e-infrastructure

CAPACITIES

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

European Grid Infrastructure
Towards a sustainable grid infrastructure

User Forum 2011, Vilnius

e-infrastructure

CAPACITIES

A Worldwide e-Infrastucture for NMR and structural biology

Project Coordinator:
Prof. Alexandre M.J.J. Bonvin, Utrecht University, NL
a.m.j.j.bonvin@uu.nl

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

The team

Universiteit Utrecht

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

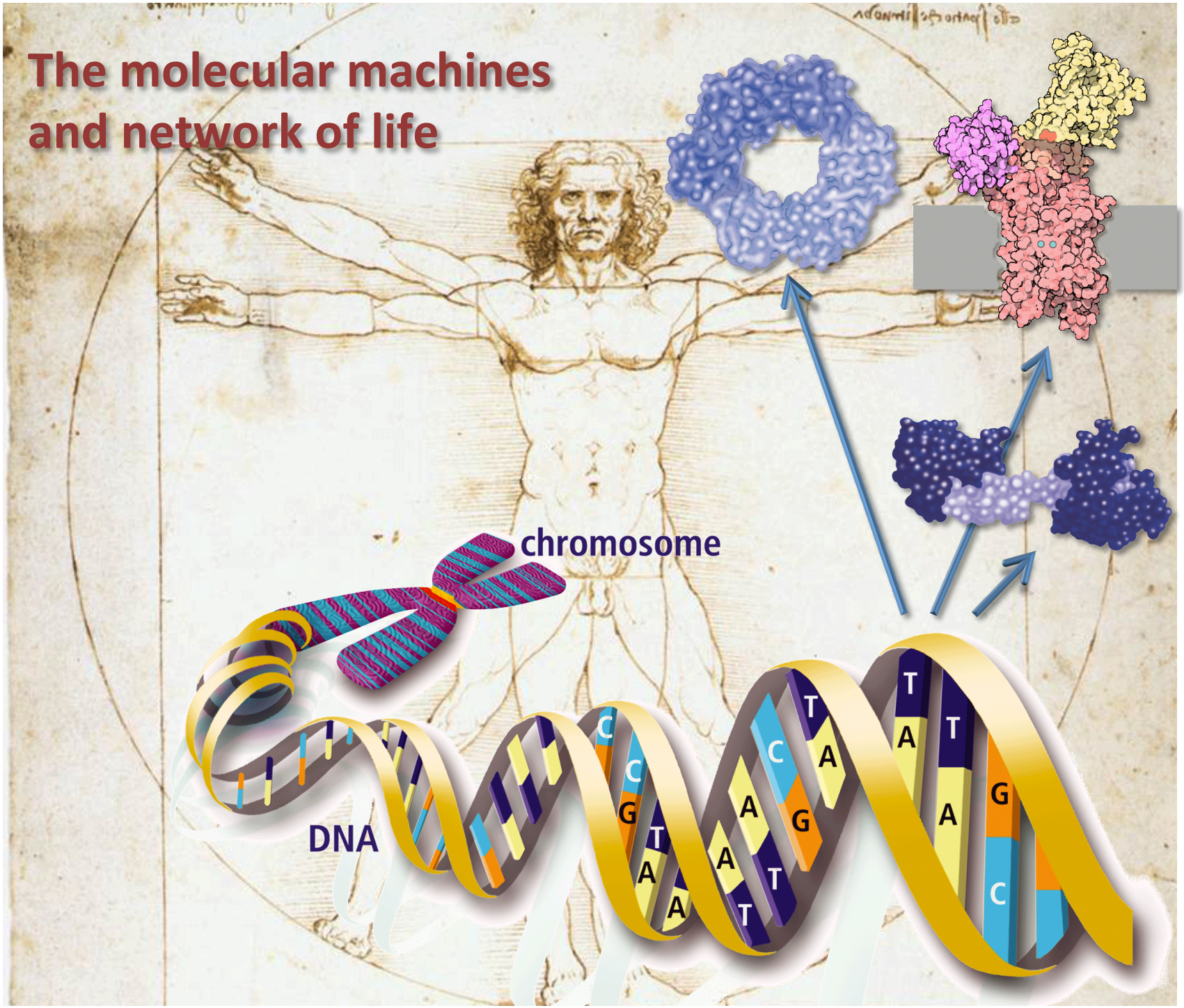
Raboud University, Nijmegen, NL

University of Cambridge UK

European Molecular Biology Laboratory, Hamburg, DE

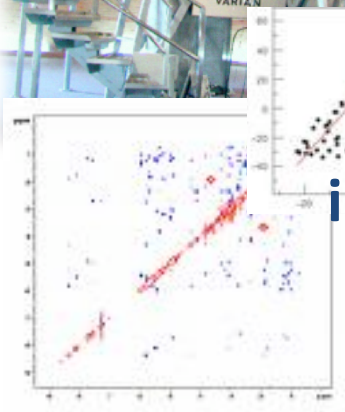
Spronk NMR Consultancy, LT

The molecular machines and network of life



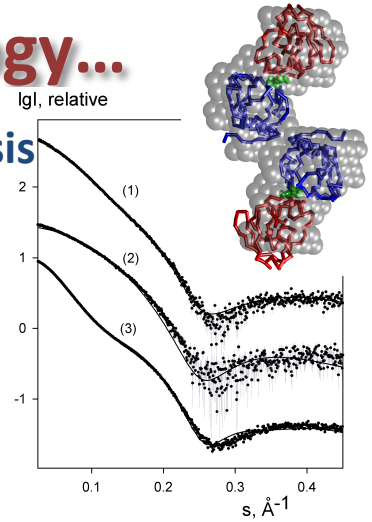
Exploiting GRID resources in structural biology…

NMR data collection and processing

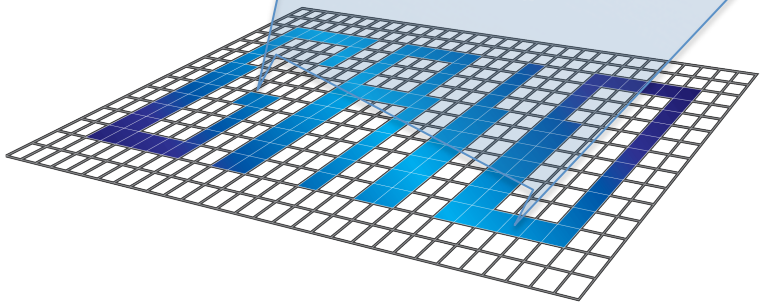


Data interpretation

SAXS data analysis



Computations



Structure, dynamics & interactions

➔ impact on research and health:

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

European Grid Infrastructure
Towards a sustainable grid infrastructure
e-infrastructure

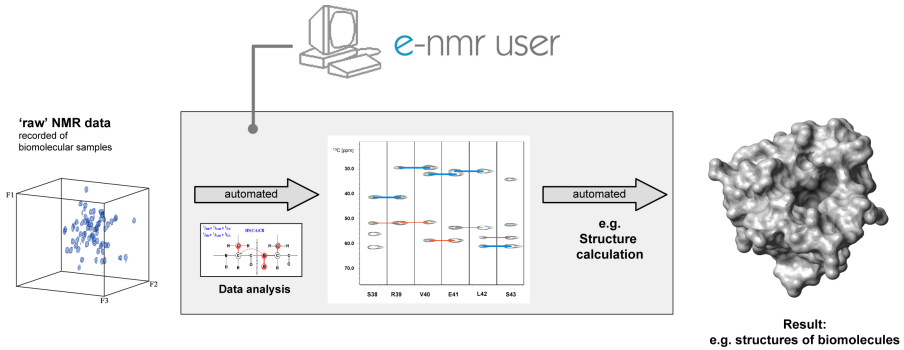
Main objectives

- Operate and further develop a user-friendly **e-Science gateway for the NMR and SAXS communities**
- 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

Builds upon the eNMR project

“Deploying and unifying the NMR e-Infrastructure in System Biology”

e-NMR allows researchers to enjoy all of the benef"its of bio-NMR with only minimal efforts for the set-up of data analysis & calculations.



The e-NMR web portal is accessible through the web and exploits GRID technology to provide users with high computational capacity and a secure protocol for access

The team:

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

University of Florence, Magnetic Resonance Center , Italy. Subcontractor: Spronk NMR, Vilnius, Lithuania

Utrecht University, The Netherlands- Bijvoet Center for Biomolecular Research. Subcontractor: CNRS Lyon

European Bioinformatics Institute, Hinxton, UK

Istituto Nazionale di Fisica Nucleare , Padova, Italy

e-infrastructure

WeNMR platform operational and well used!

