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

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e-infrastructure

CAPACITIES

The Project

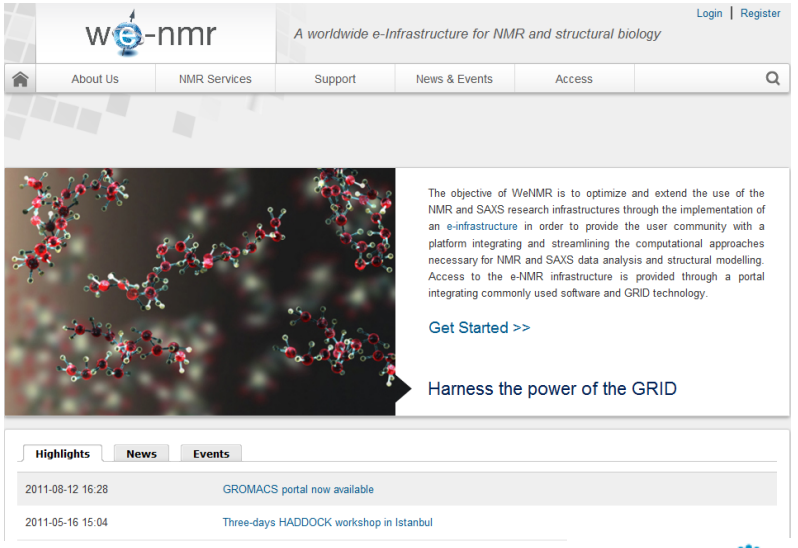
A Worldwide e-Infrastructure for NMR and structural biology

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

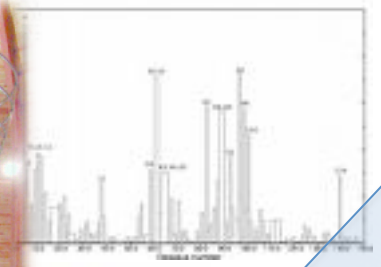


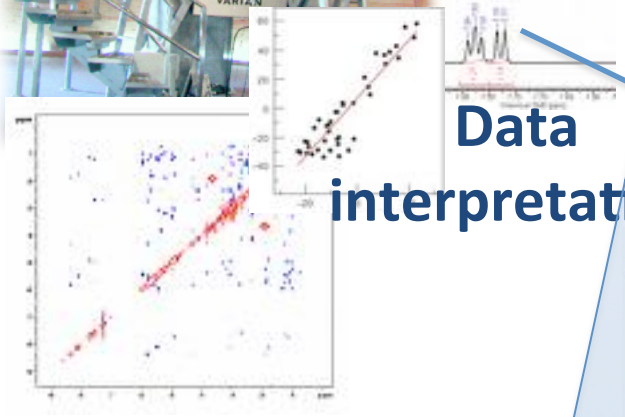
1st VRC recognized by EGI

Science Gateway → www.wenmr.eu

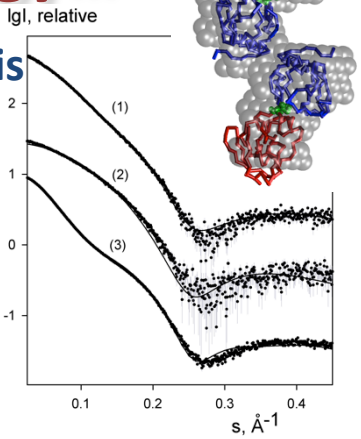
Exploiting GRID resources in structural biology…

NMR data collection and processing



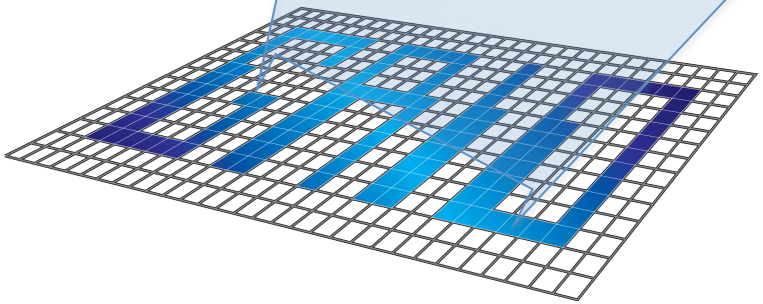


SAXS data analysis



Data interpretation

Computations



Structure, dynamics & interactions

➔ impact on research and health:

