

EGI Technical Forum 2011
September 19th-23th, Lyon, France



Workshop

we-nmr update report

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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



Radboud University, Nijmegen, NL

University of Cambridge UK



European Molecular Biology Laboratory, Hamburg, DE

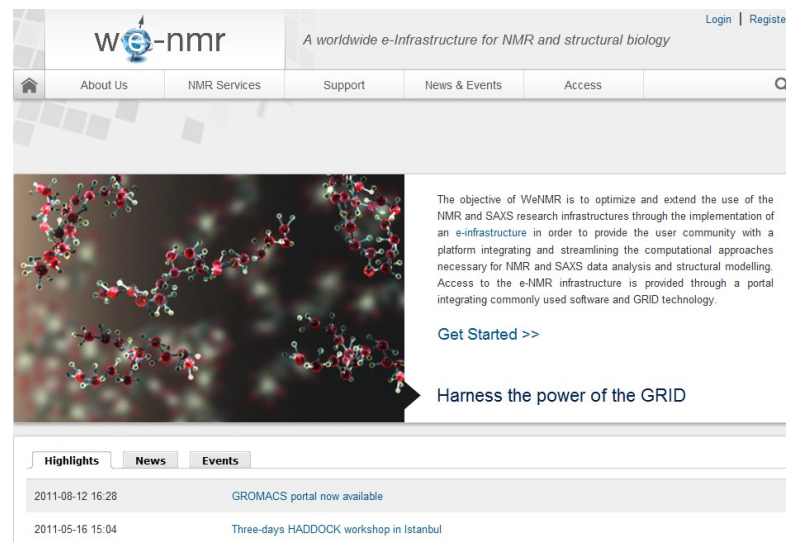
Spronk NMR Consultancy, LT



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

1st VRC recognized by EGI

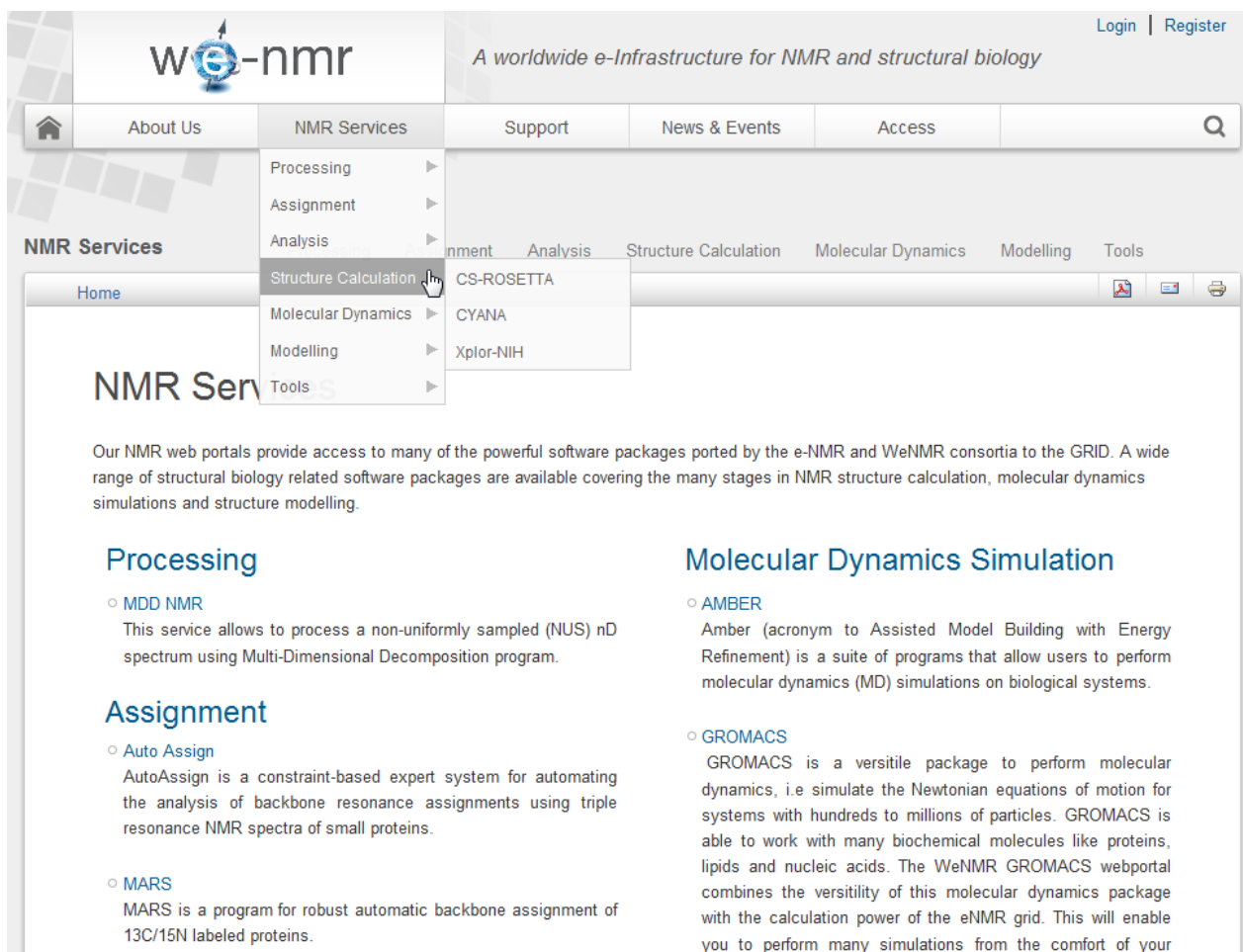
Science Gateway → www.wenmr.eu



The screenshot shows the WeNMR website homepage. At the top, there is a navigation bar with the WeNMR logo and the tagline "A worldwide e-Infrastructure for NMR and structural biology". Below the navigation bar, there is a search bar and a list of menu items: "About Us", "NMR Services", "Support", "News & Events", and "Access". The main content area features a large image of a molecular structure with a red and white color scheme. To the right of the image, there is a text block describing the project's objective: "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." Below this text, there is a "Get Started >>" link. At the bottom of the page, there is a "Highlights" section with a table of recent news items:

Highlights	News	Events
2011-08-12 16:28	GROMACS portal now available	
2011-05-16 15:04	Three-days HADDOCK workshop in Istanbul	

The WeNMR service portal



The screenshot shows the WeNMR service portal interface. At the top left is the WeNMR logo and the tagline "A worldwide e-Infrastructure for NMR and structural biology". On the top right are links for "Login" and "Register". A navigation menu includes "Home", "About Us", "NMR Services", "Support", "News & Events", and "Access". A search bar is located on the right side of the menu. The "NMR Services" dropdown menu is open, showing sub-categories: "Processing", "Assignment", "Analysis", "Structure Calculation", "Molecular Dynamics", "Modelling", and "Tools". The "Structure Calculation" sub-menu is further expanded, listing "CS-ROSETTA", "CYANA", and "Xplor-NIH".

