High Performance Molecular Dynamics

7th -9th April 2020

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

Agenda

Day 1

9.30 – 11.00	Introduction to HPC architectures and parallelism (A. Emerson)
11.00 – 11.30	Coffee break
11.30 – 12.30	Introduction to Classic Molecular Dynamics (A. Grottesi)
12.30 – 14.00	Lunch break
14.30 - 15.00	Tutorial 1:MD on M100 (A. Grottesi)
15.00 – 15.30	Coffee break
15.30 – 17.30	Practical Session

Day 2

9.30 – 10.15	MD on GPU Architectures (A. Grottesi)
10.15 – 11.00	Tutorial 2: MD @ CINECA, scripts and benchmarks (A. Grottesi & N. Besker)
11.00 – 11.30	Coffee break
11.30 – 12.30	**Invited talk (TBA)**
12.30 – 14.00	Lunch break
14.00 – 15.30	Tutorial 3: Job optimisation (A. Grottesi)
15.30 – 16.00	Coffee break
16.00 – 17.30	Practical Session

Day 3

9.30 – 11.00	Cluster Analysis with GROMACS (A. Emerson & G. Frumenzio).
11.00 – 11.30	Coffee break
11.30 – 13.00	Tutorial 4. Cluster Analysis of a simulation.
13.00 – 14.00	Lunch Break
14.00 – 14.30	Virtual Screening and MD Simulation in the Exscalate4Cov project (A. Emerson).
14.30 - 14.45	How to apply for HPC resources (A. Emerson)
14.30 – 17.30	Practical Session