



A Worldwide e-Infrastructure for NMR in structural biology

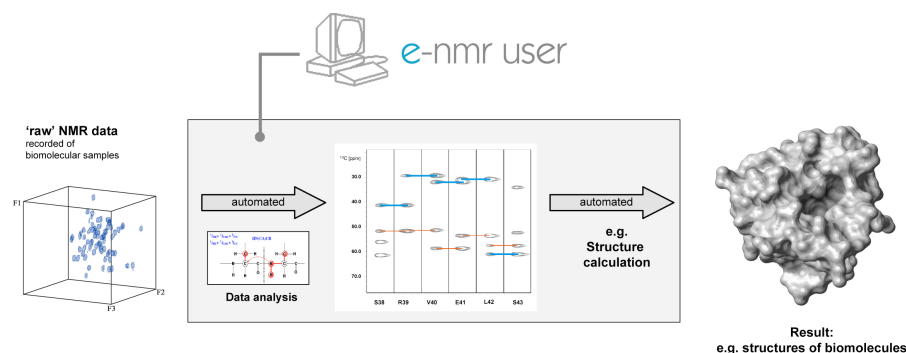
Project Coordinator:
Prof. Alexandre M.J.J. Bonvin
Bijvoet Center for Biomolecular Research
Utrecht University
a.m.j.j.bonvin@uu.nl

Talk by:
Marco Verlato
INFN
Padova Unit
Marco.Verlato@pd.infn.it

Deploying and unifying the NMR e-Infrastructure in System Biology



e-NMR will allow researchers to enjoy all of the benefits 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



Universiteit Utrecht

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



eNMR platform operational and well used!

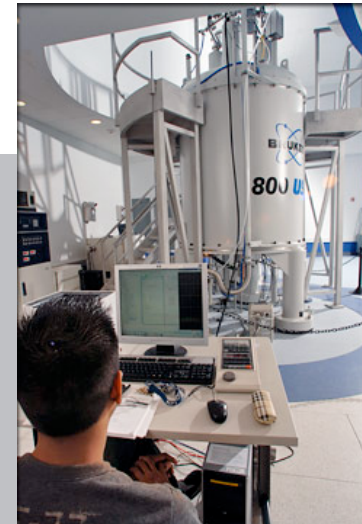
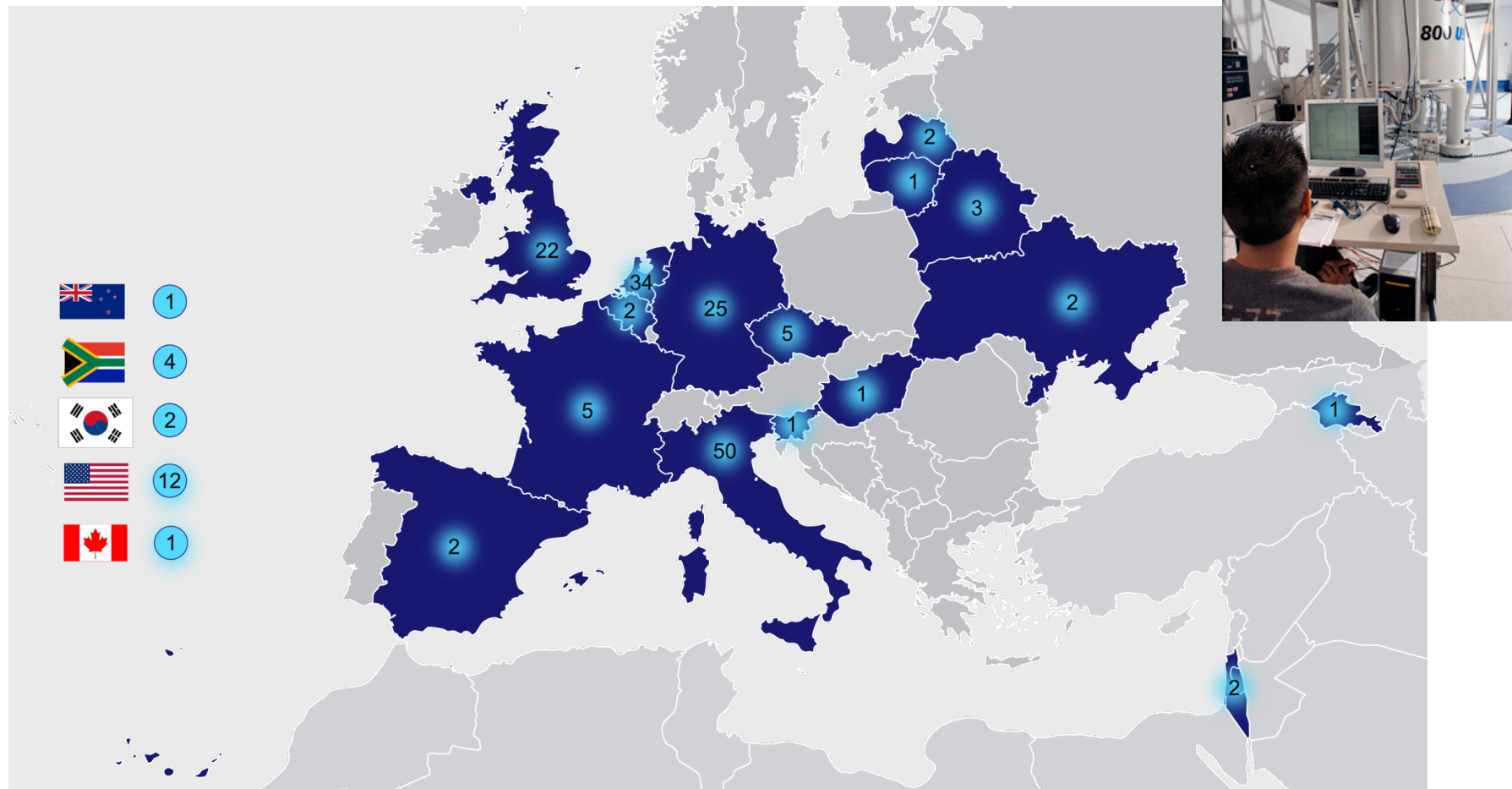
- **2nd largest VO in the life sciences**
- **Over 190 registered users and growing**
- **>13000 CPUs**
- **>350 CPU years over the last 12 months**
- **20% of Life Sciences on the Grid**
- **User-friendly access to e-Infrastructure via web portals**

