Pushing the frontiers of molecular dynamics simulations

October 7, 2024 - October 9, 2024
CECAM-HQ-EPFL, Lausanne, Switzerland & online
Registration deadline: August 30, 2024

Monday 7th October 2024 - Day 1

09:30 to 10:30	**Registration & coffee**
10:30 to 11:00	**Inaugural**: Prof. Modesto Orozco; Prof. Andrea Cavalli
Session I	
11:00 to 11:45	**Lecture 1** – Gerhard Hummer - Molecular simulations as windows into cellular dynamics
11:45 to 12:30	**Lecture 2** – Karissa Sanbonmatsu - Large-scale simulations of nucleic acid-based systems
12:30 to 13:30	**Lunch**
13:30 to 14:15	**Lecture 3** – Alberto Pérez - Synergizing simulations and experiments: Faser exploration of biologically relevant states
14:15 to 15:00	**Lecture 4** – Vittorio Limongelli - Learning the functional mechanism of G protein-coupled receptors from free-energy calculations
15:00 to 15:30	**Coffee Break**
15:30 to 16:15	**Lecture 5** – Gregory Voth - Going big: Combining ultra-coarse-graining with high performance computing to access very large length and timescales
16:15 to 17:00	**Lecture 6** – Adrian Mulholland - Dynamical non-equilibrium molecular dynamics to analyse and engineer enzyme activity and inhibition
17:00 to 17:30	**Short Lecture** – Josep Lluís Gelpí - MDDB. Molecular Dynamics Data Bank. The Repository for Biosimulation Data
17:30 to 19:00	**Poster session & aperitif**

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Tuesday 8th October 2024 - Day 2

Session II	
09:00 to 09:45	**Lecture 7** – Tamar Schlick - Heterogeneous complex pathways in RNA frameshifting conformational transitions
09:45 to 10:30	**Lecture 8** – Helmut Grubmueller - Flying, freezing and wet proteins
10:30 to 11:00	**Coffee Break**
11:00 to 11:45	**Lecture 9** – Aleksei Aksimentiev - Resolving the structure of viral genomes through multi-resolution simulations
11:45 to 12:30	**Lecture 10** – Gregory Bowman - Adaptive sampling and distributed computing
12:30 to 13:30	**Lunch**
Session III	
13:30 to 14:15	**Lecture 11** – Stefano Piana-Agostinetti - Ribosome simulations on the millisecond timescale
14:15 to 15:00	**Lecture 12** – Bert de Groot - Molecular dynamics of binding, gating and permeation
15:00 to 15:30	**Coffee Break**
15:30 to 16:15	**Lecture 13** – Matteo Dal Peraro - Integrating simulations and experiments to understand aerolysin pore-forming toxins
16:15 to 17:00	**Lecture 14** – Paolo Carloni - Massively parallel QM/MM MD simulations in the exascale era
17:00 to 17:30	**Short Lecture** – Anna Lappala - The X factor: Unveiling the secrets of the X-chromosome with data-driven 3D modelling
19:00 to 23:00	**Workshop Dinner**

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Wednesday 9th October 2024 - Day 3

Session IV	
09:00 to 09:45	**Lecture 15** – Andrea Cavalli - Molecular dynamics and related methods in drug discovery
09:45 to 10:30	**Lecture 16** – Jan Stevens - The minimal cell under a computational microscope
10:30 to 11:00	**Coffee Break**
11:00 to 11:45	**Lecture 17** – Giovanni Bussi - Towards precise and accurate simulations of RNA dynamics
11:45 to 12:15	**Short Lecture** – Laura Orellana - Conformational transitions of extremely large systems through coarse-grained simulations
12:15 to 12:30	**Closing Remarks:** Erik Lindahl

** All meals in the programme are provided by MDDB.*

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