High Performance Molecular Modelling

8-10th May 2024, Rome

Teachers: Andrew Emerson, Neva Besker, Alessandro Grottesi, Giorgia Frumenzio, Balasubramanian Chandramouli,

Agenda

Day 1

10.00 – 10.30	Registration
10.30 – 11.15	Introduction to HPC architectures and parallelism (A. Emerson)
11.15 – 11.30	Coffee break
11.30 – 12.30	Introduction to Classic Molecular Dynamics (N. Besker)
12.30 – 14.00	Lunch break
14.00 – 15.00	Parallel Molecular Dynamics (G. Frumenzio)
15.00 – 15.30	Coffee break
15.30 – 17.30	Hands-On: Introduction to CINECA HPC (A. Grottesi and N. Besker)

Day 2

9.30 – 10.15	MD on GPU Architectures (A. Grottesi)
10.15 – 11.00	Hands-on: MD practice with scripts and benchmarks (A. Grottesi & N. Besker)
11.00 – 11.30	Coffee break
11.30 – 12.30	Hands-on: Single node, Multi-replica simulations
12.30 – 14.00	Lunch break
14.00 – 15.30	Hands-on: .
15.30 – 16.00	Coffee break
16.00 – 17.30	Hands-on: job optimization for a long trajectory on Leonardo. using ligand-protein complexes from LIGATE.

Commentato [AG1]: togliere M100

Commentato [AG2]: Che sistemi e che hands-on? Decidere insieme

Day 3

9.30 – 11.00	Analysis of MD trajectories (G. Frumenzio and B. Chandramouli).
11.00 – 11.30	Coffee break
11.30 – 13.00	Hands-on. Analysis of MD simulations with Python Notebooks on Galileo100(B. Chandramouli)
13.00 – 14.30	Lunch Break
14.30 – 15.15	Invited speaker: Atomistic MD simulations for macromolecules in solution (Dssa. Sara del Galdo, Uni. Roma 3)
15.15 - 16.00	How to apply for HPC resources (N. Besker)

15.00 – 17.00	FREE