www.enmr.eu








Users distribution

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



The eNMR infrastructure

 GStat 2.0											
<div> Geo View LDAP View Site Views Service View VO View </div>											
<div> :: Home :: Site Summary </div> <div> Filters: VO Values: enmr.eu </div>											
<div> Show 25 entries Go to a site: --SELECT A SITE NAME-- </div> <div>     Search: <input type="text"/> </div>											
Name	Status	CPUs			Online Storage Space (GB)		Nearline Storage Space (GB)		Grid Jobs		
		Physical	Logical	SI2000	TotalSize	UsedSize	TotalSize	UsedSize	Total	Running	Waiting
BCBR	CRITICAL	44	176	424,160	1,964	<div><div></div></div> 5%	0	<div><div></div></div> 0%	28	<div><div></div></div> 6%	<div><div></div></div> 57%
BMFZ-FRANKFURT	WARNING	11	44	148,280	968	<div><div></div></div> 11%	0	<div><div></div></div> 0%	50	<div><div></div></div> 63%	<div><div></div></div> 44%
CIRMP	CRITICAL	8	32	88,960	528	<div><div></div></div> 7%	0	<div><div></div></div> 0%	20	<div><div></div></div> 6%	<div><div></div></div> 90%
CNR-ILC-PISA	WARNING	2	4	1,556	431	<div><div></div></div> 86%	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	<div><div></div></div> 0%
HTC-BIGGRID	CRITICAL	412	1,648	3,198,768	6,594	<div><div></div></div> 9%	0	<div><div></div></div> 0%	186	<div><div></div></div> 1%	<div><div></div></div> 90%
INFN-BARI	N/A	274	1,045	1,254,000	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	<div><div></div></div> 0%
INFN-CATANIA	CRITICAL	440	774	1,137,780	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	<div><div></div></div> 0%
INFN-LNL-2	CRITICAL	176	656	1,675,424	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	228	<div><div></div></div> 14%	<div><div></div></div> 57%
INFN-PADOVA	WARNING	54	82	84,624	7,499	<div><div></div></div> 18%	0	<div><div></div></div> 0%	54	<div><div></div></div> 58%	<div><div></div></div> 11%
INFN-TRIESTE	CRITICAL	106	350	246,750	2,684	<div><div></div></div> 72%	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	<div><div></div></div> 0%
NIKHEF-ELPROD	CRITICAL	2,064	7,464	16,719,360	107	<div><div></div></div> 25%	0	<div><div></div></div> 0%	782	<div><div></div></div> 0%	<div><div></div></div> 99%
UKI-SCOTGRID-DURHAM	CRITICAL	168	672	1,424,640	17,820	<div><div></div></div> 31%	0	<div><div></div></div> 0%	512	<div><div></div></div> 19%	<div><div></div></div> 73%
ZA-NWU	CRITICAL	24	1	1,000	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	<div><div></div></div> 0%
ZA-UCT-ICTS	CRITICAL	16	16	43,648	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	<div><div></div></div> 0%
ZA-UJ	WARNING	20	80	30,480	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	0	<div><div></div></div> 0%	<div><div></div></div> 0%
Total		3,819	13,044	26,479,430	38,595	10,278	0	0	1,860	342	1,518

