

WeNMR

Summary: 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 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 will consolidate the operation of the current services and provide an e-Infrastructure platform and Science Gateway for structural biology towards EGI for the users of existing infrastructures. It will involve researchers from around the world and will build bridges to other areas of structural biology. Integration with SAXS, a rapidly growing and highly complementary method, is directly included in WeNMR, but links will also be established to related initiatives. WeNMR will serve all relevant INSTRUCT communities in line with the ESFRI roadmap.

Objectives: 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.

Action plan: WeNMR will operate and further consolidate the e-Infrastructure deployed within the eNMR project. A virtual research community platform will be established in the first year to serve as the central entry point for all communities and the main dissemination portal of the project. 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 in the second year of the project. WeNMR will further establish and promote best practices in life sciences and offers (virtual) training services to worldwide researchers throughout the entire duration of the project.

Networking activities: The Networking Activities (NA) build on the extensive human collaboration network successfully implemented within the e-NMR project. They aim at extending it 1) geographically, i.e. involving users and other stakeholders from many new countries, 2) in size, i.e. by increasing the number of users in all countries, and 3) scientifically, i.e. by involving new scientific communities that share an interest in structural biology in its broader sense. In addition to individual laboratories and research teams, a crucial role in this process will also be carried out by National and Regional Grid Initiatives, as well as by



Project acronym:
WeNMR

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2'434'000 €

Funding from the EC:
2'150'000 €

Total funded effort in person-month:
264.5

Web site:
www.wenmr.eu

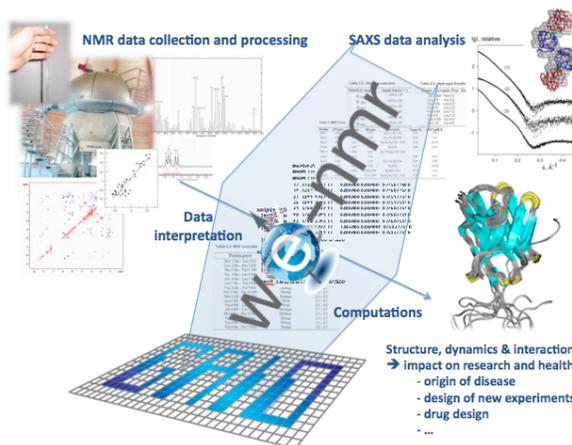
Contact person:
Prof. Alexandre Bonvin
email: a.m.j.bonvin@uu.nl
tel.: +31 30 2533859
fax.: +31 30 2537623

Project participants:

BCBR	NL
BMRZ	DE
CIRMMP	IT
INFN	IT
RUN	NL
UCAM	UK
EMBL	DE
SpronkNMR	LT

Keywords:
Nuclear Magnetic Resonance spectroscopy (NMR), Small Angle X-ray Scattering (SAXS), structural biology, life sciences, proteins, DNA, complexes, web portals

Collaboration with other EC funded projects:
East-NMR, contract no. 228461
Bio-NMR, contract no. 261863
EU-IndiaGrid2, contract no. 246698
Gisela, contract no. 261487
CHAIN, contract no. 260011
eScienceTalk contract no. 260733



researchers in Industry. NA further aim at establishing sustainability measures for future operation, both in terms of continuous feedback and quality control as well as in financial form. A large variety of disseminative actions will target stakeholders including the e-Science, bio-NMR and SAXS communities, the more general structural biology and life sciences communities, industrial researchers, as well as the general public.

Service activities: The computational GRID infrastructure is central to the services offered by WeNMR; its operation, maintenance and consolidation are therefore core Service activities. The infrastructure will be expanded to worldwide Grid initiatives, which is an important factor to both increase the available computational resources and the user community. WeNMR will also operate 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 will be deployed.

Joint Research activities: The WeNMR Joint Research activities (JRA) aim at improving the integrated services offered by the project in order to reflect the latest scientific developments. To enhance the possibilities for actual experimentation, the project will develop remote, secure access to experimental SAXS facility. Finally, to ensure an efficient usage of the WeNMR web portals and services, systematic attention will be paid to user-interaction with- and communication between the portals and the services. The JRA main three objectives are: 1) to provide a multidisciplinary approach (NMR/SAXS/validation) to the characterization of biomolecular interactions 2) to provide a secure remote access to SAXS instrumentation and 3) to provide web services and end user tools.

User communities: The NMR community in the Life Sciences is composed of a large number of research teams that tackle a vast portfolio of different biological problems. We estimate its size to around 1000 research groups worldwide; their size and expertise vary from a few researchers with access to limited instrumentation to large research units with extensive, state-of-the-art equipment (e.g. the European, North American and Japanese large-scale NMR research infrastructures). The SAXS community is similarly diverse: thousands of research groups worldwide employ SAXS as a method to obtain structural information of a wide variety of non-crystalline objects, including, but not limited to, biological macromolecules in solution. Only few dozens of these groups however maintain instruments, which range from small lab sources to full-scale third generation synchrotron radiation facilities themselves; most users visit the large synchrotron facilities with SAXS beamlines. The research teams making use of NMR and/or SAXS often collaborate with a large number of scientific groups that are skilled in molecular and cell biology and provide samples for the experimental measurements. The outcomes of these studies are of interest for an even wider community of scientists, because of the biological and biomedical implications of the results attained.

International aspects: As the title of the project states, WeNMR aims at providing a *worldwide e-Infrastructure* for NMR and structural biology. As such, it is a strongly internationally oriented project that reaches far outside Europe. International aspects are embedded in all activities of the project.