- Largest global VO in the life sciences
- Over 280 registered users and growing
- >10000 CPUs
- >500 CPU years over the last 12 months
- ~20% of Life Sciences on the Grid
- User-friendly access to e-Infrastructure via web portals

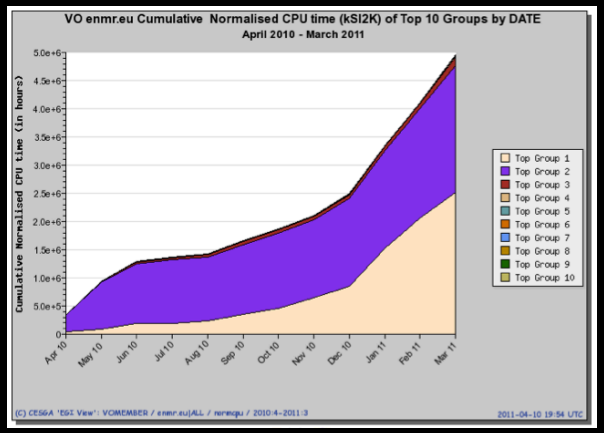
www.wenmr.eu

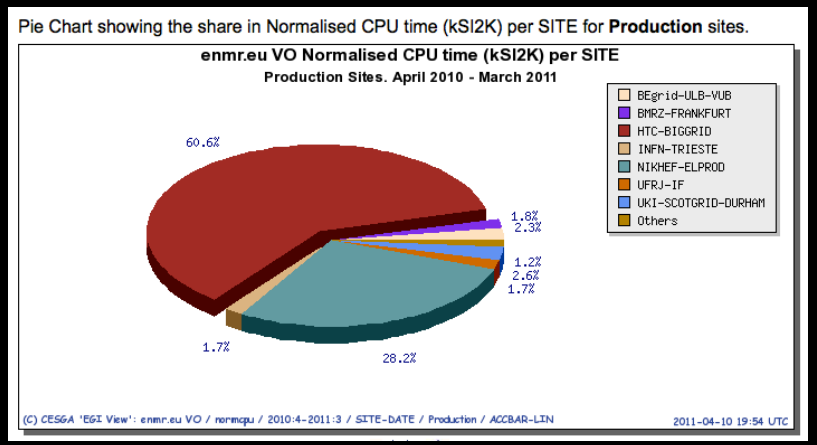
Some usage statistics

Top 10 Groups ordered by Normalised CPU time (kSI2K)														
Group/Role		Jobs		CPU time		*Norm. CPU time*		WCT		Norm. WCT		CPU Efficiency	Avg. CPU time	Avg. WCT
#	ID	#	%	Hrs	%	*Hrs*	*%*	Hrs	%	Hrs	%	%	Hrs	Hrs
1	/enmr.eu/csrosetta/Role=NULL	422,695	45.7%	1,212,683	28.4%	***2,514,876***	***50.8%***	1,237,578	28.6%	2,567,619	51.0%	98.0	2.87	2.93
2	/enmr.eu/Role=NULL	289,413	31.3%	2,982,580	69.7%	***2,244,978***	***45.3%***	2,995,670	69.3%	2,254,102	44.8%	99.6	10.31	10.35
3	/enmr.eu/haddock/Role=NULL	148,273	16.0%	64,840	1.5%	***154,340***	***3.1%***	68,891	1.6%	166,996	3.3%	94.1	0.44	0.46
4	/enmr.eu/amber/Role=NULL	2,821	0.3%	14,057	0.3%	***28,158***	***0.6%***	14,613	0.3%	29,257	0.6%	96.2	4.98	5.18
5	/enmr.eu/cyana/Role=NULL	34,745	3.8%	2,280	0.1%	***7,687***	***0.2%***	2,576	0.1%	8,681	0.2%	88.5	0.07	0.07
6	/enmr.eu/mddnmr/Role=NULL	15,635	1.7%	307	0.0%	***1,037***	***0.0%***	1,032	0.0%	3,477	0.1%	29.7	0.02	0.07
7	/enmr.eu/cns/Role=NULL	45	0.0%	308	0.0%	***595***	***0.0%***	313	0.0%	607	0.0%	98.4	6.84	6.96
8	/enmr.eu/mars/Role=NULL	130	0.0%	90	0.0%	***304***	***0.0%***	113	0.0%	380	0.0%	79.6	0.69	0.87
9	/enmr.eu /bcbr/Role=SoftwareManager	11,903	1.3%	160	0.0%	***131***	***0.0%***	507	0.0%	403	0.0%	31.6	0.01	0.04
10	/enmr.eu/gromacs/Role=NULL	5	0.0%	4	0.0%	***17***	***0.0%***	9	0.0%	29	0.0%	44.4	0.80	1.80
Total		**925,665**		**4,277,309**		***4,952,123***		**4,321,302**		**5,031,551**		**99.0**	**4.62**	**4.67**

Click here for a csv dump of this table

Key: 0% <= eff < 50%; 50% <= eff < 60%; 60% <= eff < 75%; 75% <= eff < 90%; 90% <= eff < 100%; eff >= 100% (parallel jobs)



