Enabling Grids for E-sciencE

Introduction to EGEE

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www.eu-egee.org

Information Society

Acknowledgement

Based on presentations given by Fabrizio Gagliardi

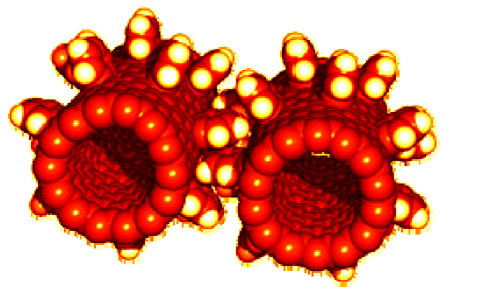
Director EGEE project

Presentation overview

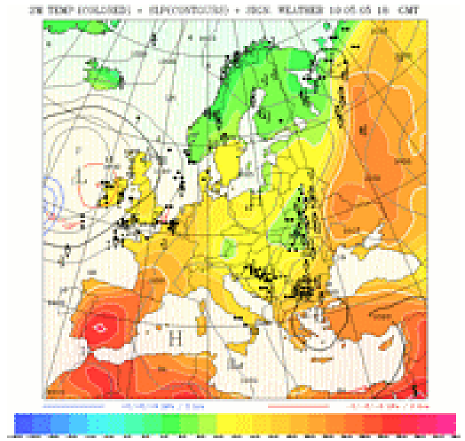
- **Data intensive science and rationale for Grid computing**
- **Particle physics and bio-informatics examples**
- **General description of the EGEE project and relations to HEP CERN LCG project**
- **EGEE operates a production infrastructure:**
  - Operations
  - Middleware
  - Applications
- **Establish new user communities**
- **Promote and enable international collaboration**

Computing intensive science

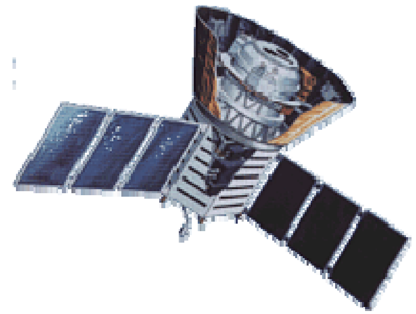
- **Science is becoming increasingly digital and needs to deal with increasing amounts of data**



- **Simulations get ever more detailed**
  - Nanotechnology – design of new materials from the molecular scale
  - Modelling and predicting complex systems (weather forecasting, river floods, earthquake)
  - Decoding the human genome

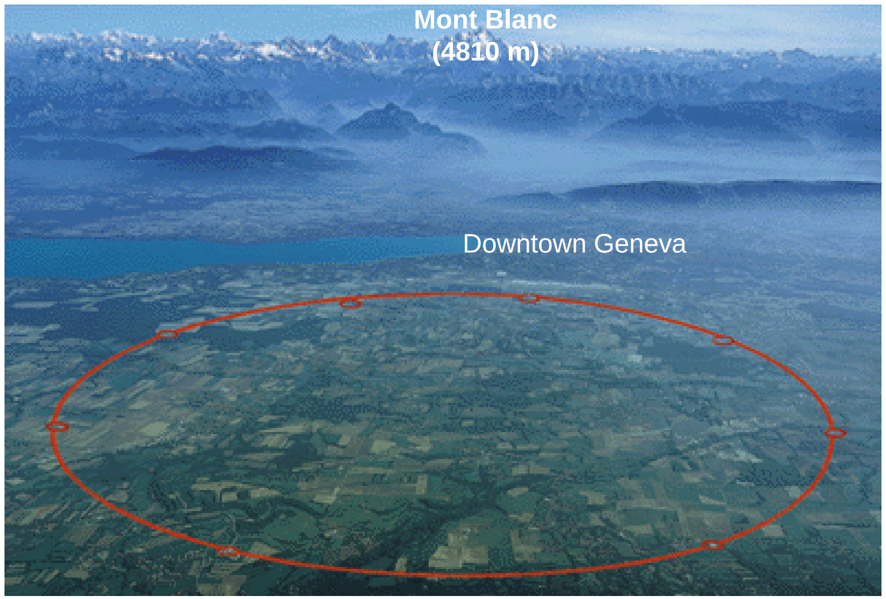


- **Experimental Science uses ever more sophisticated sensors to make precise measurements**
  → Need high statistics
  → Huge amounts of data
  → Serves user communities around the world



