

First Baltic Grid Conference: EGEE induction

The EGEE project: enabling e-Science



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Acknowledgements



This presentation includes slides and information from :

- Fabrizio Gagliardi and Bob Jones (UK AHM 2004 talk)
- Roberto Barbera (Slides on applications)
- Other colleagues in EGEE
- Additional slides and preparation by Mike Mineter



Contents

• EGEE

- The vision why EGEE got started
- Where are we now?
- Where are we going? (project goals)
- How will we get there? (project structure and activities)
- Current virtual organisations (i.e. application communities)
- Some other important questions about EGEE





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Despite its name, EGEE has a scope much wider than Europe: it is an International project with partners world-wide



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Some other important questions about EGEE

Despite its name EGEE has a scope much wider than e-Science. It is a an international project with partners world-wide, and is intended to also support non-scientific research and collaborations in industry, the public sector, ...



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However, "EGEE" is much better than "EGERIPSEWW"



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Some other important questions about EGEE

Despite having very clear targets for March 2006, the goal of EGEE is to create an infrastructure that will be sustainable, far beyond the end of its initial phase of funding.

What is our vision of "the Grid"?

- The World Wide Web provides access to information that is stored in many millions of different geographical locations
- "The Grid" is an infrastructure which provides access to computing power and data distributed over the globe and supports collaboration within virtual organisations
- The name Grid is chosen by analogy with the electric power grid
- Enabled by middleware: the "operating system of the Grid"







What is driving grid development?

Data and compute intensive sciences are next generation applications that have extreme needs but are likely to become mainstream in the next 5 years (Increasingly, also: collaboration intensive)

- Physics/Astronomy: data from different kinds of research instruments
- Medical/Healthcare: imaging, diagnosis and treatment
- **Bioinformatics:** study of the human genome and proteome to understand genetic diseases
- Nanotechnology: design of new materials from the molecular scale
- Engineering: design optimization, simulation, failure analysis and remote Instrument access and control
- Natural Resources and the Environment: weather forecasting, earth observation, modeling and prediction of complex systems: river floods and earthquake simulation



Enabling Grids for E-science in Europe



Access to a production quality GRID will change the way science and much else is done

A geneticist at a conference, inspired by a talk she hears, will be able to launch a complex biomolecular simulation from her mobile phone

A team of engineering students will be able to run the latest 3D rendering programs from their laptops using the Grid.

model a new flood of the Danube in real time, using meteorological and geological data from several centers across Europe

An international network of scientists will be able to

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The Vision

The Grid: why now?



- Networking, commodity computing and distributed software tools are ripe for Grid technology
- Science more digital oriented and dominated by data
- Many public funded projects in the US and in the EU
- Also industrial and commercial Grids (for examples: <u>www.cern.ch/gridcafe</u> and <u>www.gridstart.org</u>)
- Consequently: the EU has set the goal of creating e-Infrastructure



EGEE – towards e-infrastructure



Build a large-scale production grid service to:

- Underpin European science and technology
- Link with and build on national, regional and international initiatives
- Foster international cooperation both in the creation and the use of the e-infrastructure



After the vision: where are we now?



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Part of the Grid "ecosystem"





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Part of the Grid "ecosystem"







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CMS Data Challenge



Running with LCG-2 and CMS resources world-wide (US Grid3 was a major component)

Pre-Challenge (Phase 1)

- After 8 months of continuous running:
 - 750,000 jobs
 - 3,500 KSI2000 months
 - 700,000 files
 - 80 TB of data

Data Challenge (Phase 2)

- 2,200 jobs/day (about 500 CPU's)
- Total 45,000 jobs
- 0.4 files/s registered to RLS
- Total 570,000 files registered to RLS
- 4 MB/s produced and distributed





Grid deployment has entered a new phase

- Basic middleware is working
 - responsible now for a small fraction of the problems

Outstanding performance/functionality issues

- RLS, RB / little modularity & lack of consistent interfaces ...
- some solutions are being developed but many cannot be addressed in current software/architecture - set priorities for new middleware (gLite)

Many operational issues

- mis-configuration, out of date mware, single points of failure, failover, mgmt interfaces ...
- resources unsuitable for applications needs (e.g. insufficient disk space)
- slow response by sites to problems (holiday periods, security concerns)
- new middleware will not help for many of these issues grid partners must think **Service**

The grid still does not appear as a single coherent facility

applications must adapt to the current service to gain maximum profit

but result has been very effective for LHCb - ~3000 concurrent jobs (August)

Grids for elnfrastructure...



