



The tale of a Virtual Research Community in NMR and structural Biology

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The Project

A Worldwide e-Infrastructure for NMR and structural biology

Project Coordinator:
Prof. Alexandre M.J.J. Bonvin, Utrecht University, NL

Contract n°: RI-261572
Project type: CP-CSA
Duration: 36 months (Oct.2013)
Total budget: 2' 434' 000 €
EC Funding: 2' 150' 000 €

The team



Utrecht University, Bijvoet Center for Biomolecular Research, NL



Johann Wolfgang Goethe Universität Frankfurt a.M., Center for Biomolecular Magnetic Resonance DE



University of Florence, Magnetic Resonance Center, IT

Istituto Nazionale di Fisica Nucleare, Padova, IT



Raboud University, Nijmegen, NL

University of Cambridge UK



European Molecular Biology Laboratory, Hamburg, DE

Spronk NMR Consultancy, LT



+ Institute of Biological Chemistry, Academia Sinica, TW
expected November 2011

1st VRC recognized by EGI

Science Gateway → www.wenmr.eu

we-nmr A worldwide e-Infrastructure for NMR and structural biology [Login](#) | [Register](#)

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The objective of WeNMR is to optimize and extend the use of the NMR and SAXS research infrastructures through the implementation of an e-infrastructure in order to provide the user community with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modelling. Access to the e-NMR infrastructure is provided through a portal integrating commonly used software and GRID technology.

[Get Started >>](#)

Harness the power of the GRID

Highlights **News** **Events**

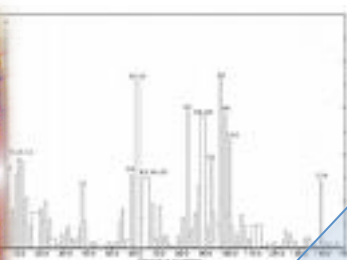
2011-08-12 16:28 GROMACS portal now available

2011-05-16 15:04 Three-days HADDOCK workshop in Istanbul

Exploiting GRID resources in structural biology...

NMR data collection and processing

SAXS data analysis



Data interpretation

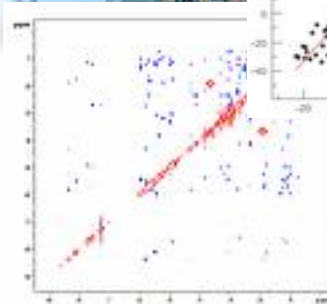


Table 2.1: NOE restraints

Proton pairs		Distance (Å)	Strength
Met 1 H α - Leu 2 HN		4.5	Medium
Leu 2 H α - Phe 3 HN		4.5	Weak
Phe 3 H α - Val 4 HN		4.5	Weak
Pro 5 H α - Ala 6 HN		4.5	Medium
Ala 6 H α - Leu 7 HN		2.5	Medium
Leu 7 H α - Val 8 HN		2.5	Medium
Val 8 H α - Val 9 HN		2.5	Medium
Val 9 H α - Phe 10 HN		2.5	Medium
Met 1 HN - Leu 2 HN		4.5	Medium
Leu 2 HN - Val 9 HN		4.5	Medium
Val 4 HN - Leu 7 HN		4.5	Medium
Ala 6 HN - Val 9 HN		4.5	Medium
Met 1 H α - Val 9 H α		2.5	Medium
Phe 3 H α - Val 9 H α		1.8 - 2.5	Strong
Val 4 H α - Pro 5 H α		1.8 - 2.5	Strong
Val 4 H α - Pro 5 H α		1.8 - 2.5	Strong

Table 2.2: Dihedral restraints

Dihedral	Angle limits (°)
ϕ Leu 2	-160 to -80
ϕ Phe 3	-160 to -80
ϕ Leu 4	-160 to -80
ϕ Val 8	-160 to -80
ϕ Val 9	-160 to -80

Table 2.3: Hydrogen Bonding (Å)

Donor	Acceptor Pair	Distance
Leu 7 HN	- Val 9 O	3.0
Leu 7 HN	- Val 9 O	3.0
Val 9 HN	- Leu 2 O	3.0
Val 9 HN	- Leu 2 O	3.0
Val 4 HN	- Leu 7 O	3.0
Val 4 HN	- Leu 7 O	3.0
Leu 7 HN	- Val 4 O	3.0
Leu 7 HN	- Val 4 O	3.0