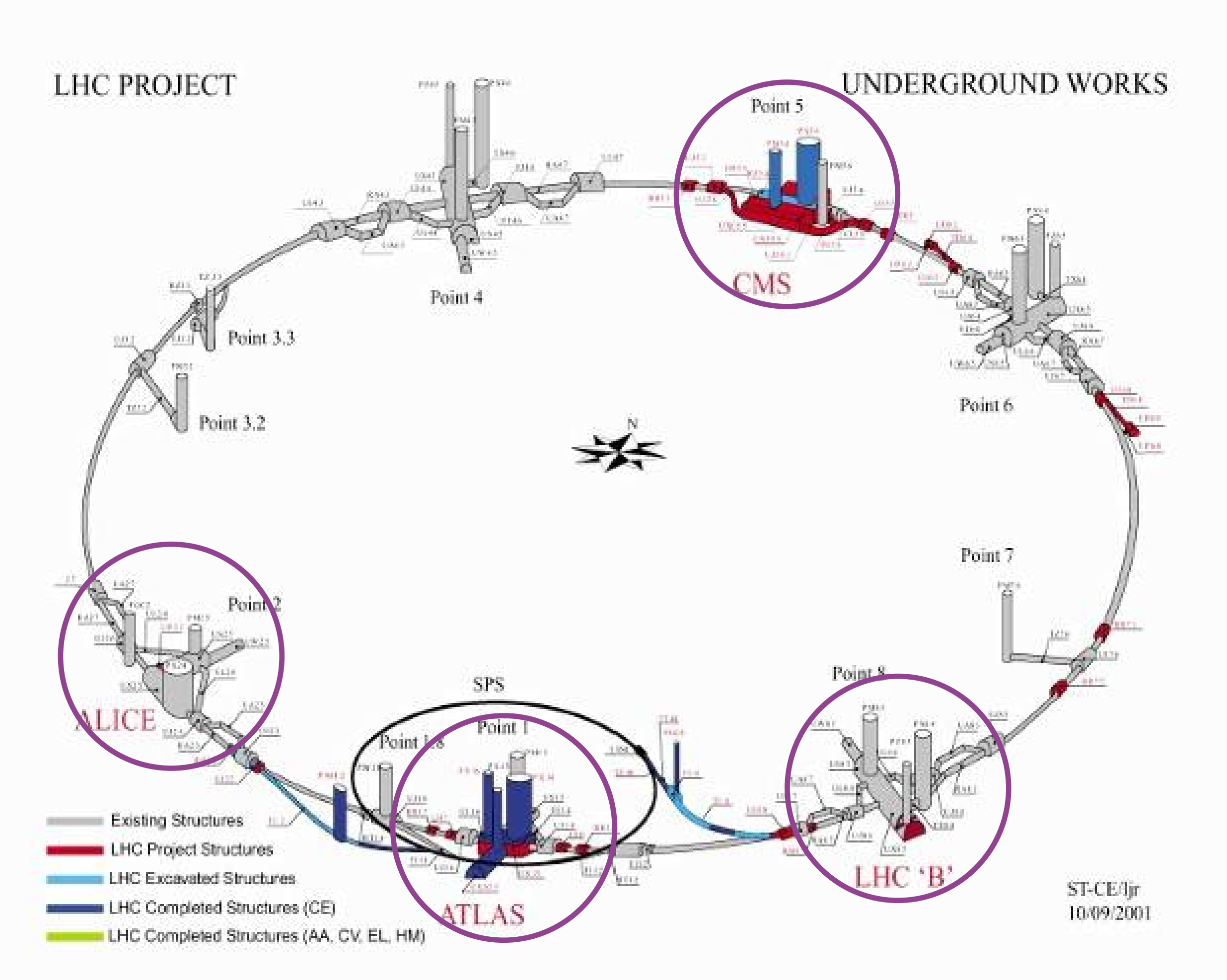
A good example: Particle Physics

- Large amount of data produced in a few places: CERN, FNAL, KEK…
- Large worldwide organized collaborations (i.e. LHC CERN experiments) of computer-savvy scientists
- Computing and data management resources distributed world-wide owned and managed by many different entities
- **Large Hadron Collider (LHC) at CERN in Geneva Switzerland:**
  - One of the most powerful instruments ever built to investigate matter



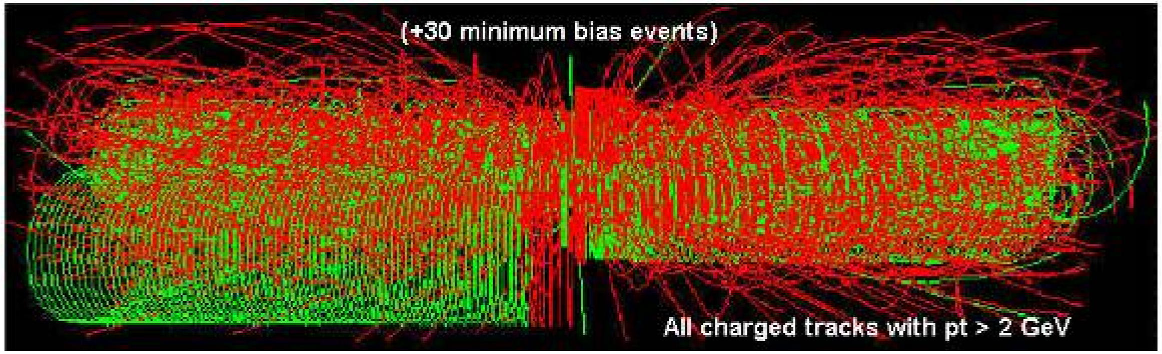
The LHC Experiments

- **Large Hadron Collider (LHC):**
  - four experiments:
    - ALICE
    - ATLAS
    - CMS
    - LHCb
  - 27 km tunnel
  - Start-up in 2007

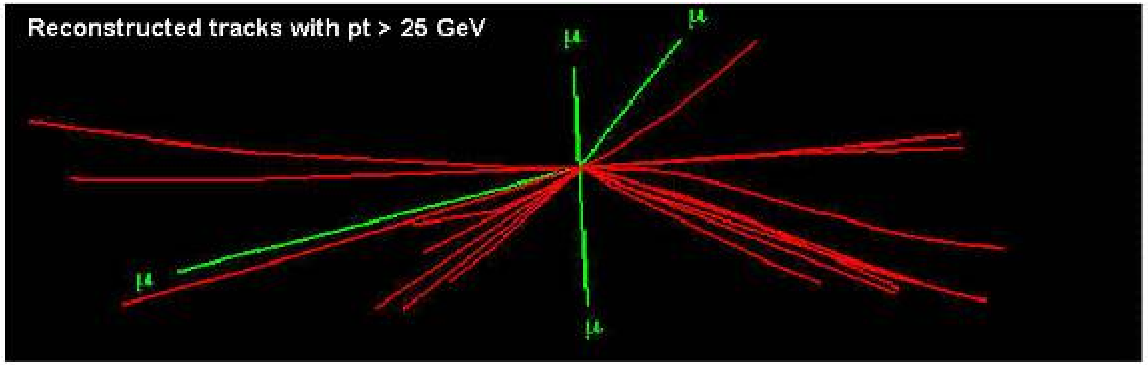


The LHC Data Challenge

Starting from this event



Looking for this "signature"