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

The WeNMR service portfolio

Recently deployed portals



The image displays a collection of web portals for various bioinformatics services. On the left, there is a grid of portals including Xplor-NIH, AMBER, CYANA, HADDOCK, CS-ROSETTA, MDD, AutoAssign, TALOS, MARS, and AnisoFIT. On the right, there are larger screenshots of the MAXOCC and GROMACS portals. The GROMACS portal includes a navigation menu with 'Home', 'About Us', 'MDS Services', 'Support', 'News & Events', and 'Access'. Below the menu, there are sections for 'Tools' and 'SHIFTX2', with a small image of a bird and a molecular model.

Users distribution

The project leverages on EU-NMR (FP6), EAST-NMR, and the new Bio-NMR (FP7) Research Infrastructures projects to enlarge its users basis in Europe

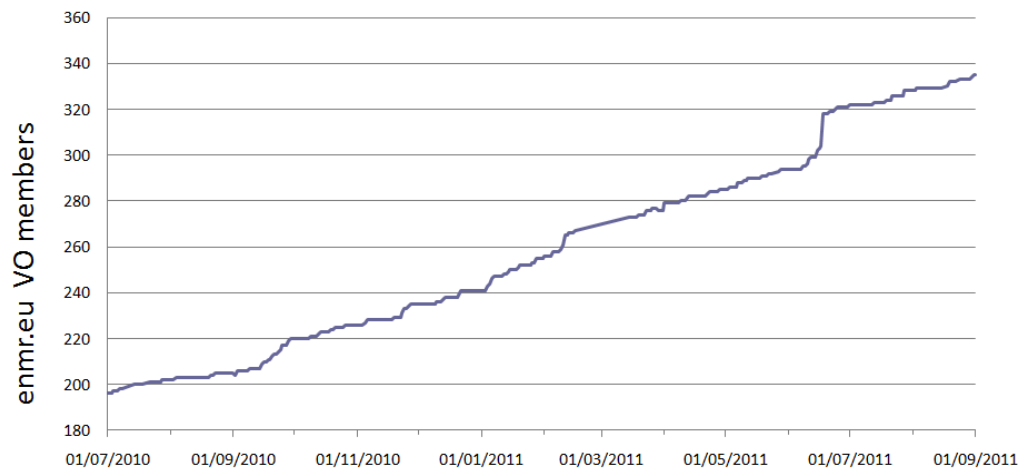
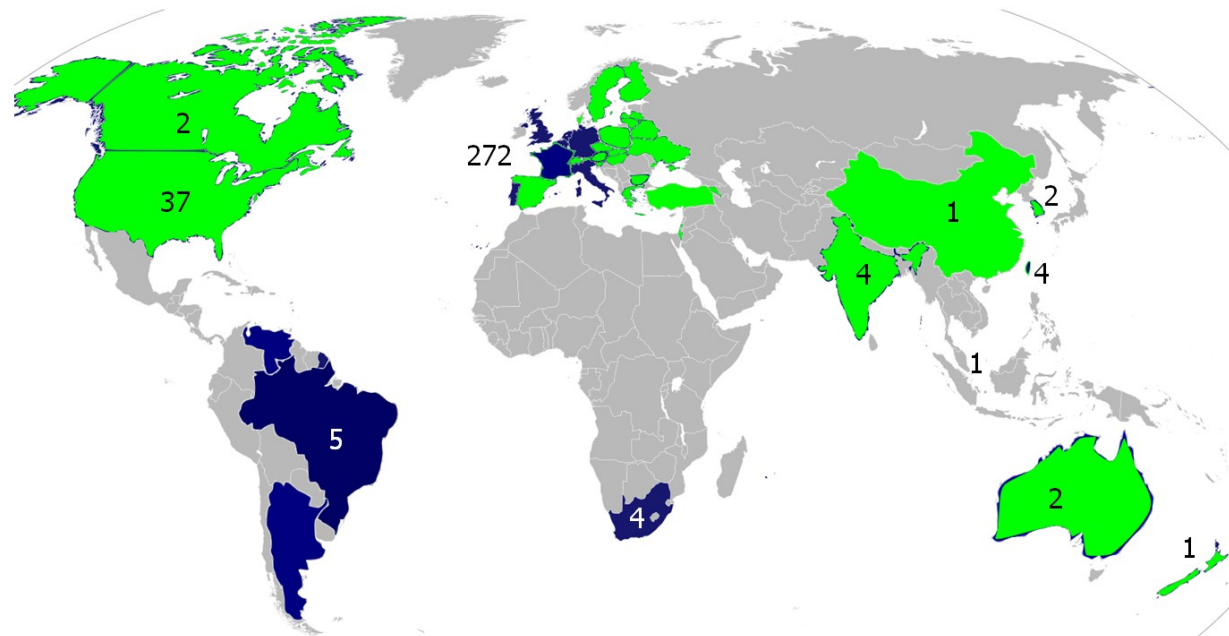
linked to ESFRI INSTRUMENT

1st largest VO in the Life Sciences

335 users (19% outside EU)

Recently joined users from:

- Centro Nacional de Ressonância Magnética Nuclear - UFRJ, Rio de Janeiro (**Brazil**)
- Centre for Cellular and Molecular Biology and Indian Institute of Chemical Technology, Hyderabad (**India**)
- TIFR National NMR Facility, Mumbai (**India**)
- Institute of Biological Chemistry and Institute of Biological Sciences, AS Taipei (**Taiwan**)
- University of Science and Technology of China, Hefei (**China**)



Training & dissemination

- Training center

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

- Recent events (May-Aug.)

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

- Coming soon

- 3rd CCPN/EU Conf., Lisbon, 28-30/9/11
- Bio-NMR workshop, Vilnius, 4-7/10/11
- WeNMR keynote & workshop at ISCG 2012, Taipei

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 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 CcpNmr Analysis, CYANA, TALOS+, YASARA, CING, HADDOCK and AMBER. Several computationally intensive procedures will be run on the e-NMR GRID.

Technology	>
Policy	>
Infrastructure	>
Publications	>
Projects	>
Collaborations	>



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

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>).



