

e-nmr

e-NMR Annual Meeting
Padova, 4 November 2008

INFN
GRID

WP2 e-NMR Grid deployment and operations

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Outline

- Overview
- WP2 Mandate
- Tasks
- Milestones & Deliverables
- Conclusions

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Overview

From the DoW:

"The main objective of this project is to optimise and extend the use of the EU-NMR Research Infrastructures through the implementation of an e-Infrastructure, e-NMR. This e-Infrastructure will provide the European bio-NMR user community with a platform that integrates and streamlines the computational approaches necessary for bio-NMR data analyses. **The e-NMR infrastructure will be based on the Grid infrastructure**"

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WP2 Mandate

- Objective 1: "Deploy and support an interoperable Grid infrastructure at the three NMR infrastructures to be later integrated with EGEE"
- Measure of success:
 1. the completion of the installation of the middleware at the three NMR research infrastructures
 2. the number of services provided by the e-NMR platform; the evaluation of the effective use of the infrastructure (n.of jobs, CPU.hours, etc.)
 3. number of new JRA components deployed

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e-nmr **WP2 tasks** INFN GRID

- Start date: PMO
- Duration: 36 Months
- WP leader: INFN
- Tasks:
 - **T2.1:** Deployment of the e-NMR grid infrastructure
 - **T2.2:** e-NMR Grid Operation Centre (GOC)
 - **T2.3:** Integration of JRA components

Part.	BMRZ	CIRMMP	BCBR	INFN
PMs	10	10	10	22

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e-nmr **T2.1: Deployment of the e-NMR grid infrastructure** INFN GRID

- **First year achievements:**
 - The NMR sites identified (or became) Registration Authority (RA) of their national Certification Authority (CA)
 - BCBR → Dutchgrid CA/O=universiteit-utrecht/OU=chem
 - BMRZ → GermanGrid CA/OU=UniFrankfurt
 - CIRMMP → INFN CA/L=CIRMMP
 - The enmr.eu VO was established and registered on the EGEE Operations Portal (cic.gridops.org)
 - The basic gLite services at sites (CE+WNs, SE and MON-box) were deployed and kept updated
 - A set of basic e-NMR dedicated grid services (VOMS, BDII, LFC, WMS, LB, etc.) were deployed at CIRMMP and INFN

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e-nmr **e-NMR gLite Infrastructure** INFN GRID

CEs, SEs and UIs at sites:

- 28 WNs
- 220 CPU-cores
- 3.1 TB storage

+ 359 CPU-cores
4.5 TB storage shared with INFN-GRID

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e-nmr **T2.2: e-NMR Grid Operation Centre** INFN GRID

- The deployed grid infrastructure has to be managed, monitored and supported
- It means:
 - Complement the basic grid services deployed with further tools to proactively monitor and account the usage of the infrastructure (e.g. gridICE, SAM, DGAS, gStat, etc.)
 - Provide support to both users and project's developers and resource managers through documentation, wiki, trouble ticketing system, mailing lists, middleware repository, bug tracking system, etc., typically accessed via the project web portal
 - Implement mechanisms to address operational problems and answer support requests
- Leveraging as much as possible on already existing operational procedures and tools adopted by EGEE


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gridICE snapshot





GridICE >> Site:ALL

General | **Grids** | Host | Job | Charts | Network | XML

Overview | Computers | Management

Computing Resources | Storage Resources


Site	Region	Q1#	Q2	RunJob	WaitJob	JobLoad	Power	W/MF	CEU#	CPUload	Available	Total	%	ML#
BCBR	NorthEU	1	5	0	2	0%	457K	4	32	0%	1.7 TB	1.7 TB	0%	24
BMRZ-FRANKFURT	SouthEU	1	4	0	0	0%	80K	1	4	0%	876.1 GB	478.3 GB	0%	5
CIRMP	Italy	1	5	0	0	0%	0	4	32	0%	477.7 GB	478.3 GB	0%	8
CNR-ILC-PISA	Italy	1	6	2	39	0%	3K	2	4	0%	376.8 GB	-	-	4
INFN-CATANIA	Italy	1	13	329	440	0%	402K	90	287	0%	-	-	-	119
INFN-PADOVA	Italy	2	14	114	460	0%	60K	19	58	0%	0.3 TB	0 TB	0%	42
TOTAL: 6		3	3	7	47	0%	1M	120	417	0%	11.8 TB	11.2 TB	0%	202

