

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

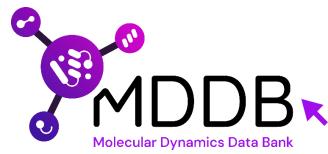


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Tuesday 8th October 2024 - Day 2

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





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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