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

WeNMR developers workshop, Utrecht, NL

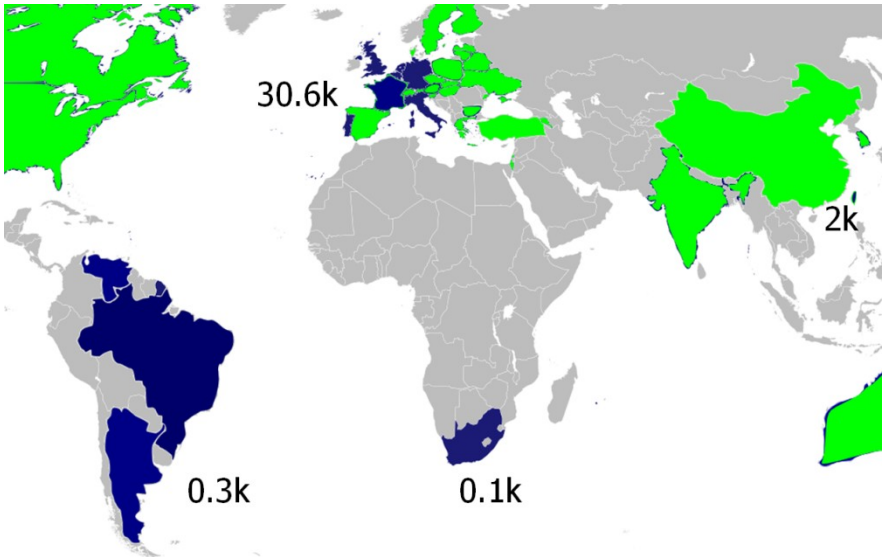
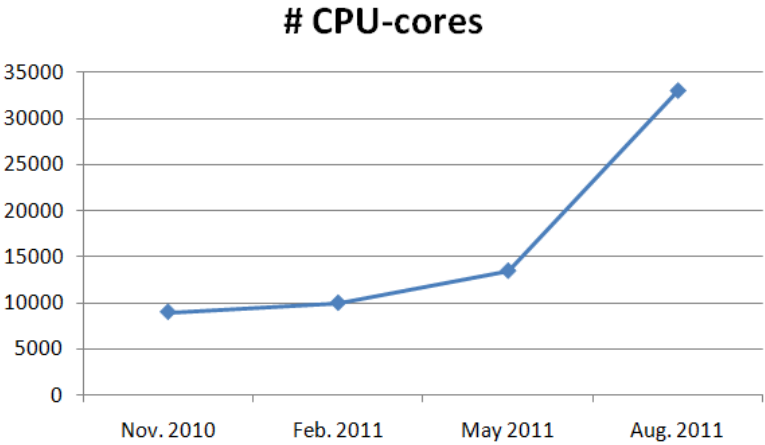
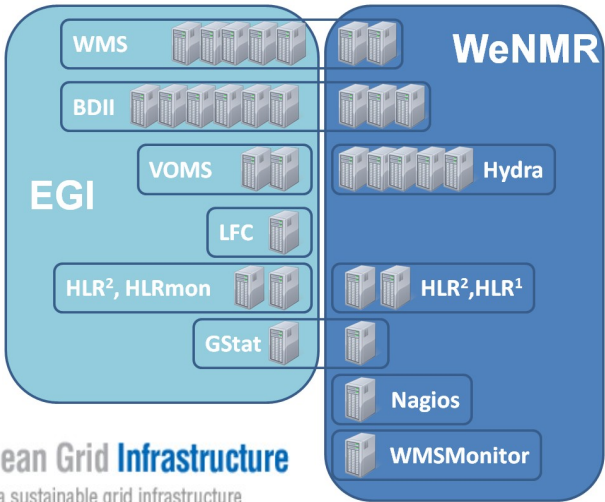
I was invited to take part in the WeNMR developers workshop held in the headquarters of this consortium at Utrecht, Netherlands. WeNMR was the first Virtual Research Community (VRC) to engage with EGI.eu, and soon after they became the largest community in the area of Life Sciences.

Resource distribution

32 central grid services
 > 33000 CPU-cores
 29 resource centres

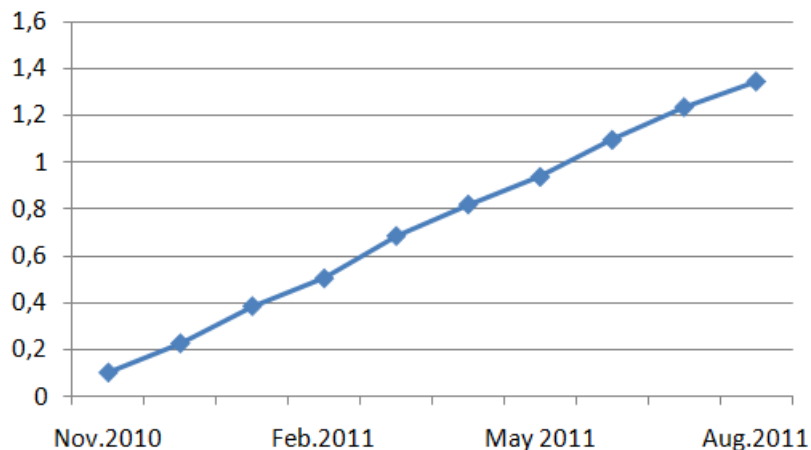
Recently added:

- DESY+FZK (19k), Germany
- TW-eScience (2k), Taiwan
- OBSPM+UNIV-LILLE (0,7k), France
- UNLP+UFRJ+ULA (0,3k), GISELA