Showing 1 to 15 of 15 entries

Easy access to Grid resources via eNMR application web portal

[home >>](#)



e-NMR

NMR computational infrastructure

[Home](#) [HADDOCK](#) [Xplor-NIH](#) [CYANA](#) [CS-ROSETTA](#) [FormatConverter](#) [eNMR-database](#) [eNMR-Grid](#) [RSS](#)

[Software](#) [eNMR Wiki](#)

[WELCOME TO THE E-NMR WEB PORTAL >>](#)

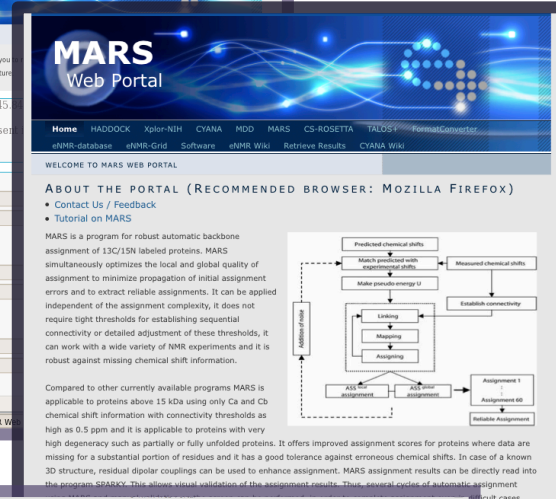
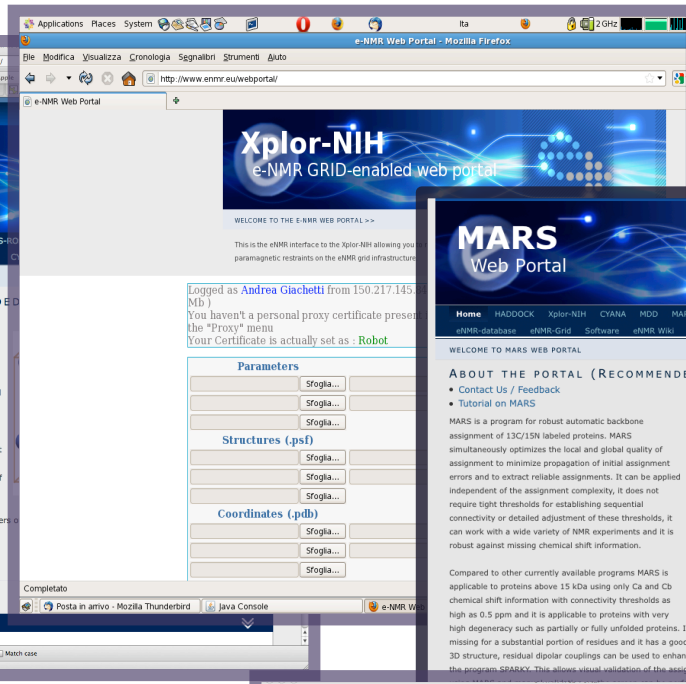
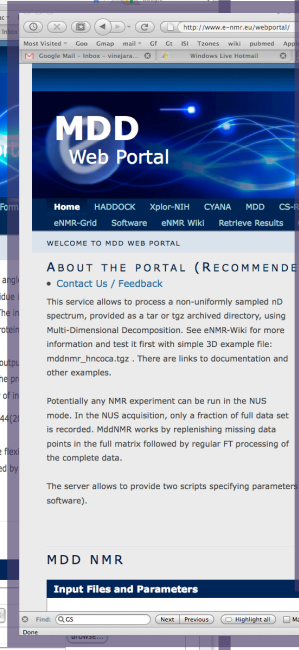
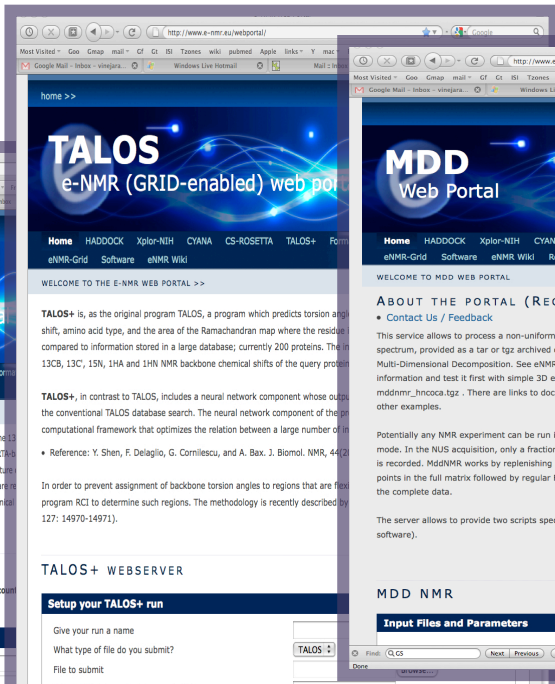
e-NMR aims at deploying and unifying the NMR computational infrastructure in system biology, a project funded under the 7th framework program of the European Union (Contract no. 213010 - e-NMR).