• What is missing?

- Production-quality (stable, mature) Grid middleware
- Production-quality operational support
 - Grid Operation Centres, Helpdesks, etc.
- Multi-discipline grid-enabled application environment
 - Now led by HEP, Bio-info
- Administrative and policy decision framework in order to share resources at pan-European scale (and beyond)
 - Areas such as AAA (Authentication, Authorisation, Accounting)
 - End-to-end issues (Network related)
 - Funding Policies (Grid economics)
 - Resource Sharing Policies
 - Usage Policies

• EGEE project will tackle most of the above issues



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What will EGEE provide?

- Simplified access (access to all the operational resources the user needs)
- On demand computing (fast access to resources by allocating them efficiently)
- Pervasive access (accessible from any geographic location)
- Large scale resources (of a scale that no single computer centre can provide)
- Sharing of software and data (in a transparent way)
- Improved support (use the expertise of all partners to offer in-depth support for all key applications)





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In 2 years EGEE will:

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Establish production quality sustained Grid services

- 3000 users from at least 5 disciplines
- over 8,000 CPU's, 50 sites
- over 5 Petabytes (10¹⁵) storage
- Demonstrate a viable general process to bring other scientific communities on board

• **Propose a second phase** in mid 2005 to take over EGEE in early 2006



In 2 years EGEE will:

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- Establish production quality sustained Grid services
 - Reliable and secure
 - 24 hr/day; 7 day/week
 - Sustained: ~20 years
- Demonstrate a viable general process to bring other scientific communities on board

• **Propose a second phase** in mid 2005 to take over EGEE in early 2006







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EGEE Figures & Organization



- Coordinator: European Organization for Nuclear Research CERN
- 70 leading institutions in 27 countries, federated in regional Grids
- 32 M € EU funding in 2004-2005 (twice from partners)



- CERN
- Central Europe (Austria, Czech Republic, Hungary, Poland, Slovakia, Slovenia)
- France
- Germany and Switzerland
- Ireland and UK
- Italy
- Northern Europe (Belgium, Denmark, Estonia, Finland, The Netherlands, Norway, Sweden)
- Russia
- South-East Europe (Bulgaria, Cyprus, Greece, Israel, Romania)
- South-West Europe (Portugal, Spain)

EGEE Activities



32 Million Euros EU funding over 2 years starting 1st April 2004

- 48 % service activities (Grid Operations, Support and Management, Network Resource Provision)
- 24 % middleware re-engineering (Quality Assurance, Security, Network Services Development)
- 28 % networking (Management, Dissemination and Outreach, User Training and Education, Application Identification and Support, Policy and International Cooperation)



Emphasis in EGEE is on operating a production grid and supporting the end-users



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 - Middleware current and future
 - Operations providing a production service
 - Networking enabling multiple effective VO's
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- "gLite" the new EGEE middleware (under test)
- Service oriented components that are :
 - Loosely coupled (by messages)
 - Accessible across network; modular and self-contained; clean modes of failure
 - So can change implementation without changing interfaces
 - Can be developed in anticipation of new uses
- ... and are based on standards.
 Opens EGEE to:
 - New middleware (plethora of tools now available)
 - Heterogeneous resources (storage, computation...)
 - Interact with other Grids (international, regional, national and thematic)



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EGEE Service Activities

- Create, operate, support and manage a production quality infrastructure
- Offered services:
 - Middleware deployment and installation
 - Software and documentation repository
 - Grid monitoring and problem tracking
 - Bug reporting and knowledge database
 - VO services
 - Grid management services



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Regional Operations Centre



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Bringing new applications to the grid



- 1. Outreach events inform people about the grid / EGEE
- 2. Application experts discuss *specific characteristics* with the users
- **3.** *Migrate application* to EGEE infrastructure with the help of EGEE experts
- 4. Initial deployment for testing purposes
- Production usage user community contributes computing resources for heavy production demands - "Canadian dinner party"
- Supported by training and regional operations as well as by applications experts



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EGEE pilot application: Large Hadron Collider

- Data Challenge:
 - 10 Petabytes/year of data !!!
 - 20 million CDs each year!
- Simulation, reconstruction, analysis:
 - LHC data handling requires computing power equivalent to ~100,000 of today's fastest PC processors!
- Operational challenges
 - Reliable and scalable through project lifetime of decades



