

NGMM2026

SUMMER SCHOOL JULY 27 - 31

PROGRAM

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 - <i>D.Estrin</i>
11:45 - 13:00	Lecture: Introduction to modeling 2 - <i>A. Laaksonen</i>
13:00 - 14:30	Lunch Break
14:30 - 16:15	Tutorial 1: Basic introduction to linux - <i>CRS4 and UNICA</i>
16:15 - 16:45	Coffee Break
16:45 - 18:15	Tutorial 2: Classical molecular dynamics modeling - <i>S. Di Lella</i>

WEDNESDAY

Time	Activity
09:15 - 10:15	Lecture: Inverse methods to bridge scales - <i>A. Laaksonen</i>
10:15 - 10:45	Coffee Break
10:45 - 11:45	Lecture: Coarse-grained simulations - <i>Lu Zhong Yuan</i>
11:45 - 12:45	Lecture: Modern enhanced sampling - <i>V. Rizzi</i>
12:45 - 13:45	Lunch Break
13:45 - 14:45	Lecture: GPU computing - <i>M. Oppel</i>
15:00 - 15:45	Poster Session & Coffee Break
15:45 - 17:30	Tutorial 5: OPES and OneOPES - <i>V. Rizzi</i>
18.30	Social trip to archaeological site Nora
20:30	Social dinner

FRIDAY

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

TUESDAY

Time	Activity
09:15 - 10:15	Lecture: Advanced modeling - <i>D. Estrin</i>
10:15 - 10:45	Coffee Break
10:45 - 11:45	Lecture: AI-assisted nucleic-acid force fields - <i>P. Kührová</i>
11:45 - 12:45	Lecture: Free energy methods with PLUMED - <i>G. Tribello</i>
12:45 - 14:15	Lunch Break
14:15 - 16:00	Tutorial 3: Enhanced sampling with PLUMED - <i>G. Tribello</i>
16:00 - 16:30	Coffee Break
16:30 - 18:15	Tutorial 4: Simulating G - Quadruplexes - <i>P. Kührová</i>

THURSDAY

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

Organized by



UNIVERSITÀ DEGLI STUDI
DI CAGLIARI

Funded by



The school is funded by "Progetto T4-AN-10 Hybrid Hub (H2UB), Finanziamento a valere sul PSC Salute, – FSC 2014-2020 – Traiettorie 4 – Biotecnologie, bioinformatica e sviluppo farmaceutico, Ministero della Salute".

Sponsored by



TENUTE FARAGÒ