Table 1: NMR Param

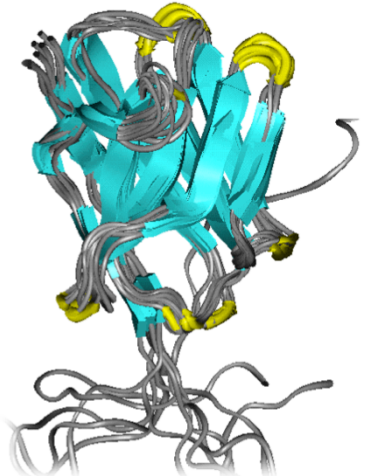
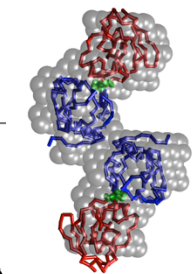
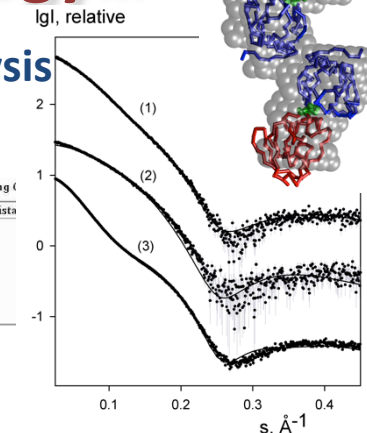
Residue	HN ppm	HB ppm	others ppm	χ^2_{resid}	ASA Type	K
Met1	6.66	1.76	H ₂ , 2.3, H ₁ , 1.94	8.42		-6.92
Leu2	8.06	4.64	H ₁ , 4.8, H ₂ , 0.88	9.00		-6.10
Phe3	8.53	5.31	H ₁ , H ₂ , 7.05-7.22	9.30		-10.37
Val4	4.47	2.09	H ₁ , 0.92	9.60		-6.02
Pro5	4.45	2.21	H ₁ , 1.99, H ₂ , 3.65, 3.76			
Ala6	8.93	4.71		7.60		-9.35
Leu7	8.30	1.77	H ₁ , 6.0, H ₂ , 0.94	8.60		-2.70
Val9	8.31	4.47	H ₁ , 0.92	9.13		-10.03
Met10	8.69	4.51	H ₁ , 0.92, 0.84	9.31		-5.12
Met10	8.69	4.51	H ₁ , 0.92, 0.84	9.31		-5.12

Number 1
INAME 1
INAME 2

assign (resid 501 and name OO)
(resid 501 and name)
(resid 501 and name X)
(resid 501 and name Y)

CA) -0.1400 0.15000

100 0.15000



Computations

Structure, dynamics & interactions

- impact on research and health:
- origin of disease
 - design of new experiments
 - drug design...

wE-nmr **Main objectives**

- Operate and further develop a user-friendly **e-Science gateway for the NMR and SAXS communities** (link to ESFRI Instruct)
- Establish a **virtual research platform** for (interaction with) the user community
- **Provide support** to software developers, users and other e-Infrastructure projects
- **Foster the adoption and use of e-Infrastructure** in a wide range of flanking disciplines within the life sciences
- **Operate and consolidate the eNMR Grid infrastructure** and to extend it to interoperate with other **worldwide Grid initiatives**
- Develop a model to ensure **sustainability** of the project

Collaborations established so far

Collaborations (**MoU**) already established with several other FP7 projects:

- **OpenAIRE** www.openaire.eu
- **e-ScienceTalk** www.e-sciencetalk.org
- **Erina+** www.erinaplus.eu
- **Gisela** www.gisela-grid.eu
- **CHAIN** www.chain-project.eu
- **EUMEDGRID** www.eumedgrid.eu
- **EMI** www.eu-emi.eu
- **EGI** www.egi.eu



The WeNMR philosophy for interacting with the Grid

- Our policy is to **shield as much as possible the end user from the Grid** and all middleware related issues and commands
- For this, we chose to develop mainly web portal providing **“protocolized” access to the Grid**
- To facilitate operation, we **use when possible robot certificates**
- Experienced users can still interact directly with the Grid via UI and we **provide “ready-to-go” customized UI distributions (MILU) for download**