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EGEE pilot application: BioMedical

BioMedical

- Bioinformatics (gene/proteome databases distributions)
- Medical applications (screening, epidemiology, image databases distribution, etc.)
- Interactive application (human supervision or simulation)
- Security/privacy constraints
 - Heterogeneous data formats Frequent data updates - Complex data sets - Long term archiving
- BioMed applications deployed
 - GATE Geant4 Application for Tomographic Emission
 - GPS@ genomic web portal
 - **CDSS** Clinical Decision Support System



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http://egee-na4.ct.infn.it/biomed/applications.html



- BLAST is the first step for analysing new sequences: to compare DNA or protein sequences to other ones stored in personal or public databases.
- Ideal as a grid application trivial to parallelise as independent concurrent jobs on one or more CEs.
 - Requires resources to store databases and run algorithms
 - Large user community

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BLAST gridification





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Monte carlo simulation for radiotherapy planning





A look at the future: the HealthGrid vision



In this context "Health" does not involve only clinical practice but covers the whole range of information from molecular level (genetic and proteomic information) over cells and tissues, to the individual and finally the population level (social healthcare).

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Earth Sciences in EGEE



• Research

- Earth observations by satellite
 - (ESA(IT), KNMI(NL), IPSL(FR), UTV(IT), RIVM(NL), SRON(NL))
- Climate :
 - DKRZ(GE),IPSL(FR)
- Solid Earth Physics:
 - IPGP (FR)
- Hydrology:
 - Neuchâtel University (CH)
- Industry
 - CGG : Geophysics Company (FR)

Climate Applications in EGEE



Model: Atmosphere, Ocean, Hydrology, Atmospheric and Marine chemistry....

Goal: Comparison of model outputs from different runs and/or institutes

- Large volume of data (TB) from different model outputs, and experimental data
- Run made on supercomputer
 - => Link the EGEE infrastruture with supercomputer Grids (DEISA)



EXAMPLE: For the IPCC Assessment reports many experiment are performed with different models (different spatial resolution, different timestep, different "physics" ..) and various sites.

The generated data need to be compared in a comprehensive and "unified" way.





Earth Observation Application: Approach to Data and Metadata deployment on European DataGrid testbed and on EGEE

IPSL: M. Petitdidier, S. Godin, C. Boonne, C. Leroy KNMI: W. Som de Cerff ESA-ESRIN: L. Fusco, J. Linford



Earth Observation: Ozone

- Building on European Datagrid experience
- To produce and store the Ozone profiles or columns
 - Enhance availability
- To extend the processing capabilities
 - Validation against other data
 - Mid-latitude ozone studies
 - ...
- To facilitate collaboration
 - Including with emerging large scale European projects



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GOME instrument (~75 GB - ~5000 orbits/y)

~28000 profiles/day

Resources added to EGEE



Starting point:

ESA: UI, CE (15 nodes), SE (1.4 TB)

*IPSL+IPGP at Paris University Computer Center : 4PC, SE (500Gb), UI

✤IPGP: UI

DKRZ: UI, CE (2nodes), SE up to several TB as a function of the application

*KNMI: UI + possibility to use VO NIKHEF and Sara facilities for the Research ES

As new applications are ported new resources will be added

Solid Earth Physics Application

Objectives : demonstration to drive the community, and production of scientific results

GPS data: final goal: workflow with data storage, processing, analysis and visualisation

Synthetic seismograms

Numerous data and computations, access to databases

Strategy Earth Core dynamo

Demonstrate the secure and restricted access to database

Propose tests inside EU project like SPICE

Obtain scientific results to constitute databases and propose to the concerned community access via the Grid



Geophysics Applications

Seismic processing Generic Platform:

- Based on Geocluster, an industrial application – to be a starter of the core member VO.

- Include several standard tools for signal processing, simulation and inversion.