- origin of disease
- design of new experiments
- drug design…

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

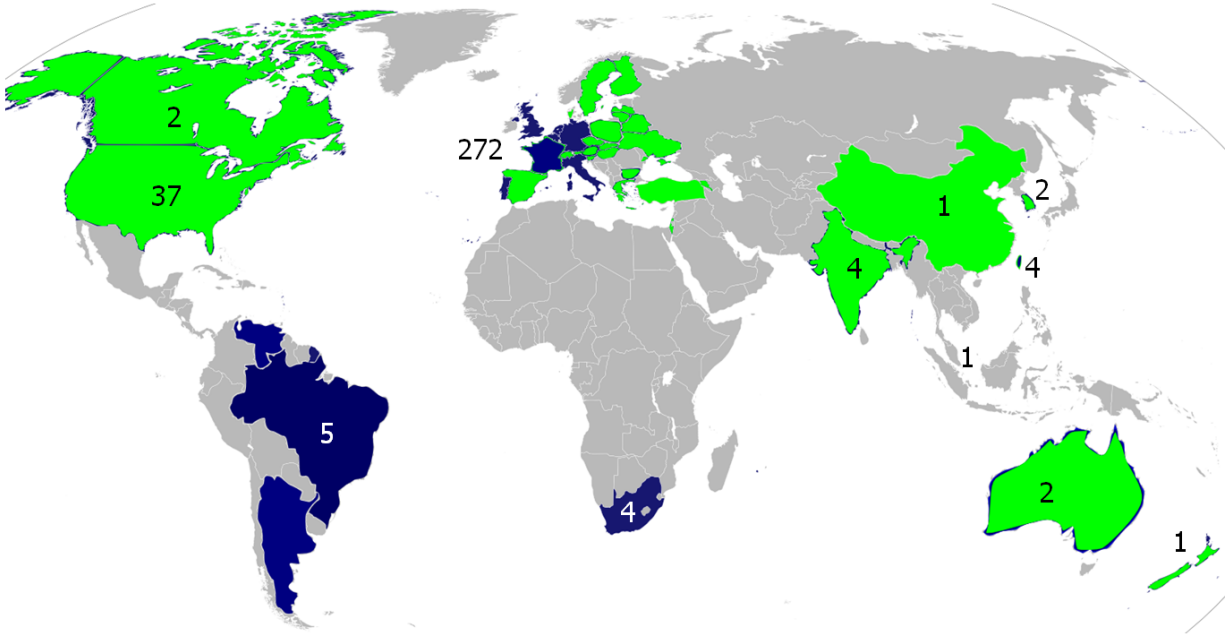
The project leverages on

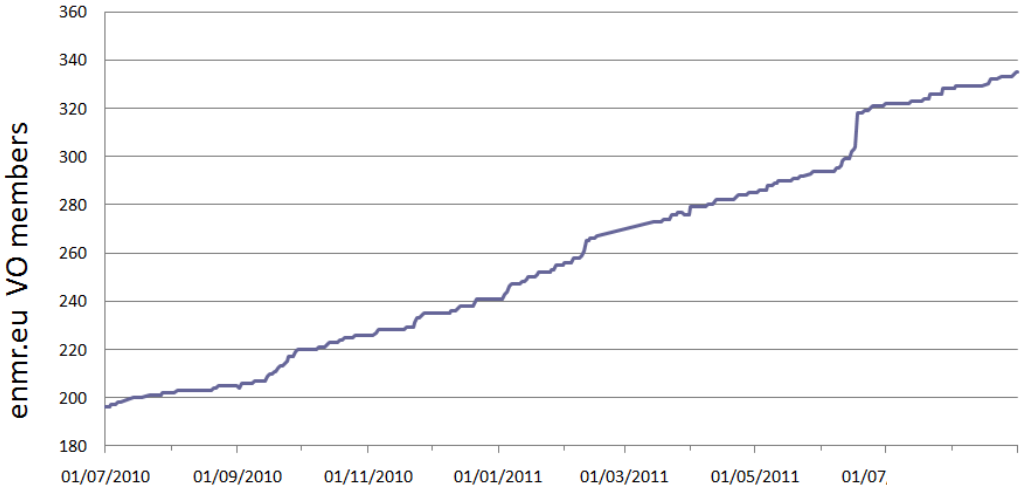
- **The previous eNMR e-Infrastructure project (FP7)**
- **EU-NMR (FP6)**
- **EAST-NMR (FP7) RI**
- **Bio-NMR (FP7) RI**

