SEVENTH FRAMEWORK PROGRAMME

Research Infrastructures

Deliverable 3.1

Joint NMR-SAXS Workshop

Grant Agreement number:	RI-261572
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Due Date	June 30th, 2011
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Section 1: Summary of Deliverable

Background

The aims of the WeNMR project are to consolidate the operation of the current computing services, extend them to interoperate with other worldwide Grid initiatives and provide an e-Infrastructure platform and structural biology Science Gateway as part of the EGI for the NMR and Small Angle X-ray Scattering (SAXS) communities. NMR and SAXS are complementary techniques to study biomolecules and their interactions in solution. The extension to include SAXS represents our first step in broadening the user community towards the larger structural biology community.

To achieve these goals, NMR and SAXS will be integrated to make best use of their complementary aspects, resulting in new joint protocols and tools for studying large macromolecular assemblies. Further, the establishment of a SAXS Grid-enabled infrastructure including secure remote access to SAXS instrumentation is envisaged. We will investigate the possibility of adopting the remote instrument framework available within the EGEE infrastructure to allow secure remote access to the SAXS beamline at EMBL-Hamburg.

Goal

The goal of the workshop was "*to discuss the ways of the joint use of SAXS and NMR in the daily routine of structural biologists and to define the computational needs for the broader integration*".

Additionally, it was expected to provide an account on the recent methodological developments and on advanced computational tools including grid computing and remote experiments.

Section 2: Workshop

Programme

The full programme can also be found at the following link:
http://www.wenmr.eu/wenmr/wenmr-workshop-computational-aspects-joint-use-saxs-and-nmr

Section 1 Complementarity of (We)NMR and SAXS

- 11:30 Alexandre Bonvin (Utrecht University): "WeNMR: the tale of a virtual research community in structural biology"
- 12:00 Dmitri Svergun (EMBL, Hamburg): "The use of NMR-SAXS complementarity in ATSAS"
- 12:30 Javier Perez (SOLEIL, Paris): "Dadimodo : a software designed to refine multimodular protein structures against SAXS and possibly NMR-RDC experimental data"
- 13:00 – 14:00 Lunch

Section 2 Grid computing for SAXS/NMR

- 14:00 Daniel Franke (EMBL, Hamburg): "Enabling SAXS for the NMR Community: Grid Tools for SAXS and Remote Instrument Access"
- 14:30 Giacomo Parigi (CERM, Florence): "Maximum occurrence of conformations with an integrated SAXS-paramagnetic NMR approach"

Section 3 Joint SAXS/NMR applications

- 15:00 Ad Bax (NIH, Bethesda): "Chemical shifts, dipolar couplings and SAXS, how can they help?"
- 15:30 Michael Sattler (Technische Universität München): "Combining NMR and small-angle scattering for structural analysis of protein complexes in solution"
- 16:00 - 16:30 Coffee break
- 16:30 Pau Bernado (Institute for Research in Biomedicine, Barcelona): "A more Complete Picture of Protein Dynamics from the combined use of NMR and SAXS"
- 17:00 Jan Skov Pedersen (University of Aarhus): "Unfolding States of an Integral Membrane Protein by NMR, light scattering and SAXS: TFE-induced Disintegration of Surfactant-KcsA Complexes"
- 17:30 Hartmut Oschkinat (Leibnizinstitut fur Molekulare Pharmakologie, Berlin):"An integrated view on the structure and activation mechanisms of alphaB crystallin"
- 18:00 – 19:00 Round-table discussion, “Present state and future directions”, Chair: A.Bonvin

List of speakers

First Name	Last Name	Affiliation	Country	*
Alexandre	Bonvin	Utrecht University	Netherlands	proj.
Giacomo	Parigi	CERM	Italy	proj.
Dmitri	Svergun	EMBL Hamburg	Germany	proj.
Daniel	Franke	EMBL Hamburg	Germany	proj.
Javier	Perez	SOLEIL	France	ext.
Ad	Bax	NIH	USA	ext.
Michael	Sattler	TU München	Germany	ext.
Pau	Bernado	IRB	Spain	ext.
Jan Skov	Pedersen	University of Aarhus	Denmark	ext.
Hartmut	Oschkinat	FMP	Germany	ext.