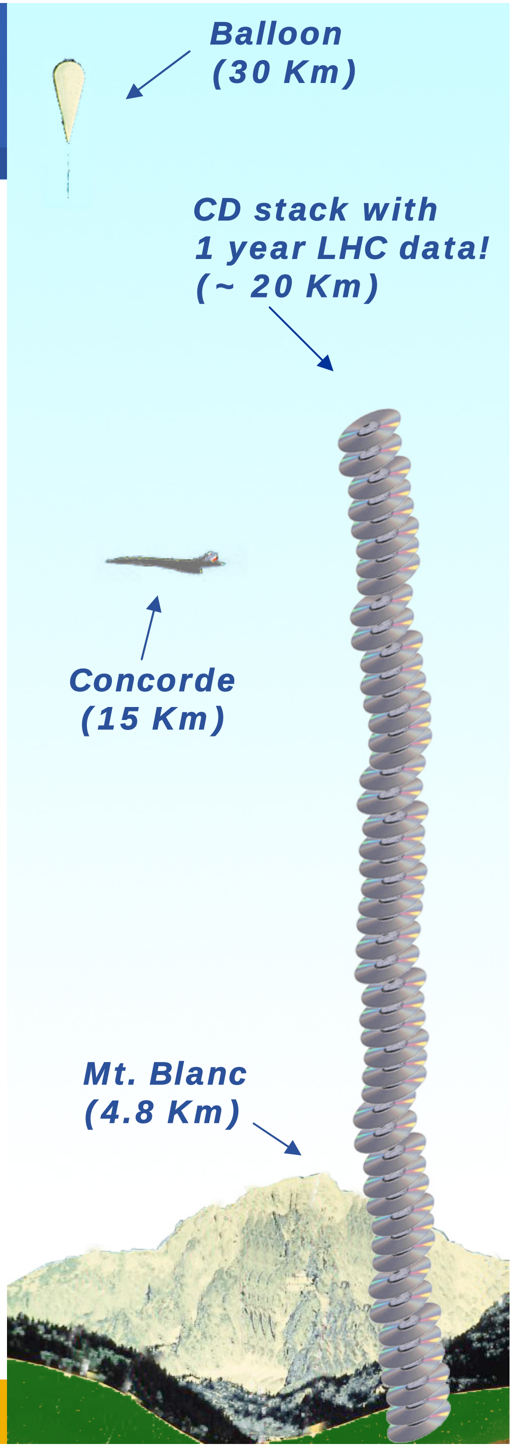


→ **Selectivity: 1 in 10^{13}**

(Like looking for a needle in 20 million haystacks)

LHC Data

- 40 million collisions per second
- After filtering, 100 collisions of interest per second
- A Megabyte of data for each collision = recording rate of 0.1 Gigabytes/sec
- 10^{10} collisions recorded each year
- ~ 10 Petabytes/year of data
- LHC data correspond to about 20 million CDs each year!
- ~ 100,000 of today's fastest PC processors



The solution: the Grid

- Integrating computing and storage capacities at major computer centres
- 24/7 access, independent of geographic location

→ Effective and seamless collaboration of dispersed communities, both scientific and commercial

→ Ability to use thousands of computers for a wide range of applications

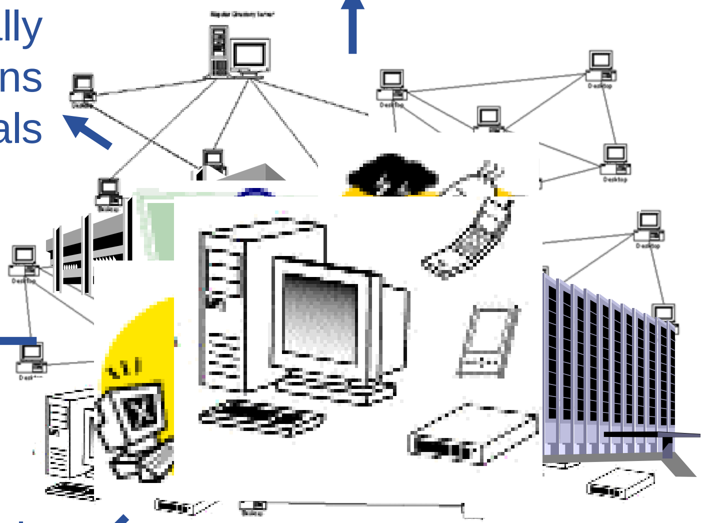
- Best cost effective solution for HEP LHC Computing Grid project (LCG) and from this the close integration of LCG and EGEE projects

What are the characteristics of a Grid system?

Numerous Resources

Ownership by Mutually Distrustful Organizations & Individuals

Different Security Requirements & Policies Required



Potentially Faulty Resources

Resources are Heterogeneous

What are the characteristics of a Grid system?

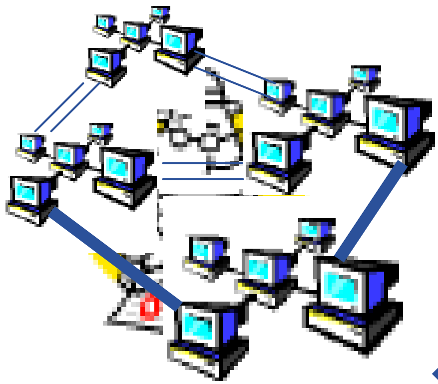
Standards

Numerous Resources

Ownership by Mutually Distrustful Organizations & Individuals

Connected by Heterogeneous, Multi-Level Networks

Different Security Requirements & Policies Required



Different Resource Management Policies

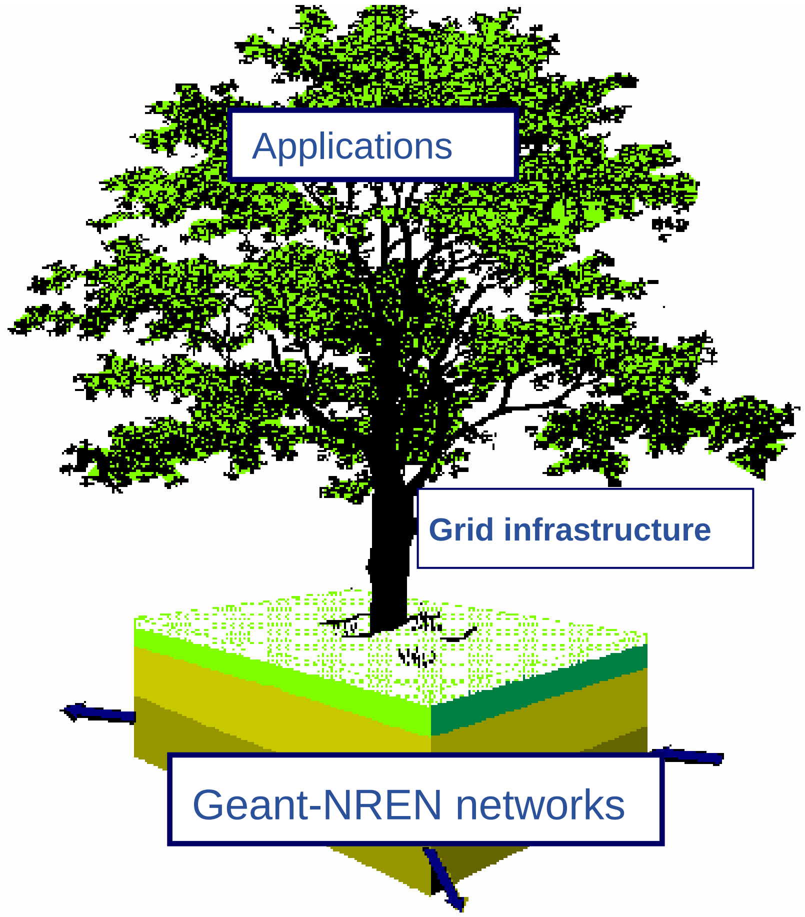
Potentially Faulty Resources

Geographically Separated

Resources are Heterogeneous

EGEE Overview

- Goal:
  - Create a ***world-wide production-quality Gid infrastructure for e-Science***
    - on top of present and future EU Research Networking infrastructure
- Build on**:**
  - EU and EU member states major investments in Grid Technology
  - International connections (US and AP)
  - Several pioneering prototype results
  - Large Grid development teams in EU require major EU funding effort
- Approach
  - Leverage current and planned national and regional Grid initiatives and infrastructures
  - Work closely with relevant industrial Grid developers, NRENs and US-AP projects



