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
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