ESI Erwin Schrödinger International Institute for Mathematics and Physics

universität wien

DVR 0065528

"E-CAM State-of-the Art Workshop: Large Scale Activated Event Simulations"

October 1 – 3, 2018

organized by

Peter Bolhuis (U of Amsterdam), Christoph Dellago (ESI, U Vienna), Gerhard Kahl (TU Vienna)

- **Monday, October 1, 2018**

  10:00 – 13:00 **Registration**

  Session 1

  13:00 – 13:15 **Welcome and Introduction**

  13:15 – 13:50 **Ben Leimkuhler**
  Advanced algorithms for sampling problems in chemistry and statistics

  13:50 – 14:25 **Bettina Keller**
  Girsanov reweighting for path ensembles and Markov state models

  14:25 – 15:00 **Michele Ceriotti**
  Atomic-structure representations between supervised and unsupervised learning

  15:00 – 15:30 *Coffee / Tea Break*

  15:30 – 16:05 **Mónica García Mota**
  SIMUNE and SIESTA-PRO: Professional atomistic simulation software ready for industry

  16:05 – 16:40 **Pratyush Tiwary**
  Three birds with one stone: reaction coordinate, free energies and kinetics in biomolecules with rare events

  16:40 – 17:40 **Discussion**

  17:45 – 19:30 **Poster Session**

- **Tuesday, October 2, 2018**

  Session 2

  09:00 – 09:35 **Gerhard Hummer**
  Can machine learning make rare events more frequent?

  09:35 – 10:10 **Andreas Singraber**
  High-dimensional neural network potentials in action: large-scale simulations of water and ice

  10:10 – 10:45 **Christine Peter**
  Dimensionality reduction aides scale-bridging in multi-resolution simulations of conformational landscapes

  10:45 – 11:15 *Coffee / Tea Break*

  11:15 – 11:50 **Tim Conrad**
  Modelling, Simulation and Data Analysis in an Industrial Context

  11:50 – 12:25 **John Chodera**
  Rare events and large-scale conformational changes in drug discovery

  12:25 – 14:15 *Lunch Break*

  Session 3

  14:15 – 14:50 **David Swenson**
  Path sampling of medically relevant biomolecular systems: New and old tricks using OpenPathSampling

  14:50 – 15:25 **Albert Pan**
  Atomic-level characterization of protein-protein association

  15:25 – 15:55 *Coffee / Tea Break*

  15:55 – 17:00 **Discussion**

  19:00 – 23:00 **Social Dinner**

- **Wednesday, October 3, 2018**

  Session 4

  09:00 – 09:35 **Baron Peters**
  Isolated catalyst sites on amorphous supports: a wild frontier for ab initio calculations

  09:35 – 10:10 **Jutta Rogal**
  Reaction coordinate analysis for nucleation in metals

  10:10 – 10:45 **Titus van Erp**
  Path sampling and machine learning to identify reaction triggers

  10:45 – 11:15 *Coffee / Tea Break*

  11:15 – 11:50 **Fabio Pietrucci**
  Wide-spectrum collective variables for condensed matter transformations and efficient enhanced sampling schemes

  11:50 – 12:25 **Peter Bolhuis**
  At the limits of path sampling: protein dissociation and gas hydrate nucleation

  12:25 – 14:30 *Lunch Break*

  14:30 – 15:30 **Discussion**

  15:30 – 15:40 **Closing Word**

All talks take place at ESI, Boltzmann Lecture Hall!