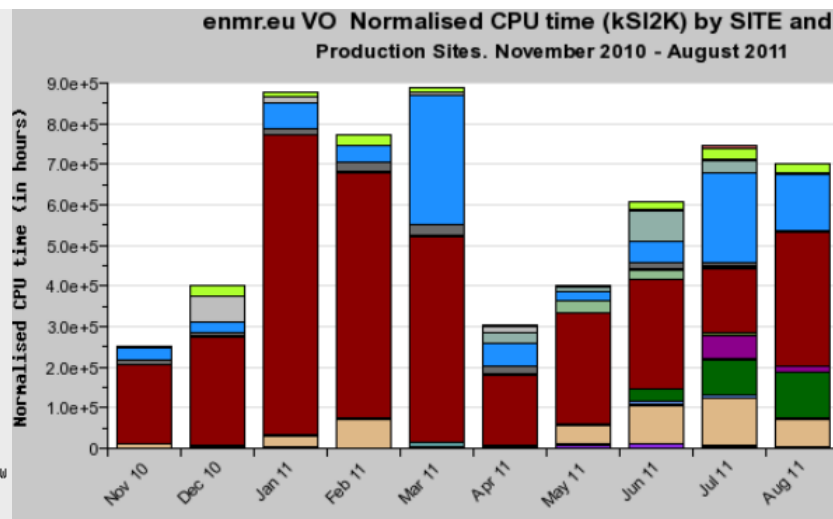
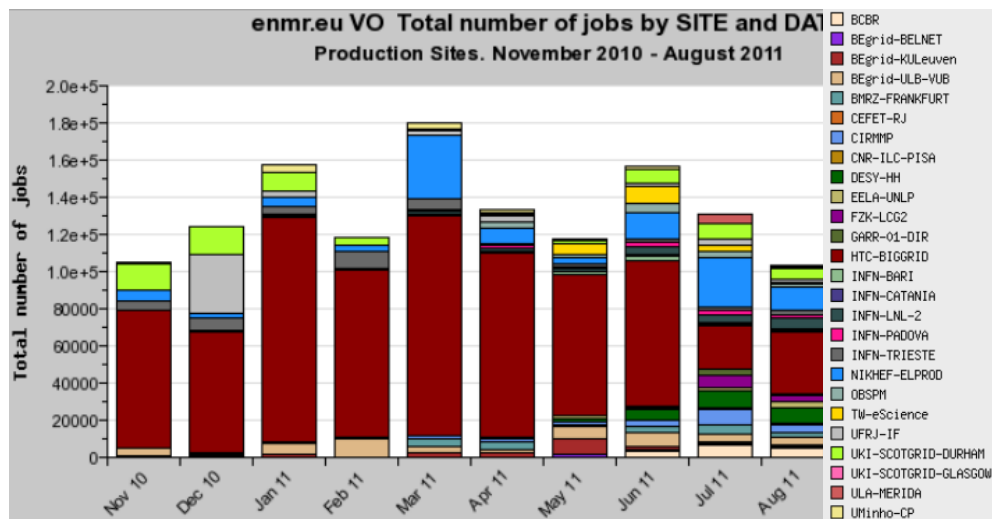
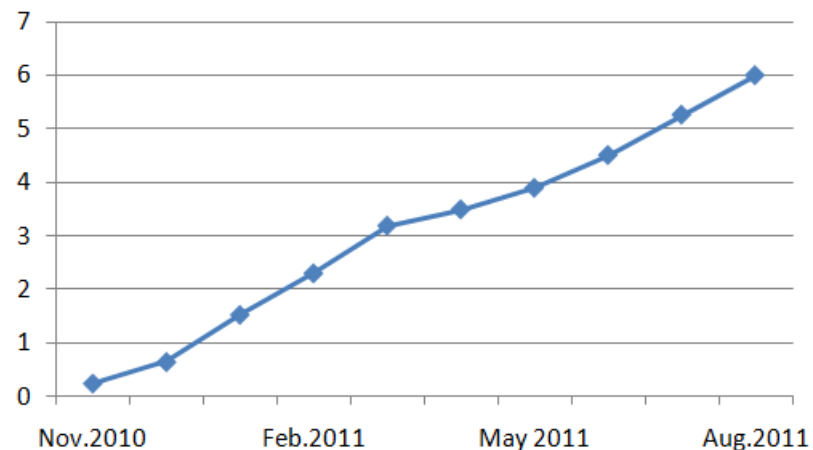


Resource usage

jobs (Millions)



CPU-hours (Millions)



Resource usage

Taiwan and GISELA resources usage comparable to EU sites of the same size

Total number of jobs run by SITE and DATE for Production sites												
SITE	Nov 10	Dec 10	Jan 11	Feb 11	Mar 11	Apr 11	May 11	Jun 11	Jul 11	Aug 11	Total	%
BCBR	0	0	0	0	0	0	0	3,090	6,703	5,365	15,158	1.13%
BEgrid-BELNET	0	0	0	0	172	300	1,307	1,408	652	477	4,316	0.32%
BEgrid-KULeuven	955	964	1,544	36	1,963	1,839	8,883	1,009	963	411	18,567	1.38%
BEgrid-ULB-VUB	3,805	894	5,666	9,559	3,438	2,355	6,066	7,818	4,540	4,487	48,628	3.62%
BMRZ-FRANKFURT	169	72	14	1,209	4,700	3,567	1,083	3,510	4,306	2,595	21,225	1.58%
CEFET-RJ	0	0	0	0	0	0	34	11	0	0	45	0.00%
CIRMMP	17	206	1,197	122	1,117	1,770	1,565	3,375	8,874	4,344	22,587	1.68%
CNR-ILC-PISA	0	0	0	2	79	87	123	134	561	803	1,789	0.13%
DESY-HH	0	0	0	0	0	0	2,172	5,786	9,379	8,120	25,457	1.90%
EELA-UNLP	0	0	0	0	168	1,219	936	934	1,889	3,189	8,335	0.62%
FZK-LCG2	0	0	0	0	0	0	0	103	6,467	3,282	9,852	0.73%
GARR-01-DIR	0	0	0	0	0	0	0	41	3,032	1,190	4,263	0.32%
HTC-BIGGRID	74,056	65,686	120,972	90,173	118,589	99,195	76,304	78,917	23,830	33,358	781,080	58.17%
INFN-BARI	0	85	555	34	98	450	1,364	2,134	1,250	2,097	8,067	0.60%
INFN-CATANIA	0	0	0	14	224	151	28	779	838	938	2,972	0.22%
INFN-LNL-2	9	49	100	324	1,598	1,628	1,640	4,093	5,359	6,368	21,168	1.58%
INFN-PADOVA	2	40	831	29	1,072	1,206	846	2,295	4,675	4,199	15,195	1.13%
INFN-TRIESTE	4,848	6,927	3,833	9,475	5,737	1,644	1,997	2,319	1,509	1,706	39,995	2.98%
NIKHEF-ELPROD	6,261	2,849	5,492	3,181	34,747	8,042	2,804	13,507	26,697	12,545	116,125	8.65%
OBSPM	0	0	0	0	3	3,376	2,178	5,611	3,562	2,344	17,074	1.27%
TW-eScience	0	0	0	0	0	0	5,553	9,328	3,467	435	18,783	1.40%
UFRJ-IF	0	31,590	3,093	67	2,525	3,357	344	1,368	3,166	1,665	47,175	3.51%
UKI-SCOTGRID-DURHAM	13,992	14,979	10,339	4,027	700	1,007	1,435	7,219	8,083	6,276	68,057	5.07%
UKI-SCOTGRID-GLASGOW	0	0	0	0	0	0	0	61	171	226	458	0.03%
ULA-MERIDA	0	0	0	0	135	225	0	373	5,041	1,030	6,804	0.51%
UMinho-CP	954	31	4,210	34	3,312	2,308	615	2,339	4,165	1,544	19,512	1.45%
Total	105,068	124,372	157,846	118,286	180,377	133,726	117,277	157,562	139,179	108,994	1,342,687	
Percentage	7.83%	9.26%	11.76%	8.81%	13.43%	9.96%	8.73%	11.73%	10.37%	8.12%		

Application accounting

EGI ACCOUNTING PORTAL



GLOBAL View

VO MANAGER View

VO MEMBER View

SITE ADMIN View

USER View

REPORTS

METRICS PORTAL

[LINKS](#)

November 2010 - August 2011.

