



## **Deliverable 1.6**

### **Report on connections established with the e-Science community**

INFRA-2007-1.2.2 - Deployment of eInfrastructures for scientific communities

**Grant agreement for:      Combination of Collaborative projects &  
  Coordination and support actions**

Proposal/Contract no.: 213010 – **e-nmr**

Project full title:   Deploying and unifying the NMR e-Infrastructure in System Biology

Project coordinator: Prof. Dr. Harald Schwalbe

Project website: <http://www.enmr.eu/>

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## Introduction

e-NMR started out as a project complementing the EGEE II P project. For a better synergy between these two initiatives, a specific task within WP 1 was devoted to establishing connections between the e-science and the bio-NMR communities (Task 1.2). One of the aims was to make NMR experts, both within and outside the e-NMR partnership, aware of a grid platform could provide to them in terms of resources and support, and how it could foster the development of new applications. In addition, the ICT and software experts at the various bio-NMR infrastructures needed to become familiar with the EGEE middleware also to evaluate the possible needs of enhancements specific for the NMR domain or to identify solutions already in use within the bio-NMR community that could be beneficial to the e-Science community. Throughout the project a continuous interaction between these two communities has occurred, pushed by a continuing effort especially of the INFN partner. This has allowed the e-NMR partnership to promote the project results among the EGEE and e-Science community, supporting the project participation to the main conferences and workshops with posters, lectures and live demonstrations of the achieved results (Milestone M1.2: "Demonstration of e-NMR at e-Science event"). In addition, the connections that have been established are instrumental to permit a smooth transition from the EGEE to the EGI model, particularly with respect to the Life Sciences grid community, through cooperation with the various relevant EGI bodies as well as the NGIs.

## Activities toward the e-Science community

The table below lists the main events targeting e-Science community (scientific, or of any other nature) in which the e-NMR project has been involved.

Date	Title/subject of meeting	Location	Website address
22 <sup>nd</sup> – 26 <sup>th</sup> September 2008	<b>EGEE'08 Conference</b>	Istanbul (Turkey)	<a href="http://egee08.eu-egee.org">egee08.eu-egee.org</a>
12 <sup>th</sup> -16 <sup>th</sup> May 2008	Biomed Grid School	Varenna (IT)	<a href="http://www.biomedgrid.it">www.biomedgrid.it</a>
2 <sup>nd</sup> -6 <sup>th</sup> March 2009	4 <sup>th</sup> EGEE User Forum/OGF 25 and OGF Europe's 2nd International Event Search	Catania (IT)	<a href="http://egee-uf4.eu-egee.org">egee-uf4.eu-egee.org</a>
7 <sup>th</sup> -8 <sup>th</sup> May 2009	Research Connection 2009	Prague (CZ)	<a href="http://ec.europa.eu/research/conferences/2009/rt-d-2009">ec.europa.eu/research/conferences/2009/rt-d-2009</a>
10 <sup>th</sup> -15 <sup>th</sup> May 2009	Biomed Grid School	Varenna (IT)	<a href="http://www.biomedgrid.it">www.biomedgrid.it</a>
21 <sup>st</sup> -25 <sup>th</sup> Sept, 2009	<b>EGEE'09 Conference "Enabling Grids for E-sciencE '09"</b>	Barcelona (ES)	<a href="http://egee09.eu-egee.com">egee09.eu-egee.com</a>

Date	Title/subject of meeting	Location	Website address
1 <sup>st</sup> December 2009	GEANT launch event - Panel discussion "Keeping Europe at the cutting edge of Science Discovery"	Stockholm (S)	<a href="http://www.geant.net/Events/LaunchEvent/Pages/EventAgenda.aspx">http://www.geant.net/Events/LaunchEvent/Pages/EventAgenda.aspx</a>
2 <sup>nd</sup> – 3 <sup>rd</sup> March 2010	EGI VRC Support Meeting	Amsterdam (NL)	<a href="https://www.egi.eu/indico/conferenceDisplay.py?confId=1">https://www.egi.eu/indico/conferenceDisplay.py?confId=1</a>
18 <sup>th</sup> March 2010	ICTDelta 2010	Rotterdam (NL)	<a href="http://www.ictdelta2010.nl">www.ictdelta2010.nl</a>
12 <sup>th</sup> -16 <sup>th</sup> April 2010	5 <sup>th</sup> EGEE User Forum	Uppsala (S)	<a href="http://egee-uf5.eu-egee.org">egee-uf5.eu-egee.org</a>
24 <sup>th</sup> – 27 <sup>th</sup> May 2010	IBERGRID 2010	Braga (P)	<a href="http://www.ibergrid.eu/2010/">www.ibergrid.eu/2010/</a>
28 <sup>th</sup> June 2010	LS VRC workshop at Healthgrid conference	Paris (F)	<a href="http://indico.in2p3.fr/sessionDisplay.py?sessionId=1&amp;slotId=0&amp;confId=2504#2010-06-28">http://indico.in2p3.fr/sessionDisplay.py?sessionId=1&amp;slotId=0&amp;confId=2504#2010-06-28</a>

The above events constituted occasions to demonstrate the achievements of the e-NMR project to audiences whose main focus was e-Science applications. In particular, the e-NMR contribution at the 4<sup>th</sup> EGEE User Forum (March 2009) constituted of a live demonstration that was a début for the project in the e-Science arena, after other demonstrations held to audiences comprising mainly or only bio-NMR scientists. Instead, the meeting in Catania was primarily attended by GRID facility managers, developers and users from a number of different scientific fields, including life sciences: The demo of the e-NMR portal was awarded '[Best demonstration of an application](#)' with the following motivation: **"it represented a unique and important application, was adopted to grid very fast, had a clear development strategy and most importantly brought new resources to the grid"**. A short video of the presentation is [available](#). This constituted the project milestone M1.2: "Demonstration of e-NMR at e-Science event".

