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eGee News
Enabling Grids for E-sciencE

July 2005   **Hot topics**   **Newsletter # 8**
(.pdf)

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Two new applications running on the EGEE infra-structure: Drug Discovery and Earthquake Analysis

Welcome

Its summer at last and the weather, over most of Europe at least, has been hot! We have lots of news for you in this issue of the EGEE Newsletter, both within the project and in the wider world. As always, you can access an online version of the latest newsletter, as well as all back issues, at http://egee-intranet.web.cern.ch/egee-intranet/newsletter/Newsletter.html

4th EGEE Conference Announced

Pisa will host the 4th EGEE conference later on this year. This high profile event will be held at the Palazzo dei Congressi di Pisa from 24-28 October 2005. Featuring speakers from the European Union and Italian Government, as well as CERN's Director General, the conference looks certain to live up to the excellent standard of the last conference in Athens.As with the last three conferences, this will be an opportunity both to reflect on the achievements of the last 6 months and to plan for the future. The website for the conference is available at http://public.eu-egee.org/conferences/4th/ and registration is now open!

Departure of Project Director

Project Director Fabrizio Gagliardi announced his departure from EGEE on 12 June in an email to all members of the project. Having been highly successful in both EGEE and its predecessor, European DataGrid, he is now moving on to take a senior position in Industry. Many project members will have experienced his dynamic management style and seemingly limitless energy for promoting EGEE and Grid technology over the past years, and we all wish him well in the future.

Fabrizio will continue to lead the project until 31 October 31, and so will remain in charge of the planning for the next phase of EGEE. The project will bid him farewell at the 4th conference in Pisa.

Using a JAX-RPC generated java stub interface you can dynamically the service end point for your client by calling the get_Property(), _setProperty() methods to change the ENDPOINT_ADDRESS_PRO This allows you to have alternative producers in the case of failure.

Globus Toolkit 4 released

Since the last newsletter, The Globus Alliance has released the lates of their extremely widespread Globus Toolkit (GT). GT4 features a new features, such as a state-of-the-art Web service hosting envi

for Java, Python and C, as well a long list of other improvements.

EGEE already makes use of a number of GT components in middleware stack, and is constantly assessing the Globus software modules that will make gLite more effective and more compatible v global grid efforts. EGEE already plans to make use of the improved functionality in GT4 (which includes backward compatibility with G more information, or to download GT4, see the Globus Toolkit http://www.globus.org/toolkit/.

Training News

FORTHCOMING TRAINING EVENTS
For full event listings, see http://www.egee.nesc.ac.uk .

EMBRACE biomed tutorial, Clermont-Ferrand, France, 25-27 June
This joint Embrace / EGEE tutorial is mainly dedicated to new EGEE application developers as well as Embrace PhD students and I workers. Programme and registration can be fou http://tutorial.healthgrid.org

FURTHER EDUCATION

Two new applications running on the EGEE infrastructure: Drug Discovery and Earthquake Analysis

Continuing its mission to support as many scientific disciplines as possible, EGEE has added two more applications to its portfolio, Drug Discovery and Earthquake Analysis, both with the potential to save lives around the world.

The Drug Discovery application aims to find potential new drugs to combat malaria, a disease which kills a million people per year and affects 300 million more. In this application, scientists carry out "in silico" docking, which enables researchers to compute the probability that potential drugs will dock with a target protein - in this particular case with the active site of one of the malaria parasite proteins. On a single computer, a study like this, with 100,000 potential drugs, would normally require six months to complete - but on the EGEE Grid it was achieved in just two days. The next step is to increase the performance of the application and compute millions of potential drugs in only a few weeks, a real possibility with the EGEE grid. Working at this rate, researchers hope to take a significant step towards finding a new drug to treat this widespread and socially devastating disease.

In comparison, the Earthquake Analysis application takes a slightly more long term view. Understanding the exact parameters of when, where and how an earthquake occurs brings researchers closer to comprehending why earthquakes happen. This may make it possible to predict earthquakes in the future and to make the assessment of the potential impact they could have on a specific region much easier. Rapid analysis is particularly important for the relief efforts after a major earthquake, where those in charge need to have accurate information about the epicenter, magnitude and mechanism of the earthquake. Using the advanced grid infrastructure of EGEE, researchers at the Paris Geophysical Institute (IPGP), France, were able to complete analysis of the large Indonesian earthquake that occurred on 28 March 2005, just 30 hours after it occurred.

