christoph Dellago (U Vienna), Gerhard Hummer (MPI Biophysics, Frankfurt)

- **Wednesday, September 16, 2015**

  08:30 – 08:50 **Registration**

  08:50 – 09:00 **Welcome**

  09:00 – 09:25 **Ron Elber**
  Milestoning Networks in Search for Reaction Pathways

  09:30 – 09:55 **Michele Ceriotti**
  Automatically recognizing molecular patterns in atomistic simulations

  10:00 – 10:15 **Carla Molteni**
  Exploring the Effects of Mutations on the Neurotransmitter Binding Free Energy Landscape of Ligand-Gated Ion Channels

  10:20 – 10:35 **Srabani Taraphder**
  Determination of the Reaction Coordinate for a Key-Conformational Fluctuation in Human Carbonic Anhydrase II

  10:40 – 11:10 *Coffee break*

  11:10 – 11:35 **William A. Eaton**
  Protein Folding Transition Paths: Single Molecule Experiments, Theory and All-Atom MD Simulations

  11:40 – 12:05 **Michael Woodside**
  Direct observation of transition paths during the folding of proteins and nucleic acids

  12:10 – 12:35 **Robert Best**
  Reduction of all-atom folding dynamics to one-dimensional diffusion

  12:40 – 14:30 *Lunch break*

  14:30 – 14:55 **Swetlana Jungblut**
  Caveats of mean first-passage time methods applied to crystallization

  15:00 – 15:25 **Francesco Gervasio**
  Investigating Allosteric Regulation Through Enhanced Sampling Simulations.

  15:30 – 15:55 **Jordi Marti**
  Computer Simulation Study of DMPC-Cholesterol Biomembranes in Aqueous Solution: Diffusion, Spectroscopy and Free Energy Surfaces

16:00 – 16:30 *Coffee break*

16:30 – 16:55 **Aaron Dinner**
Understanding Error in Umbrella Sampling

17:00 – 17:25 **Chris Oostenbrink**
Protein-Ligand Binding from Distancefield Distances and Hamiltonian Replica Exchange Simulations

17:30 – 20:00 *Poster Session*

- **Thursday, September 17, 2015**

  09:00 – 09:25 **Carsten Hartmann**
  Cross entropy minimization for rare events based on optimal control of reaction coordinates

  09:30 – 09:55 **Frank Noe**
  pyEMMA: Estimation and analysis of Markov models from molecular dynamics and thermodynamic simulations

  10:00 – 10:15 **Jan-Hendrik Prinz**
  OpenPathSampling (OPS): An open Python framework for path sampling simulations

  10:20 – 10:35 **Omar Valsson**
  Variationally-Enhanced Sampling

  10:40 – 11:10 *Coffee break*

  11:10 – 11:35 **Richard Sear**
  Crystallisation via an intermediate that is neither liquid nor crystalline

  11:40 – 12:05 **Ivan Coluzza**
  Transferable Coarse-grained potential model for quantitative protein folding and design

  12:10 – 12:35 **Eduardo Sanz**
  A seeding approach to the crystal nucleation problem

  12:40 – 14:30 *Lunch break*

  14:30 – 14:55 **Titus van Erp**
  Analyzing complex reaction mechanisms using path sampling

  15:00 – 15:25 **Baron Peters**
  From path sampling to mechanistic hypothesis testing

  15:30 – 15:55 **Pietro Faccioli**
  Using the Renormalisation Group theory to rigorously construct Markov State Models of adjustable time-resolution from atomistic trajectories

  16:00 – 16:30 *Coffee break*

  16:30 – 16:55 **Modesto Orozco**
  Towards and integrative approach to the exploration of the conformational landscape

  17:00 – 17:25 **Christine Peter**
  Making Sense of a Mess: Conformational Equilibria of (Partially) Disordered Systems

  17:30 – 18:30 *Round table discussion*

- **Friday, September 18, 2015**

  09:00 – 09:25 **Yannis Kevrekidis**
  Some twists in the use of diffusion maps for data mining of atomistic simulations

  09:30 – 09:55 **Daniel Munoz-Santiburcio**
  Simulating Prebiotic Peptide Synthesis with ab initio Metadynamics

  10:00 – 10:15 **Marco Saitta**
  Miller Experiments in Atomistic Computer Simulations

  10:20 – 10:35 **Pratyush Tiwary**
  Towards predictive pharmacokinetics simulations with recent developments in enhanced sampling

  10:40 – 11:10 *Coffee break*

  11:10 – 11:35 **Cristian Micheletti**
  Self-assembling knots of controlled topology by designing the geometry of patchy templates

  11:40 – 12:05 **Sergei Krivov**
  Optimal Reaction Coordinates.

  12:10 – 12:35 **Giovanni Bussi**
  RNA dynamics in stop motion: from crystal structures to trajectories

  12:40 – 14:30 *Lunch break*

  14:30 – 14:55 **Christof Schütte**
  A complete theory of how to select the optimal reaction coordinates

  15:00 – 15:25 **John Chodera**
  TBA

  15:30 – 15:55 **Edina Rosta**
  Asymmetric activation of RAF Kinase Dimers

  16:00 – 16:30 *Coffee break*

  16:30 – 16:55 **Fabio Pietrucci**
  Exploiting Topological Coordinates to Explore Reactive Pathways in Gas Phase and Solution in a Unified Way

  17:00 – 17:25 **Bernd Ensing**
  Describing the Environment Reorganization that Governs Charge Transfer Reactions

All talks take place at the ESI, Boltzmann Lecture Hall!