- **http://www.eu-egee.org**

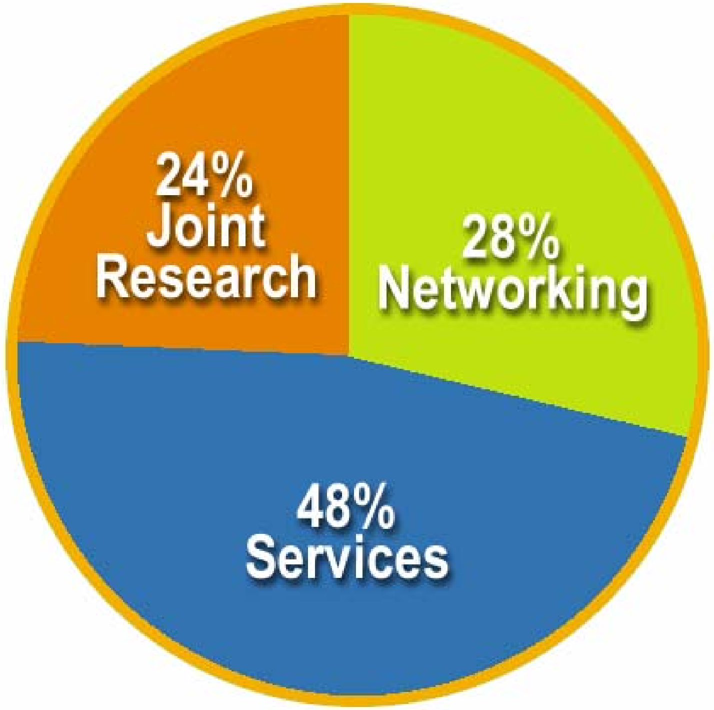
The largest e-Infrastructure: EGEE

- **Objectives**
  - consistent, robust and secure service grid infrastructure
  - improving and maintaining the middleware
  - attracting new resources and users from industry as well as science

- **Structure**
  - 71 leading institutions in 27 countries, federated in regional Grids
  - leveraging national and regional grid activities worldwide
  - funded by the EU with ~32 M Euros for first 2 years starting 1st April 2004