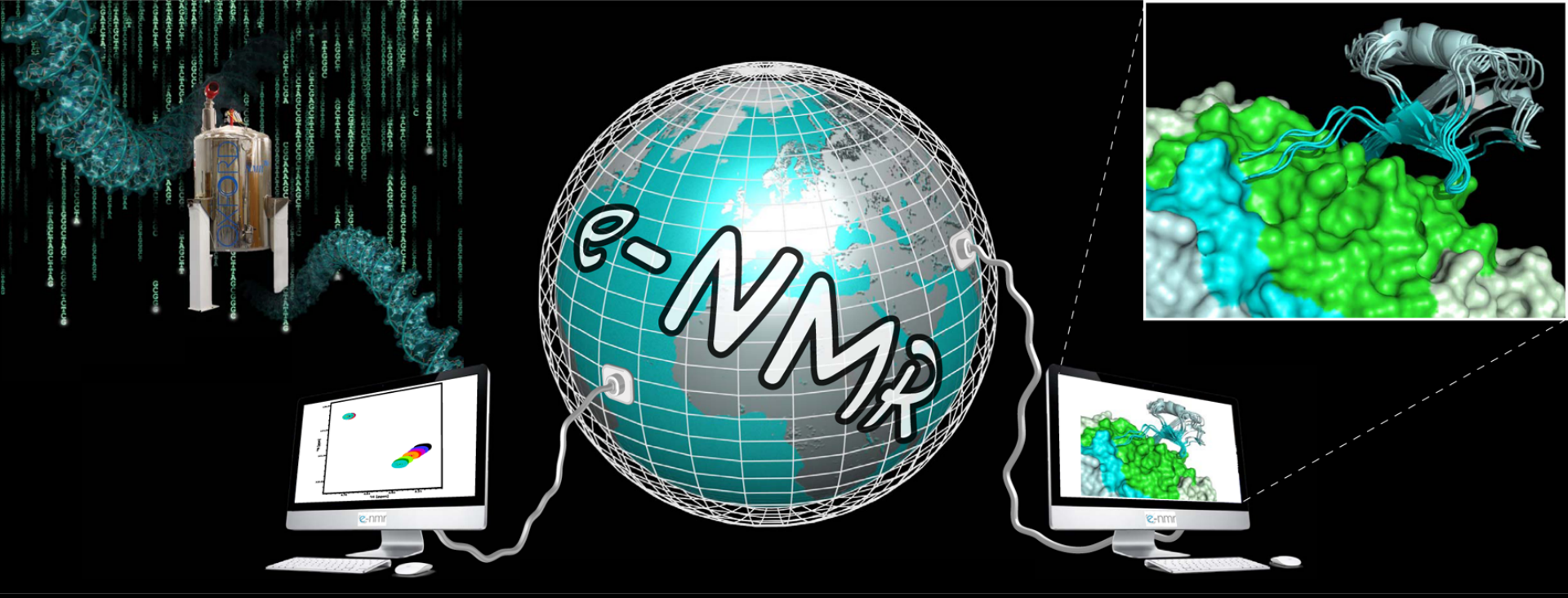
Linked to ESFRI INSTRUCT

Steady growth

~20% of users from outside Europe







WeNMR platform operational and well used!

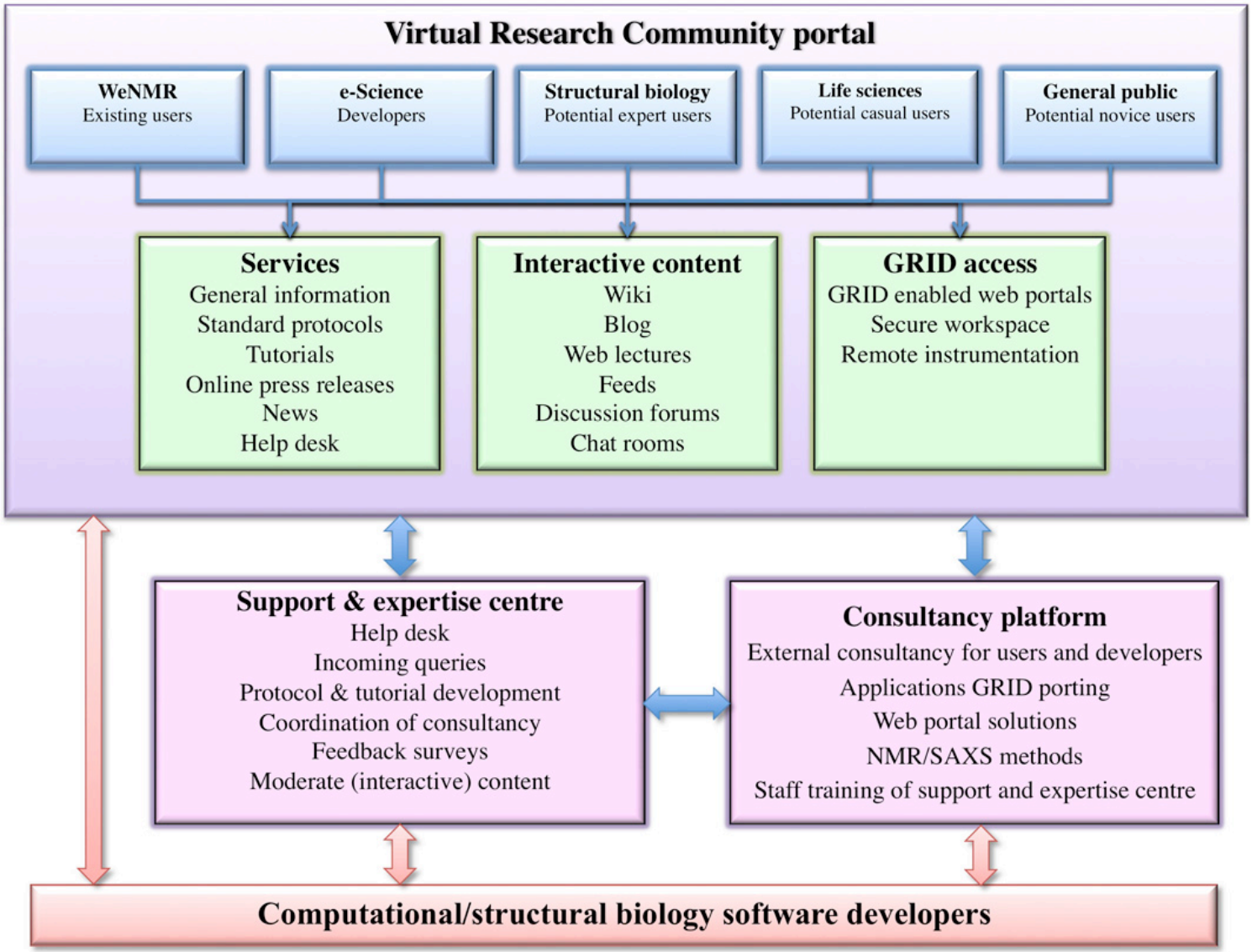
- Largest VO in the life sciences
- Over 338 registered users from 38 nationalities, and growing
- >33 000 CPUs
- >700 (normalized) CPU years over the last 12 months
- 1.4 million jobs over the last 12 months
- 150Tb of storage space
- ~20% of Life Sciences on the Grid
- User-friendly access to e-Infrastructure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