In both of these cases, EGEE offers a shortcut to calculations that previously would have taken much longer to complete. In Drug Discovery this allows researchers to test many more possible treatments than before, while on Earthquake Analysis it allows rapid responses to one of the most destructive kinds of natural disaster.

gLite update

Since the first release of gLite at the end of March this year, both the Middleware Reengineering Activity (JRA1) and the Operations Activity (SA1) have been very busy deploying and improving this new lightweight middleware solution. SA1 has spent much of this time certifying the middleware and testing it on the new Pre-Production Service, as well as keeping the main production service running smoothly. Through several stress tests and a deployment on a wider scale, the Operations Activity has provided a lot of valuable feedback to JRA1. The middleware developers, integrators and testers have responded quickly, releasing several fixes and critical updates, all of which will also be included in the soon be released gLite v1.2. This new release will also include a brand new File Transfer Service for gLite users, due to be severely stress tested this summer as part of the 3rd set of LCG Service Challenges.

Developer tips for composing web services

WSDL can be downloaded from a UDDI registry. If the service uses JAXRPCServlet you can attach ?WSDL (or ?model) to the URL request to get the WSDL (or model file).
E.g. http://localhost:8080/Service/Servicename?WSDL

MSc. In eScience, University of Edinburgh
This course will begin at the start of the next academic year. For furth details, see
http://www.ph.ed.ac.uk/postgraduate/degrees/msc_escience.html.

GRID SUMMER SCHOOLS

3rd International Summer School on Grid Computing, Vico Equense, 10-22 July
The School will be held in Vico Equense, Italy (near Naples) from 10 2005. It will consist of lectures by experts in various aspects of grid middleware and grid applications, and laboratory sessions in which th students will carry out practical exercises. For details, see
http://www.dma.unina.it/~murli/GridSummerSchool2005/.

Regional EGEE Summer School Budapest, Budapest, Hungary, 11-
The Regional EGEE Grid Summer School aims at introduc technology to potential users and at studying and practicing ap developments on the EGEE infrastructure. The Regional school is anyone interested in the use of EGEE for one's e-Science rese particular, researchers and students from the Central European a European regions are expected but anyone interested is warmly w For details, see http://www.egee.hu/grid05/.

GirdKa Summer School, FZK, Karlsruhe, Germany, 26-30 Septembe
This event will feature tutorials on gLite Introduction and Installation, Application Development and ROOT/PROOF.

TRAINING MATERIAL

A great deal of training material can be found in the NA3 Training Ma Archive at: http://www.egee.nesc.ac.uk/trgmat/index.html.

Current course material is available in:

- EGEE Induction
- Globus Toolkit
- LCG2 APIs
- LCG2 Installation and Administration
- UML for developing web services
- Web Services

We expect to be adding the first gLite material in the coming months

Endnotes

A general feedback form on EGEE websites and information service available on the EGEE public website at http://public.eu-egee.org/fee If you have the time, please consider filling it in to help us improve ou service.

If you have comments on the newsletter, or any submissions for futu issues, please contact owen.appleton@cern.ch. Thanks for reading, enjoy the summer!
On 5-6 July, CERN will host an EGEE All Activity meeting to look at t proposal for EGEE phase II. For those planning to attend, please se Laure an email to ask for an access card. Make sure to arrange accommodation early as this is likely to be a particularly well attende meeting.

EGEE in Numbers
100 Sites pass daily tests

On 9 June, for the first time, 100 sites on the EGEE production service passed their daily functional tests. Every day, SA1 put all sites through a wide and rigorous that check almost all aspects of the Grid middleware. In general, a number of sites will not pass each day, be it because they cannot be reached, problems component or scheduled downtime for upgrades. Having 100 sites pass their daily tests is an important step towards the smoothly running production service nece EGEE and LCG. Even better for the project, while some days are inevitably better than others, since reaching this milestone, the total number of sites passing their frequently climbed even higher!

Interested in reading more? Please refer to the other newsletters

Russia JINR in Russia JSI in Slovenia KFKI RMKI in Hungary KIAM RAS in Russia KTH in Sweden KU-NATFAK in Denmark LIP in Portugal MT Hungary NeSC in the United Kingdom NIIF in Hungary PNPI in Russia PPARC in the United Kingdom PSNC in Poland RED.ES in Spain RRC KI in R in the Netherlands SINP-MSU in Russia TAU in Israel TCD in Ireland TERENA in the Netherlands UCY in Cyprus UH HIP in Finland UiB in Norway Un UNIINNSBRUCK in Austria UniLe in Italy UniNa in Italy University of Chicago in the United States UPV in Spain USC in the United States Netherlands VR in Sweden VUB in Belgium Wisconsin University in the United States.