

High Performance Molecular Dynamics

18 - 19 - 20 November 2015
Cineca - Casalecchio di Reno (BO)

Trainers: A. Emerson, G. Chillemi, N. Besker, A. Grottesi.
Invited Speaker: Massimiliano Bonomi, Univ. Cambridge.
Trainer for Tutorial: Alejandro Gil Ley.

AGENDA

18th November 2015

09.30 - 10.15 *Registration*
10.15 - 11.00 *Introduction to HPC Architectures (A. Emerson)*
11.00 - 11.30 *Break*
11.30 - 12.30 *Introduction to Classical Molecular Dynamics (G. Chillemi)*
12.30 - 14.00 *Lunch*
14.00 - 15.00 *Parallel Molecular Dynamics - Parallelism and Parallel Algorithms (A. Emerson)*
15.00 - 17.30 *Tutorial T1: Introduction to Unix: modules, job scripts, PBS (A. Grottesi)*

19th November 2015

09.30 - 10.15 *Running MD on HPC Clusters and Hybrid Clusters.(A. Grottesi)*
10.15 - 11.00 *Tutorial T2: MD @CINECA: scripts and benchmarks.*
11.00 - 11.30 *Break*
11.30 - 12.30 *Tutorial T3: Scalability tests for biological systems. (N. Besker, A. Grottesi)*
12.30 - 14:00 *Lunch*
14:00 - 15:30 *Tutorial T4: Analysis of MD trajectories: Essential Dynamics (N. Besker)*
15:30 - 16:00 *Break*
16.00 - 17.30 *Tutorial T4: Continued (N. Besker)*

20th November 2015

09.30 - 12.30 *PLUMED Session: Talk and Tutorial*
 9.30 -10.15 *“Metainference Metadynamics with PLUMED”, (Massimiliano Bonomi, Univ. Cambridge)*
 10.45-12.30 *Hands-on tutorial (Trainer, Alejandro Gil Ley).*
12.30 - 14.00 *Lunch*
14.00 - 15.00 *How to obtain HPC resources (A. Emerson)*
15.00 - 17.30 *Practical session or FREE.*