Contribution ID: **7** Type: **Demonstration**

e-NMR: Computational NMR Infrastructure in life science and system biology

Monday 12 April 2010 17:00 (10 minutes)

In order to enable the life science community to make full use of the EGEE computing resources we have developed an e-infrastructure named 'eNMR'(EU 7th FP, Contract no. 213010).

eNMR deploys and integrates biomolecular NMR applications into a platform, so that EU scientists can easily access it via a standard browser interface and use it at every step of their research process.

The sequence of available web-portals covers all aspects of bio-NMR: data acquisition, processing, analysis, protein/DNA/RNA structure calculation, molecular docking, validation, deposition etc.

Detailed analysis

Life-science researchers require the full range of advanced computational techniques in order to analyze complex biological data acquired experimentally at the EU NMR facilities. It becomes increasingly impossible to fulfill all of their requirements using the local computing resources.

eNMR is part of EGEE has developed solutions for performance computing, data access, authentication, security, accounting and usage statistics. Thus the e-NMR platform has all the strength of Grids, however, its focus is "science-driven". For example, in addition to already available applications, new ones are being identified and ported continuously, aiming to cover all aspects of bio-NMR; the enhancements to the grid middleware (gLite) are carried out to match the requirements of the applications.

Since the e-NMR portals have the same look and feel as bioinformatics web-gateways that have been available to the Life Science community for years, biologists can easily use the portals to execute their data analysis and structure calculation tasks without extensive knowledge of Grid technologies. The portals include documentation, tutorials and sets of use-cases from the worldwide labs.

Conclusions and Future Work

An NMR e-Infrastructure has been successfully deployed at the various EU partner sites: the Universities of Utrecht, Frankfurt, Padova, Florence, and EBI-EMBL. The e-Infrastructure tests, compares, integrates and provides access to the computational tools for NMR structural biology community. Streamlined protocols and efficient workflows are being developed that enable the researcher to run in parallel their calculations, and to perform all the steps from the basic data to the structures of biomolecules and to a better understanding of biological systems and living organisms.

Impact

Biomolecular NMR is truly a multi-disciplinary science comprised of all bio – physics/chemistry/informatics/tech/nano/omics etc. This has resulted in the fragmentation of research methods, preventing full interoperability among different labs, and thereby limiting the scientific impact of European bio-NMR research.

The eNMR by integrating applications enables scientists to address complex inter-disciplinary problems. Comparing the efficiency of different methods (CASD) leads to a more thorough and consistent analysis of exper-

imental data, and thus a higher reliability of structural information.
The eNMR includes both established and emerging applications, so that scientists can depend on it to achieve their research and education goals and eventually could conduct potentially all of their computational work using it.
To use eNMR e-infrastructure capabilities via a user-friendly web-browser interface does not require extensive knowledge of Grid and IT technologies, thus increasing the potential user base from just bioinformatics to across life sciences. The number of users is growing and currently eNMR is the second largest VO in EU life sciences as measured by the volume of computation.

Keywords

Life sciences, NMR, biomolecules, structure calculation, pipeline, web portals, structural biology

URL for further information

http://www.enmr.eu

Justification for delivering demo and/or technical requirements (for demos)

We'd like to demonstrate the sequence of the web-portals implementing the applications for biomolecular-NMR; we shall need a big screen (preferably on a stand; to be connected to our computer).

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Session Classification: Demo Session 1, Welcome Drink

Track Classification: Experiences from application porting and deployment