Users distribution and growth

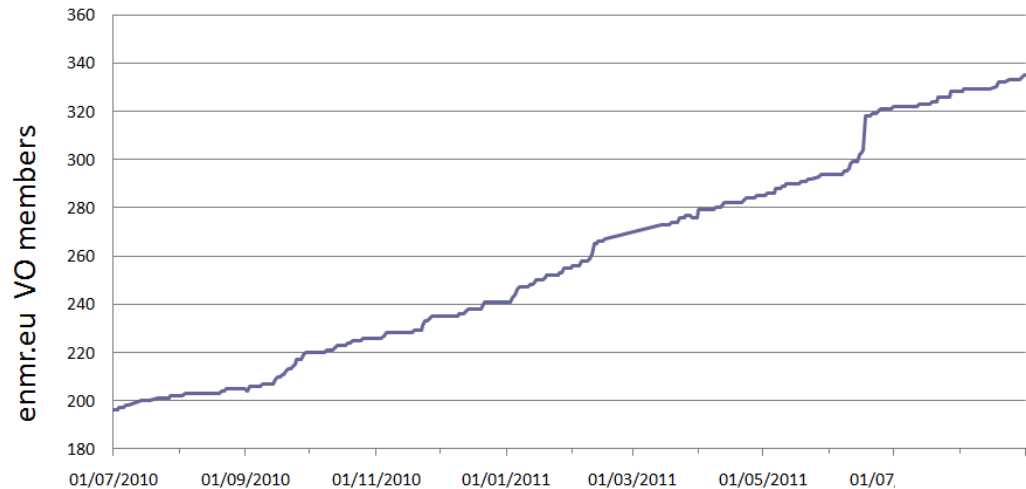
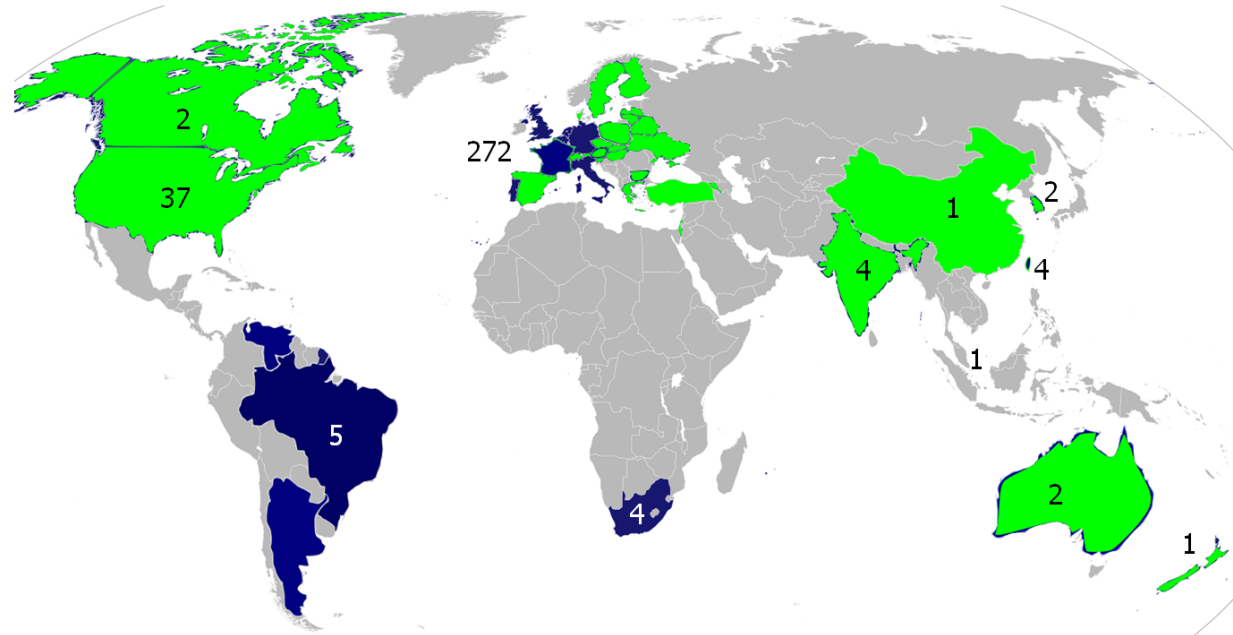
The project leverages on

- The previous eNMR e-Infrastructure project (FP7)
- EU-NMR (FP6)
- EAST-NMR (FP7) RI
- Bio-NMR (FP7) RI

Linked to ESFRI
INSTRUCT

Steady growth

~20% of users from outside Europe





WeNMR platform operational and well used!