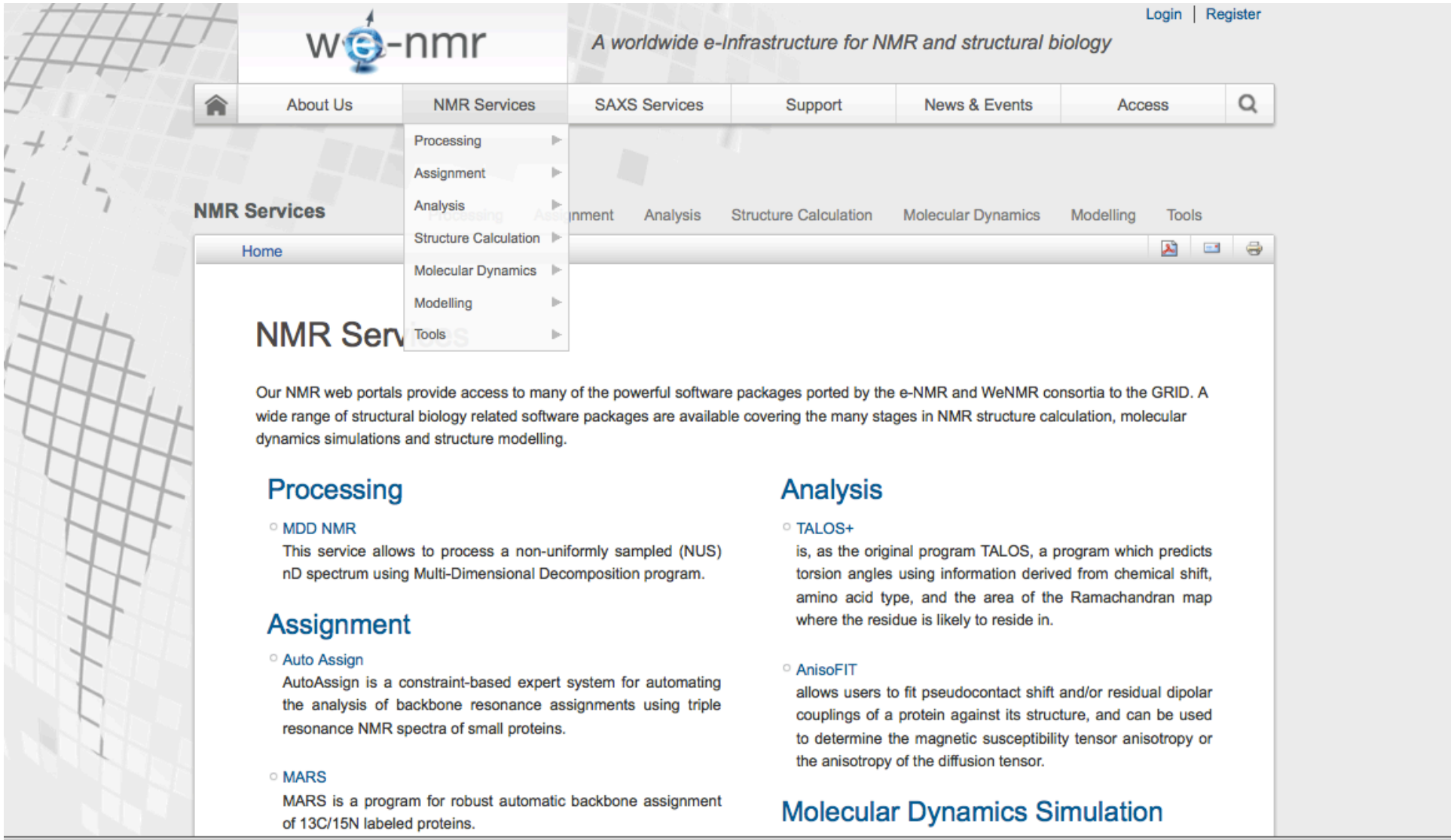


BiG Grid

The WeNMR philosophy for interacting with the Grid

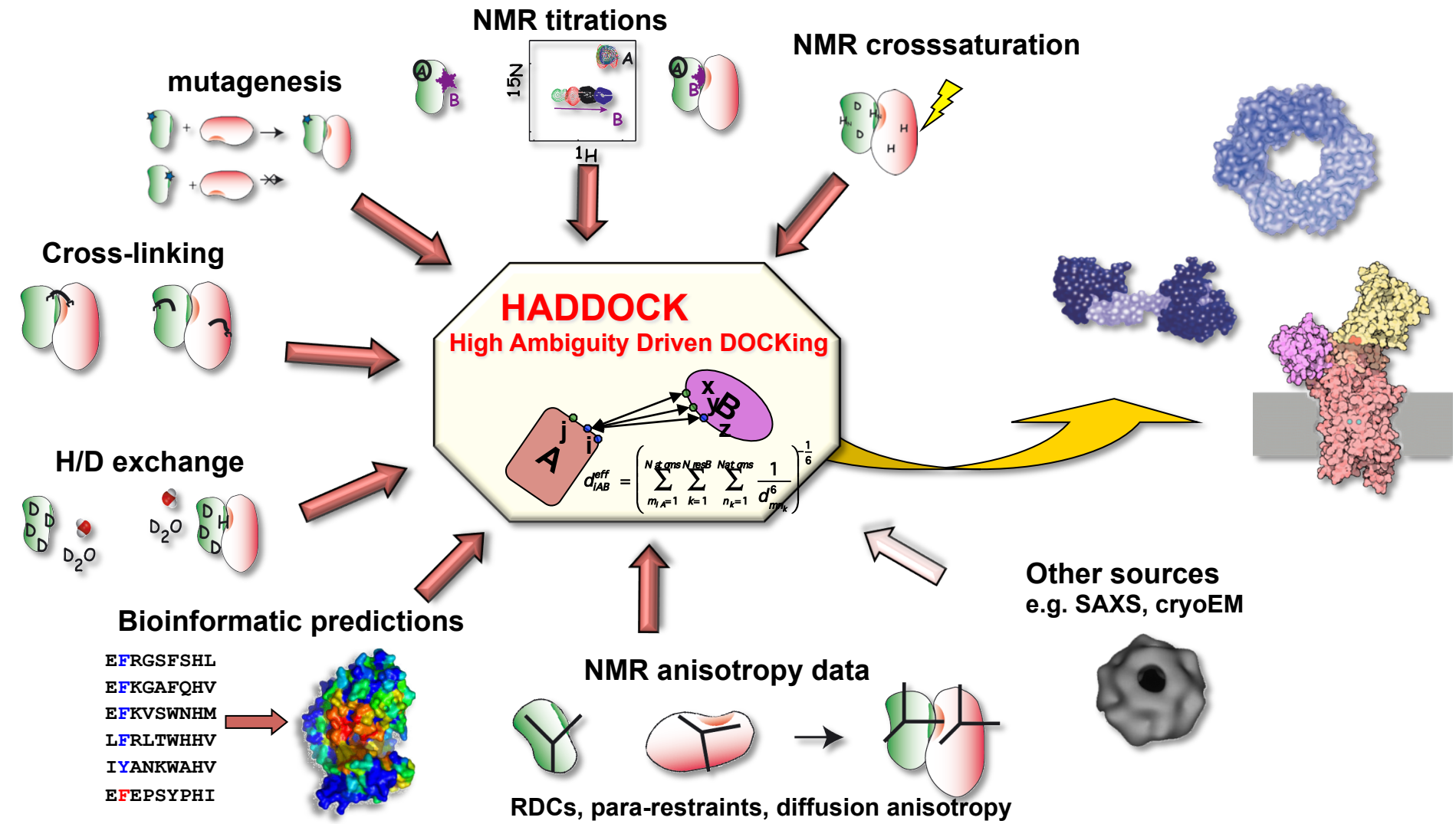
- Our policy is to shield as much as possible the end user from the Grid and all middleware related issues and commands.
- For this, we chose to develop mainly web portal providing "protocolized" access to the Grid
- To facilitate operation, we use when possible robot certificates
- Experienced users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

The WeNMR service portal



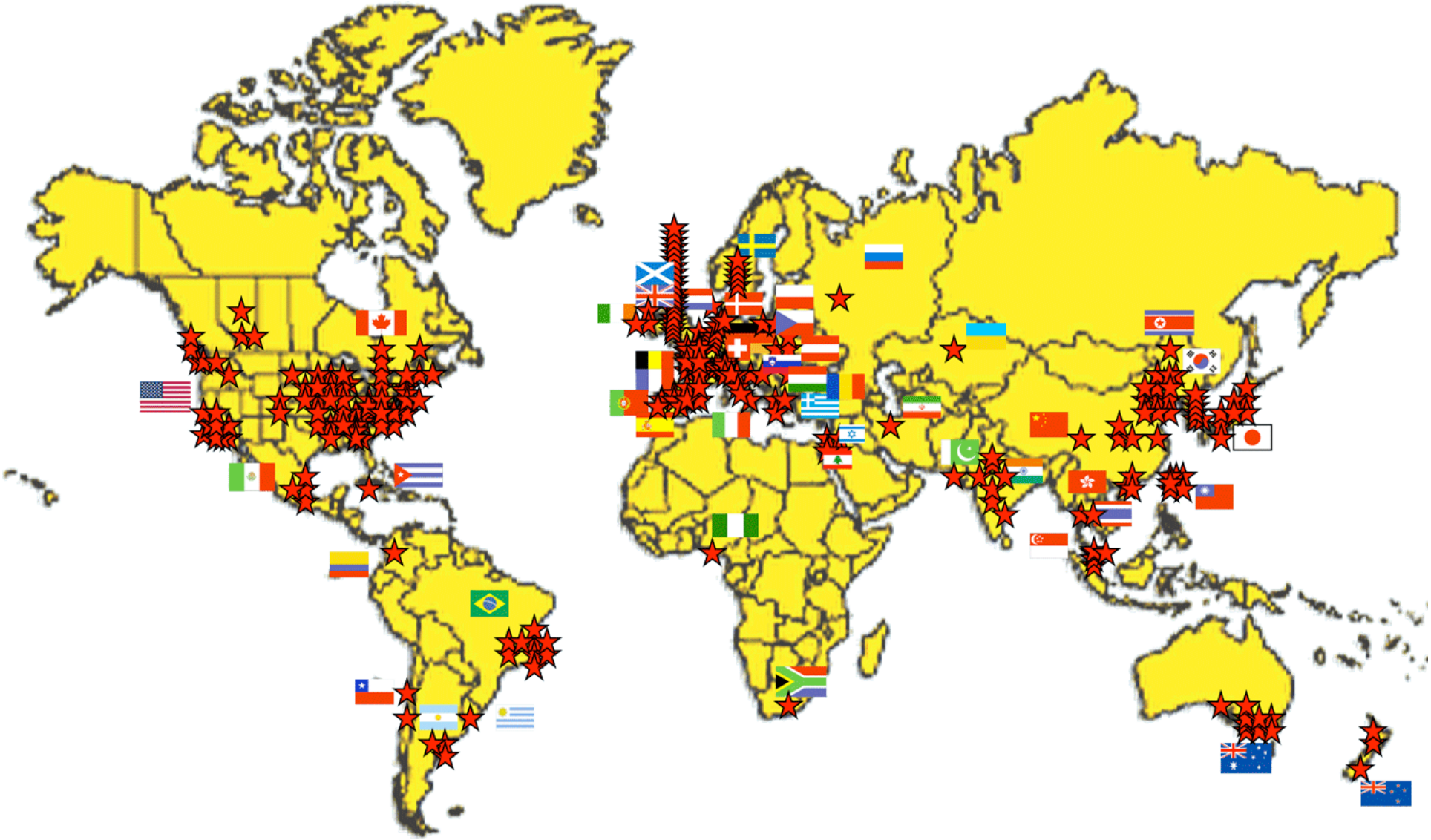
CS-ROSETTA
e-NMR GRID-enabled web portal
TALOS
e-NMR (GRID-enabled) web p
MDD
Web Portal
AMBER
e-NMR GRID-enable
Xplor-NIH
e-NMR GRID-enabled web portal
MARS
Web Portal
CCPN format converter
e-NMR web portal
AutoAssign
Web Portal
CCPN
NMR FormatConverter
3DDART
e-NMR (GRID-enabled) web portal
Cyana
Web Portal
HADDOCK
e-NMR GRID-enabled