NMR plays an important role in life sciences (biomolecular NMR), and structural biology in particular, at both European and international levels. Our main objective is to optimize and extend the use of the NMR Research Infrastructures of EU-NMR through the implementation of an e-Infrastructure in order to provide the biomolecular NMR user community with a platform integrating and streamlining the computational approaches necessary for NMR data analysis and structural modelling (e-NMR).

[PROFILE >>](#)



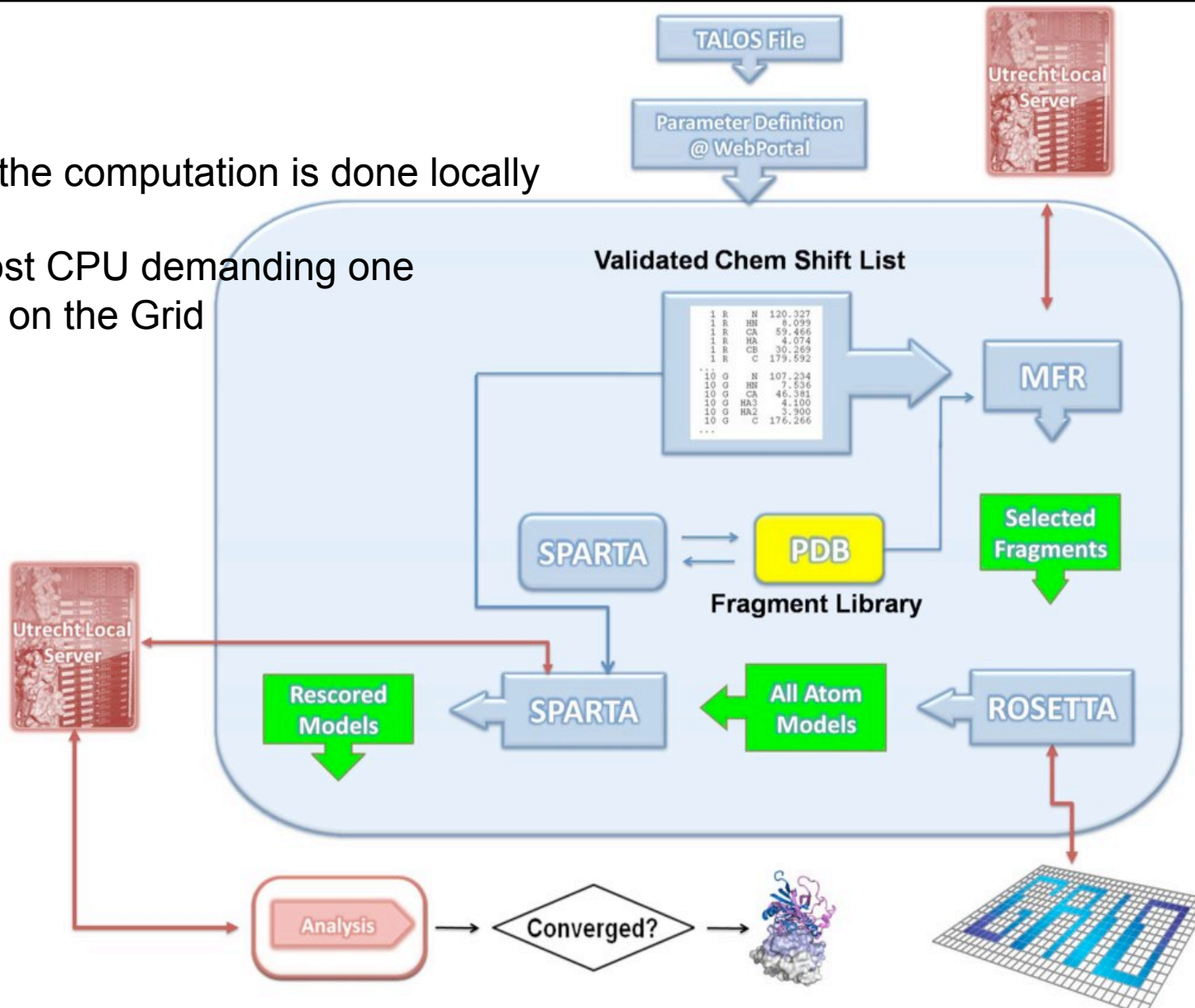
<http://www.enmr.eu/webportal>



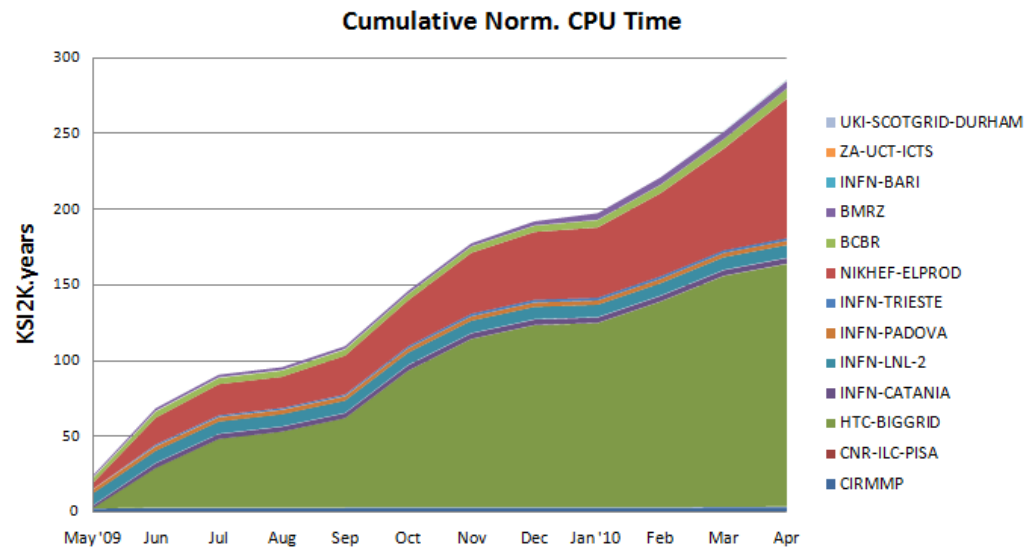
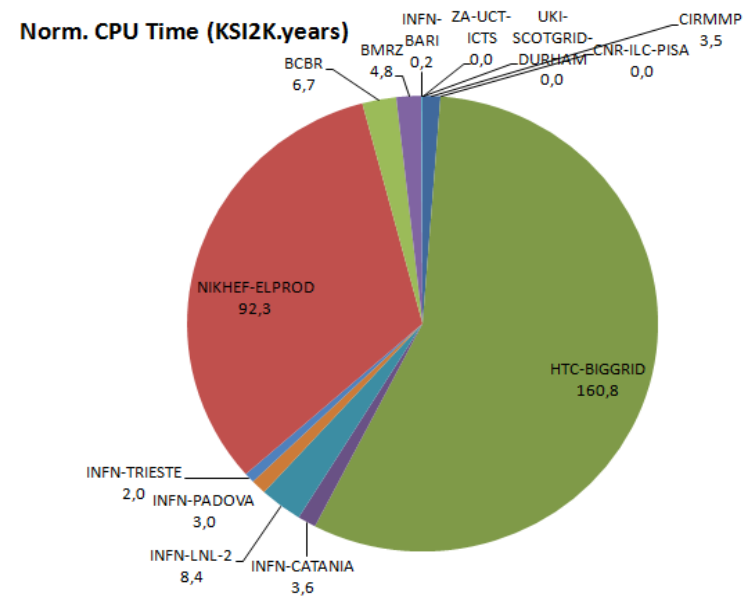
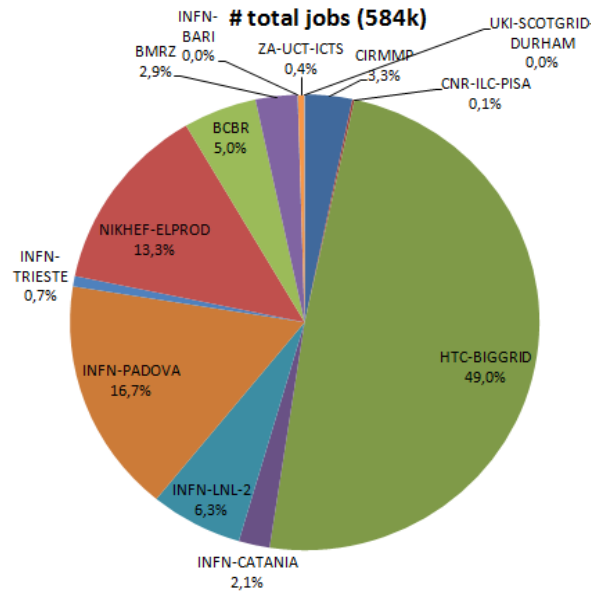
Example: the CS-Rosetta web portal flowchart