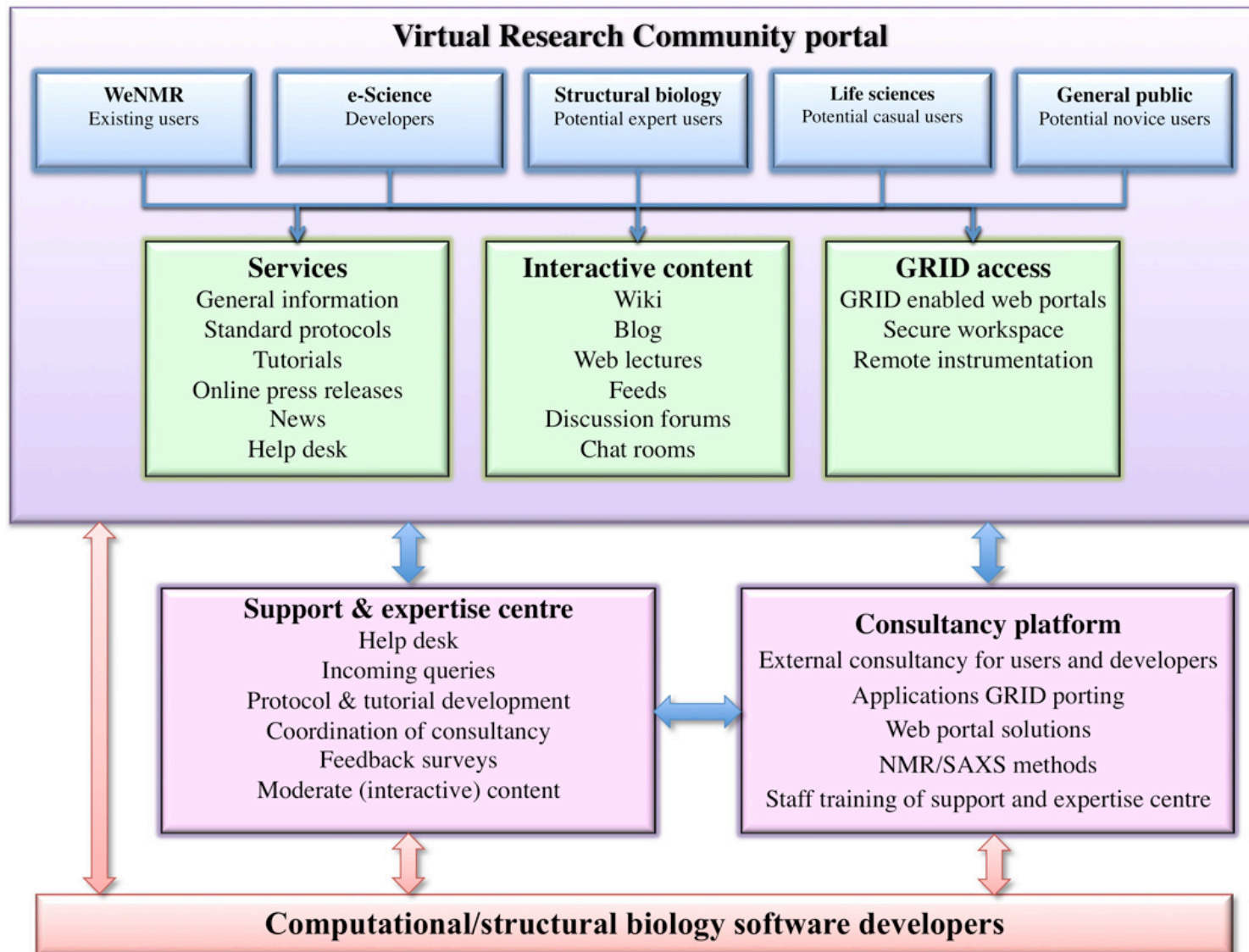
- Largest VO in the life sciences
- Over 338 registered users from 38 nationalities, and growing
- >33 000 CPUs
- >700 (normalized) CPU years over the last 12 months
- 1.4 million jobs over the last 12 months
- 150Tb of storage space
- ~20% of Life Sciences on the Grid
- User-friendly access to e-Infrastructure via web portals