Data-driven HADDOCKing

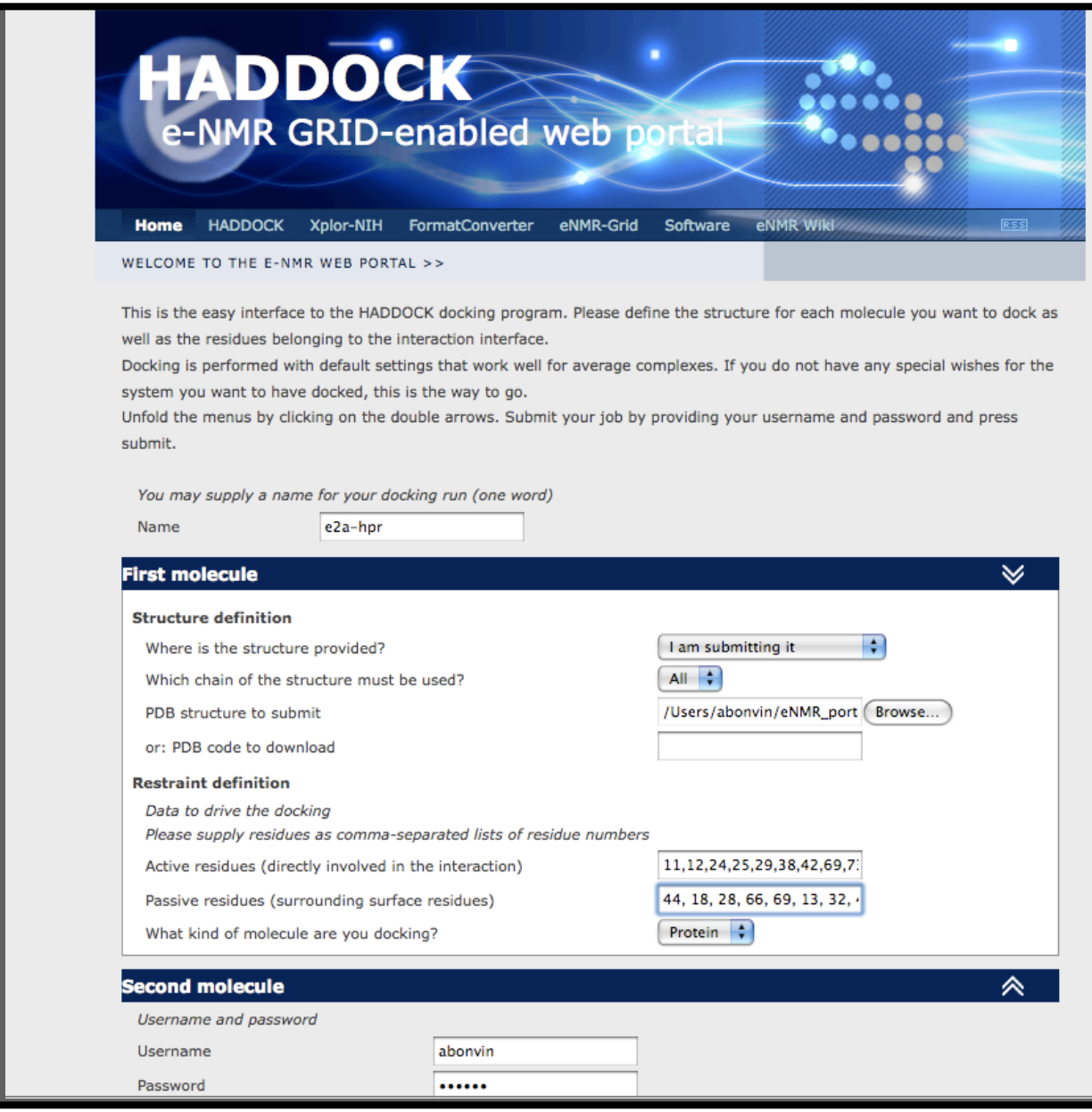


Dominguez, Boelens & Bonvin. *JACS* 125, 173 (2003).

HADDOCK world map



User friendly easy interface

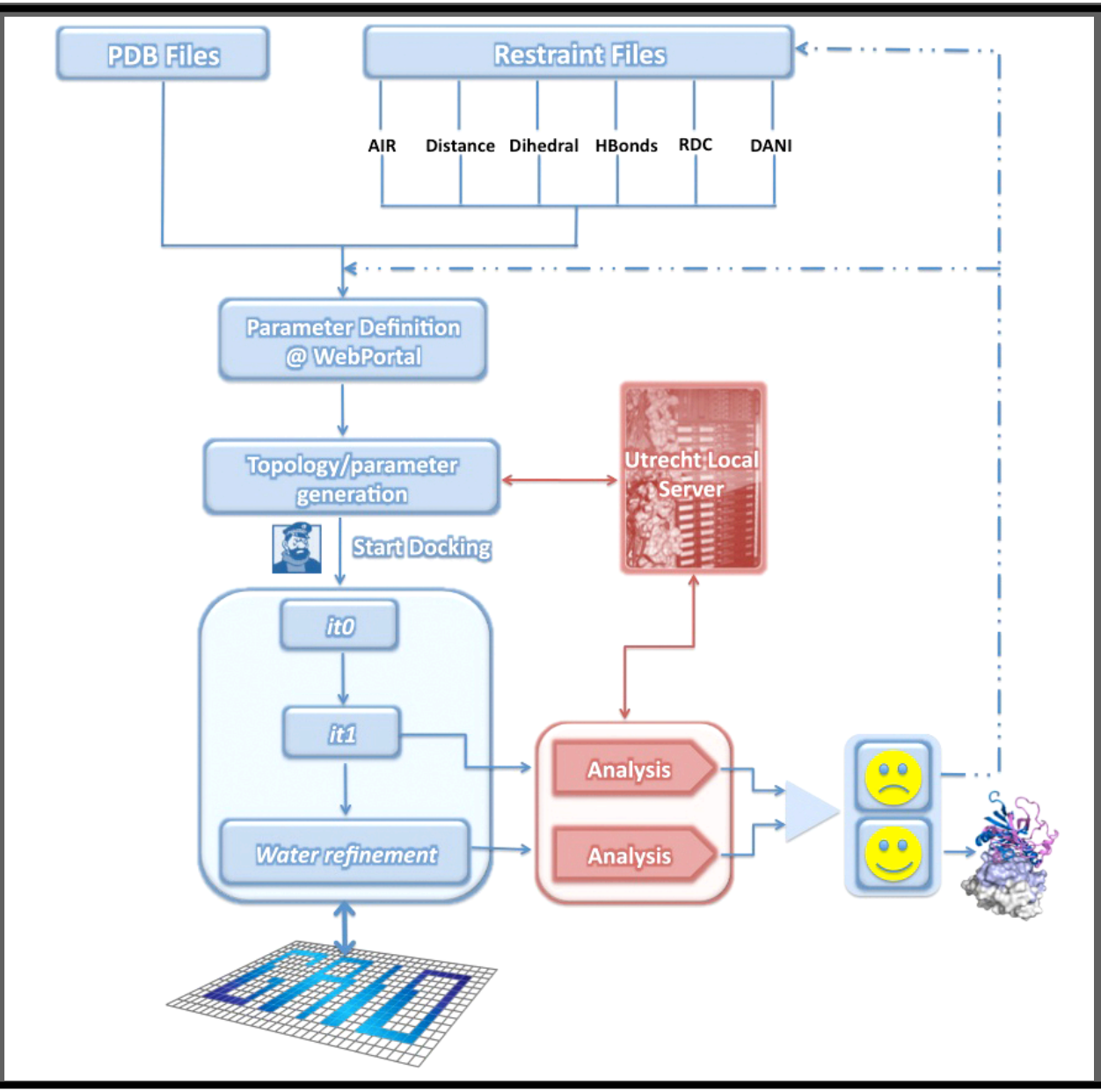


~ 1400 registered users

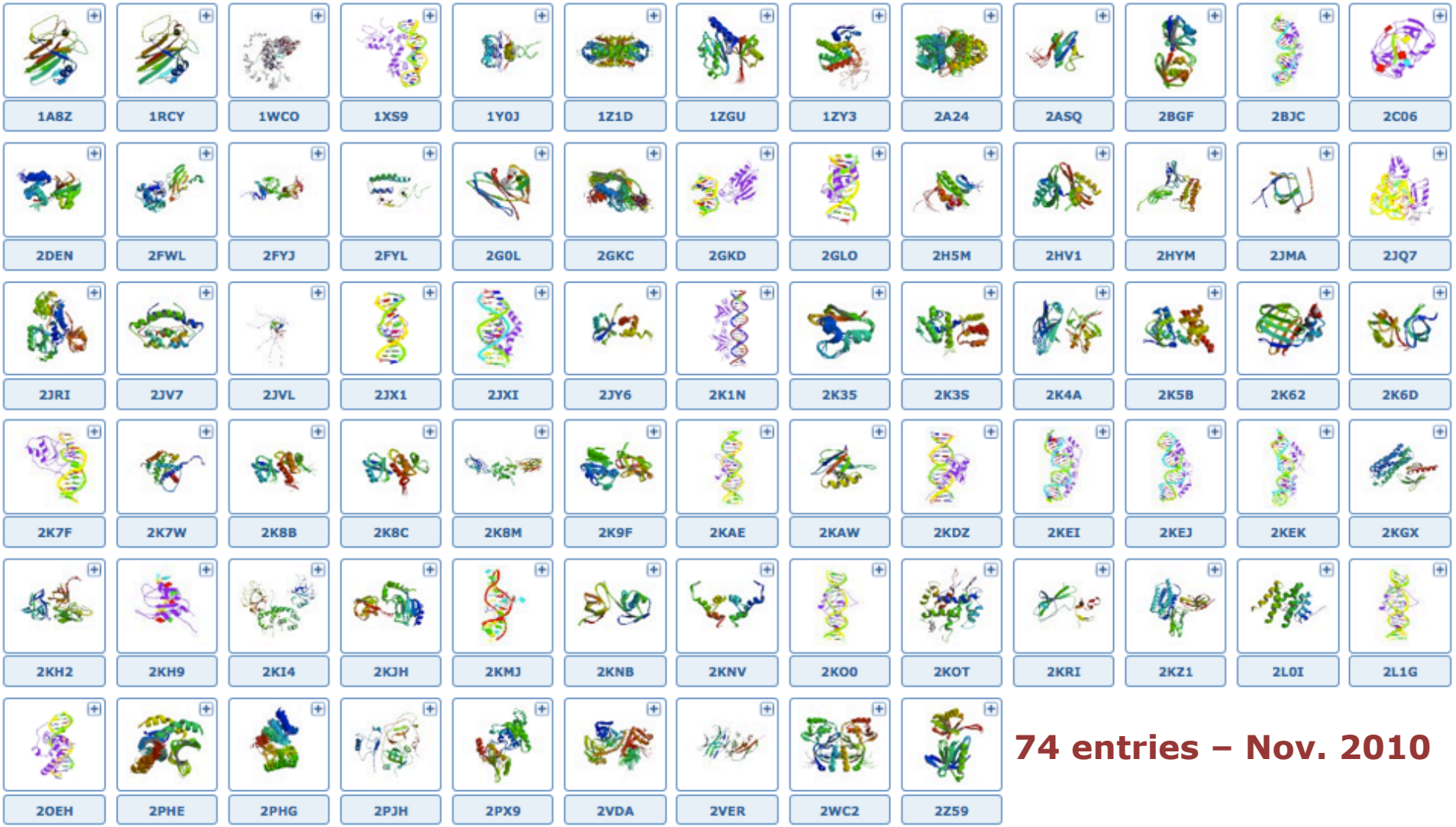
> 15500 served runs since June 2008

~ 7.5% on the GRID

What is happening behind the scene?