- Opened: any user can write new algorithms in new modules (shared or not)

- Free for academic research

-Controlled by license keys (opportunity to explore license issue at a grid level)

- initial partners F, CH, UK, Russia, Norway





Computational Chemistry: molecular simulator





eGee

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Critical Features of the Individual Programs

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- AB INITIO METHODS (molpro, gamess, adc, gaussian,) resource requests are proportional to N³ (N is the number of electrons) and to M^D (M is the number of grid points per dimension D) for CPU and disc demand.
- EMPIRICAL FORCE FIELDS (Venus, dl_poly, ...) resource requests are proportional to P! (P is the number of atoms)
- DYNAMICS (APH3D, TIMEDEP, ...) these programs use as input the output of the previous module most critical dependence is on the total angular momentum **J** value that can increase up to several hundred units and the size of the matrices depend on 2J+1
- KINETICS PROGRAMS use dynamics results for integrating relevant time

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The MAGIC telescope

CGCC Enabling Grids for E-science in Europe

- Largest Imaging Air Cherenkov Telescope (17 m mirror dish)
- Located on Canary Island
 La Palma (@ 2200 m asl)
- Lowest energy threshold ever obtained with a Cherenkov telescope
- Aim: detect γ-ray sources in the unexplored energy range:
 30 (10)-> 300 GeV





Data Acquisition Rate & Storage



- Event Size:
 - 577 PM x 1 Byte x 30 samples
 ⇒ ~ 20 kByte/event
- Data Acquisition Rate:
 - 500 Hz typical trigger rate
 ⇒ ~ 10 MByte/sec
- Data Storage Requirements:
 - ~ 1000 h / year useful moonless observation time ⇒ ~ 36 TByte/year



MAGIC Summary



MAGIC:

- is a new generation gamma ray Cherenkov telescope
- has large discovery potential both in astrophysics and fundamental physics
- just started data taking
- has large computing requirements
 - > 100 CPU
 - > 50 TB / year
- is well suited to join and test GRID technology with 16 participating institutions over all Europe (and beyond) some with strong links to mayor GRID sites (Bologna, Barcelona)



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Who else can benefit from EGEE?

- EGEE Generic Applications Advisory Panel:
 - For new applications
- EU projects: MammoGrid, Diligent, SEE-GRID ...
- Expression of interest: Planck/Gaia (astroparticle), SimDat (drug discovery)

http://agenda.cern.ch/age?a042351





Links to industry?



- EGEE Industry Forum
 - raise awareness of the project in industry to encourage industrial participation in the project
 - foster direct contact of the project partners with industry
 - ensure that the project can benefit from practical experience of industrial applications
- For more info:

http://public.eu-egee.org/industry/



Private or Federated Resources?



For applications that must operate in a closed environment, EGEE middleware can be downloaded and installed on closed infrastructures Approach being used by MammoGrid



EGEE sites are administered/owned by different organisations

Sites have ultimate control over how their resources are used Limiting the demands of your application will make it acceptable to more sites and hence make more resources available to you

Intellectual Property

- The existing EGEE grid middleware (LCG-2) is distributed under an Open Source License developed by EU DataGrid
 - Derived from modified BSD no restriction on usage (academic or commercial) beyond acknowledgement
 - Same approach for new middleware (gLite)
- Application software maintains its own licensing scheme
 - Sites must obtain appropriate licenses before installation



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How to access EGEE (III)



- Where to go for an accredited certificate?
- Everyone (almost) in Europe has a national CA



- Green: CA Accredited
- Yellow: being discussed

Other Accredited CAs:

- DoEGrids (US)
- GridCanada
- ASCCG (Taiwan)
- ArmeSFO (Armenia)
- CERN
- Russia (HEP)
- FNAL Service CA (US)
 - Israel
 - Pakistan

EGEE Plans for the coming year



• November

2nd EGEE conference (Den Hague) in common with DEISA, SEE-GRID, DILIGENT etc.

December

Application migration reports

• February 2005

1st EU review

• March 2005

Large-scale deployment of gLite software Annual report

To read more about EGEE...



- Explore the web site!
- <u>www.eu-egee.org</u>



Summary

- EGEE is the first attempt to build a worldwide Grid infrastructure for data intensive applications from many scientific domains
- A large-scale production grid service is already deployed and being used for HEP and BioMed applications with new applications being ported
- Resources & user groups will rapidly expand during the project
- A process is in place for migrating new applications to the EGEE infrastructure
- A training programme has started with events already held
- Prototype "*next generation*" middleware is being tested (**gLite**)
- Plans for a **follow-on project** are being discussed

Further Information



EGEE <u>www.eu-egee.org</u> LCG <u>lcg.web.cern.ch/LCG/</u>

NeSC <u>www.nesc.ac.uk</u>

The Grid Cafe <u>www.gridcafe.org</u>