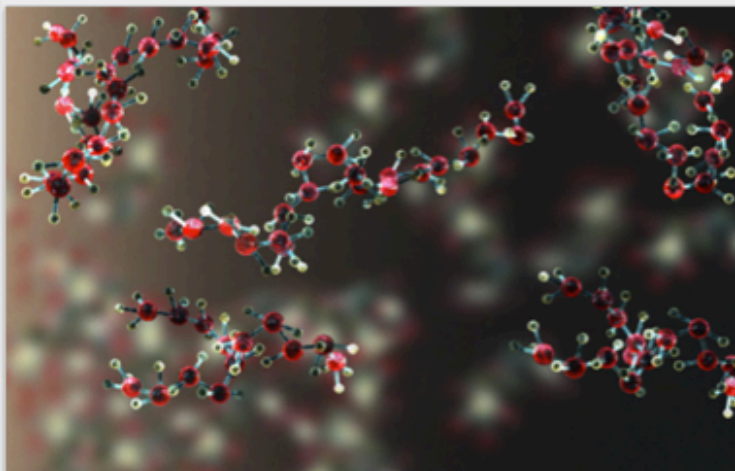




The Virtual Research Community

The VRC portal



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The objective of WeNMR is to optimize and extend the use of the NMR and SAXS research infrastructures through the implementation of an [e-infrastructure](#) in order to provide the user community with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modelling. Access to the e-NMR infrastructure is provided through a portal integrating commonly used software and GRID technology.

Harness the power of the GRID

Highlights

[WeNMR demo - EGI User Forum, Vilnius 2011](#)

[WeNMR Workshop - NMR applications on the GRID](#)

[WeNMR Workshop - Computational aspects of the joint use of SAXS and NMR](#)

[CASD-NMR](#)

The VRC portal: www.wenmr.eu

The WeNMR service portal

we-nmr Login | Register

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NMR Services

- Processing
- Assignment
- Analysis
- Structure Calculation
 - CS-ROSETTA
 - CYANA
 - Xplor-NIH
- Molecular Dynamics
- Modelling
- Tools

Home

NMR Services

Our NMR web portals provide access to many of the powerful software packages ported by the e-NMR and WeNMR consortia to the GRID. A wide range of structural biology related software packages are available covering the many stages in NMR structure calculation, molecular dynamics simulations and structure modelling.

Processing

- MDD NMR**
This service allows to process a non-uniformly sampled (NUS) nD spectrum using Multi-Dimensional Decomposition program.

Assignment

- Auto Assign**
AutoAssign is a constraint-based expert system for automating the analysis of backbone resonance assignments using triple resonance NMR spectra of small proteins.
- MARS**
MARS is a program for robust automatic backbone assignment of ¹³C/¹⁵N labeled proteins.

Molecular Dynamics Simulation

- AMBER**
Amber (acronym to Assisted Model Building with Energy Refinement) is a suite of programs that allow users to perform molecular dynamics (MD) simulations on biological systems.
- GROMACS**
GROMACS is a versatile package to perform molecular dynamics, i.e simulate the Newtonian equations of motion for systems with hundreds to millions of particles. GROMACS is able to work with many biochemical molecules like proteins, lipids and nucleic acids. The WeNMR GROMACS webportal combines the versatility of this molecular dynamics package with the calculation power of the eNMR grid. This will enable you to perform many simulations from the comfort of your

European egi Towards a sustainable infrastructure

The WeNMR services portofolio

Recently deployed portals

Xplor-NIH e-NMR GRID-enabled web portal

AMBER e-NMR GRID-enabled web portal

CYANA Web Portal

HADDOCK e-NMR GRID-enabled web portal

CS-ROSETTA e-NMR GRID-enabled web portal

MDD Web Portal

AutoAssign Web Portal

TALOS e-NMR (GRID-enabled) web portal

MARS Web Portal

3DDART e-NMR (GRID-enabled) web portal

3D-DART

AnisoFIT WeNMR GRID-enabled web portal

Antechamber GRID-enabled web portal

MAXOCC WeNMR GRID-enabled web portal

GROMACS e-NMR (GRID-enabled) web portal

INTRODUCTION TO MAXOCC WEB PORTAL

THE GROMACS WEB SERVER

Welcome to the GROMACS web server! The GROMACS web server is a versatile package to perform molecular dynamics (MD) simulation. It simulates the Newtonian equations of motion for systems with hundreds to millions of particles. GROMACS is able to work with many biochemical molecules like proteins, lipids and nucleic acids. The WeNMR GROMACS web server provides a convenient interface to the GROMACS web server.

