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WeNMR: the tale of Virtual Research Community in NMR and structural biology

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Overview

Structural biology and life sciences in general, and NMR in particular, have always been associated with advanced computing. The current challenges in the post-genomic era call for virtual research platforms that provide the worldwide research community with both user-friendly tools, platforms for data analysis and exchange, and an underlying e-infrastructure. WeNMR, a three year EC co-funded project started in November 2010, groups different research teams into a worldwide virtual research community. It builds on the established eNMR e-Infrastructure and its steadily growing virtual organization, which is currently the second largest VO in the area of life sciences. WeNMR provides an e-Infrastructure platform and Science Gateway for structural biology. It involves researchers from around the world and will build bridges to other areas of structural biology.

Impact

WeNMR will strengthen the European ties with National Grid Initiatives, the new EGI and PRACE initiatives toward an effective sharing of the offered service. Collaborations will be established with the Asian, South-African, South- and North-American GRID initiatives, in close contact with existing EC projects, to extend and open the WeNMR Life-Science Gateway at a global level. WeNMR will further establish and promote best practices in life sciences and offers (virtual) training services to worldwide researchers.

Description of the work

The main objective of WeNMR is to establish an e-Infrastructure-based global virtual research community for structural biology in the life sciences.
To this end six objectives are defined:
1) to operate, maintain and further develop a user-friendly science gateway for the NMR and SAXS communities,
2) to establish a virtual research platform to serve as a digital knowledge repository, data exchange medium, and forum for (interaction with) the user community,
3) to provide support to software developers, users and other e-Infrastructure projects in an e-Science knowledge and training centre,
4) to foster the adoption and use of e-Infrastructure on a global scale by supporting a wide range of flanking disciplines within the life sciences,
5) to operate and consolidate the eNMR Grid infrastructure in line with NGIs and the EGI, and to extend it to interoperate with other worldwide Grid initiatives,
6) to develop a model to ensure sustainability of the project.

The computational GRID infrastructure is central to the services offered by WeNMR; its operation, maintenance and consolidation are therefore core Service activities. The infrastructure is being expanded to worldwide Grid initiatives, which is an important factor to both increase the available computational resources and the user community. WeNMR also operates a Virtual Research Community portal that will address the needs of the various user communities, from general public to experienced users and software developers. For each community, a number of services, information channels and communication tools is being deployed. WeNMR also aims at expanding the extensive human collaboration network successfully implemented within the e-NMR project geographically, i.e. involving users and other stakeholders from many new countries, in size and scientifically by involving new scientific communities. The inclusion of the SAXS community is a first step in that direction.

URL

www.wenmr.eu

Conclusions

WeNMR has established itself as a lively and growing Virtual Research Community in the life sciences and structural biology area. It already represents one of the largest if not the largest Virtual Research Organization (VO), accounting for about 20% of the CPU on the GRID within the life science area. Its global character is well illustrated by the international nature of its user community covering more than 30 countries, including South Africa and Latin America. To date, more than 10% of the users come from outside Europe. WeNMR has thus developed into a successful Virtual Research Community in structural biology for researchers from around the world.

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