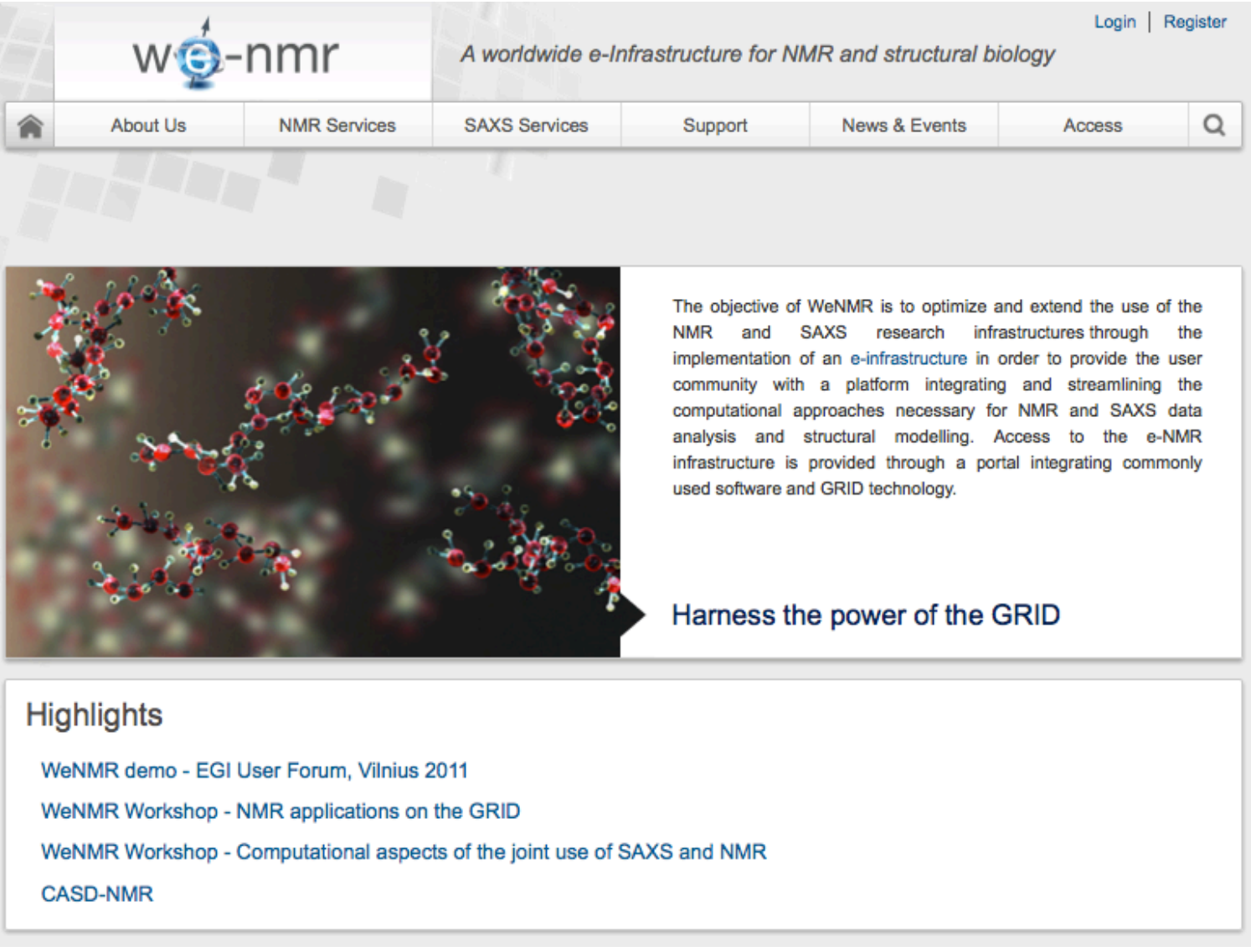
www.wenmr.eu

BiG Grid

The Virtual Research Community

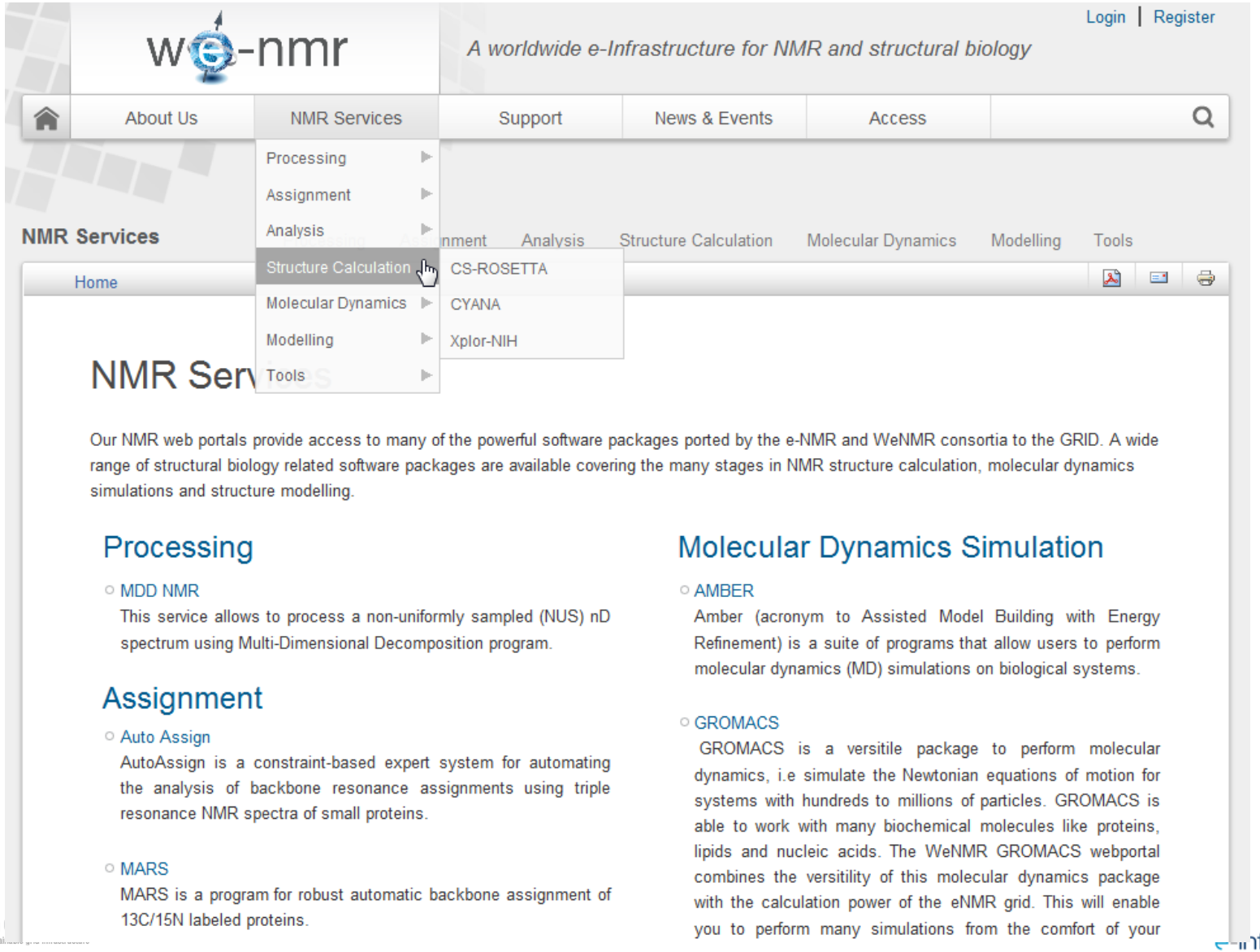
The VRC portal





The VRC portal: www.wenmr.eu

The WeNMR service portal