The HADDOCK PDB structure gallery

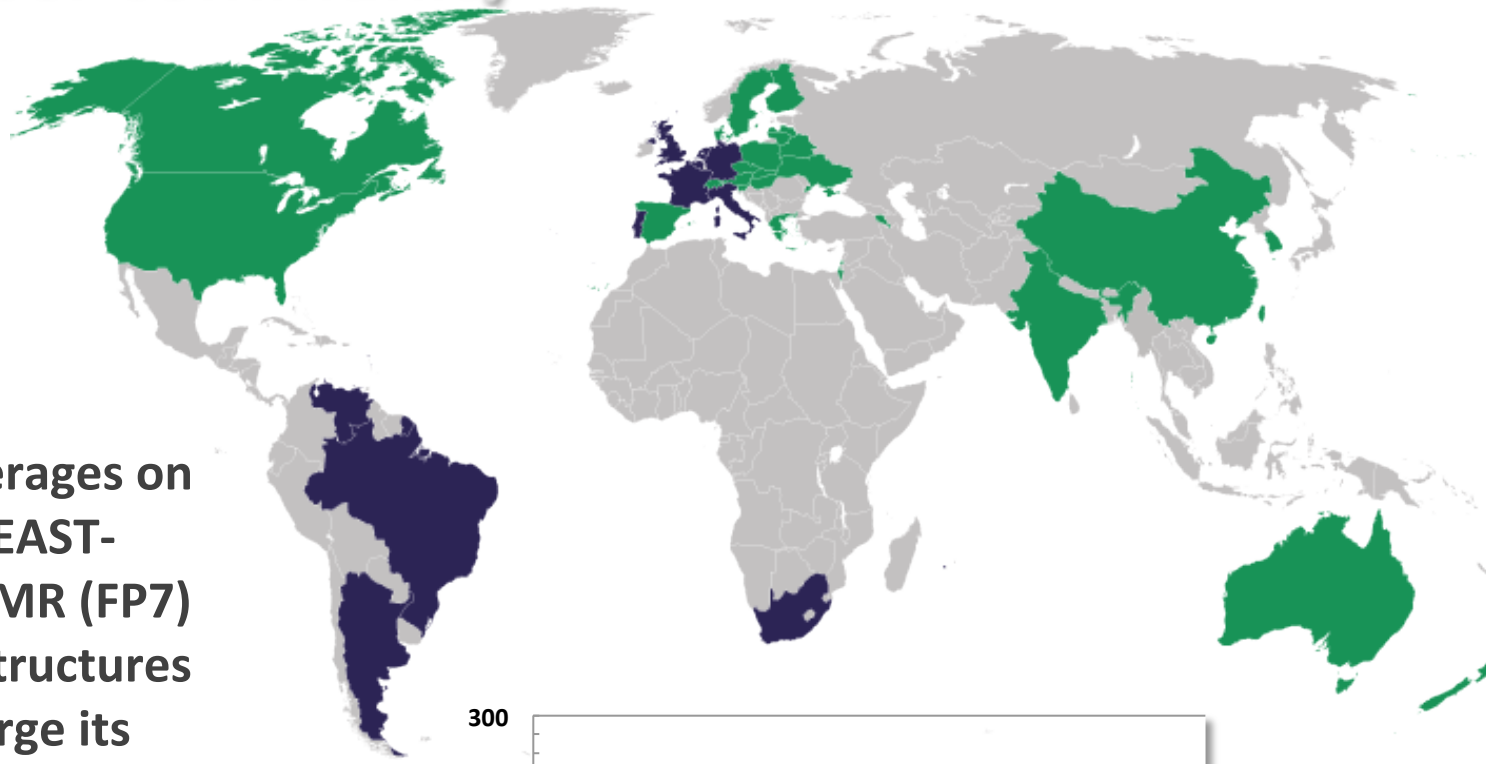


74 entries – Nov. 2010

Image collage from http://www.pdb.org

The User Community

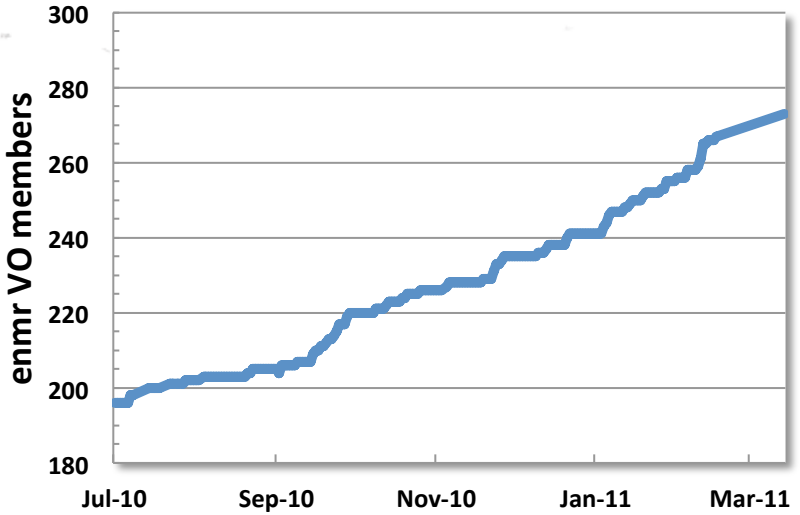
The User community



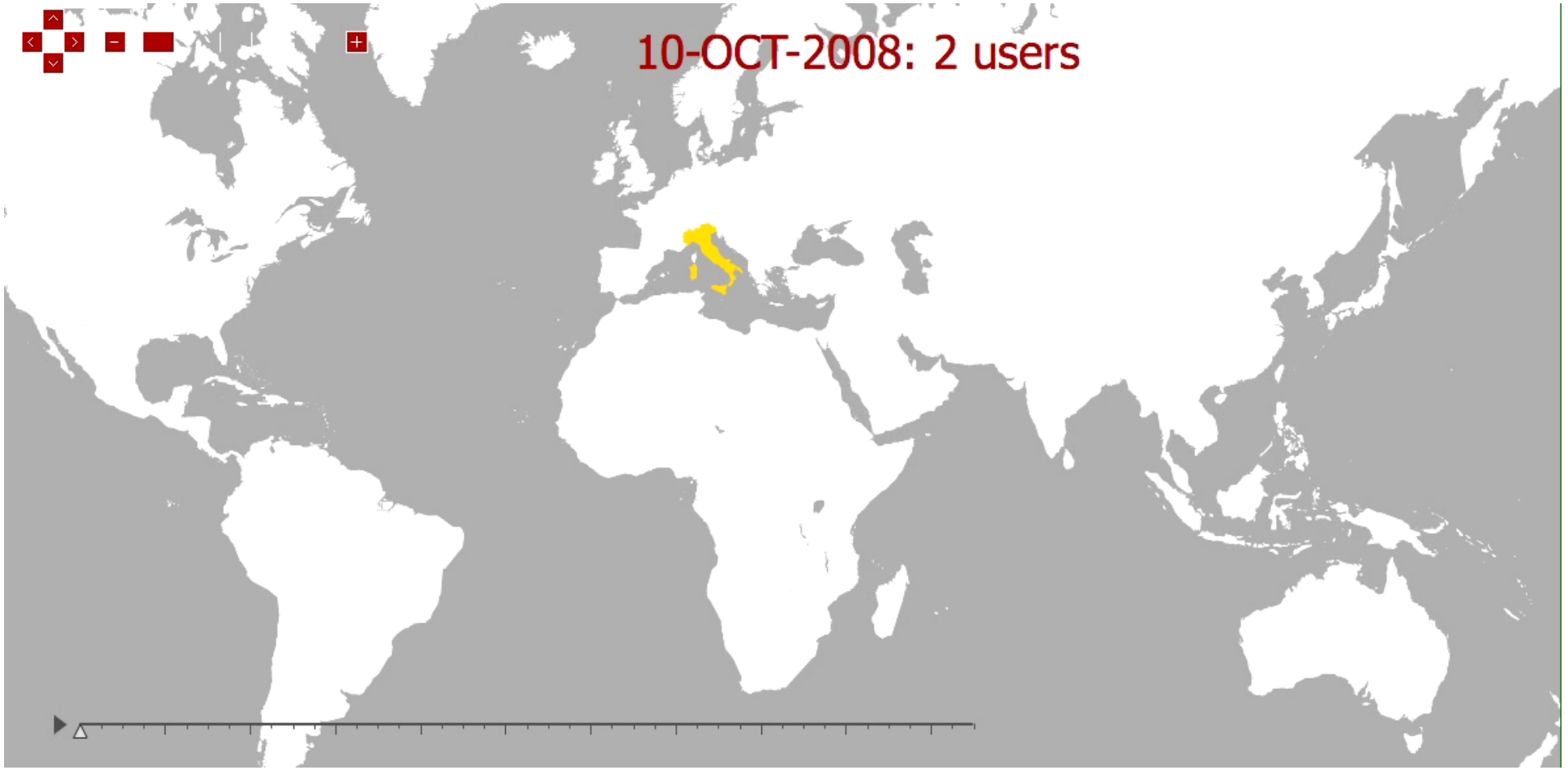
The project leverages on EU-NMR (FP6), EAST-NMR, and BioNMR (FP7) Research Infrastructures projects to enlarge its users basis

