# **CGCC** Enabling Grids for E-sciencE

## Newsletter May 2006

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#### WELCOME TO EGEE-II

In April we began EGEE-II, and while much of the project will remain the same as under EGEE, I wanted to take this opportunity to welcome both new and old partners to EGEE-II and explain some of the key changes we have made.

The most dramatic change to the project is the number of partners, with a total of 91 contractors and an additional 48 through membership of Joint Research Units. This expanded consortium, along with close relationship with related projects, further extends the scope of this global project, and we are particularly happy to be able to welcome US and Asian institutes, with whom we have worked for some time, as full partners in the project. I would also like to thank all the partners who attended the Transition meeting in April; the meeting was very successful with many talks providing useful information on the project, and plenty of lively discussion. For those that could not attend, the slides from the talks are all available at http://agenda.cern.ch/fullAgenda.php?ida=a061190.

For EGEE-II we have restructured our efforts in several areas, increasing efforts in application support and dissemination in order to maintain the rapid growth in the size of the user community we saw during EGEE. We have also renewed our commitment to industrial relations, with a revised Industry Forum (now under the care of NA2) and the EGEE Business Associate programme, which provides a framework for collaborative research alliances between EGEE and industry. Along with a formalised relationship with the CERN openlab, a highly successful research project combining CERN and leading IT firms, we hope to dramatically increase the opportunities for industry to learn about our work and make use of our infrastructure.

For the EGEE middleware, this month we are testing a new combined release of the LCG-2 and gLite stacks, to be called the gLite 3.0 distribution. Recognising the excellent work in the area of middleware carried out by projects around the world, for EGEE-II we will be incorporating a greater number of middleware components from outside sources, moving further toward providing a global reference implementation for middleware.

Looking to the future, in September we will hold the EGEE'06 conference, the first of EGEE-II. Registration is now open, and we hope this event will be considerably larger than previous EGEE conferences, attracting more users, members of industry and representatives from the international organisations in the Geneva area, such that they can learn about the Grid and its potential to help them in their work. We will also soon be planning the next User Forum, following on from the very successful event organised by NA4 in March. As mentioned later in this newsletter, we are open to bids to host the next User Forum, as well as the EGEE'07 conference.

Once again, welcome to EGEE-II. I look forward to working with you all over the next two years, and am sure EGEE-II will prove as successful as EGEE has been.

Regards,

Bob Jones EGEE-II Project Director



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#### EGEE GRID ATTACKS AVIAN FLU

During April, a collaboration of Asian and European laboratories analysed 300,000 possible drug components against the avian flu virus H5N1 using the EGEE Grid infrastructure. The goal was to find potential compounds that can inhibit the activities of an enzyme on the surface of the influenza virus, the so-called neuraminidase, subtype N1.



The binding pocket of Neuraminidase, the box shows the region investigated in the study. Photo from Ying-Ta Wu.

The drug discovery process is being greatly accelerated by the use of the EGEE and associated computing Grid infrastructures. For the docking of 300,000 compounds against 8 different target structures of Influenza A neuraminidases, 2000 computers were used during 4 weeks in April – the equivalent of 100 years on a single computer. More than 60 000 output files with a data volume of 600 Gigabytes were created and stored in a relational database. Potential drug compounds against avian flu are now being identified and ranked according to the binding energies of the docked models.

"With the help of the high-speed computing and huge data managing capabilities of the Grid, possible drug components can be screened and studied very rapidly by the available computer modeling applications," says Ying-Ta Wu, biologist at the Genomics Research Center of the Academia Sinica in Taipei. "This will free up medicinal chemists' time to better respond to instant, large-scale threats. Moreover, we can concentrate our biological assays in the laboratory on the most promising components, the ones we expect to have the greatest impact." is a powerful and reliable resource for scientists, opening up new research possibilities and improving existing methods," said Viviane Reding, European Commissioner responsible for Information Society and Media. "I am very grateful to see that the European flagship Grid infrastructure is contributing to solving current and socially important problems such as avian flu."

Taking advantage of the experience acquired in the previous WISDOM data challenge on malaria, the Grid-enabled in silico process was implemented in less than a month on three different grid infrastructures: AuverGrid, EGEE, and TWGrid, paving the way for a virtual drug screening service at a large scale. The majority of computing is conducted on the WISDOM platform; in addition, a light-weight application framework called DIANE was also adopted in this challenge and used to perform a sizeable fraction of the total activity to enable efficient computing resource integration and usage. The next WISDOM data challenge against several targets of neglected diseases will take place in autumn 2006.

