



H2UB
COMETA

NGMM2026

Next-Generation Molecular Modeling Summer School

Pula, Sardinia – July 27–31, 2026

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
11:45–13:00	Lecture: Introduction to modeling 2 – Aatto Laaksonen
13:00–14:30	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	09:15–10:15 Lecture: Advanced modeling – Dario Estrin
10:15–10:45	Coffee Break
10:45–11:45	10:45–11:45 Lecture: AI-assisted nucleic-acid force fields – Petra Kührová
11:45–12:45	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 – Petra Kührová

Wednesday

Time	Activity
09:15–10:15	Lecture: Inverse methods to bridge scales – Aatto Laaksonen
10:15–10:45	Coffee Break
10:45–11:45	Lecture: Coarse-grained simulations – Lu Zhong Yuan
11:45–12:45	Lecture: Modern enhanced sampling – Valerio Rizzi
12:45–13:45	Lunch Break
13:45–14:45	Lecture: GPU computing – Markus Opper
15:15–16:00	Poster Session & Coffee Break
16:00–17:45	Tutorial 5: OPES and OneOPES – Valerio Rizzi
18.30	Social trip to archaeological site Nora
20:30	Social dinner

Thursday

Time	Activity
09:15-10:15	Lecture: DFT and machine learning MD – Claudio Melis
10:15-10:45	Coffee Break
10:45-11:45	Lecture: Glycobiology – Santiago Di Lella
11:45-12:45	Lecture: MD in electronic excited states (Part 1) – Leticia González
12:45-14:15	Lunch Break
14:15-16:00	Tutorial 6: Quantum & non-equilibrium MD – Melis & Dettori
16:00-16:30	Coffee Break
16:30-18:15	Tutorial 7: QM/MM – Estrin & Di Lella

Friday

Time	Activity
09:15-10:15	Lecture: MD in electronic excited states (Part 2) – Leticia González
10:15-10:45	Coffee Break
10:45-11:45	Lecture: Electronic & optical properties – Giancarlo Cappellini
11:45-12:45	Lecture: Hybrid methods in drug discovery – Paola Fossa
12:45-14:15	Lunch Break
14:15-15:15	Lecture: Polymer-grafted nanoparticles – Lu Zhong Yuan
15:15-16:15	Lecture: Structural modeling of melanin – Roberto Cardia
16:15-17:30	Coffee Break & Poster Session & Awards
17:30-18:15	Round Table Discussion