Linked to Instruct (ESFRI)

To date: >280 VO members, >14% outside Europe

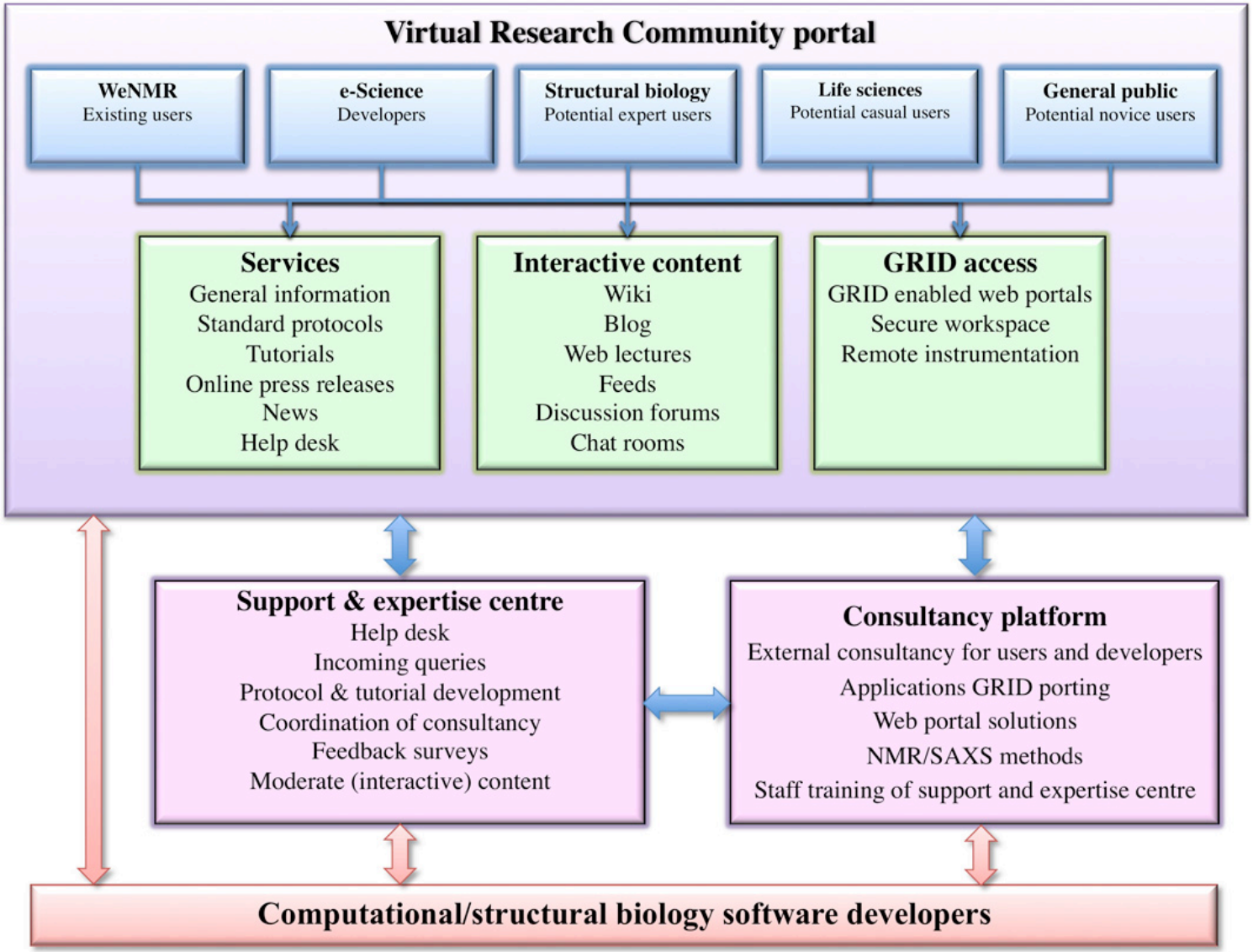


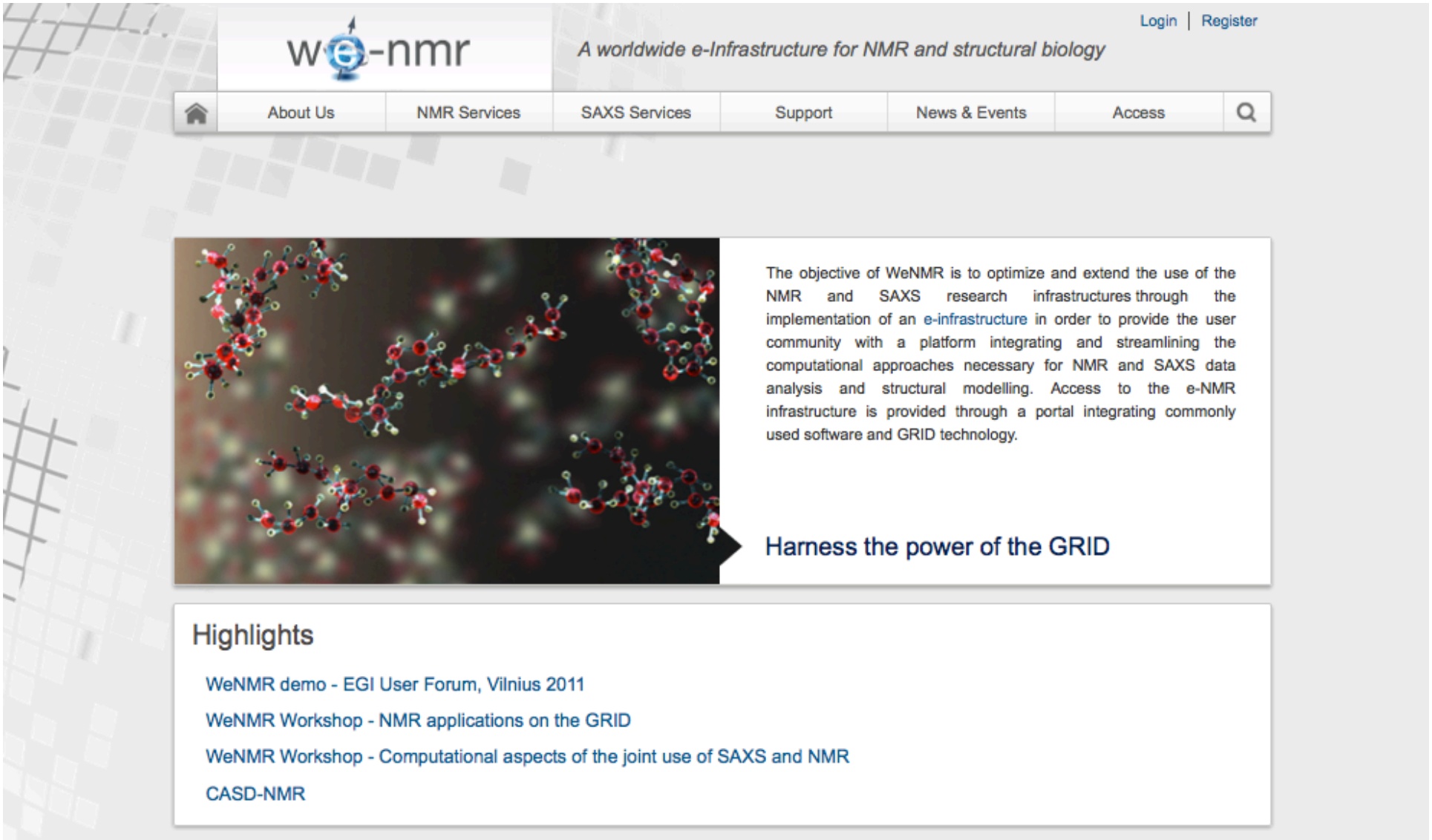
The User community over the last 3 years



