



Contribution ID: 27

Type: **not specified**

Extending WeNMR e-Infrastructure outside Europe

Wednesday, 28 March 2012 11:00 (20 minutes)

Description of the Work

During the last year the WeNMR operations team has worked to integrate into the WeNMR grid a number of resource centres from South Africa, Latin America, North America, Mediterranean and Asia-Pacific areas. The integration of one centre in South Africa (University of Cape Town), three centres in Latin America (UFRJ in Brasil, ULA in Venezuela and UNLP in Argentina) and one centre in Taiwan (ASGC of Taipei) has run quite smoothly being these centres deployed with the UMD/gLite middleware. In order to monitor the proper configuration and functioning of these grid sites WeNMR has leveraged on the VO-specific instances of the EGI operational tools deployed at one of its partners' site. In North America the situation is different. WeNMR has been in contact since its beginning with the SBGrid Consortium, which is serving the Structural Biology user community in the US. SBGrid is also a VO of the Open Science Grid (OSG), the US national distributed computing grid for data-intensive research, which is interoperable with the EGI grid. At the beginning of 2011 it has been agreed between WeNMR and SBGrid that every US user registering with SBGrid VO is given the option to register with the enmr.eu VO too, allowing him to use the WeNMR services.

Moreover, OSG, SBGrid and WeNMR representatives designed a technical plan aiming at setting up a test-bed for allowing the submission of WeNMR grid jobs towards the OSG resource centres supporting the SBGrid VO.

The first proof of concept has been achieved through the use of dedicated UMD/gLite middleware services components deployed in Europe and configured to submit WeNMR jobs to OSG. A further step is planned to enable the job submission from Europe making use of the Condor based glideinWMS system services deployed in OSG and properly configured to receive WeNMR jobs.

Conclusions

A number of resource centres belonging to NGIs located outside Europe have been successfully integrated in the WeNMR grid infrastructure. A more challenging effort has started to extend the WeNMR grid to the OSG grid in US, through the collaboration with the SBGrid VO. The first tests of WeNMR job submission have been successful carried out using dedicated UMD/gLite based grid services deployed in Europe. A second phase of testing is currently ongoing with the goal of exploiting the existing Condor based glideinWMS system services deployed at OSG. The whole testing phase is expected to be completed before the end of 2012. After that, if successful, the WeNMR production portals will have the technical possibility to route their workload in US, exploiting potentially a few additional tens of thousands of CPU-cores provided by OSG resource centres and making the extension of WeNMR grid infrastructure to OSG grid a reality.

Impact

The collaboration with the relevant ROCs and/or NGIs outside Europe together with the EU FP7 projects like GISELA, EUMEDGRID-Support and CHAIN has been formally agreed by exchanging Letters of Support and/or

by signing Memorandum of Understanding describing a more detailed joint work plan, motivated by the fact that the local NMR/SAXS user community would greatly benefit of the support from the NGIs established in their country. During its lifetime in fact the WeNMR community has grown up to become the largest EGI VO in Life Science, counting more than 350 registered users, around 20% of them being affiliated in Institutions outside Europe. In particular, the large majority of them are located in the US. In the last year about 2400 CPU-cores have been added to the WeNMR grid from resource centres in South Africa, Latin America and Asia-Pacific areas, corresponding to around 10% of the total computing power potentially available now for the WeNMR calculations. These sites have properly run more than 100k WeNMR jobs. New sites from the Mediterranean area are also in the process to be integrated. However, a big increase in computing capacity would become available by enabling the dozens of OSG grid sites currently supporting the SBGrid VO to execute WeNMR jobs. Moreover, in the context of the collaboration with CHAIN, the project is involved in the effort to foster interoperability among EGI and those other grid infrastructures in China, India and Brasil which are not based on the UMD/gLite middleware. The adoption of the proposed standard based solutions to achieve a production level interoperability would also allow a further extension of the WeNMR grid for the benefit of the user community active in those countries.

URL

www.wenmr.eu

Overview (For the conference guide)

WeNMR brings together research teams in the Structural Biology area into a Virtual Research Community at a worldwide level, focusing on biomolecular Nuclear Magnetic Resonance (NMR) and Small Angle X-ray Scattering (SAXS). This has been achieved through the implementation of a grid based e-infrastructure, now fully integrated into EGI, aimed at providing the user community with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modelling. Nowadays more than 20% of the users come from outside Europe. Therefore, in the last year the WeNMR team has worked to extend the e-infrastructure with new resource centres from South Africa, Latin America, North America, Mediterranean and Asia-Pacific areas, with the goal of involving their NGIs to support their local NMR/SAXS community. In particular, a program to interoperate with the OSG grid in US in collaboration with their SBGrid Virtual Organisation has started.

Primary author: Dr VERLATO, Marco (INFN)

Co-author: Dr STOKES-REES, Ian (Harvard Medical School)

Presenter: Dr VERLATO, Marco (INFN)

Session Classification: Community-tailored Services

Track Classification: Users and communities