The e-NMR partnership presented live demonstrations also at the Research Connection 2009 and at the EGEE'09 Conference "Enabling Grids for E-science'09". For the latter occasion in particular, new presentation materials were developed, and shown at a booth that the e-NMR project maintained throughout the conference. The presentation included [showing a newly developed video on the project](#), also available [at higher resolution](#). The e-NMR project delivered also a lecture at a bioinformatics session in the meeting. Finally, the EGEE'09 conference additionally provided a further opportunity to discuss about the Life Sciences SSC. Further discussion on this matter took place in June 2010 at a meeting in Paris that focused on the role and future of the Life Sciences Virtual Research Community, after the proposal to the EC to fund the establishment and support of various SSC's, including that for the Life Sciences in which eNMR was involved, was rejected. At the 2010 Paris meeting, it was proposed that a

Life Sciences VRC be formally created by the Healthgrid organization. The e-NMR project will maintain close interactions with this VRC. A booth with new videos of the project achievements, focusing on the use of the eNMR web portal (e.g., [http://www.enmr.eu/bmrz-portal/enmr/tutorial\\_videos/cyana\\_auto\\_portal.mov](http://www.enmr.eu/bmrz-portal/enmr/tutorial_videos/cyana_auto_portal.mov)), was presented also at the 5<sup>th</sup> EGEE user forum, held in Uppsala in 2010. All e-NMR movies are available at <http://www.enmr.eu/Video>. A demo was additionally presented (<http://www.youtube.com/watch?v=axqn08-JybE&feature=digest>). A paper and an oral presentation were instead the two components of the e-NMR contribution to IBERGRID 2010 (see for example the paper at <http://www.enmr.eu/eNMR-news-events>); participation in this conference was deemed by the e-NMR partnership as being important to spread awareness of the project in the Iberian countries and resulted in the addition of a Portuguese GRID site to the list of sites supporting the eNMR VO.

The Biomedgrid school in Varenna provided a completely different environment with respect to the aforementioned events, in that this is a small-scale event involving only people closely working on Life science and biomedical applications that are Grid-based. These events thus provide a venue for close interactions and exchanges of experience among people with different backgrounds but with an interest in related problems and often facing similar hurdles (e.g., web-based services, workflow management, etc.). E-NMR attended this school twice, once at the very beginning of the project, in order mainly to obtain information on the solutions that were already in use within the community and that could be of interest to the project, but also to discuss its concept and the first guidelines for its development. At the second participation, the project had already matured significantly, enabling a detailed presentation and discussion especially of its web-based solutions.

Finally, it is important to mention meetings where eNMR has been involved in order to take part in the discussion of the transition from EGEE to EGI, which will be a crucial step for the e-Science community as well as for all those scientific communities that have been making use of grid infrastructures to address their computational needs (in full or in part). One such event took place in March in Amsterdam, aimed at fine tuning the support needed by the current EGEE communities in the perspective of the transition. A follow-up activity has already been planned in the EGI Technical Forum 2010 that will be held in Amsterdam on September 14<sup>th</sup> - 17<sup>th</sup>, 2010. eNMR (and its follow-up project WeNMR) will be represented in Amsterdam. Further, eNMR is directly involved in the organization in the person of Prof. Dr. A. Bonvin who

is a member of the programme committee for this meeting.

### *Concluding remarks*

e-NMR interacted and built links with the e-Science community by moving along three main directions:

- collecting indications on the best use of the grid infrastructure by exploiting previous experiences in the field of Life sciences as well as in other disciplines
- developing a solid reputation by setting up and presenting/demonstrating a portfolio of services carefully designed to address the needs of a community of users that were completely new to e-Science
- starting activities at the managerial / policy making level.

The well-balanced temporal planning of the above initiatives was important to ensure that the reputation of the project could be based on a solid scientific background that could be successfully presented both to the NMR community, to engage a solid base of users, and to the eScience community as a model for the presentation of an e-Infrastructure to a new user community. The reputation of the e-NMR project is demonstrated, among other things, by its involvement at the Panel discussion “Keeping Europe at the cutting edge of Science Discovery” held on the occasion of the GEANT launch event in Stockholm. In addition to the core partners reference NGIs (Italy, Germany and the Netherlands), e-NMR has obtained support by the South African, the UK, the Belgian and Portugal NGIs. On this basis, the project partnership could be usefully and successfully involved in policy making by interacting with the EGI bodies, other grid infrastructure operators as well as the management levels of the various NGIs.