The following table shows the Usage of the Top 10 Groups ordered by Normalised CPU time (kSI2K).

Top 10 Groups ordered by Normalised CPU time (kSI2K)

#	Group/Role ID	Jobs		CPU time		Norm. CPU time		WCT		Norm. WCT		CPU Efficiency	Avg. CPU time	Avg. WCT
		#	%	Hrs	%	Hrs	%	Hrs	%	Hrs	%	%	Hrs	Hrs
1	/enmr.eu/csrosetta/Role=NULL	543,287	39.7%	1,451,489	48.9%	2,947,952	48.2%	1,486,759	47.1%	3,019,548	46.1%	97.6	2.67	2.74
2	/enmr.eu/Role=NULL	414,483	30.3%	1,294,455	43.6%	2,682,141	43.8%	1,433,231	45.4%	3,004,077	45.9%	90.3	3.12	3.46
3	/enmr.eu/haddock/Role=NULL	328,930	24.1%	192,122	6.5%	434,404	7.1%	202,949	6.4%	462,925	7.1%	94.7	0.58	0.62
4	/enmr.eu/amber/Role=NULL	19,866	1.5%	29,989	1.0%	51,511	0.8%	33,058	1.0%	55,203	0.8%	90.7	1.51	1.66
5	/enmr.eu/gromacs/Role=NULL	69	0.0%	258	0.0%	780	0.0%	433	0.0%	1,454	0.0%	59.6	3.74	6.28
6	/enmr.eu/cns/Role=NULL	44	0.0%	145	0.0%	371	0.0%	146	0.0%	375	0.0%	99.3	3.30	3.32
7	/enmr.eu/ops/Role=NULL	59,731	4.4%	125	0.0%	295	0.0%	2,372	0.1%	6,237	0.1%	5.3	0.00	0.04
8	/enmr.eu/cyana/Role=NULL	158	0.0%	39	0.0%	133	0.0%	197	0.0%	664	0.0%	19.8	0.25	1.25
9	/enmr.eu/mdnrm/Role=NULL	33	0.0%	36	0.0%	122	0.0%	157	0.0%	531	0.0%	22.9	1.09	4.76
10	/enmr.eu/Role=SoftwareManager	350	0.0%	11	0.0%	29	0.0%	292	0.0%	375	0.0%	3.8	0.03	0.83
Total		1,366,951		2,968,669		6,117,738		3,159,594		6,551,389		94.0	2.17	2.31

[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)

WeNMR Monitoring

WMSMonitor >> VO view >> Single VO >> Charts::enmr.eu

Select VO data

GStat 2.0

Geo View LDAP View Site Views Service View VO View

Home :: Site Summary Filters: VO

Show 10 entries | Go to a site: --SELECT A SITE NAME--

Name	Status	CPUs			Online Storage Space (GB)		Nearline Storag (GB)
		Physical	Logical	SI2000	TotalSize	UsedSize	
BCBR	WARNING	52	208	501,280	1,964	5%	0
BEgrid-BELNET	WARNING	18	36	70,200	211	9%	0
BEgrid-KULeuven	CRITICAL	57	113	42,940	1,476	6%	0
BEgrid-ULB-VUB	CRITICAL	178	1,282	2,884,500	0	0%	0
BMRZ-FRANKFURT	WARNING	10	40	134,800	968	18%	0
CIRMWP	WARNING	8	32	72,000	528	11%	0
CNR-ILC-PISA	WARNING	2	4	5,976	431	80%	0
DESY-HH	WARNING	808	4,784	9,486,672	0	0%	0
EELA-UNLP	WARNING	5	10	30,750	630	5%	0
FZK-LCG2	CRITICAL	2,562	13,757	26,959,968	0	0%	0
Total		6,494	33,006	66,113,714	151,078	40,302	0

Showing 1 to 10 of 29 entries

- VO dedicated instances of EGI operations tools:
- SAM/Nagios
 - GStat
 - WMSMonitor

WeNMR Monitoring

Argentina (Argentina)

Host	Status	Services	Actions
ce01.unlp.edu.ar	UP	17 OK 1 CRITICAL	
se01.unlp.edu.ar	UP	8 OK	

Venezuela (Venezuela)

Host	Status	Services	Actions
cream01.cecalc.ula.ve	UP	1 OK 1 WARNING 1 CRITICAL 14 PENDING	
se.cecalc.ula.ve	UP	8 OK	

Taiwan (Taiwan)

Host	Status	Services	Actions
as-ce01.euasiagrid.org	UP	15 OK 2 WARNING	
as-ds01.euasiagrid.org	UP	8 OK	

South Africa (South Africa)

Host	Status	Services	Actions
fs01.grid.uj.ac.za	UP	8 OK	
glite-ce.grid.uj.ac.za	UP	1 WARNING 2 CRITICAL 14 PENDING	
svslng004.uct.ac.za	DOWN	1 OK 2 WARNING 14 PENDING	
svslng010.uct.ac.za	DOWN	2 WARNING	

Brazil (Brazil)

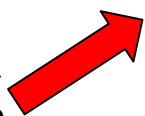
Host	Status	Services	Actions
ce01.eela.if.ufjr.br	UP	17 OK	
ce02.eela.if.ufjr.br	UP	17 OK	
lnx097.eela.if.ufjr.br	UP	8 OK	
lnx105.eela.if.ufjr.br	UP	8 OK	