The VRC

The VRC portal





The VRC portal: www.wenmr.eu

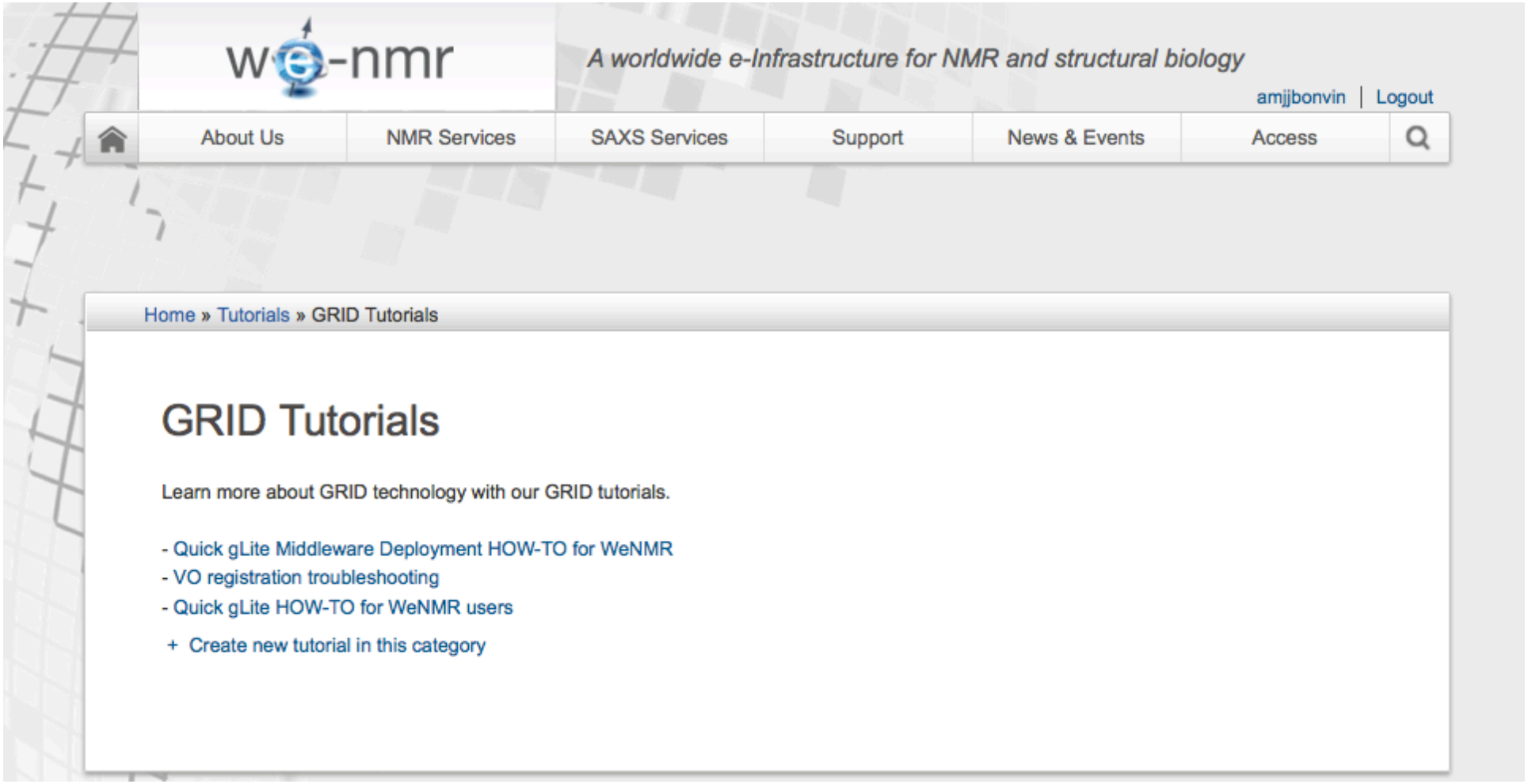
The VRC and the user community

- 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

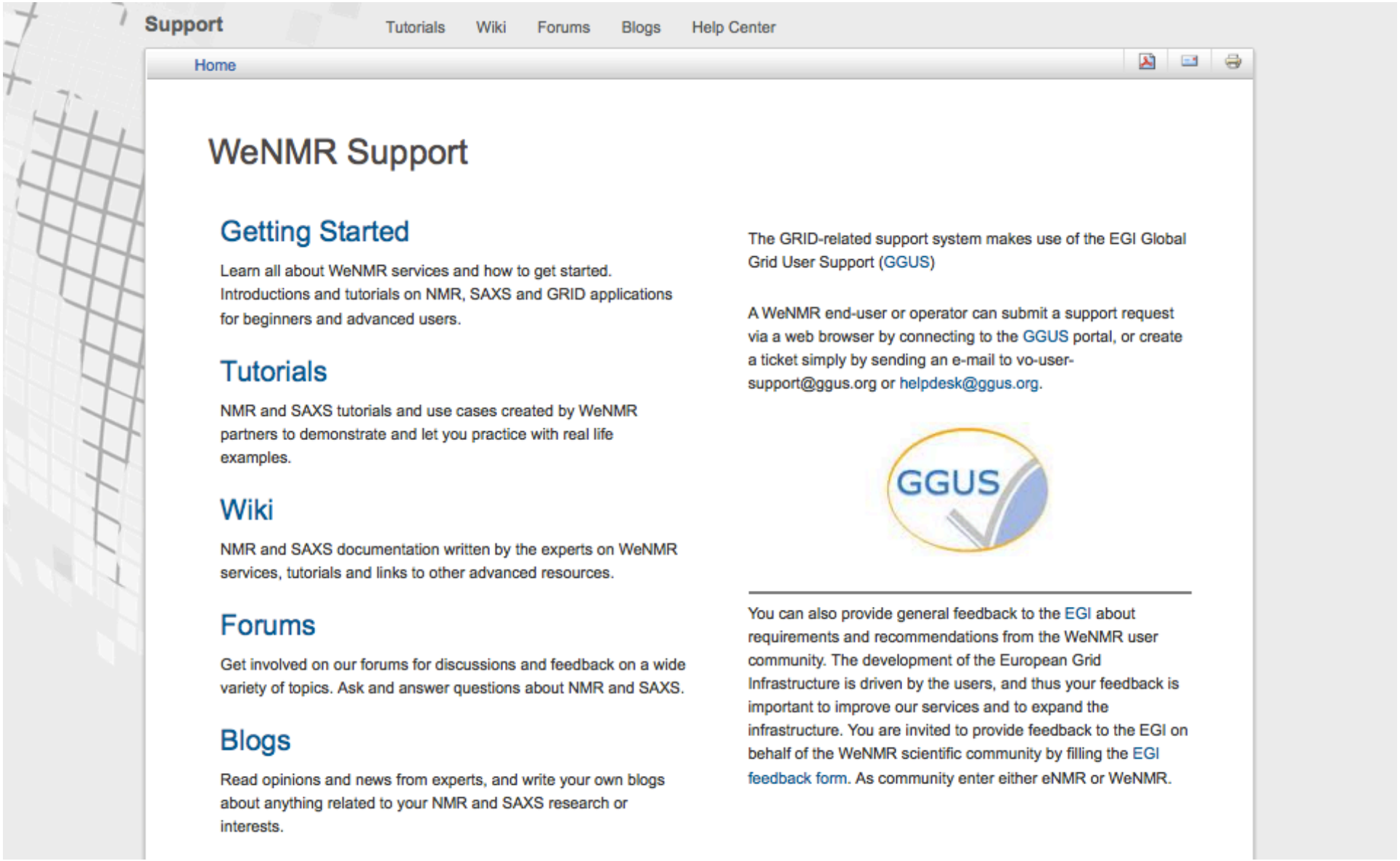
The VRC and the GRID



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



The VRC and the GRID

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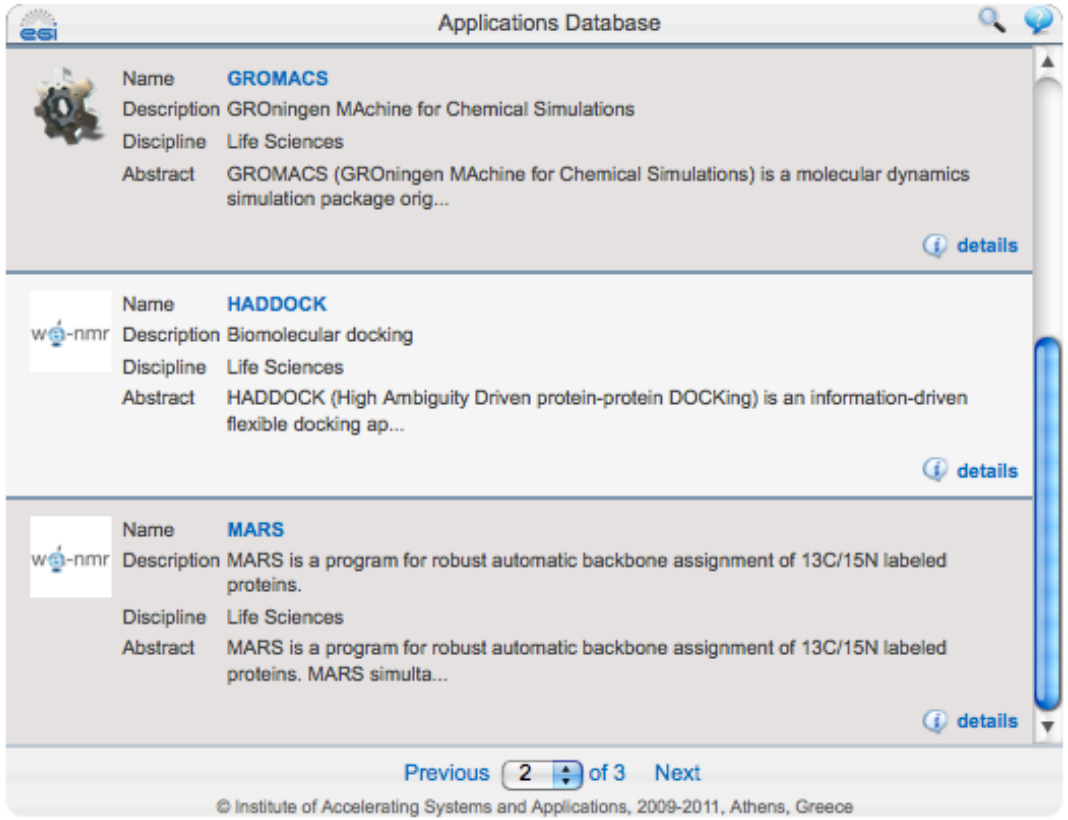
- Interface to GGUS
- **Application database applet from EGI embedded in our web portal**

The VRC and the GRID

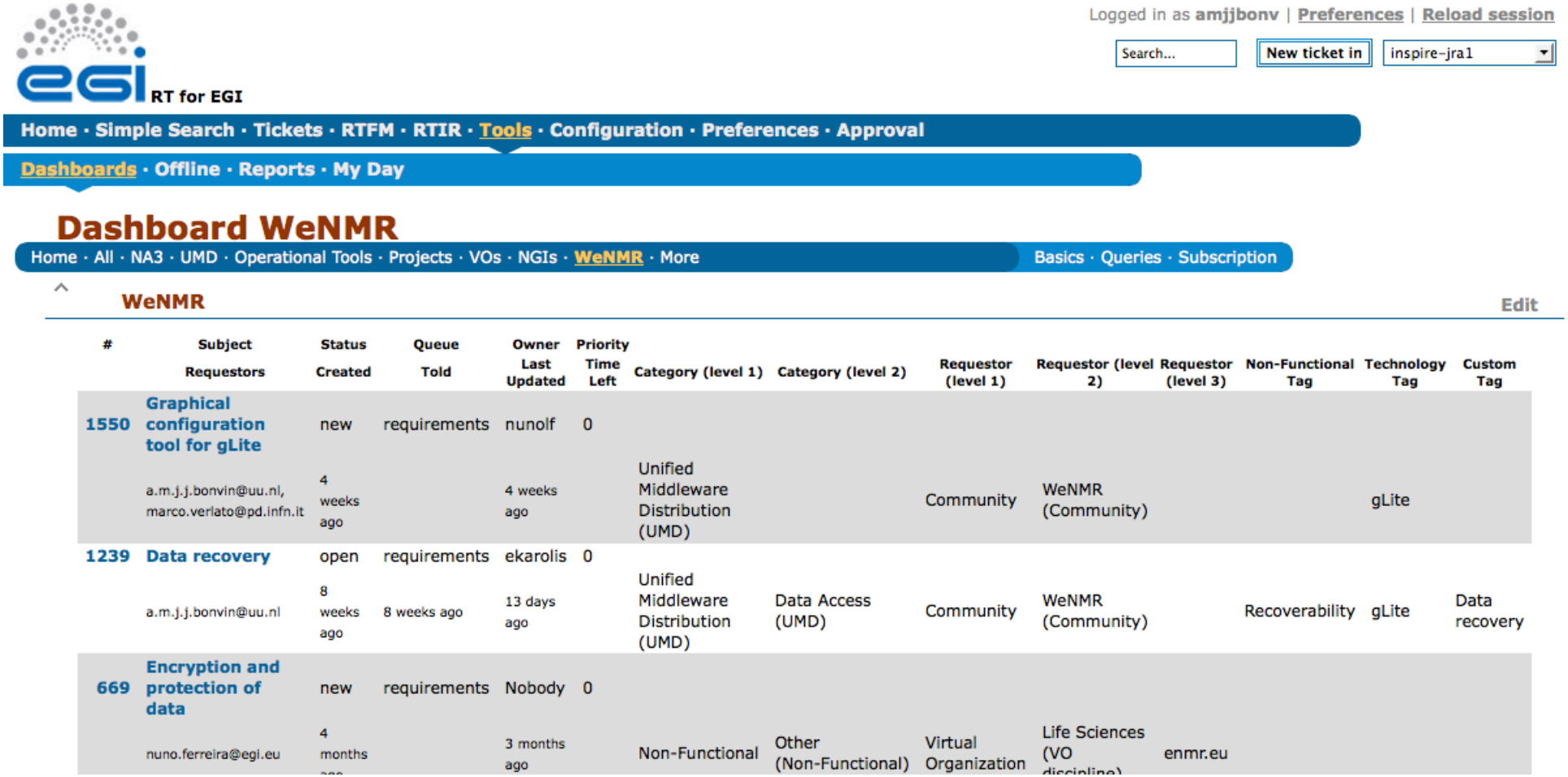
Applications



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



Logged in as **amjjbonv** | Preferences | Reload session

Search... | New ticket in | inspire-jra1

RT for EGI

Home · Simple Search · Tickets · RTFM · RTIR · Tools · Configuration · Preferences · Approval

Dashboards · Offline · Reports · My Day