Part of the computation is done locally

The most CPU demanding one
is done on the Grid



Usage statistics



eNMR training

focused on the
eNMR applications
integrated via web
portals

The Biomolecular NMR Training Center



Spronk NMR Consultancy

e-NMR - Extend-NMR Workshops

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 organized and sponsored by the e-NMR consortium with additional support from [Extend-NMR](#).



The workshop covers theory and practical aspects of state of the art NMR structure calculation techniques that are currently employed on the [e-NMR webportal](#). The participants will first be introduced to the eNMR GRID, followed by introductions and practical applications of programs such as CYANA, CING, HADDOCK and CcpNmr Analysis. Several computationally intensive procedures will be run on the eNMR GRID. In addition, the workshop includes an introduction to the integrated software pipeline [Extend-NMR](#).

Speakers and trainers (confirmed)

- › Prof. Dr. Alexandre Bonvin
- › Prof. Dr. Peter Guentert
- › Prof. Dr. Geerten Vuister
- › Dr. Rasmus Fogh
- › Dr. Henry Jonker
- › Dr. Chris Spronk
- › Dr. Wim Vranken
- › Daniel Gottstein
- › Ezgi Karaca

Registration requirements

Currently there are no requirements for registration. It is however appreciated if you have an eNMR VO (Virtual Organization) certificate, which you can obtain here: <http://www.enmr.eu/eNMR-registration>.

Workshop information

Prices	Non-profit organizations	€ 410.00
	Profit organizations	€ 1000.00

Dates

Registration progress



Prices include:

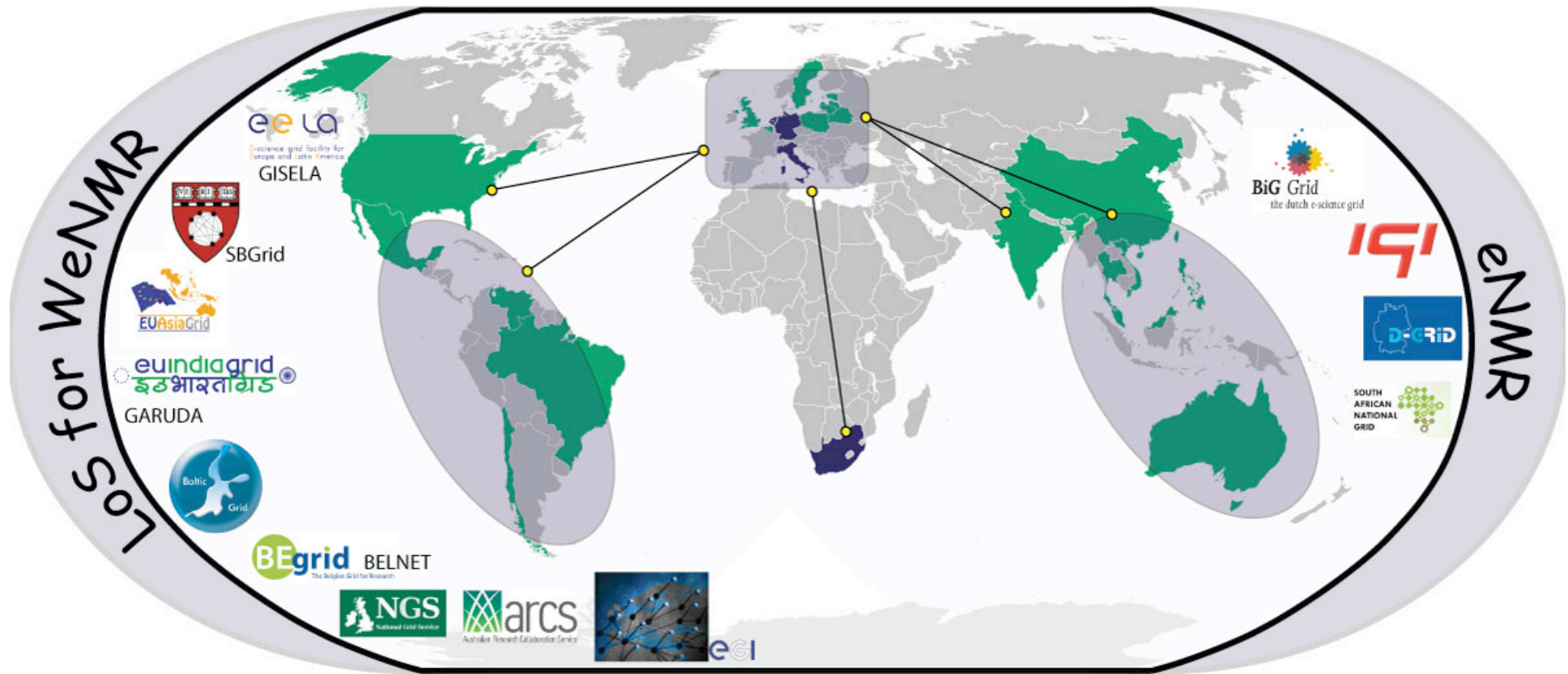
- › VAT
- › 6 nights hotel accommodation, breakfast, single room
- › 5 lunches
- › Local transfer to and from airport, hotel and course site