Hannelore Hämmerle, NA2/CERN

#### EGEE INDUSTRY DAY

Given the EGEE reputation in Grid technology it is not surprising that some of Europe's key players from Industry attended the first Industry Day in Paris on 27 April. Over 60 delegates representing over 30 European Organisations from ICT, Research, Energy, Finance, Geosciences and Physics, reflected the steadily growing Industry interest and the possibilities of using the EGEE Grid Infrastructure.

The event triggered much interest, particularly given projects increasingly industry-friendly approach, reflected by the revamped EGEE Industry Forum, Industry Task Force and EGEE Business Associates, all of which aim to open up the EGEE Grid infrastructure and know-how to Industry.

Many participants came to hear how the EGEE Grid could be used in an Industrial environment. Successful examples of EGEE technology transfer demonstrated that indeed the Grid is a viable alternative to traditional IT solutions.

The flexibility of the EGEE Grid was demonstrated



"With these results, the Grid demonstrates that it

by applications from Geosciences through to the plastics industry, where the Grid has produced real savings for SMEs, through the OpenPlast project. NICE and DATAMAT gave insight on their successful work with EGEE and Grid technology.

With the crisis of avian flu still current, demonstrating how Asian and European laboratories made use of the EGEE Grid infrastructure to develop drugs against the virus drove home the real potential of the EGEE Grid. A task that would have normally taken 100 years on a single computer was done in just 4 weeks.

Naturally the business orientation of the audience led to discussions on the real potential but also the challenges ahead for EGEE, in terms of business and return on investment, the sustainability of EGEE and security issues. These include how EGEE is now working towards certification and standardisation activities and the challenges facing EGEE in terms of industrial use of the GEANT network.

Industry days are set to become a regular feature of EGEE, following the success of this first event in Paris. The next Industry Day will take place in Cambridge, UK, organised by PPARC and will be attended by the Project Director and NA2 representatives.

For more information on the EGEE Industry Forum and Industry Days visit http://www.eu-egee.org/user-forum/industry\_forum

Douglas McKinley, NA2/Metaware

#### E-IRG OPEN WORKSHOP ON E-IN-FRASTRUCTURES

The e-Infrastructure Reflection Group (e-IRG) held their latest two-day Open e-Infrastructures Workshop at the beginning of April. With the Austrian Presidency of the European Union, EGEE's Dieter Kranzlmüller has taken the chair of the e-IRG and was hosting the meeting in his home town of Linz, with the support of the Austrian Grid Initiative.

The workshop started on 10 April with a closed meeting for e-IRG delegates in the morning and continued with a plenary session in the afternoon. The plenary session began with a description of the BELIEF project by coordinator Stephen Benians,



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Austria.

which was holding its first brainstorming event on Future Knowledge Infrastructures just after the e-IRG workshop. Mr Benians's talk was followed by a presentation from Robert Cohen from GGF and the Economic Strategy Institute on the potential value of a study of Grid adoption and research in Europe to identify future infrastructure and technology needs. Sergi Girona from BEinGrid presented the project, which is demonstrating the power of Grid computing solutions to industry through a series of business experiments.

The focus of the talks in the second plenary session of the afternoon was on sustainability. Vasilis Maglaris of GRNet discussed the future of research networking while head of DEISA Victor Alessandrini concentrated on the future for supercomputing. Leif Laaksonen of CSC, the next e-IRG chair, represented the Sustainable e-Infrastructures Task Force and spoke about its current work: preparing a paper with a set of recommendations to be given to the European Commission (EC) at the end of April. This is intended to help the EC in planning the Seventh Framework Programme (FP7), which will shape how the EC funds e-Infrastructure projects in the next seven years.

The following day was dedicated to ten discussion groups, arranged in two sets of five parallel sessions, with reports given in plenary at the end of each set of discussions. Each discussion will form the basis of a chapter in the Austrian e-IRG White Paper. The e-IRG White Paper Editors, EGEE's Fotis Karayannis and Panagiotis Louridas, have taken the decision to use an open-access wiki format to gather contributions to the White Paper, and we



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would be pleased to see EGEE members sharing their ideas and experience in this way. The address for the wiki page where you can see the titles of the chapters and make your contributions is http://wiki. e-irg.org/bin/view/Main/AustrianWhitePaper.