The WeNMR services portofolio

Recently deployed portals

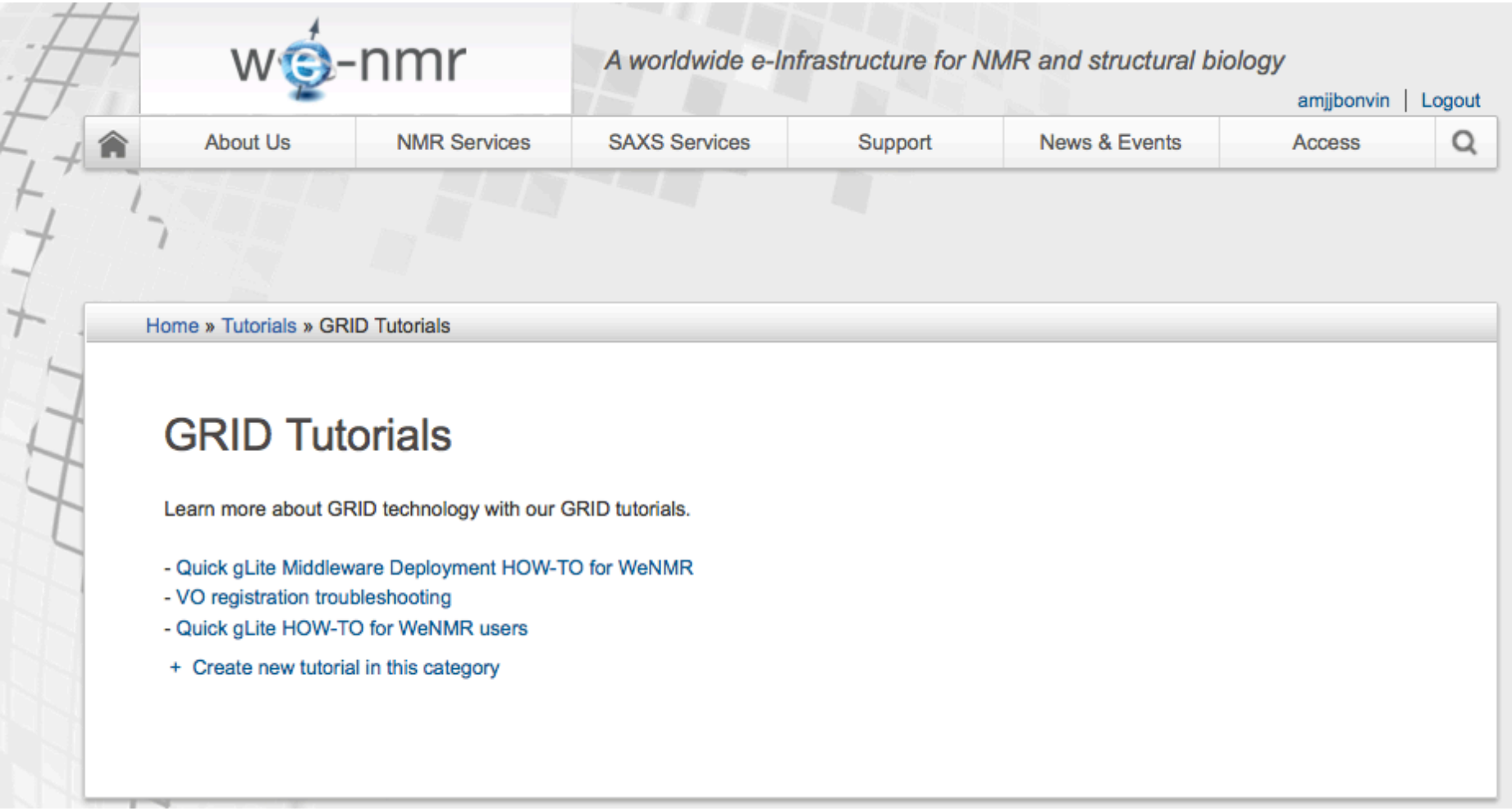
The VRC and the user community

- 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



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.

