Contribution ID: **94** Type: **Training session**

Molecular Dynamics Simulations on Grid and HPC systems

Friday, 12 April 2013 13:30 (1h 30m)

Summary

The training event includes tutorials on basic and advanced usage of two major packages for Molecular Dynamics simulations, GROMACS and AMBER, with focus on their application to modeling of biomolecular systems. In following sessions will be presented two portals for automated submission of jobs developed by the organizer EU projects WeNMR (wenmr.eu) and ScalaLife (scalalife.eu).

Impact

GROMACS and AMBER are very powerful and versatile packages but their efficient usage requires expertise that is usually gained after a long experience with them. We hope that the tutorials will greatly help both novice and advanced users to take full advantage of the capabilities of the codes, and thus accelerate their research. At the same time, the job submission portals presented here offer user-friendly tools for the most common usage scenarios that would be of great benefit for beginners in particular.

Description

Molecular Dynamics is a heavily used method for investigating the dynamic properties of systems, and has become an indispensible tool in many research areas, in particular in Life Sciences. GROMACS and AMBER are two applications that are most widely used by the scientific community. The training sessions will include:

• Introduction to Molecular Dynamics simulations
• Basic usage of GROMACS and AMBER for biomolecular modeling
• Advanced GROMACS and AMBER usage on HPC systems
- Hybrid-MPI/OpenMP execution
- Hybrid-CPU/GPU execution
• Using GROMACS and AMBER on Grid resources –WeNMR portal
• Preparing parameters for MD simulations of small organic molecules
• Writing and running your own custom scripts for MD on the grid
• Personal workspaces for structure preparation, MD simulation and trajectory analysis –MDWeb portal

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Session Classification: Training

Track Classification: Virtual Research Environments (Track Lead: G Sipos and N Ferreira)