Supported by EGI-InSPIRE NA3 and EGI.eu UCST for deploying the VO SAM



Host	Service	Status	Last Check	Duration	Attempt	Status Information
ce01.eela.if.ufjr.br	eu.wenmr.WN-CNS-/enmr.eu/ops	OK	09-14-2011 15:23:35	5d 23h 22m 51s	1/2	Inx082: CNS-probe OK - File sa_1.pdb created.
	eu.wenmr.WN-RepLCG_LOC-/enmr.eu/ops	OK	09-14-2011 15:22:29	47d 17h 27m 40s	1/2	Inx082: TEST-LCG_LOC OK - LCG_LOCATION=/usr
	eu.wenmr.WN-csRosetta-/enmr.eu/ops	OK	09-14-2011 15:23:20	6d 0h 23m 6s	1/2	Inx082: csRosetta-probe OK - DONE :: 1 starting structures built 1 (nstruct) times
	eu.wenmr.lcg-tags_probe-/enmr.eu/ops	OK	09-14-2011 17:12:58	1d 16h 19m 14s	1/3	TagProbe OK - VO-enmr.eu-CNS1.2, VO-enmr.eu-CNS1.2-PARA, VO-enmr.eu-CSROSETTA, VO-enmr.eu-GROMACS3.3.3, VO-enmr.eu-GROMACS4.5.3-rtc-r2, VO-enmr.eu-NMRPIPE, VO-enmr.eu-ROSETTA
	hr_srce.CADist-Check-/enmr.eu/ops	OK	09-14-2011 15:22:32	47d 21h 42m 55s	1/2	Inx082: CA DIST OK - The official version is 1.40. Using AAACertificateServices to get CA distribution version. CA distribution is correctly installed.
	org.sam.CREAMCE-JobState-/enmr.eu/ops	OK	09-14-2011 17:16:23	1d 0h 56m 1s	1/2	OK: [Scheduled] https://lb-enmr.cern.unifi.it:9000/LwzcytFHlulX4n-K5Xc9DQ
	org.sam.CREAMCE-JobSubmit-/enmr.eu/ops	OK	09-14-2011 15:31:26	1d 0h 50m 56s	1/2	OK: success.
	org.sam.WN-Bi-/enmr.eu/ops	OK	09-14-2011 15:22:32	47d 23h 58m 39s	1/2	Inx082: OK: getCE: ce01.eela.if.ufjr.br:8443/cream-pbs-enmr
	org.sam.WN-Csh-/enmr.eu/ops	OK	09-14-2011 15:22:34	47d 23h 58m 37s	1/2	Inx082: OK
	org.sam.WN-Rep-/enmr.eu/ops	OK	09-14-2011 15:26:41	0d 14h 52m 6s	1/2	Inx082: OK: success.
	org.sam.WN-RepCr-/enmr.eu/ops	OK	09-14-2011 15:24:23	0d 14h 53m 37s	1/2	Inx082: OK: File was copied to SE Inx097.eela.if.ufjr.br and registered in LFC lfcserver.cnaf.infn.it. CLI
	org.sam.WN-RepDel-/enmr.eu/ops	OK	09-14-2011 15:26:41	0d 14h 52m 6s	1/2	Inx082: OK: Replicas for [lfn:/grid/enmr.eu/SAM/sam-lcg-rm-cr-Inx082.110914132309.107381710] were deleted. CLI
	org.sam.WN-RepFree-/enmr.eu/ops	OK	09-14-2011 15:22:37	5d 18h 23m 34s	1/2	Inx082: OK: ok
	org.sam.WN-RepGet-/enmr.eu/ops	OK	09-14-2011 15:25:09	0d 14h 53m 14s	1/2	Inx082: OK: File was copied from SRM. Diff successful. CLI
	org.sam.WN-RepSrv-/enmr.eu/ops	OK	09-14-2011 15:22:35	47d 23h 58m 36s	1/2	Inx082: OK: LCG_GFAL_INFOSYS is set to lcg-bdii.cern.ch:2170
	org.sam.WN-RepRep-/enmr.eu/ops	OK	09-14-2011 15:26:20	0d 14h 52m 32s	1/2	Inx082: OK: File was replicated to SE(s) prod-se-02.pd.infn.it. Replicas listed successfully. CLI
	org.sam.WN-SoftVer-/enmr.eu/ops	OK	09-14-2011 15:22:36	47d 23h 58m 35s	1/2	Inx082: OK: 3.2.0

WeNMR specific Nagios probes



WeNMR 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
- Operate and **consolidate** the e-NMR Grid infrastructure and to **extend** it to **inter-operate** with other **worldwide** Grid initiatives
- 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
- Develop a model to ensure **sustainability** of the project

Extension to other Grids

- INFN is responsible of the Work Package 5 (start in Nov. 2011)
 - Worldwide grid extension outside EGI
 - Building on Network Activities aimed at involving worldwide grids and e-Science projects
 - Towards EGI UMD based infrastructures → South Africa, Latin America, DEISA/PRACE (via EMI-ES)
 - Towards non-UMD based infrastructures → SBGrid in USA (OSG), Asian grids (Garuda, CNgrid...)
- Attended networking events in 2010-2011:
 - WeNMR at CHAIN KoM (Roma, 13-14 December)
 - WeNMR at EU-IndiaGrid2 Workshop (Delhi, 13-16 December)
 - WeNMR at OSG All Hands (Boston, 7-11 March)
 - WeNMR at ISGC 2011 / OGF31 (Taipei, 21-25 March)
 - WeNMR at GISELA & CHAIN Workshop (Vilnius, 11-14 April)



Collaboration with OSG

- OSG is already inter-operating with EGI (e.g. in HEP)
- A good collaboration with SBGrid VO was already established during the previous e-NMR project
- 37 US users (DOEGrids CAs) already registered with enmr.eu VO (11% or the total)