GGUS

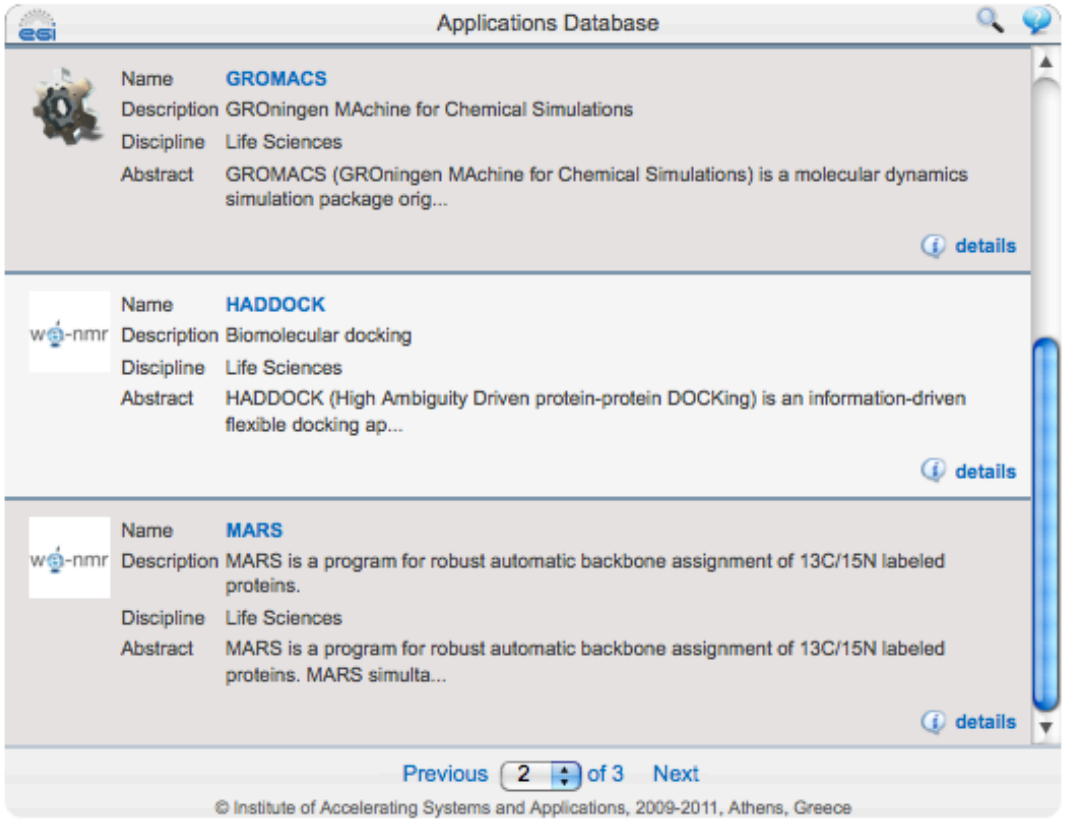
You can also provide general feedback to the EGI about requirements and recommendations from the WeNMR user community. The development of the European Grid Infrastructure is driven by the users, and thus your feedback is important to improve our services and to expand the infrastructure. You are invited 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

