

## ESI/CECAM Workshop on

## “Challenges across Large-Scale Biomolecular and Polymer Simulations”

February 21 – 24, 2017

organized by

**Ivan Coluzza (U Vienna), Barbara Capone (U Vienna), Christoph Dellago (ESI, U Vienna),  
Samuela Pasquali (IBPC & U Paris), Tamar Schlick (New York U)**

• **Tuesday, February 21, 2017****Session 1**11:30 – 12:30 *Registration*12:30 – 14:30 *Lunch Break*14:30 – 15:00 **Gerhard Hummer***Modeling Membrane Sensing and Remodeling Dynamics*15:00 – 15:30 **Ivan Coluzza***Artificial Chaperonins*15:30 – 16:00 **Angel Garcia***Free-energy landscape of a hyperstable RNA tetraloop*16:00 – 16:30 *Coffee Break*16:30 – 17:00 **Samuela Pasquali***Predicting and Exploring Complex Nucleic Acids Architectures through a Coarse-Grained Model*17:00 – 17:30 **Angelo Rosa***Chromosome organization and the Physics of crumpled polymers*17:30 – 18:00 **Jonathan Doye***Large-scale DNA simulations with oxDNA*• **Wednesday, February 22, 2017****Session 2**09:00 – 09:30 **Doros Theodorou***Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites*09:30 – 10:00 **Barbara Capone***TBA*10:00 – 10:30 **Pietro Faccioli***Self-Consistent Atomistic Calculation of Protein Folding Pathways*10:30 – 11:00 *Coffee Break*

11:00 – 11:30 **Raffaello Potestio**

*Multi-resolution modelling for biomolecular simulations*

11:30 – 12:00 **Cristian Micheletti**

*Pore translocation of knotted polymer chains: how friction depends on knot complexity*

12:00 – 12:30 **Karissa Sanbonmatsu**

*Simulating movement of the 30S head during translocation*

12:30 – 14:30 *Lunch Break*

### **Session 3**

14:30 – 15:00 **Peter Bolhuis**

*Multiscale Simulations of Patchy Particle Systems Combining Molecular Dynamics, Path Sampling and Greens Function Reaction Dynamics*

15:00 – 15:30 **Albert Pan**

*Characterizing amyloid beta monomers and oligomers with long-timescale molecular dynamics simulations*

15:30 – 16:00 **Dave Thirumalai**

*Understanding RNA folding*

16:00 – 16:30 *Coffee Break*

16:30 – 17:00 **Bert de Groot**

*Challenges and opportunities in large scale alchemical free energy simulations.*

17:00 – 17:30 **Wonpil Im**

*CHARMM-GUI Toward Large-Scale Biomolecular and Polymer Simulations*

17:30 – 18:00 **Marc Baaden**

*Large-scale Data Exploration and Analysis across Biomolecular Simulations*

19:30 *Social Dinner*

### • **Thursday, February 23, 2017**

#### **Session 4**

09:00 – 09:30 **Amos Maritan**

*TBA*

09:30 – 10:00 **Peter Freddolino**

*Modeling Protein-Nucleic Acid Interactions from Atomistic to Cellular Scales*

10:00 – 10:30 **Modesto Orozco**

*Advances and challenges in the simulation of DNA*

10:30 – 11:00 *Coffee Break*

11:00 – 11:30 **Michele Vendruscolo**

*Structural basis for the different aggregation propensities of Abeta40 and Abeta42*

11:30 – 12:00 **Chris Oostenbrink**

*Reversible guest-host interactions from extensive simulations*

12:00 – 12:30 **Ron Elber**

*Electric Fields Across Heterogeneous Membranes*

12:30 – 14:30 *Lunch Break*

### Session 3

14:30 – 15:00 **Tamar Schlick**

*In Memoriam: Klaus Schulten*

15:00 – 15:15 **Ewa Anna Oprzeska-Zingrebe**

*Interactions Between a Short DNA Oligonucleotide and Urea in the Light of Kirkwood-Buff Theory: a Molecular Dynamics Simulation Study*

15:15 – 15:30 **Martin Goethe**

*Prediction of Protein Configurational Entropy (Popcoen)*

15:30 – 16:00 **Lennart Nilsson**

*Codon Recognition on the Ribosome - Free Energy and QM/M Calculations*

16:00 – 16:30 *Coffee Break*

16:30 – 17:00 **Helmut Grubmüller**

*Atomistic Simulation of Single Molecule Experiments: Molecular Machines and a Dynasome Perspective*

17:00 – 17:30 **Jeremy C. Smith**

*Proteins: Forever Aging*

17:30 – 18:00 **Stefan Boresch**

*Playing the Devil's Advocate: Some Challenges with Respect to Large-scale Biomolecular Simulations*

### ● Friday, February 24, 2017

#### Session 6

09:00 – 09:30 **Simone Melchionna**

*Macromolecules and hydrodynamics: a simulation approach*

09:30 – 10:00 **Yasmine Chebaro**

*Role of intrinsically disordered regions in the nuclear receptors architecture*

10:00 – 10:30 **Sarah Harris**

*Multiscale Modelling of Biomolecules: From atomistic Molecular Dynamics to the continuum limit with Fluctuating Finite Element Analysis*

10:30 – 11:00 *Coffee Break*

11:00 – 11:30 **Amir Lohrasebi**

*The influence of a 2450 MHz electric field on the microtubule mechanical properties: a multi scale modeling approach*

11:30 – 12:00 **Gianluca Lattanzi**

*Challenges in computational biophysics: from membrane proteins to biosensors*

12:00 – 12:30 **Othmar Steinhauser**

*Protein in Reverse Micelles - The Dielectric Approach*

12:30 – 13:00 **Closing Word**

**The workshop will take place in the Joseph Loschmidt Hörsaal at the Faculty of Chemistry, University of Vienna, Währinger Str. 42, 1090 Vienna!**