Generated: Mon, 3 Nov 2008 12:11:55 + 0100


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SAM snapshot




No	RegionName	SiteName	NodeName	Status	enmr.eu				
					crh	ca	ver	bi	js
1	Default	bcbcr	ce-enmr.chem.uu.nl	OK	ok	crit	3.1.0	ok	ok
2	Default	bmrz-frankfurt	ce-enmr.chemie.uni-frankfurt.de	OK	ok	crit	3.1.0	ok	ok
3	Default	cirump	ce-enmr.cern.unifi.it	OK	ok	crit	3.1.0	ok	ok
4	Default	cnr-ipc-pisa	gridce.ilc.cnr.it	OK	ok	crit	3.1.0	ok	ok
5	Default	infn-catania	grid012.ct.infn.it	ERROR	na	na	na	na	error
6	Default	infn-padova	prod-ce-01.pd.infn.it	ERROR	na	na	na	na	error
7	Default	infn-padova	prod-ce-02.pd.infn.it	OK	ok	crit	3.1.0	ok	ok


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HLRMon (DGAS) snapshot





Distributed Grid Accounting System

Report | Ranking | Monthly

Your role: ROC manager

Select your Role

ROC Manager

Select your Sites

All | Name

BCBR

BMRZ-FRANKFURT

CIRMP

CNR-ILC-PISA

INFN-PADOVA

Select your VOs

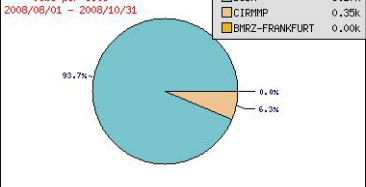
All | Name

enmr

Choose your Charts

Jobs/Site | NWT/Site | CPU/Day | CPU,W/VO | WT/VO

Jobs per Site
2008/08/01 - 2008/10/31




BCBR 5.17%
 CIRMP 0.35%
 BMRZ-FRANKFURT 0.00%
 CNR-ILC-PISA 93.78%
 INFN-PADOVA 6.33%


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GStat snapshot



GStat: 13:54:48 10/20/08 GMT - @wgc01

[home](#) [alert](#) [table](#) [service](#) [regional](#) [service](#) [metrics](#) [links](#) [prod](#) [pos](#) [test](#) [ballic](#) [sela](#) [suchina](#) [sundia](#) [sumed](#) [seogrind](#) [gilda](#) [trigrid](#) [p2s2](#) [grisu](#) [ireland](#) [eags](#) [e-nmr](#)

Color Legend

GSTAT : OK INFO NOTE WARN ERROR CRIT MAINT DEF

SFT : OK WARN ERROR CRIT SchedDown

Site List. sort by: [siteName](#) [domain](#) [maxcpu](#) [status](#)

No	Site Reports	GIS Host	hnode	cernse	apert	sanlrv	serv	serEntrv	version	schust	totalCPU	freeCPU	runJob	waitJob				
1	BCBR	ce-enmr.chem.uu.nl			ok	ok		ok	GLITE-3.1.0	Scientific Linux 3.0.9	176	142	34	4				
2	BMRZ-FRANKFURT	ce-enmr.chemie.uni-frankfurt.de			ok	ok		ok	GLITE-3.1.0	Scientific Linux 3.0.9	4	12	0	0				
3	CIRMP	ce-enmr.cern.unifi.it			ok	ok		ok	GLITE-3.1.0	Scientific Linux 3.0.9	32	29	0	0				
4	CNR-ILC-PISA	gridce.ilc.cnr.it			ok	ok	info	ok	GLITE-3.1.0	Scientific Linux 3.0.9	4	1	3	16				
5	INFN-CATANIA	grid005.ct.infn.it			ok	ok	ok	ok	GLITE-3.1.0	Scientific Linux 3.0.9	208	208	76	0				
6	INFN-PADOVA	prod-ce-01.pd.infn.it	ok	ok	ok	ok	ok	ok	GLITE-3.1.0	Scientific Linux 3.0.9	38	1	56	8				
sites countries totalCPU freeCPU runJob waitJob seAvail setJob																		
Total											6	3	462	393	169	28	14.29	119.01

