

**“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 **Sergio Decherchi**

Approximate methods for protein ligand unbinding kinetics estimation

15:25 – 15:55 *Coffee / Tea Break*

15:55 – 16:30 **Albert Pan**

Atomic-level characterization of protein-protein association

16:30 – 18:00 **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!