Erice School on Exploring and Quantifying Rough Free Energy Landscapes
Lecturers and Schedule - May 15-19, 2018

Lecturers and Affliations

Peter Bolhuis, University of Amsterdam
Giovanni Bussi, International School for Advanced Studies
Paolo Carloni, Juelich Research Center
Matteo Dal Peraro, Federal Institute of Technology, Lausanne
Christoph Dellago, University of Vienna
Bernd Ensing, University of Amsterdam
Angel Garcia, Los Alamos National Lab
Francesco Gervasio, University College London
Helmut Grubmueller, Max Planck Institute for Biophysical Chemistry
Gerhard Hummer, Max Planck Institute for Biophysical Chemistry
Michele Parrinello, ETH Zurich
Christine Peter, University of Konstanz
Edina Rosta, King's College London
John Straub, Boston University
Pratyush Tiwary, University of Maryland
Gareth Tribello, Queen's University Belfast
Omar Valsson, Max Planck Institute for Polymer Research
Gregory Voth, University of Chicago
Wei Yang, Florida State University

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Schedule

Arrival - Tuesday, May 15th

Day One - Wednesday, May 16th
Session Leader: Greg Voth

8:45am – 9:00am: Welcome, Greg Voth, Michele Parrinello

9:00am – 9:45am: Francesco Gervasio, "Investigating the binding mechanisms of allosteric ligands using enhanced sampling simulations"

9:45am – 10:30am: Gareth Tribello, "Variation on kernel density estimation"

10:30am – 11:00am: **Coffee Break**

11:00am – 11:45am: Edina Rosta, "Coarse-graining and molecular kinetics from biased simulations"

11:45am – 2:00pm: **Lunch**

Session Leader: Michele Parrinello

2:00pm – 2:45pm: Giovanni Bussi, "Combining molecular simulations and solution experiments to characterize RNA structural dynamics"

2:45pm – 3:30pm: Matteo Dal Peraro, "Integrative modeling at the protein-membrane interface"

3:30pm – 4:00pm: **Coffee Break**

4:00pm – 4:45pm: John Straub, "Role of membrane domains and interfaces in protein structure, assembly and function"

4:45pm – 5:30pm: General Discussion

7:30pm: **Group Social Dinner**

Day Two - Thursday, May 17th
Session Leader: Gerhard Hummer

9:00am – 9:45am: Greg Voth, "Ultra-coarse-graining and its applications"

9:45am – 10:30am: Christine Peter, "Consistent sampling of conformational free energy landscapes in models on different levels of resolution"

10:30am – 11:00am: **Coffee Break**

11:00am – 11:45am: Helmut Grubmueller, "Hierarchical energy landscapes: From specific to general"

11:45am – 1:00pm: **Lunch**

1:00pm: **Excursion**

Day Three – Friday, May 18th
Session Leader: Peter Bolhuis

9:00am – 9:45am: Michele Parrinello, "Path collective variables without paths"

9:45am – 10:30am: Gerhard Hummer, "Dynamic histogram analysis to determine free energies and rates from biased simulations"

10:30am – 11:00am: **Coffee Break**

11:00am – 11:45am: Christoph Dellago, "Machine learning in atomistic simulations: from reaction pathways to phase diagrams"

11:45am – 2:00pm: **Lunch**

Session Leader: Christoph Dellago

2:00pm – 2:45pm: Peter Bolhuis, "Free energy, kinetics and mechanisms of complex molecular processes from trajectory sampling"

2:45pm – 3:30pm: Bernd Ensing, "Advances in enhanced sampling along adaptive paths of collective variables"

3:30pm – 4:00pm: **Coffee Break**

4:00pm – 4:45pm: Angel Garcia, "Exploring the topography of Ras proteins and the dynamic accessibility of their effector-binding surfaces"

4:45pm – 5:30pm: General Discussion

Day Four – Saturday, May 19th
Session Leader: John Straub

9:00am – 9:45am: Paolo Carloni, "Conformational ensembles of proteins in mass spectrometry"

9:45am – 10:30am: Pratyush Tiwary, "Two birds with one shot: reaction coordinate and free energies from all-atom simulations aided by statistical mechanics and deep learning"

10:30am – 11:00am: **Coffee Break**

11:00am – 11:45am: Wei Yang, "Free energy sampling of protein hierarchical energy landscapes"

11:45pm – 12:30pm: Omar Valsson, "Bridging time scales with variationally enhanced sampling"

12:30pm – 2:00pm: **Lunch**

2:00pm – **Free Afternoon**

Departure - Sunday, May 20th