EGEE had a strong presence at the workshop itself and the editors would appreciate the active participation of EGEE members and other interested parties in the work of e-IRG.

The next e-IRG meeting will be in Finland in October this year, more information on this and other e-IRG news can be found at http://www.e-irg.org, while EGEE's contribution through the NA5 activity is documented at http://cern.ch/egee-NA5.

Joanne Lawson, NA5/CERN

### ARCHAEOGRID, A GRID FOR THE PAST

Modern archaeology is far more than trench digging, and as it gets set to embrace the Grid it is shedding its low-tech image in favour of a high-tech approach to uncovering the past.

The idea of an ArchaeoGRID, a Grid for archaeology, has been around since 2003 when it was presented to the IEEE NSS-MIC conference in Portland, USA. It was discussed again at the 2004 IEEE conference in Rome, Italy and finally in October 2005 the ArchaeoGRID proposal was submitted for approval to the EGEE Generic Applications Advisory Panel. The panel found the ArchaeoGRID proposal particularly attractive, as it adds an application from the human sciences to the EGEE portfolio. They recommended ArchaeoGRID for full approval at the March 2006 User Forum meeting. EGEE also suggested that the ArchaeoGRID consortium could profit from collaborating with the DILIGENT project (which works on digital libraries and is interested in many of the same technical challenges) and that the ArchaeoGRID community should deploy their paleoclimate application on the GILDA testbed.

EGEE is looking forward to welcoming and accommodating ArchaeoGRID: deploying an archaeological application on a Grid infrastructure presents many interesting new challenges due to the complexity and heterogeneity of archaeological data from excavations and field surveys. It includes aspects of work from fields as diverse as physics, chemistry, earth sciences, biology, geography, anthropology and social science, as well as techniques developed during the development of archaeological methods and theories.

Archaeological data also loses much of its meaning when taken out of the original spatio-temporal context in which it was discovered. This spatial and temporal context of modern archaeological research extend from the dig site itself to much larger regions and long time periods. The final stage of archaeological work is also very complex, involving the visualisation of results (digital maps, virtual worlds, 2D and 3D images, etc.) and a textual description based on the analysis of results and theoretical knowledge.

The ArchaeoGRID structure must merge these different approaches into a single system using a service-oriented architecture, also used by the gLite middleware, by DILIGENT middleware and the Open Geospatial Consortium Web Services system. The ArchaeoGRID community is now attempting to produce an integrated ArchaeoGRID structure with the help of the GILDA and DILIGENT groups.

The ArchaeoGRID proposal included an investigation into the origin of the city in the Mediterranean area as the archaeological application for the Grid. In collaboration with the GILDA group, the ArchaeoGRID community is deploying a paleoclimate application using a mesoscale model on the GILDA t-Infrastructure and testing this model with the present data. In the next step, the model will run on the archaeological data that corresponds to studied centuries.

Giuliano Pelfer, CSDC, University of Florence

### THE BELIEF PROJECT

e-Infrastructures might well be referred to as the new 'knowledge generation highways', but how can we guarantee they won't remain empty or underused? BELIEF, a new project funded under the European Commission Sixth Framework Programme, has been established to help ensure that e-Infra-



structures are effectively exploited and developed worldwide.



BELIEF brings together e-Infrastructure stakeholders, the providers and the users, to help them exchange knowledge on the technology and user needs, and to ensure that Europe collaborates effectively with other regions, especially the emerging economies of India and Latin America.

To bring these communities together, BELIEF offers its registered members an e-Infrastructures digital library, an online forum, a facility to search and contact other members, and e-Infrastructure case studies. Offline, BELIEF organises events including brainstorming meetings, networking workshops and international conferences as well as publications.

BELIEF's first brainstorming in Linz, Austria, on 11-12 April, was on Scientific Repositories. The participants, high level experts from many different disciplines, concluded that such knowledge infrastructures could "unleash scientific and academic potential worldwide", and that, though ambitious, this value-adding vision must be realised. BELIEF's first Technology Report will set out how this vision of scientific repositories can be accomplished. A concept paper on the topic can already be accessed on the BELIEF website.

BELIEF's Research-Industry handbook, soon to be published, matches supply with demand, showing industry which e-Infrastructures exist and how to access them, whilst showing to the research fields the achievements that industry has pioneered and how synergies can be created between these communities. These publications will be available via the BELIEF Digital Library, which is a rich source of e-Infrastructure documentation, collected from many projects such as EGEE and GÉANT, and itself helps to connect e-Infrastructure consumers and providers through its tailor-made search facility.

