When data science meets molecular dynamics

October 15, 2025 - October 17, 2025
Location: CECAM-HQ-EPFL, Lausanne, Switzerland

Wednesday 15th October 2025

10:00 to 10:30	**Registration & coffee**
10:30 to 11:00	**Inaugural**: Modesto Orozco; Andrea Cavalli
Session I	
11:00 to 11:45	**Lecture 1** – Siewert-Jan Marrink: Computational microscopy at the whole-cell level
11:45 to 12:30	**Lecture 2** – Phil Biggin: From sequence to mechanism: insights into proton coupling in cystinosin from multiscale molecular simulations
12:30 to 13:30	**Lunch**
13:30 to 14:15	**Lecture 3** – Zoe Cournia: Using MD simulations to understand self-assembly in biomolecular processes
14:15 to 15:00	**Lecture 4** – Paolo Carloni: Novel machine learning and simulation approaches for drug design
15:00 to 15:30	**Coffee break / Poster session**
15:30 to 16:00	**Contributing talk 1** – Aysenur Iscen: Investigation of structure-property relationships in amyloid-like supramolecular peptide nanofibrils
16:00 to 16:30	**Contributing talk 2** – Nils Strand: Adaptive tensor train metadynamics for high-dimensional free energy exploration
16:30 to 17:00	**Contributing talk 3** – Shivnandi: Crowding effects on structural preferences of amyloid oligomers
17:00 to 17:30	**Short Lecture 1** – Adam Hospital: Molecular Dynamics Data Bank. Current status of the European Repository for Biosimulation Data.
17:30 to 19:00	**Poster session & aperitif**

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Session II	
09:00 to 09:45	**Lecture 5** – Adrian Mulholland: Dynamics, electric fields and enzyme design: insights from natural and directed evolution
09:45 to 10:30	**Lecture 6** – Yuji Sugita: Integrated enhanced conformational sampling methods for biomolecular dynamics and functions
10:30 to 11:00	**Coffee break / Poster session**
11:00 to 11:45	**Lecture 7** – Marco de Vivo: Decoding biochemical complexity with simulations and AI-enhanced sampling
11:45 to 12:30	**Lecture 8** – Alberto Pérez: Predicting Rare B→A-DNA Transitions with Dynamical Graphical Models
12:30 to 13:30	**Lunch**
Session III	
13:30 to 14:15	**Lecture 9** – Samia Aci-Sèche: Predict protein-ligand binding affinity with deep-learning models based on molecular dynamics simulations
14:15 to 15:00	**Contributing talk 4** – Yasaman Karami: Toward developing dynamics-aware methods for macromolecular complexes
15:00 to 15:30	**Coffee break / Poster session**
15:30 to 16:15	**Lecture 10** – Tatiana Galochkina: Large-scale analysis and prediction of protein flexibility using molecular dynamics data
16:15 to 17:00	**Lecture 11** – Matthieu Chavent: ilLUMENating the dark matter of the MDverse
17:00 to 17:30	**Short Lecture 2** – Federica Battistini: The hexABC project, a DNA conformational study at the hexamer level
19:00 to 23:00	**Workshop Dinner**

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Session IV	
09:00 to 09:45	**Lecture 12** – Helmut Grubmueller: Disordered Proteins in Water, Air, and X-rays
09:45 to 10:30	**Lecture 13** – Thomas Cheatham: Why should we share our MD data and analysis codes? To assess reproducibility, convergence and to aid the community.
10:30 to 11:00	**Coffee break / Poster session**
11:00 to 11:45	**Lecture 14** – Anna Panchenko: Histone Alterations Influence Chromatin Structure and Dynamics at Different Scales
11:45 to 12:30	**Lecture 15** – Gregory Bowman: Cracking undruggable proteins with cryptic pockets
12:30 to 13:00	**Closing Remarks: Erik Lindahl**

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