SHIFTX2

Documentation Download Instructions Contact FAQ

SHIFTX2 predicts both the backbone and side chain ¹³C and ¹⁵N chemical shifts for proteins using their structural (PDB) coordinates as input. SHIFTX2 combines ensemble machine learning methods with sequence alignment-based methods to calculate protein chemical shifts for backbone and side chain atoms. SHIFTX2 has been trained on a carefully selected set of 187 proteins and tested on a separate set of 81 proteins. Both the training and testing sets consisted of high-resolution (≤1.5 Å) structures (21 Angstrom) with carefully vetted chemical shifts assignments. SHIFTX2 is able to attain correlation coefficients between experimentally observed and predicted backbone chemical shifts of 0.960 (1D), 0.965 (13C), 0.982 (15N), 0.974 (1H), 0.974 (1H), 0.974 (1H) and 0.985 (1H) atoms of 1105, 3,432, 8,124, 8,126, 0.1711 and 8,1271 ppb, respectively. Comparisons to other chemical shift predictors using the same testing data set indicates that SHIFTX2 is substantially more accurate (up to 30% better by correlation coefficient with an RMS error that is up to 1.3x smaller) than any other program.

The VRC and the user community

- **Wiki's**
- **Online tutorials and instruction videos**
- **Help center**
- **NMR and SAXS services**
- **Chat and video conferencing tools**
- **And much more ...**

The VRC and the GRID

- GRID tutorials for end users and site administrators
- “Ready to go” MILU UI installation for end users

The VRC and the GRID



A worldwide e-Infrastructure for NMR and structural biology

amjibonvin | Logout



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GRID Tutorials

Learn more about GRID technology with our GRID tutorials.

- [Quick gLite Middleware Deployment HOW-TO for WeNMR](#)
- [VO registration troubleshooting](#)
- [Quick gLite HOW-TO for WeNMR users](#)
- + [Create new tutorial in this category](#)

The VRC and the GRID

- GRID tutorials for end users and site administrators
- “Ready to go” MILU UI installation for end users
- **In the future: “ready to go” virtual machines with WeNMR software including end user applications, workflow management system and UI**
- **Interface to GGUS within our help center**

The VRC and the GRID

Support

Tutorials

Wiki

Forums

Blogs

Help Center

Home

WeNMR Support

Getting Started

Learn all about WeNMR services and how to get started. Introductions and tutorials on NMR, SAXS and GRID applications for beginners and advanced users.

Tutorials

NMR and SAXS tutorials and use cases created by WeNMR partners to demonstrate and let you practice with real life examples.

Wiki

NMR and SAXS documentation written by the experts on WeNMR services, tutorials and links to other advanced resources.

Forums

Get involved on our forums for discussions and feedback on a wide variety of topics. Ask and answer questions about NMR and SAXS.

Blogs

Read opinions and news from experts, and write your own blogs about anything related to your NMR and SAXS research or interests.

The GRID-related support system makes use of the EGI Global Grid User Support ([GGUS](#))

A WeNMR end-user or operator can submit a support request via a web browser by connecting to the [GGUS](#) portal, or create a ticket simply by sending an e-mail to vo-user-support@ggus.org or helpdesk@ggus.org.



You can also provide general feedback to the [EGI](#) about requirements and recommendations from the WeNMR user community. The development of the European Grid Infrastructure is driven by the users, and thus your feedback is important to improve our services and to expand the infrastructure. You are invited to provide feedback to the EGI on behalf of the WeNMR scientific community by filling the [EGI feedback form](#). As community enter either eNMR or WeNMR.




The VRC and the GRID

- GRID tutorials for end users and site administrators
- “Ready to go” MILU UI installation for end users
- In the future: “ready to go” virtual machines with WeNMR software including end user applications, workflow management system and UI
- Interface to GGUS
- Application database applet from EGI embedded in our web portal

The VRC and the GRID

Applications

The screenshot displays a web browser window titled "Applications Database" with the ESI logo in the top left corner. The page lists three applications, each with a small icon, a name, a description, a discipline, and an abstract. A "details" link is provided for each entry. At the bottom, there is a pagination control showing "Previous 2 of 3 Next" and a copyright notice: "© Institute of Accelerating Systems and Applications, 2009-2011, Athens, Greece".

Name	Description	Discipline	Abstract
 GROMACS	GROningen MAchine for Chemical Simulations	Life Sciences	GROMACS (GROningen MAchine for Chemical Simulations) is a molecular dynamics simulation package orig...
 HADDOCK	Biomolecular docking	Life Sciences	HADDOCK (High Ambiguity Driven protein-protein DOCKing) is an information-driven flexible docking ap...
 MARS	MARS is a program for robust automatic backbone assignment of ¹³ C/ ¹⁵ N labeled proteins.	Life Sciences	MARS is a program for robust automatic backbone assignment of ¹³ C/ ¹⁵ N labeled proteins. MARS simulta...