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WMSMonitor Main >> Single Instance >> Overview: wms-nmr.cern.unifi.it

Component Details from 2008-10-29 11:00:02 to 2008-10-29 11:15:01 WMS Proxy Jobs -> WMSProxy 0 Collections submitted 0 Mean nodes per coll. 0 Std nodes per coll. 0 Proxy Renewal Workload Manager WM file descriptors 0 WM queue 0 Jobs -> WM 0 Jobs Resub -> WM 0 VO Views 205 Log Monitor LM file descriptors 10 Job Controller JC queue 0 JC file descriptor 4 Jobs -> JC 0 Jobs JC -> Condor 0 Local Logger LB events queue 0 LL file descriptor 4	General Info at 2008-10-29 11:15:01 WMS HW Status Sandbox partition 26% /tmp partition 26% CPU load 0 /var/log partition 26% /var/lib/mysql partition 26% Job Stats (Condor) Running jobs 4 Idle jobs 0 Total Condor jobs 4 Info from LB lib-enmr.cern.unifi.it LB status ✔ CPU load 0 / partition 0% LB connections 0 /var/lib/mysql partition 0%
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e-nmr **Users' & operations support** INFN GRID

- INFN Wiki page for e-NMR users and site administrators + training events:
grid-it.cnaf.infn.it/e-nmr/wiki/
- mailing list for site administrators:
enmr@dist.uni-frankfurt.de
- Contact established with EGEE-NA4 DE/CH regional support representative (Dr. Torsten Rathmann)
<https://twiki.cern.ch/twiki/bin/view/EGEE/RegionalSupport>
- In the future, with the joining of the e-NRM sites to EGEE, regional helpdesks interconnected with the Global Grid User Support (GGUS) system
www.ggus.org

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e-nmr **T2.3: integration of JRA components** INFN GRID

- We deployed the latest gLite middleware release
- It is expected that JRAs will produce new middleware/software components specific for e-NMR community
- new component developed to access application web portals using the personal certificate in the browser, verifying its VO membership and then starting a job submission with robot certificate:
<https://forge.cnaf.infn.it/projects/enmrwebui/>

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e-nmr **Milestones** INFN GRID

- M2.1: Grid infrastructure operational (M 12)
- M2.2: First integration of JRA developed components (M 24)

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e-nmr **Deliverables** INFN GRID

- D2.1: e-NMR grid infrastructure operational (M 12)**
 A document describing the hardware, the middleware and the grid services deployed at the NMR sites, and the GOC supporting the infrastructure
- D2.2: Assessment of the e-NMR infrastructure and GOC report (M 18, 27, 36)**
 A document evaluating the use of the infrastructure in terms of number of users, number of jobs run, CPU time used, storage capacity used, integration level with EGEE, effectiveness of GOC procedures and users' support
- D2.3: New components' integration and deployment report (M21, 36)**
 A document listing the programming libraries, APIs, tools, applications released by the JR activities and describing the procedure adopted for their integration and deployment on the infrastructure
- D2.4: Report on e-NMR infrastructure state-of-the-art toward integration with EGEE (M27)**
- D2.5: Final report on e-NMR infrastructure usage and integration with EGEE (M36)**

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e-nmr **Milestones & Deliverables** INFN GRID

M2.1: Grid infrastructure operational

M2.2: First integration of JRA developed components

M2.3: New components' integration and deployment report

D2.1: e-NMR grid infrastructure operational

D2.2: Assessment of the e-NMR infrastructure and GOC report

D2.3: New components' integration and deployment report

D2.4: Report on e-NMR infrastructure state-of-the-art toward integration with EGEE

D2.5: Final report on e-NMR infrastructure usage and integration with EGEE

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e-nmr **Conclusions** INFN GRID

- e-NMR grid is operational at the 3 NMR sites
- More than 220 cores and 3.1 TB dedicated available (and soon additional cores and TBs from BMRZ)
- A basic support system (wiki, mailing list) and operations tools are in place, but with growing the number of users we should soon:
 - To leverage on EGEE-NA4 regional support and GGUS
 - To become part of EGEE grid through ROC affiliation of e-NMR sites
- Some development version of bio-NMR application codes already run on the grid (e.g. HADDOCK already run 5500 jobs/2 CPU.months), see next presentations

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