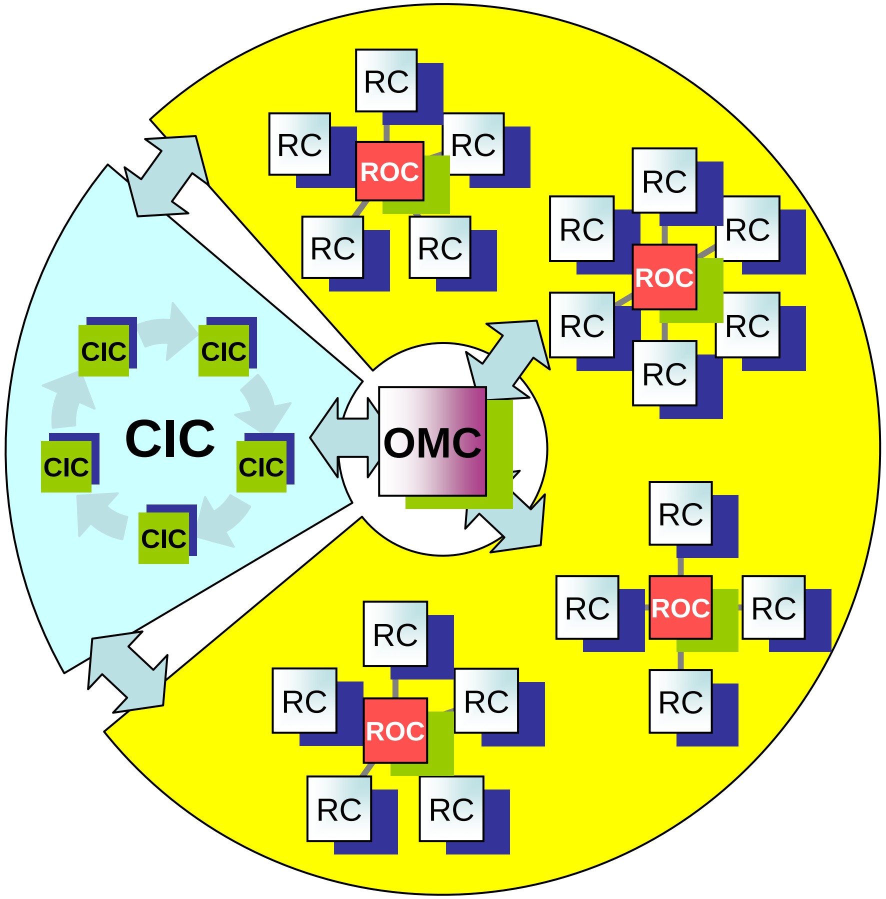
EGEE Activities

- 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

Grid Operations

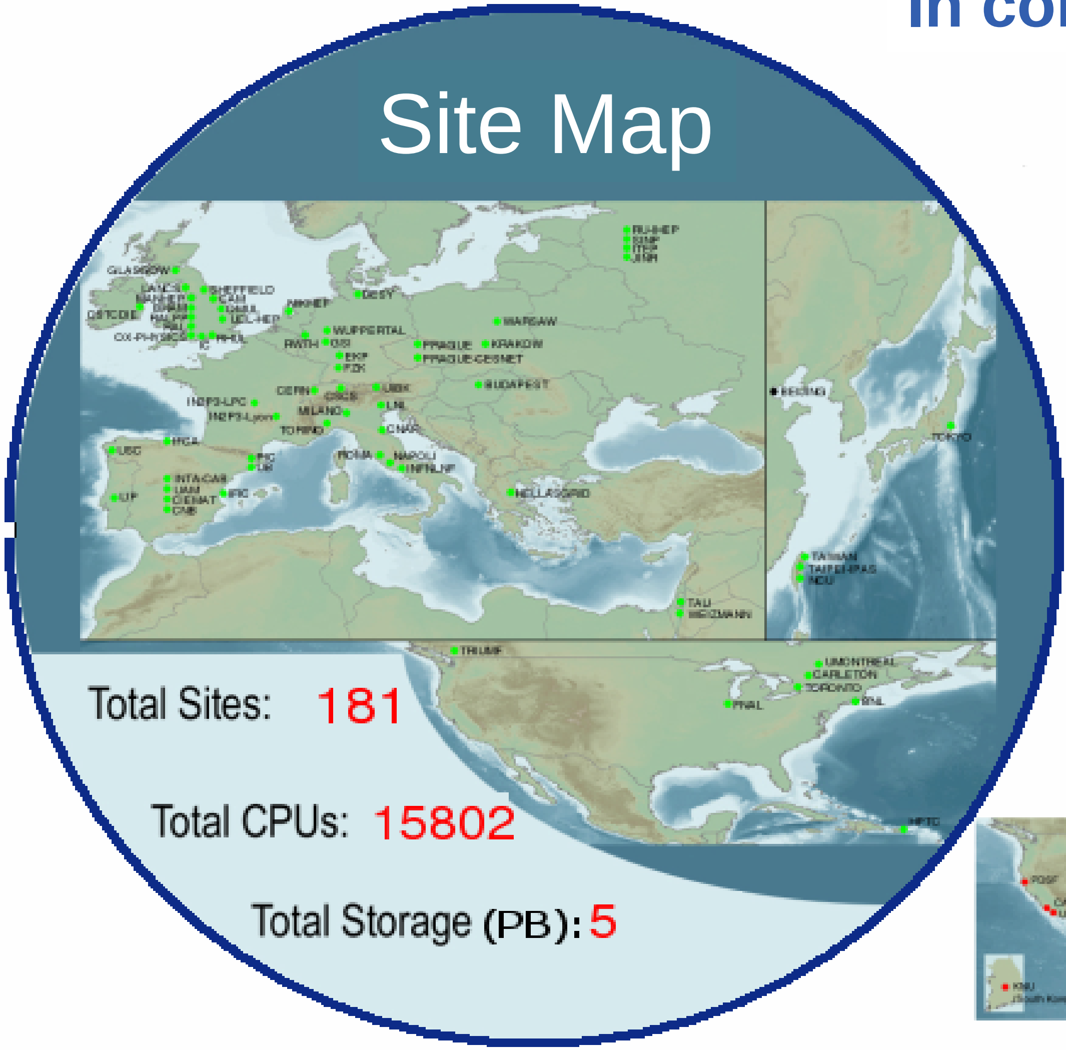


RC = Resource Centre
ROC = Regional Operations Centre
CIC = Core Infrastructure Centre
OMC = Operations Management Centre

- **The *grid* is flat, but**
- ***Hierarchy* of responsibility**
  - Essential to scale the operation
- **CICs act as a single Operations Centre**
  - Operational oversight ***(grid operator)*** responsibility
  - rotates weekly between CICs
  - Report problems to ROC/RC
  - ROC is *responsible* for ensuring problem is resolved
  - ROC oversees regional RCs
- **ROCs responsible for organising the operations in a region**
  - Coordinate deployment of middleware, etc
- **CERN coordinates sites not associated with a ROC**