A milestone of the project was set at October 2012

Project Number ¹	261572	Project Acronym ²	WeNMR
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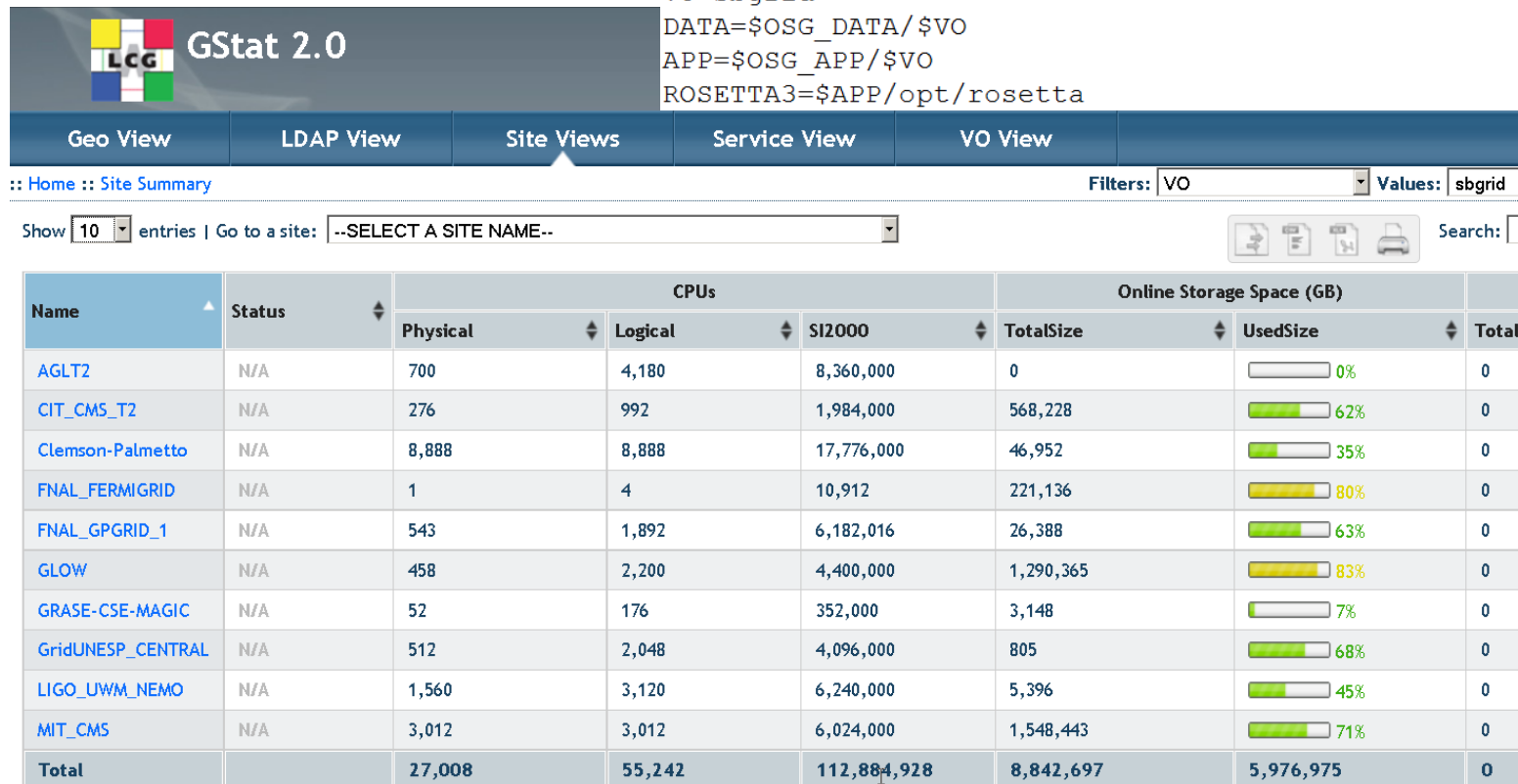
List and Schedule of Milestones

Milestone number ⁵⁹	Milestone name	WP number ⁵³	Lead beneficiary number	Delivery date from Annex I ⁶⁰	Comments
MS23	Extension to SBGrid implemented	WP4, WP5	4	24	WeNMR applications run on SBGrid resources

OSG/SBGrid resources

- 26 OSG sites supporting SBGrid VO
- Potentially >50k CPU-cores shared with other VOs
- gLite clients and application software path available on WNs, e.g.:

```
OSG_HOSTNAME=osggrid01.hep.wisc.edu
GLITE_LOCATION=/afs/hep.wisc.edu/osg/wnclient/glite
VO=sbgrid
DATA=$OSG_DATA/$VO
APP=$OSG_APP/$VO
ROSETTA3=$APP/opt/rosetta
```



The screenshot shows the GStat 2.0 interface for the SBGrid VO. The 'Site Views' tab is selected, displaying a table of 26 sites. The table columns include Name, Status, CPUs (Physical, Logical, S12000), Online Storage Space (GB) (TotalSize, UsedSize, Total), and a Total column. The 'UsedSize' column includes progress bars and percentage values.