The VRC and the GRID

- GRID tutorials for end users and site administrators
- “Ready to go” MILU UI installation for end users
- In the future: “ready to go” virtual machines with WeNMR software including end user applications, workflow management system and UI
- Interface to GGUS
- Application database applet from EGI embedded in our web portal
- **WeNMR custom dashboard within the EGI site**
 - Allows to input VRC-specific requirements and track them

The VRC and the GRID

Dashboard WeNMR

WeNMR

[Edit](#)

#	Subject Requestors	Status Created	Queue Told	Owner Last Updated	Priority Time Left	Category (level 1)	Category (level 2)	Requestor (level 1)	Requestor (level 2)	Requestor (level 3)	Non-Functional Tag	Technology Tag	Custom Tag
1550	Graphical configuration tool for gLite a.m.j.j.bonvin@uu.nl, marco.verlato@pd.infn.it	new 4 weeks ago	requirements	nunolf 4 weeks ago	0	Unified Middleware Distribution (UMD)		Community	WeNMR (Community)			gLite	
1239	Data recovery a.m.j.j.bonvin@uu.nl	open 8 weeks ago	requirements 8 weeks ago	ekarolis 13 days ago	0	Unified Middleware Distribution (UMD)	Data Access (UMD)	Community	WeNMR (Community)		Recoverability	gLite	Data recovery
669	Encryption and protection of data nuno.ferreira@egi.eu	new 4 months ago	requirements	Nobody 3 months ago	0	Non-Functional	Other (Non-Functional)	Virtual Organization	Life Sciences (VO discipline)	enmr.eu			

The VRC and the EGI

- **WeNMR on the EGI User Community Board**
- **WeNMR coordinator on External Advisory Board of EGI-Inspire**
- **Do contact us (me) for any user-related issue / requirements /wishes concerning the Grid**

Training and dissemination

- **Training center**

- Focus on applications integrated in the web portals
- Modular format developed by SpronkNMR

- **Recent events (May-Aug.)**

- EMBO course **Beijing**
- Workshop at National Tsing Hua University, **Taiwan**
- Workshop at Bogazici University, **Istanbul**
- **Gordon NMR Conference Lucca**
- **NMR & SAXS Workshop, Florence**
- **IWSG-Life 2011, London**
- **HealthGrid 2011, Bristol**
- **3DSIG - Structural bioinformatics and computational biophysics, Vienna**
- **Workshop at EUROMAR Conf., Frankfurt**

The Biomolecular NMR Training Center



We-NMR

Select a workshop:

NMR structure calculation - GRID applications and integrated tools

NMR structure calculation - GRID applications and integrated tools

The workshop „NMR structure calculation - GRID applications and integrated tools“ is a workshop that will be organized by the We-NMR consortium, and is a continuation of the successful e-NMR workshop series.



The world's leading research centers of excellence in the field of NMR structure calculation - GRID applications and integrated tools, from the e-NMR consortium, as Ccp4, AMBER, and GRID.



European Grid Infrastructure
Towards a sustainable grid infrastructure

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- Policy
- Infrastructure
- Publications
- Projects
- Collaborations

Training marketplace

[Home](#) > [User Support](#) > Training marketplace

The EGI Training Marketplace exists as a service. The Training Marketplace enables trainers to advert material and events that meet their needs.

[Return to Training Marketplace](#)

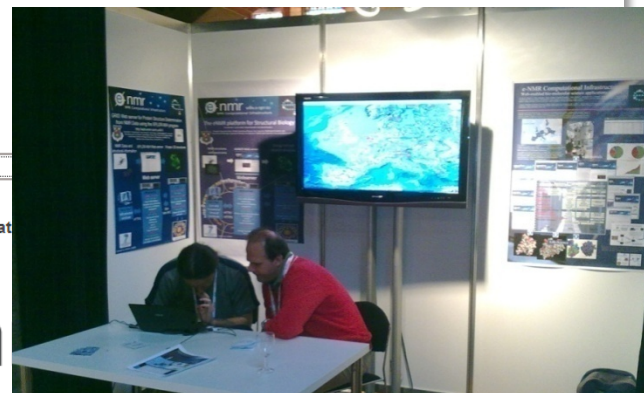
WeNMR Workshop -

Start: 2011-08-19 09:00

Timezone: Europe/Amsterdam

Abstract

The workshop „NMR applications on the Grid“ is Frankfurt and is organized by the WeNMR consortium. The workshop provides training on how to use some of the widely used processing and analysis to structure determinat integrated in WeNMR webportals. The program



The EGI blog
Behind the scenes of EGI

<< Web widgets for the EGI Community | Blog Home | Horizon 2020 - a new dawn for e-

A successful software workshop in Istanbul

The WeNMR project (see www.wenmr.eu) organized in June a [three days workshop](#) in Istanbul around the grid-enabled software HADDOCK. HADDOCK is an information-driven docking software for the modelling of biomolecular complexes which is made available to end users as a friendly and grid-enabled web portal (see <http://www.wenmr.eu/wenmr/modelling-software>).



