

The WeNMR VRC: operating a worldwide e-Infrastructure for structural biology

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Printable Summary

WeNMR (Worldwide e-Infrastructure for Nuclear Magnetic Resonance and Structural Biology) is a European Union funded project that brings together research teams in the structural biology area into a Virtual Research Community at a worldwide level, focusing on bio-molecular Nuclear Magnetic Resonance (NMR) and Small Angle X-ray Scattering (SAXS). This has been achieved starting six years ago through the implementation of a grid based e-Infrastructure, now fully integrated into EGI. Conventional calculation of structures requires the use of various software packages, considerable user expertise and ample computational resources. In order to shield as much as possible the end user from the grid technicalities and all middleware related issues and commands, WeNMR chose to develop mainly web portals providing “protocolized” access to the grid. These portals distribute automatically the high CPU demanding parts of the calculations over the grid. Moreover, a IaaS cloud provisioning system has been recently made available to meet specific use cases that required more flexibility. The proper monitoring of the infrastructure has been implemented by adopting the VO-specific instances of the EGI operational tools deployed locally by its partners’ sites. New developments in the last project year include the implementation of a Single Sign On system for authentication and central user management and accounting, and the enable of the application software provisioning through the CVMFS service. With more than 550 registered users, 30% of them from non-European countries, WeNMR is now the largest Virtual Organization of EGI in life sciences. A status report of the project mainly focusing on the operational aspects will be given.

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