Refunds

Participants from non-profit organizations are eligible for a refund up to €250 for travel and other expenses. Application forms for refunds will be made available during the workshops.

[Apply »](#)

The future



3 new partners joined the consortium:

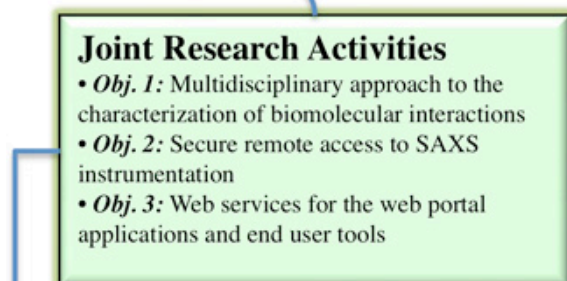
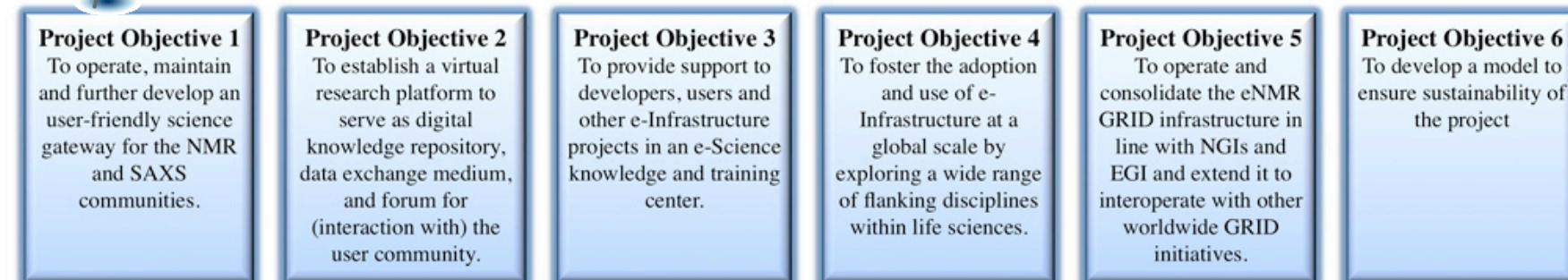
Radboud Universiteit Nijmegen, Netherlands

EMBL, Hamburg Outstation, Germany (brings in SAXS)

University of Cambridge, UK

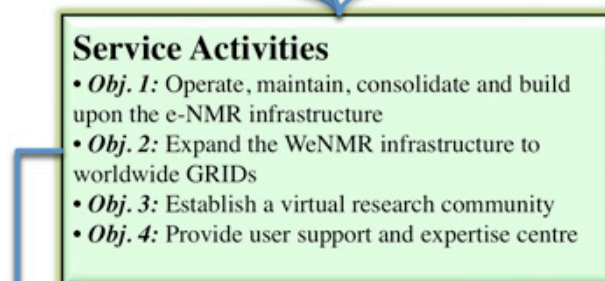


WeNMR Main Objective
Establish an e-Infrastructure-based global virtual research community for structural biology in life sciences