Dashboard WeNMR

Home · All · NA3 · UMD · Operational Tools · Projects · VOs · NGIs · WeNMR · More | Basics · Queries · Subscription

WeNMR

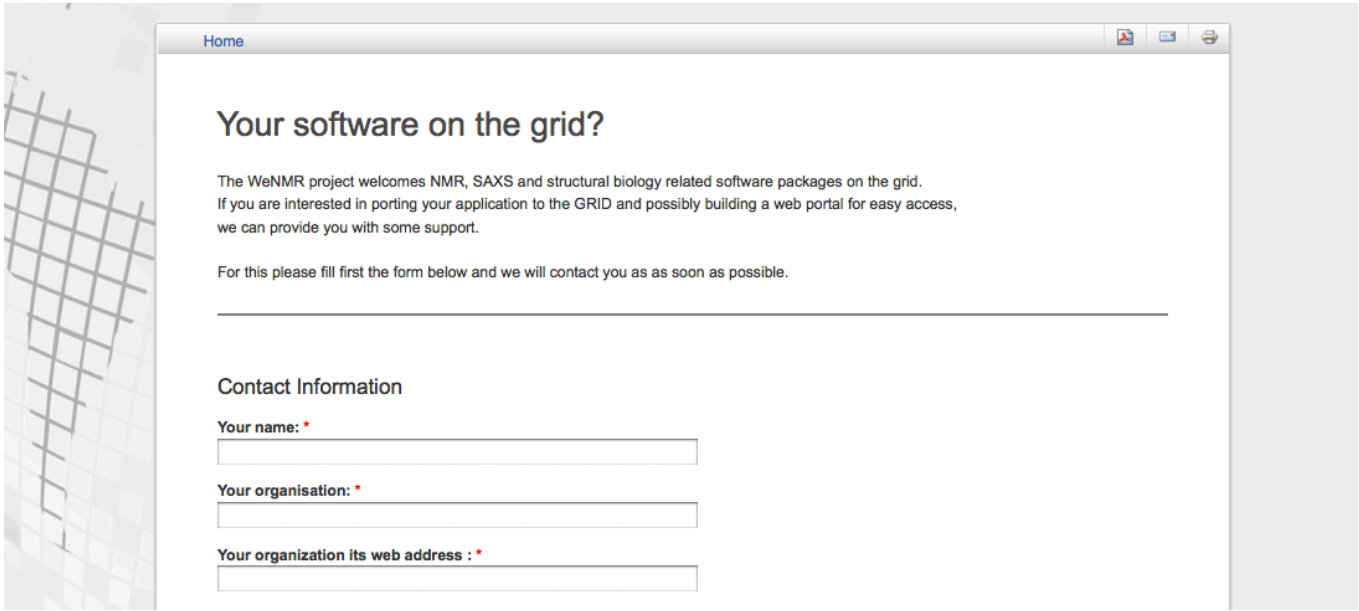
Edit

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

And beyond…

WeNMR Support center

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



- **Consultancy services for third parties**

Collaborations established so far

- Collaborations already established with several other FP7 projects:
  - OpenAIRE www.openaire.eu
  - e-ScienceTalk www.e-sciencetalk.org
  - Gisela www.gisela-grid.eu
  - CHAIN www.chain-project.eu
  - Erina+ www.erinaplus.eu
  - EMI www.eu-emi.eu

- WeNMR is the 1st VRC officially recognized by the EGI

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e-infrastructure

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

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