Through these offline and online activities, BELIEF helps to ensure the knowledge generation highways are well developed and effectively exploited, adding value to research and industry worldwide. Register with BELIEF at www.beliefproject.org to spread the word about your activities, exchange your knowledge and find out more about e-Infrastructures.

#### Stephen Benians, BELIEF



#### SOUTH-EASTERN EUROPE REACHES **OUT TO ASIA-PACIFIC**

EGEE is rightly proud of its worldwide scope: recently our international approach has been reaping benefits not only for the Grid community but also for a talented group of Serbian physics students who travelled to Taiwan as part of the World Year of Physics 2005 celebrations. During 2005, physics societies all over the world hosted events to celebrate and promote physics, including the 'Young Talents in Physics Search', an international competition for high school students.



Min-Hong Tsai of Academica Sinica showing the Grid to the Serbian students.

In Serbia, the Serbian Physical Society organized this competition at the national level and sent EGEE contributor Antun Balaz as their representative to escort the winning team of students to the 'International Young Physics Ambassadors Symposium', held at Takmang University in Taiwan, from 30 December 2005 to 5 January 2006.

At the Taiwan Symposium, the students were treated to lectures by Nobel laureates and visits to several research and development institutions in Taiwan, including Tamkang University, Taiwan National University, and the Institute of Physics of Academia Sinica. For the lucky Serbian students the event also took on a significant Grid dimension, thanks to the efforts of Antun Balaz and EGEE's Asia-Pacific partners.





Since Antun Balaz represents Serbia in the EGEE-SEE ROC and acts as one of the SEE-GRID GIMs, he organized an additional visit to EGEE Asia-Pacific CIC/ROC (located at the Academia Sinica Computing Center), where the Serbian team was hosted by Asia-Pacific ROC Managers Min-Hong Tsai and Jason Shih. The students were introduced to the Grid world and the basics of Grid computing and received an explanation of the development of the GStat monitoring tool. Antun Balaz also took time to discuss current and future collaborations with Asia-Pacific colleagues on the EGEE-II, SEE-GRID and SEE-GRID-2 projects. Our congratulations go to the Serbian students, and we hope they enjoyed playing a part in EGEE's international collaboration during their visit to the Asia-Pacific CIC/ROC.

Antun Balaz, Institute of Physics, Belgrade

#### **NEWS IN BRIEF**

#### EGEE'06 REGISTRATION GOES LIVE

Registration for EGEE'06 is now open! To be held on 25-29 September 2006 in Geneva, Switzerland, this should be the largest EGEE conference thus far, featuring increased participation from users, industry and the international organisations in the Geneva area. Delegates are encouraged to register early to qualify for a reduced price by logging on to http:// www.eu-egee.org/egee06. Any parties wishing to apply for exhibition space should also make sure to look at the information at http://cern.ch/egee-intranet/conferences/EGEE06/programme.html in order to reserve space.

EGEE FINAL REVIEW: 23-24 MAY 2006, CERN

While work has already begun in earnest for EGEE-II, we are still in parallel completing final reporting for the EGEE project, culminating in the Final Review on 23-24 March which will be held at CERN. In the coming weeks, the activity leaders will be preparing their presentations on the important achievements made since the last review and how EGEE has addressed the reviewers' previous recommendations. The reviewers will shortly be receiving their reading list, which will include all the deliverables and reports from EGEE project months 19 to 24, as well as information about our relationship with industry and a short film about EGEE. Attendance at the review is by invitation, and activity leaders will nominate those individuals they feel should attend.

### EGEE-II PROJECT CONFERENCE AND USER FORUM: OPEN FOR OFFERS!

With preparations well under way for the EGEE'06 project conference on the 25-29 September in Geneva, thoughts are already turning to the EGEE'07 conference and the next User Forum. The User Forum will take place in spring 2007, and the EGEE conference in autumn 2007. Any partners who are interested in hosting either event are encouraged to get in touch with the Project Office for further details.