* proj.: speaker from the WeNMR project; ext.: External speaker

List of participants

First Name	Last Name	Affiliation	Country	*
Marc	van Dijk	Utrecht University	Netherlands	proj.
Henry	Jonker	University of Frankfurt	Germany	proj.
Antonio	Rosato	CERM	Italy	proj.
Claudio	Luchinat	CERM	Italy	proj.
Ivano	Bertini	CERM	Italy	proj.
Lucia	Banci	CERM	Italy	proj.
Enrico	Ravera	CERM	Italy	proj.
Geerten	Vuister	University of Leicester	UK	proj.
Iulia	Danciu	EMBL Hamburg	Germany	proj.
Michal	Gajda	EMBL Hamburg	Germany	proj.
Chris	Spronk	Spronk NMR	Lithuania	proj.
Simonas	Jurksa	Spronk NMR	Lithuania	proj.
Abel	Garcia-Pino	Vriie University Brussel	Belgium	ext.
Valentina	Zorzini	Vriie University Brussel	Belgium	ext.
Nico	van Nuland	Vriie University Brussel	Belgium	ext.
Lukasz	Skora	University of Basel	Switzerland	ext.
Amanda	Altieri	University of Maryland	USA	ext.
Matthias	Buck	Case Western Reserve U.	USA	ext.
Ada	Prochnicka-Chalufour	Institute Pasteur	France	ext.
Yann	Sterckx	Vriie University Brussel	Belgium	ext.
Muruga	Karuppiah	Madurai Kamaraj Univ.	India	ext.
Adam	Round	EMBL Grenoble	France	ext.
Vytautas	Lesmantavicius	University of Copenhagen	Denmark	ext.
Andras	Boeszoermenyi	University of Graz	Austria	ext.
Guy	Montelione	Rutgers University	USA	ext.

* proj.: participant from the WeNMR project; ext.: External participant

Summary

The workshop was scheduled right after the Gordon NMR conference on computational aspects of biomolecular NMR taking place in Il Ciocco, Italy (22-27.05), and was thus attended by several delegates of the Gordon conference. The leaders of the major groups developing software for the joint SAXS-NMR applications from both the NMR field and the SAXS field were represented at the workshop, such that all the main novel approaches were covered. The talks were given by scientists from the Netherlands, Germany, Italy, Denmark, France and USA. Of all people attending the workshop, 16 (45%) were affiliated with WeNMR and 19 (55%) were from other research institutes in Europe, India and the USA.

In addition to the planned access to the ATSAS program suite from Hamburg (as a part of the WeNMR activity), interest has been expressed to provide grid portals for the Dadimodo software of J. Perez (Eur Biophys J, 2007, 37:95–104) and M. Sattler's implementation in CNS (Gabel F, J Biomol NMR. 2008 41:199-208).

The possibilities of the GRID access and the challenges in setting up GRID services at EMBL-Hamburg were discussed, in particular those related to certificates and authentication. At current time, the German certification authority does not support robot certificates. This issue has now been brought up at the EGI User Community Board meeting.

The general question of how to deposit SAXS experimental data, possibly together with NMR data, for public access was raised. It was mentioned that it is possible to deposit SAXS data as a restraints files together with a NMR PDB coordinate deposition through the ADIT-NMR deposition system. This point will be brought to the attention of the PDB Validation Taskforce for NMR.

Throughout the day, discussion among participants and between participants and speakers was lively and fruitful. The program developers had a chance to better understand the needs of the end users from both NMR and SAXS field, which will help in the further implementation of the SAXS and NMR protocols.