WP7: Research Platform

2.4 FTEs

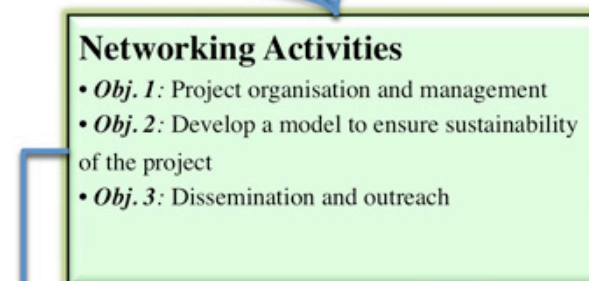


WP4: Operation & maintenance

WP5: Worldwide GRID deployment / extension

WP6: Virtual Research Community gateway

5.7 FTEs



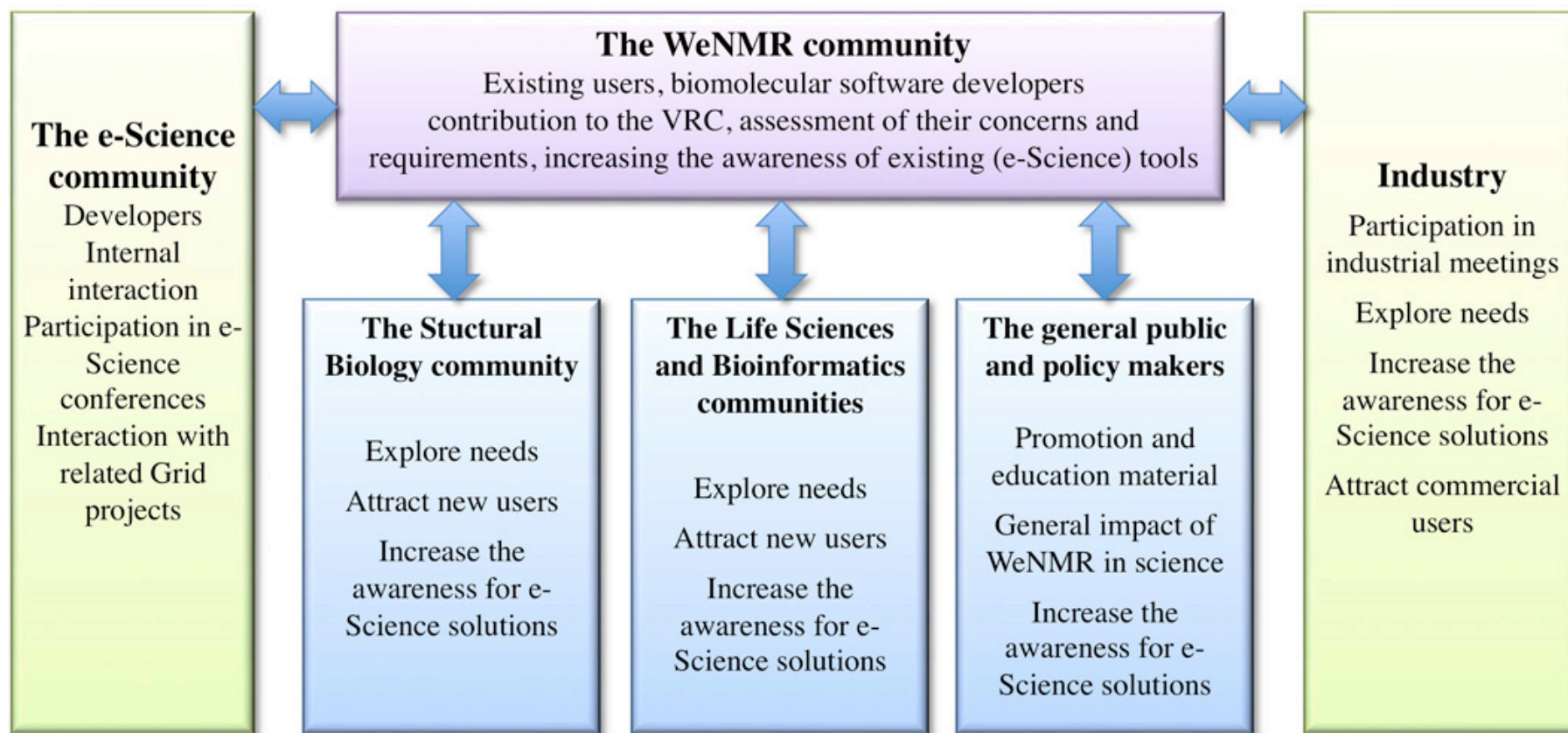
WP1: Management

WP2: Sustainability.

WP3: Outreach to stakeholders

1.3 FTEs

Outreach



Expectations from a LS VRC

- **eNMR deployed originally its own Grid infrastructure following the EGEE standards**
- **eNMR and WeNMR leverage on the NGIs for support**
- **WeNMR is interested to see if synergies are possible in the support of standards LS services**
- **Organization of workshops and schools (more Grid-oriented) where to exchange experiences and train the newcomers**
- **Other discipline-specific workshops should be kept at the level of the VRCs (e.g. like the current eNMR training workshops)**
- **Interaction with EGI / EMI for representing LS common instances:**
 - **Need to lower the barrier for grid adoption (e.g. via SLCS)**
 - **Security, data protection**