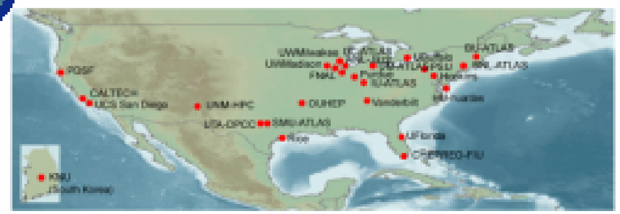
EGEE Infrastructure

In collaboration with LCG



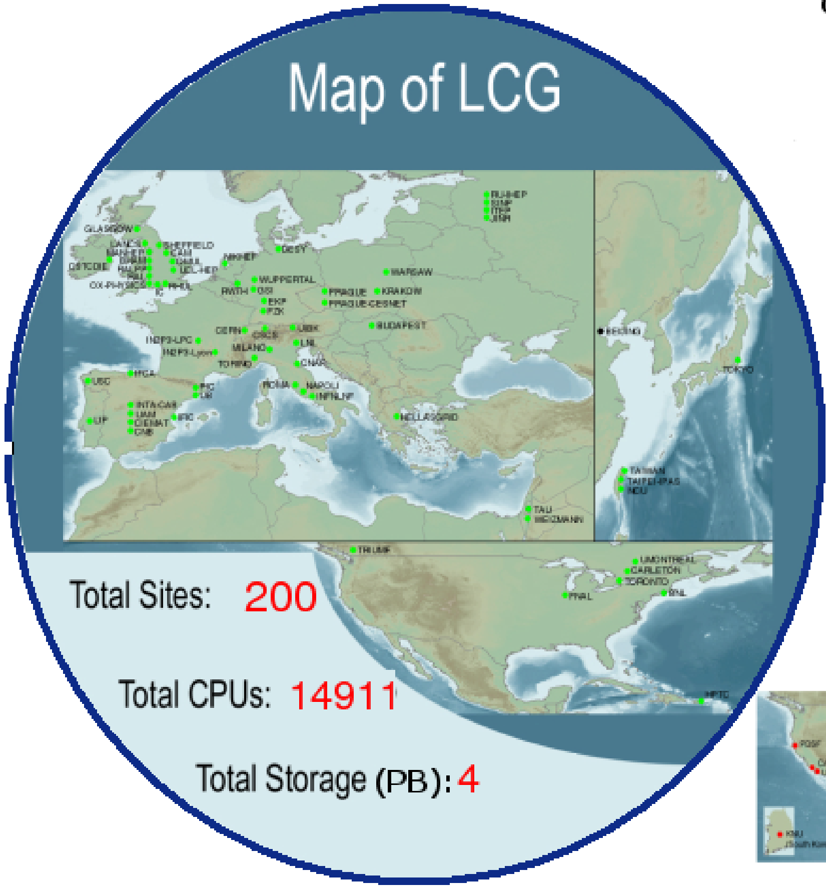
NorduGrid

Grid3/OSG

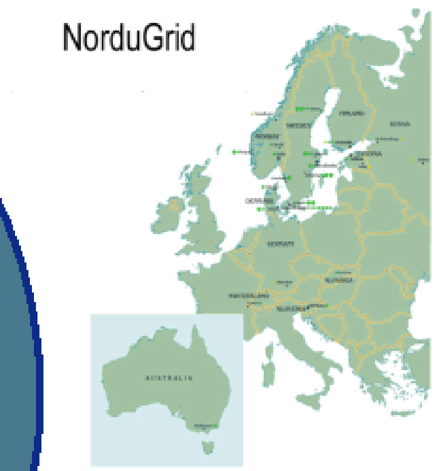


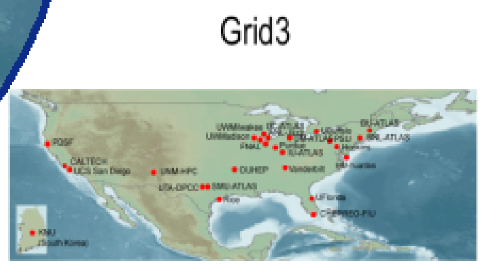
Status 25 July 2005

Launched Sept'03 with 12 sites, now more than 100 sites and continues to grow



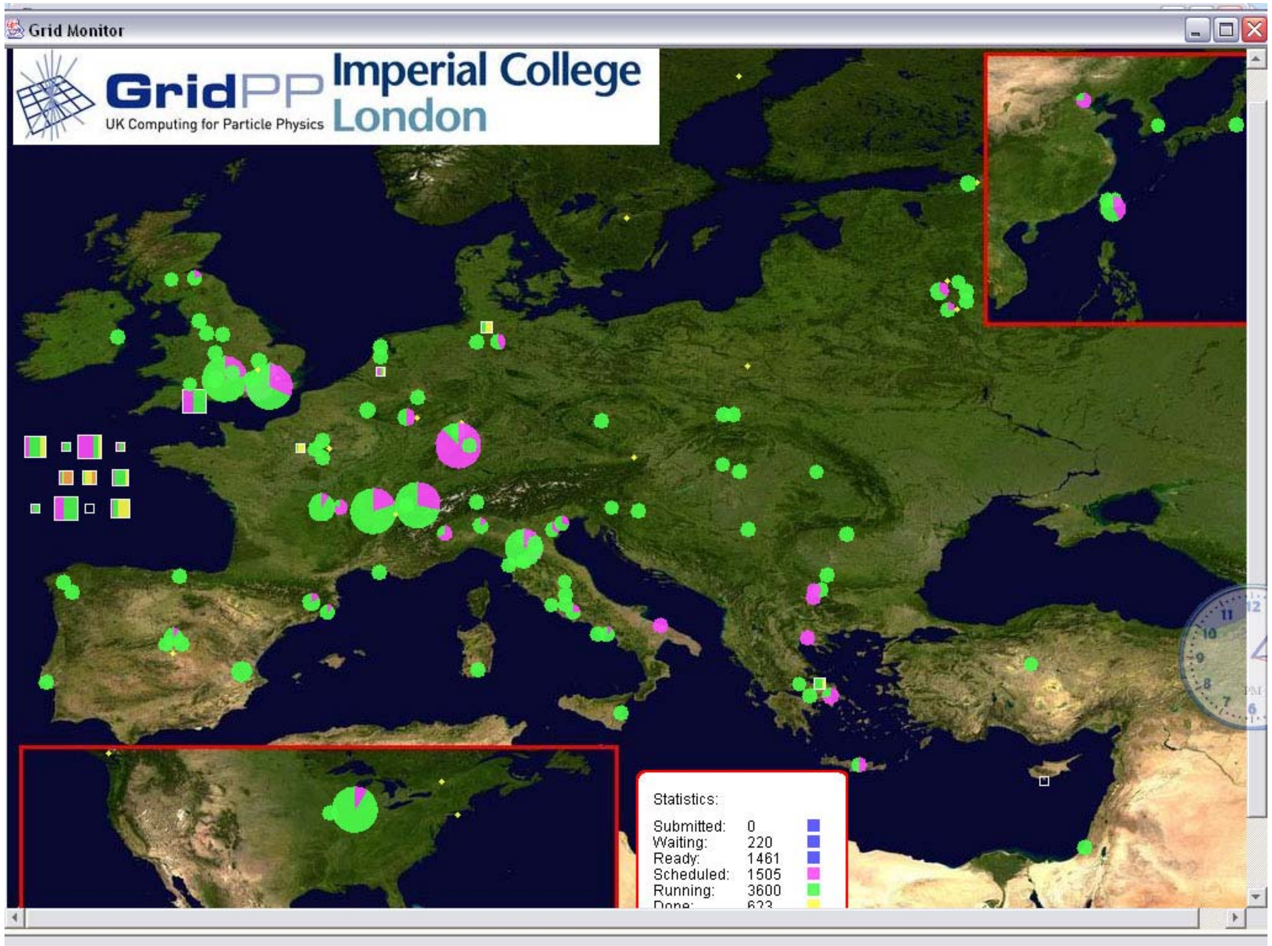
Collaborating with LCG





Production grid service

Launched Sept'03 with 12 sites, now more than 100 sites and continues to grow