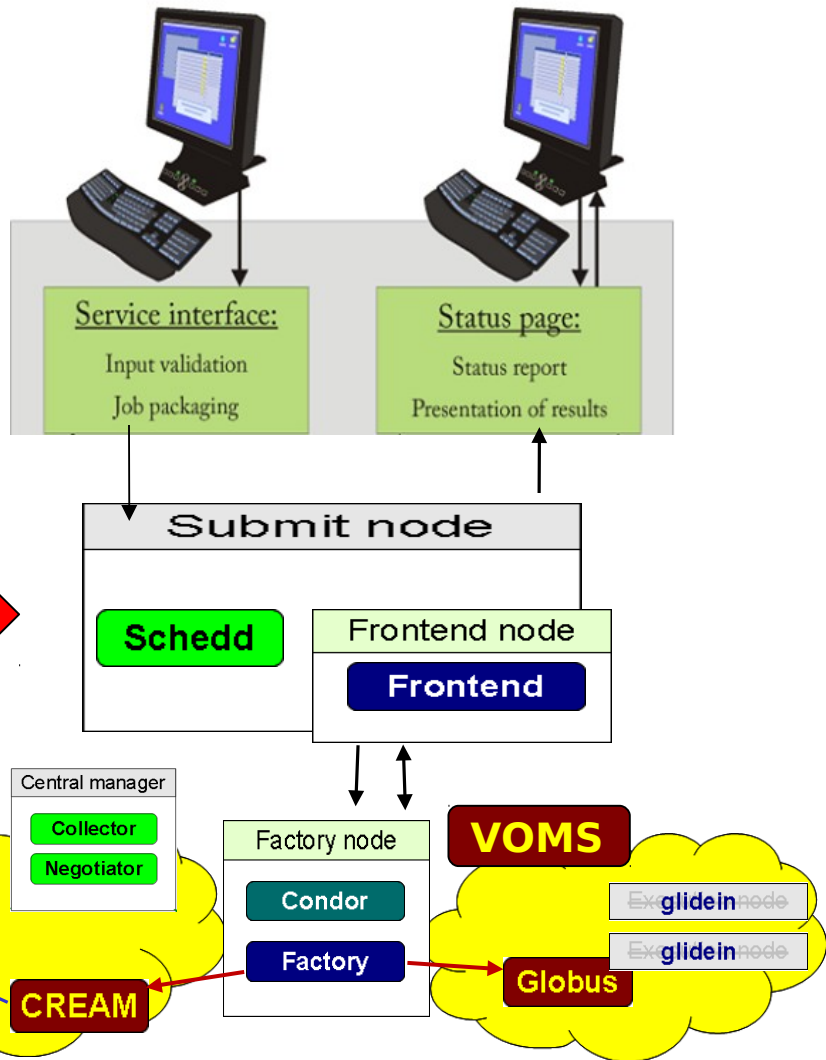
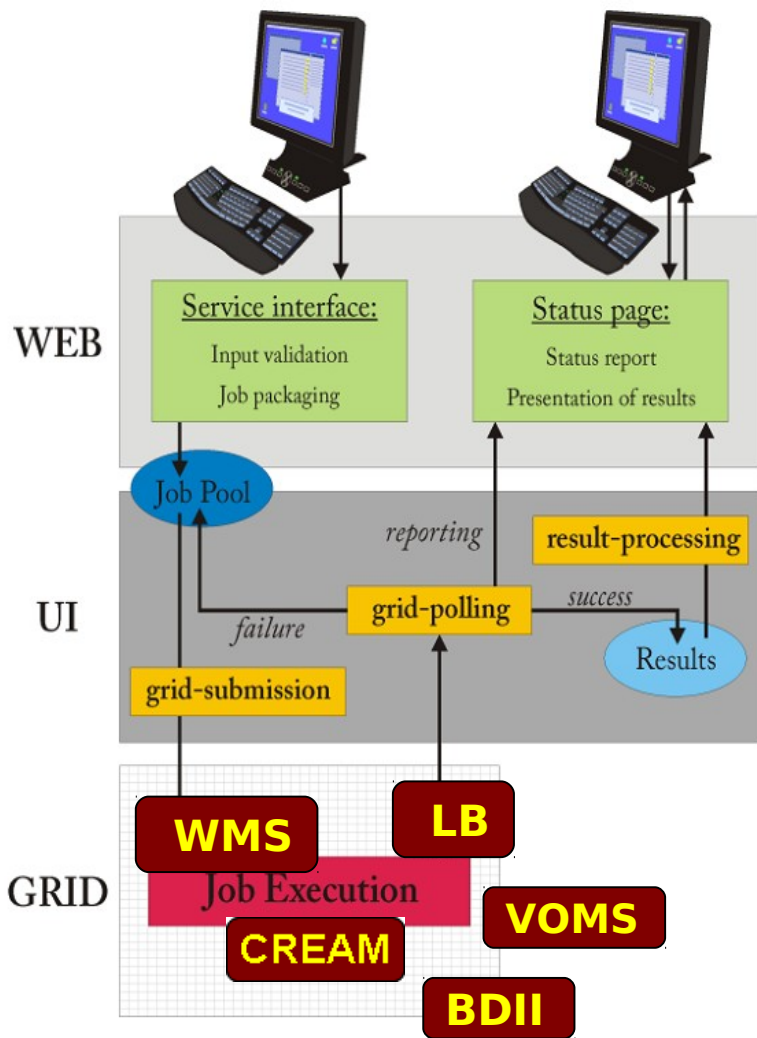
Name	Status	CPUs			Online Storage Space (GB)			Total
		Physical	Logical	S12000	TotalSize	UsedSize	Total	
AGLT2	N/A	700	4,180	8,360,000	0	0%	0	
CIT_CMS_T2	N/A	276	992	1,984,000	568,228	62%	0	
Clemson-Palmetto	N/A	8,888	8,888	17,776,000	46,952	35%	0	
FNAL_FERMIGRID	N/A	1	4	10,912	221,136	80%	0	
FNAL_GPGRID_1	N/A	543	1,892	6,182,016	26,388	63%	0	
GLOW	N/A	458	2,200	4,400,000	1,290,365	83%	0	
GRASE-CSE-MAGIC	N/A	52	176	352,000	3,148	7%	0	
GridUNESP_CENTRAL	N/A	512	2,048	4,096,000	805	68%	0	
LIGO_UWM_NEMO	N/A	1,560	3,120	6,240,000	5,396	45%	0	
MIT_CMS	N/A	3,012	3,012	6,024,000	1,548,443	71%	0	
Total		27,008	55,242	112,884,928	8,842,697	5,976,975	0	

Showing 1 to 10 of 26 entries

WeNMR-SBGrid Interoperability Plan

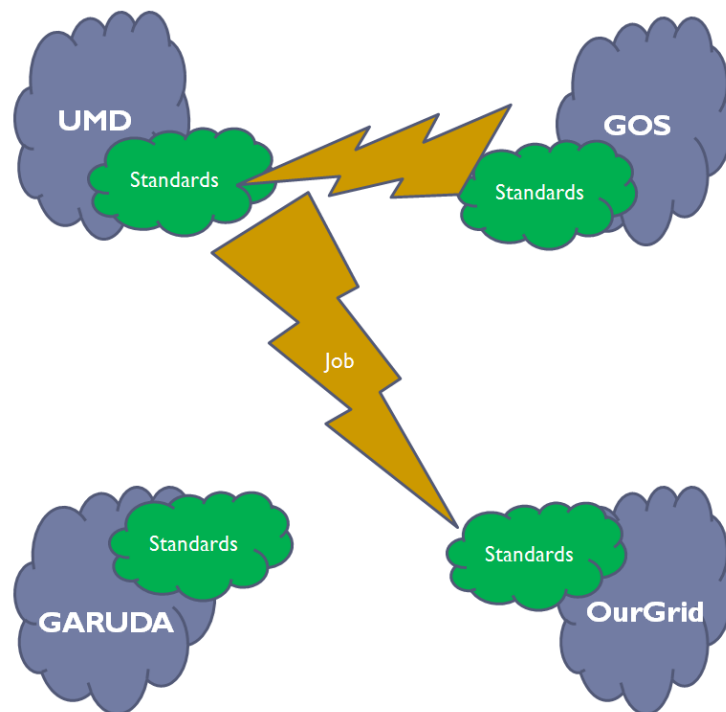
- Discussed at OSG AHM and at EGI-UF with OSG, EGI and SBGrid directors:
 - joint team with OSG-SBGrid-WeNMR-EGI personnel set up
 - use of **SBGrid VO** to access OSG/SBGrid resources
 - testing WeNMR jobs on OSG through gLite-WMS
 - configuring of a **glideinWMS** submission system for WeNMR
- Current status:
 - existing gLite UI and WMS enabled with SBGrid VO, new LFC server set up for SBGrid VO at INFN-Padova centre
 - Data transfer from/to 10 OSG SEs with registration on LFC successful using lcg-utils from both gLite UI and OSG WNs
 - CS-Rosetta software installed from remote in 14 OSG CEs
 - CS-Rosetta test jobs successful submitted through gLite-WMS (with minimal changes of bash scripts) and run on OSG WNs
 - Condor submit node (schedd) installed at INFN-Padova, configuration started

Using glideinWMS



Interoperability perspectives

- CHAIN is proposing an interoperability plan
- Application-level vs Service-level interoperability
- Based on OGF standards:
 - OGSA-BES, JSDL, SAGA (job manag.)
 - GLUE (info system)
 - SAML (security)
 - SRM (data management)
- A possible solution for WeNMR



Using standards

