

## The MoBrain Competence Center for Translational Research from Molecule to Brain

*Wednesday, 6 April 2016 16:00 (30 minutes)*

The MoBrain CC (<https://mobrain.egi.eu/>) has been designed with the aim to allow scientists access to the best e-Science environments from micro to macro scales. It builds on solid basis and expertise provided by the N4U, WeNMR and INSTRUCT initiatives. The aim of MoBrain is to lower barriers for scientists to access modern e-Science solutions to investigate and simulate life science processes. To this end, MoBrain has focused on the development of accelerated computing solutions as well as of cloud-based approaches for specific applications in Structural biology. These solutions, and their integration, will constitute the core of a virtual research environment accessible via a unified web interface. To date, the MoBrain CC has deployed and benchmarked various applications on GPGPU's, most notably in the field of molecular dynamics simulations, and showed that such computations can be successfully submitted with gLite to GPGPU supporting CREAM-CE. This allowed us to extend some of the WeNMR web portals to include both CPU- or GPGPU-environments as options for the user. The same applications have been implemented as containers for Docker, for usage in a cloud environment. This provides a connection to work currently underway in the INDIGO-DataCloud project. In addition, the Scipion package (<http://scipion.cnb.csic.es/>) for the analysis of cryo-electron microscopy data is being deployed both on the EGI Federated Cloud and SurfSARA HPC cloud.

In summary, the MoBrain CC will provide an integrated infrastructure based on a variety of e-Infrastructure solutions, including grid, cloud and accelerated computing systems accessible through cloud interfaces and a virtual research environment to serve translational research from molecule to brain.

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**Session Classification:** Competence centres, user communities