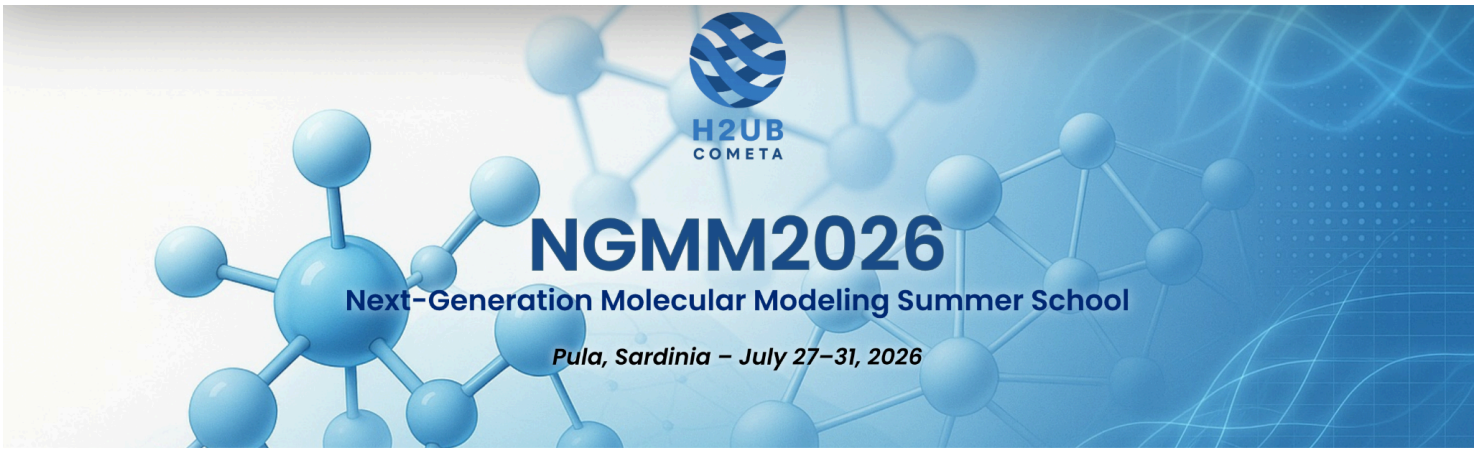

Preliminary Schedule

Monday

Time	Activity
09:00–10:00	Registration + Poster Hanging
10:00–10:30	Opening Session & Welcome Talks
10:30–11:30	Lecture: Introduction to modeling 1 - Dario Estrin
11:30–12:00	Coffee Break
12:00–13:15	Lecture: Introduction to modeling 2 - Bridging time, length, and beyond: inverse & integrative multiscale modelling - Aatto Laaksonen
13:15–14:30	Lunch Break
14:30–16:15	Tutorial 1: Basic introduction to linux - CRS4 and UNICA
16:15–16:45	Coffee Break
16:45–18:15	Tutorial 2: Classical molecular dynamics modeling - Santiago Di Lella

Tuesday

Time	Activity
09:15–10:15	Lecture: Advanced modeling: enhanced sampling, force field parametrization, QM/MM- Dario Estrin
10:15–10:45	Coffee Break
10:45–11:45	Lecture: From pre-AI to AI-assisted nucleic-acid force fields: validation that matters - Petra Kührová
11:45–12:45	Lecture: Free energy methods with PLUMED - Gareth Tribello
12:45–14:15	Lunch Break
14:15–16:00	Tutorial 3: Enhanced sampling with Plumed - Gareth Tribello
16:00–16:30	Coffee Break
16:30–18:15	Tutorial 4: Simulating G-Quadruplexes: best practices with enhanced sampling - Petra Kührová

Wednesday

Time	Activity
09:15–10:15	Lecture: Bottom-up meets top-down: Inverse methods to bridge scales - Aatto Laaksonen
10:15–10:45	Coffee Break
10:45–11:45	Lecture: Coarse-grained simulations of biomolecular condensate formation via liquid–liquid phase separation - Lu Zhong Yuan
11:45–12:45	Lecture: Modern enhanced sampling in the face of suboptimal collective variables, from OPES to OneOPES - Valerio Rizzi
12:45–14:15	Lunch Break
14:15–15:15	Lecture: GPU computing - Markus Oppel
15:15–16:30	Poster Session & Coffee Break
16:30–18:15	Tutorial 5: Practical application of OPES and OneOPES from fundamental systems to real-world biophysical problems, as protein-ligand binding and protein folding - Valerio Rizzi

Thursday

Time	Activity
09:15–10:15	Lecture: Combined use of DFT and machine learning MD for the study of heat and charge transport in functional materials, the case of Cu_3BHT, a 2D metal–organic framework with tunable thermal and electronic properties - Claudio Melis
10:15–10:45	Coffee Break
10:45–11:45	Lecture: Glycobiology and post-translational modifications of biomolecules: impact on their dynamics and function - Santiago Di Lella
11:45–12:45	Lecture: Molecular dynamics in the electronic excited states: from gas phase to condense phase - Leticia González (part 1)
12:45–14:15	Lunch Break
14:15–16:00	Tutorial 6: Integration of semiclassical, quantum and non-equilibrium MD simulations to characterize thermal transport properties, the role of defects, and electronic properties - Claudio Melis and Riccardo Dettori
16:00–16:30	Coffee Break
16:30–18:15	Tutorial 7: QM-MM - Dario Estrin, Santiago Di Lella

Friday

Time	Activity
09:15–10:15	Lecture: Molecular dynamics in the electronic excited states: from gas phase to condense phase - Leticia González (part 2)
10:15–10:45	Coffee Break
10:45–11:45	Lecture: Electronic and optical properties of clusters adsorbed on solid surfaces: organic and biological molecules on Si(001) - Giancarlo Cappellini
11:45–12:45	Lecture: Application of hybrid methods in drug discovery. A case study: the development of CFTR modulators - Paola Fossa
12:45–14:15	Lunch Break
14:15–15:15	Lecture: Multiscale simulation of polymer-grafted nanoparticles - Lu Zhong Yuan
15:15–16:15	Lecture: Chemical disorder and structural modeling of melanin: a computational perspective - Roberto Cardia
16:15–17:30	Coffee Break & Poster Session & Awards
17:30–18:15	Round Table: Shaping tomorrow: trends, challenges, and inspirations in multiscale molecular modeling - Open discussion with Dario Estrin, Aatto Laaksonen, Lu Zhong Yuan, Leticia Gonzalez