HPC Molecular Dynamics Course

17-19 November 2014

PRACE link

http://events.prace-ri.eu/conferenceDisplay.py?confId=313

https://hpc-forge.cineca.it/files/CoursesDev/public/2014/Molecular_dynamics_in_an_HPC_environment/Bologna/

Programme

	Day-1	*Day -2*	*Day -3*
9.30 - 10.15	*Registration. L1 HPC architectures I (* **A.Emerson***)*	*L4.Running MD on HPC architectures I. Clusters and Hybrid clusters. (***A. Grottesi***)*	*L5 Running MD on HPC architectures II. Bluegene/Q. (***G. Chillemi)**
10.15 - 11.00	*L1. Introduction to HPC architectures II (***A. Emerson***)*	*Invited lesson 1. (***R. Gnudi, Uni. Modena***) Porting of an MD code on Xeon PHI.*	*Tutorial T3. Analysis of MD trajectories: Essential Dynamics (***A. Grottesi***)*
11.00 - 11.30	*Break*	*Break*	*Break*
11.30- 12.30	*L2.Introduction to Classical Molecular Dynamics (***G. Chillemi***)*	*Invited Lesson 2. (***I. Eberini, Uni. Milano***) Simulation of urea-induced protein unfolding: a lesson from bovine β-lactoglobulin*	*Invited Lesson 3. PLUMED (***G. Bussi, SISSA***)*
12.30 - 14.00	*LUNCH*	*LUNCH*	*LUNCH*
14.00 - 15.00	*L3. Parallel Molecular Dynamics: Atom, Force and Domain decomposition (***A. Emerson***)*	*Tutorial T2. Running and analysing Gromacs on a GPU cluster. (***A. Grottesi***)*	*L6. A guide for accessing computer resources from funding bodies such as PRACE. (***A. Emerson***)*
15.00 - 17.30	*Tutorial T1. Analysis of a parallel program.*	*T2. continued (***A. Grottesi***)*	*Practical session or FREE*