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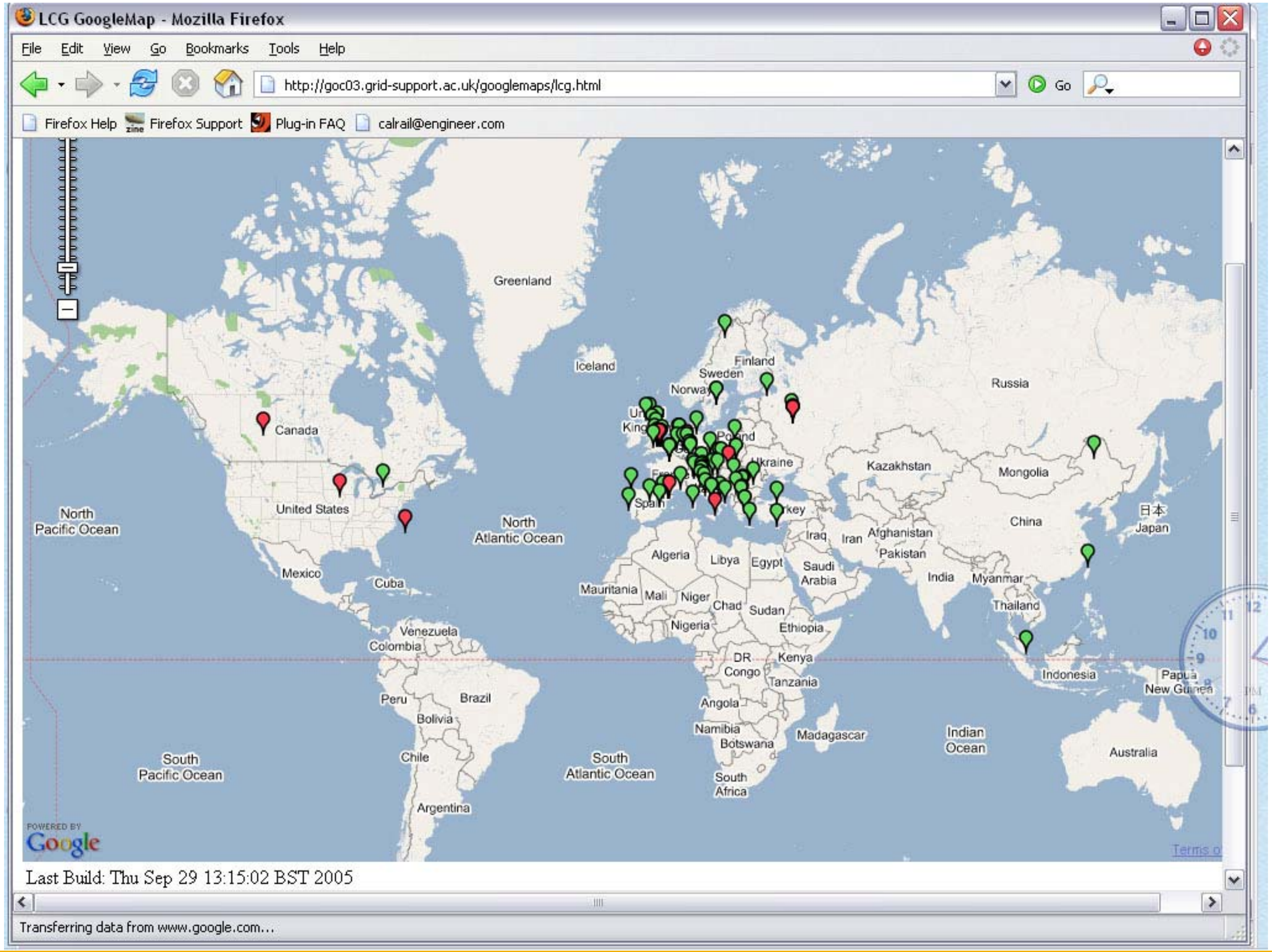
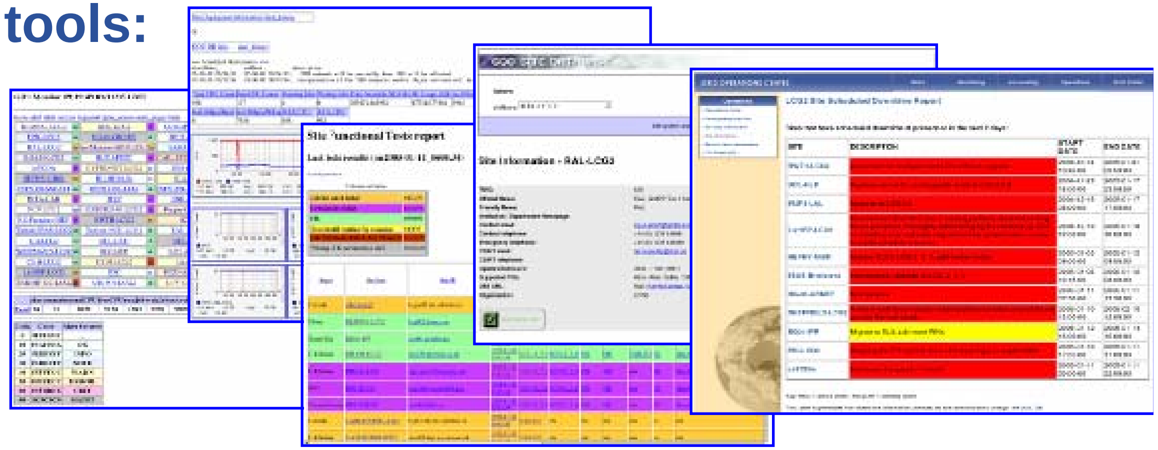
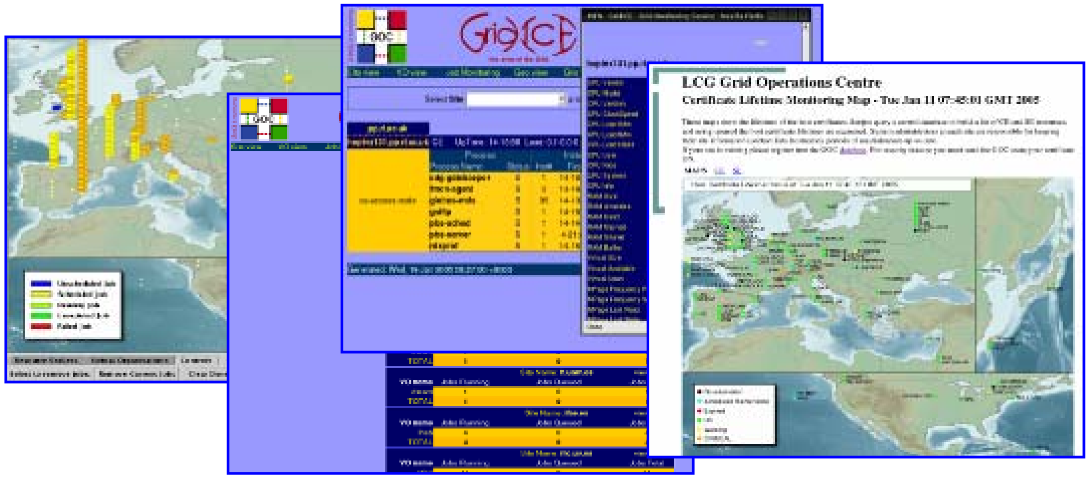


Grid monitoring

- **Operation of Production Service: real-time display of grid operations**
- **Accounting Information**
- **Selection of Monitoring tools:**
  - GIIS Monitor + Monitor Graphs
  - Sites Functional Tests
  - GOC Data Base
  - Scheduled Downtimes

