# High Performance Molecular Dynamics

March 26th - 27th - 28th  2018

CINECA – Roma, Sala Corsi, via dei Tizii 6B

## Teachers: Andrew Emerson, Giovanni Chillemi, Neva Besker, Alessandro Grottesi

### Agenda

**March 26th**

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|---|---|
| 9.30 – 10.15 | Registration |
| 10.15 – 11.00 | Introduction to HPC architectures I (A. Emerson) |
| 11.00 – 11.30 | Coffee break |
| 11.30 – 12.30 | Introduction to Classic Molecular Dynamics (G.Chillemi) |
| 12.30 – 14.00 | Lunch break |
| 14.00 – 15.10 | MD: Atom, Force and Domain Decomposition (A. Emerson) |
| 15.10 – 15.30 | Coffe break |
| 15.30 – 17.30 | Tutorial 1: UNIX Environment@ CINECA: PBS and SLURM scheduler (A. Grottesi & N. Besker) |

**March 27th**

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|---|---|
| 9.30 – 10.15 | MD on HPC Architectures: GPU, Intel Xeon Phi, KNL, Skylake (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 | Tutorial 3: scalability test for biological systems (A. Grottesi & N. Besker) |
| 12.30 – 14.00 | Lunch break |
| 14.00 – 15.00 | Tutorial 4: Analysis of MD trajectories (N. Besker) |
| 15.00 – 15.30 | Coffee break |

| 15.30 – 17.30 | Tutorial 5: Running and analysis using GROMACS and NAMD (A. Grottesi & N. Besker) |

## March 28th

| 9.30 – 11.00 | Advanced Molecular Dynamics techniques and benchmarks (A. Emerson & A. Grottesi |
| 11.00 – 11.30 | Coffee break |
| 11.30 – 13.00 | Tutorial 6: Essential Dynamics of Proteins (N. Besker) |
| 13.00 – 14.00 | Lunch Break |
| 14.00 – 14.30 | Access to CINECA HPC resources @ CINECA (A. Emerson) |
| 14.30 - | Free exercises and tutorials. |