The EGI blog
Behind the scenes of EGI

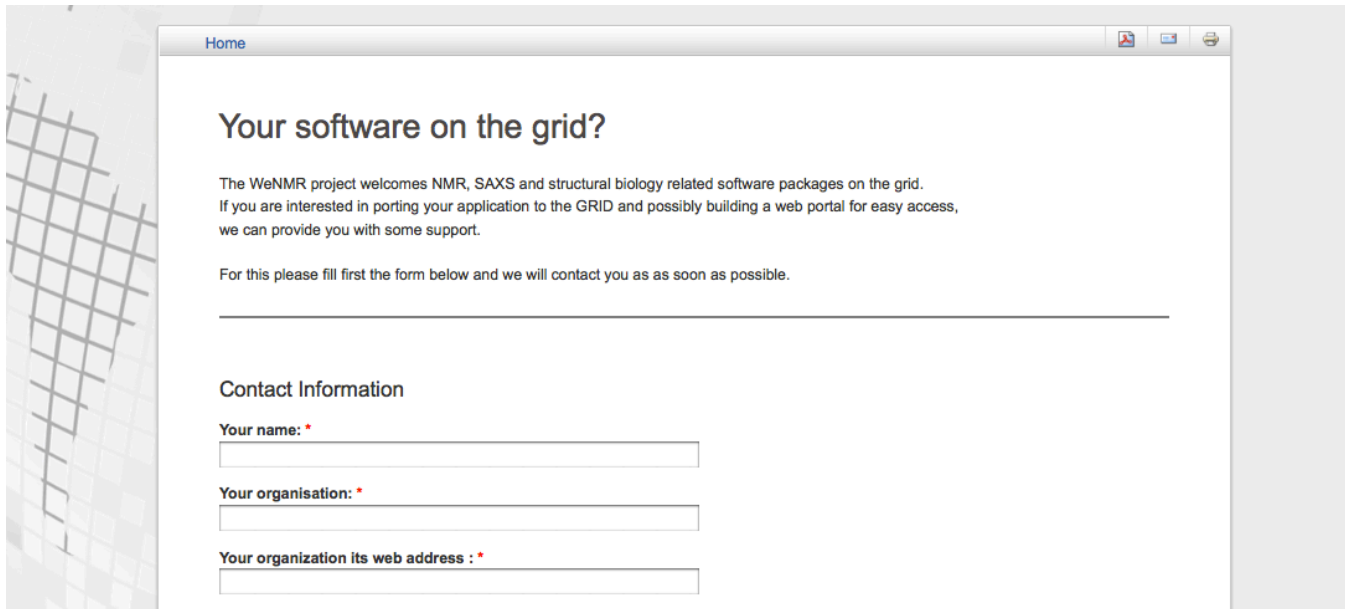
<< Horizon 2020 - a new dawn for e-Infrastructures? | Blog Home | User Community Board me

WeNMR developers workshop, Utrecht, NL

I was invited to take part in the WeNMR developers workshop held in the headquarters of this consortium at Utrecht, Netherlands. WeNMR was the first Virtual Research Community (VRC) to engage with EGI.eu, and soon after they became the largest community in the area of Life Sciences.

WeNMR Support center

- Support to software developers in the structural biology area to port their applications to the grid



The screenshot shows a web browser window titled "Home" with a grid pattern in the background. The main heading is "Your software on the grid?". Below this, the text reads: "The WeNMR project welcomes NMR, SAXS and structural biology related software packages on the grid. If you are interested in porting your application to the GRID and possibly building a web portal for easy access, we can provide you with some support. For this please fill first the form below and we will contact you as as soon as possible." Below the text is a horizontal line. Underneath, the section is titled "Contact Information" and contains three input fields: "Your name: *", "Your organisation: *", and "Your organization its web address : *".

- Consultancy services for third parties (e.g. web design, hosting, training, support, ... a SpronkNMR SME activity)