#### **RECENT DELIVERABLES**

All public deliverables are available online through the CERN EDMS system at https://edms.cern.ch/ under the EGEE and EGEE-II sections. The latest deliverables are the final batch from EGEE and provide a full overview of our activities over the past two years:

- DNA1.4: Report on Gender Action Plan
- DNA2.7: Final Dissemination & Usage Report addressing the issues of public participation and awareness
- DNA3.3.3: Training Progress Report update
- DSA1.9: Release notes corresponding to expanded production Grid infrastructure operational
- DSA2.3: Revised SLAs and policies
- DJRA2.3: 2nd Annual report on EGEE Quality Status, including software and Grid operations
- DJRA3.4: Assessment of security infrastructure report
- DJRA1.7: Final report on middleware re-engineering
- DJRA4.6: Report on bandwidth allocation and reservation
- DJRA4.7: Report on network monitoring
- DNA4.4: combined with DNA4.3.3
- DNA4.3.3: Final Report of Application Identification and Support Activity with revision of EGEE Application Migration Progress report
- DNA5.5: Final progress report on International Cooperation Activities
- DSA1.8: Assessment of production infrastructure operation
- DNA1.1.8: Quarterly report
- DNA1.3.2 combined with DNA1.3: Periodic report.

#### THE TECHNICAL REPORT SERIES

The project has recently implemented a new system for collecting published and unpublished technical articles about the EGEE and EGEE-II projects to



make them easily accessible to both project members and our external contacts. This, the EGEE Technical Reports (TR) series is accessible via the CERN Document Server on http://cdsweb.cern. ch/?c=EGEE and the first documents have already been uploaded:

- Security of Distributed Data Management by Frohner, A; Kunszt, P; Brito Da Rocha, R; Laure, E

Implementation of a Medical Data Manager on top of gLite services by Montagnat, J;
Jouvenot, D; Pera, C; Frohner, Á; Kunszt, P;
Koblitz, B; Santos, N; Loomis, C
Network and Grid : the EGEE use-case by
Goutelle, Mathieu; Gautier, Jean-Paul
Programming the Grid with gLite by Laure, E et al.

- Middleware for the next generation Grid infrastructure by Laure, E et al.

#### FORTHCOMING EVENTS

#### MAY

10-12 May 2006, Tokyo, Japan GGF17 http://www.ggf.org/GGF17/ggf\_events\_ggf17.htm

#### June

19 June 2006, Paris, France EGEE Workshop on Rights Management in Production Grids HPDC 15 http://cern.ch/egee-intranet/HPDC-Workshop/

19-23 June 2006, Singapore Euro-Southeast Asia 2006 (EUSEA2006) conference http://www.eusea2006.org/createMember

20-23 June 2006, Singapore Euro-Southeast Asia 2006 (EUSEA2006) Exhibition http://www.eusea2006.org/createMember

26-30 June, Dubna, Russia Distributed computing and Grid technologies in science and education http://grid2006.jinr.ru

Thanks for reading this newsletter, which will keep you up to date on events within the project and the European Grid community in general.

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#### JULY

3-6 July 2006, Cetraro, Italy HPC and Grid, HPC 2006-05-04 www.hpcc.unical.it/hpc2006

#### SEPTEMBER

19-21 September 2006, Brussels, Belgium European Grid Technology Days http://www.cordis.lu/ist/grids/agenda\_15\_09\_04.htm

21-23 September 2006 Austrian Grid Symposium, Innsbruck, Austria http://www.austriangrid.at/austriangrid/

25-29 September 2006, Geneva, Switzerland EGEE'06 conference http://www.eu-egee.org/egee06

#### **CALLS FOR PAPERS AND PARTICIPATION**

21-23 September 2006, Innsbruck, Austria 6th Austrian-Hungarian Workshop on Distributed and Parallel Systems Deadline 16 June http://www.lpds.sztaki.hu/dapsys

1-4 December 2006, Sorrento, Italy The 2006 International Symposium on Parallel and Distributed Processing and Applications (ISPA 2006) Deadline for papers 31 May, closed for workshops http://www.ispa-conference.org/2006/

4-6 December 2006, Amsterdam, The Netherlands Second IEEE International Conference on e-Science Deadline for papers 15 June, closed for workshops http://www.escience-meeting.org/eScience2006

#### **TRAINING EVENTS**

9-21 July 2006, Ischia, Near Naples, Italy Fourth International Summer School on Grid Computing http://www.dma.unina.it/~murli/ISSGC06/

11-15 September 2006, Karlsruhe, Germany GridKa School 2006-03-20 http://www.fzk.de/gks06

You are receiving this newsletter as you have expressed an interest in the EGEE project. If you have any questions, comments or suggestions for the next issue, please feel free to contact owen.appleton@cern.ch.

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