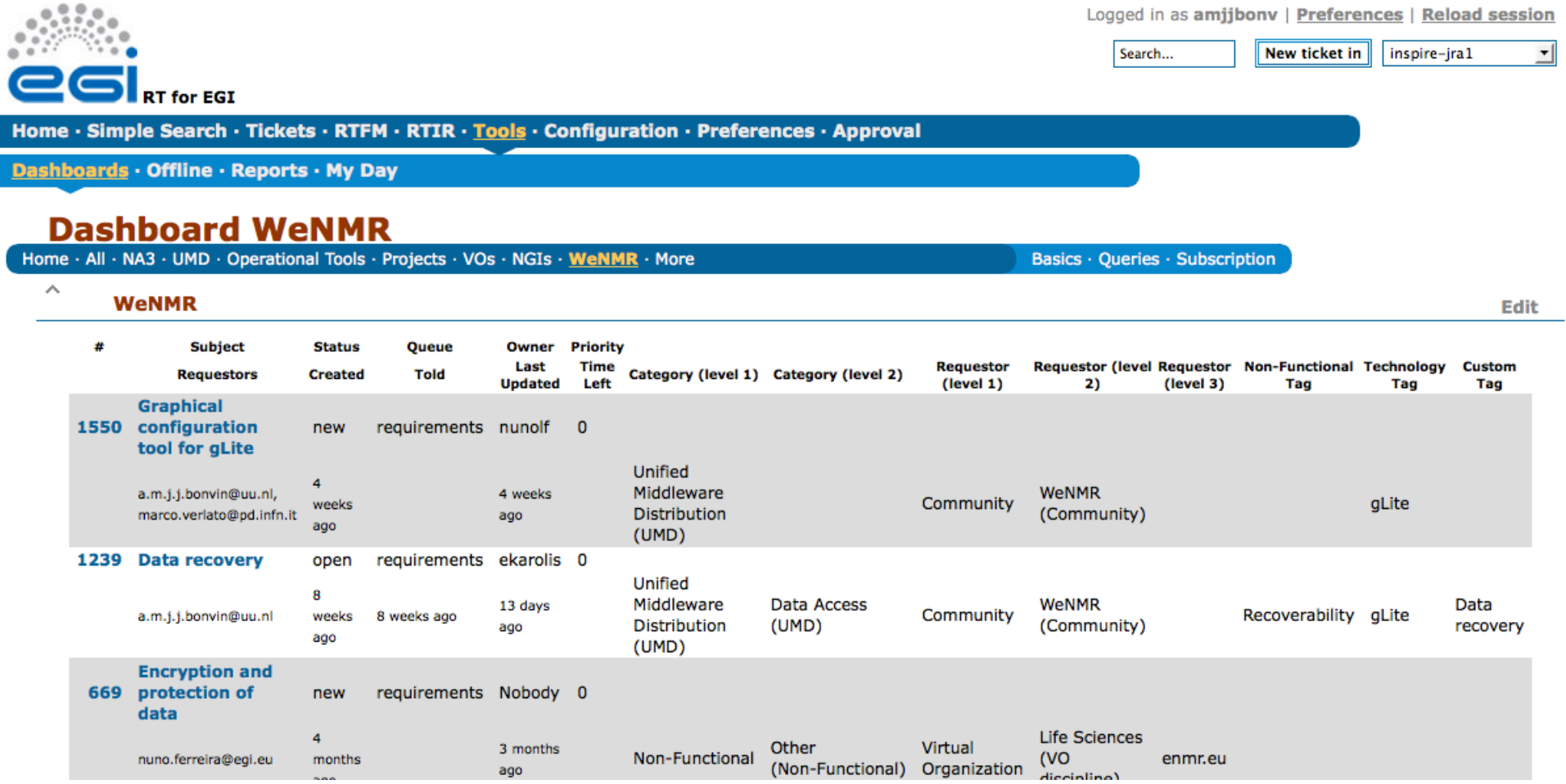
Applications



The 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



#	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	requirements	Nobody 3 months ago	0	Non-Functional	Other (Non-Functional)	Virtual Organization	Life Sciences (VO	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

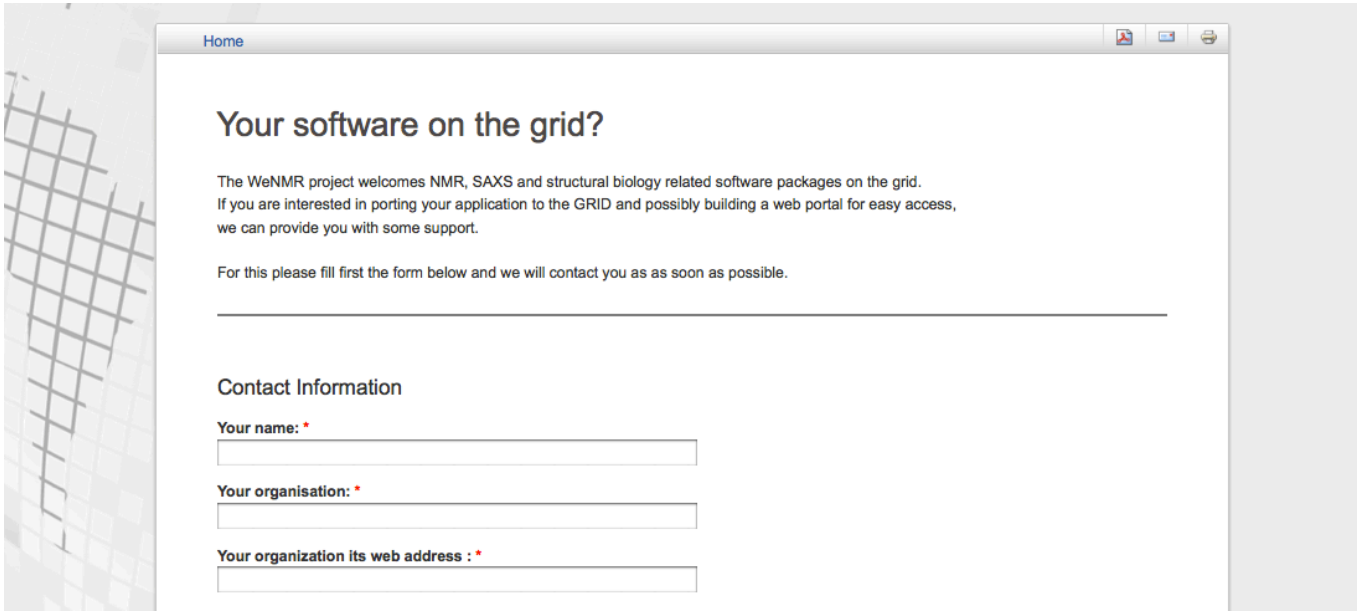
Training and dissemination

- **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**

WeNMR Support center

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



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


WeNMR
research
community
project
biology
worldwide
SAXS
communities
e-Infrastructure
structural
services
provide
activities
sciences
virtual
NMR
researchers
groups
initiatives
users
life
teams
large
number
general
established
infrastructure
scientific
operation
user
develop
access
offered
Grid
Research
well
within
global
eNMR
operate
consolidate
platform
establish
biological
sustainability
main
size
method
different
objectives
deployed
computational
infrastructures
Networking
experimental
web
exchange
existing
also
Gateway
growing
remote
new
use
serve
maintain
build
training
information
International
user-friendly
data
NA
portal
central
platforms
portals
aim
knowledge
communication
Joint
National
i.e
secure
tools
facilities
range
software
synchrotron
ensure
year
JRA
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aspects
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projects
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countries
GRID
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current
including
around
wide
public
involving
extend
limited
stakeholders
extensive
developers
European
Initiatives
interest
Service
variety

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