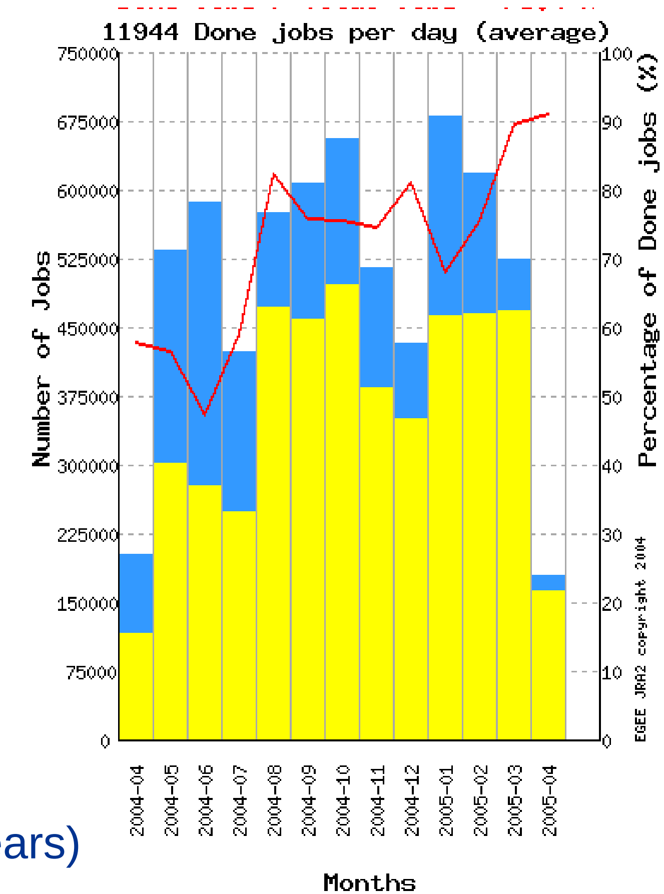


  - Live Job Monitor
  - GridIce – VO + Fabric View
  - Certificate Lifetime Monitor



Service Usage

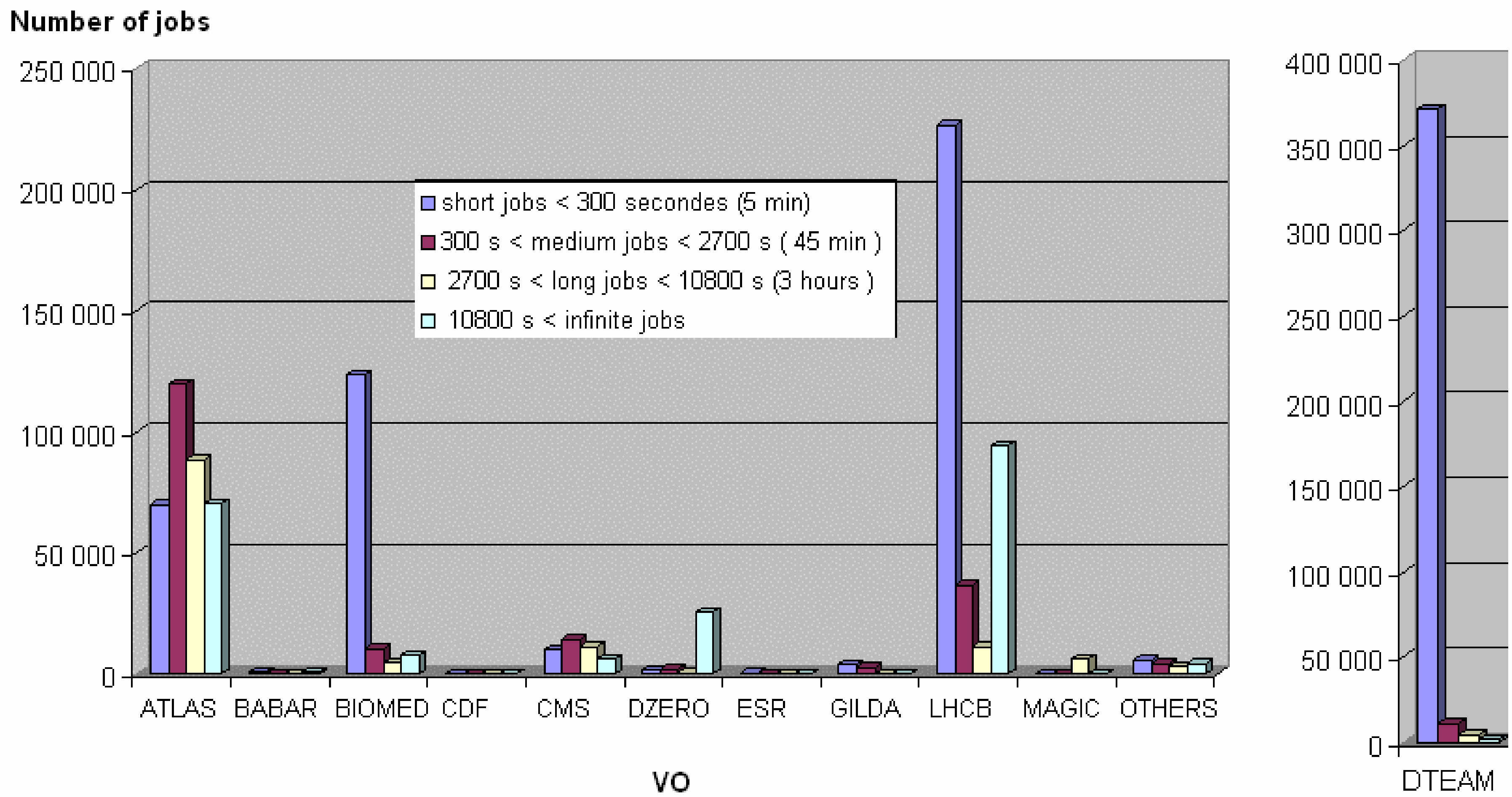
- **VOs and users on the production service**
  - Active VOs:
    - HEP: 4 LHC, D0, CDF, Zeus, Babar
    - Biomed
    - ESR (Earth Sciences)
    - Computational chemistry
    - Magic (Astronomy)
    - EGEODE (Geo-Physics)
  - Registered users in these VO: 600
  - \+ Many local VOs, supported by their ROCs
- **Scale of work performed:**
  - LHC Data challenges 2004:
    - >1 M SI2K years of CPU time (~1000 CPU years)
    - 400 TB of data generated, moved and stored
    - 1 VO achieved ~4000 simultaneous jobs (~4 times CERN grid capacity)



Number of jobs processed per month (April 2004-April 2005)

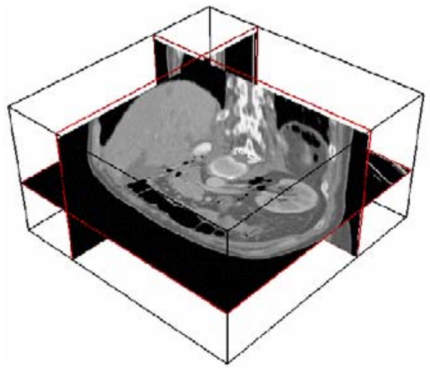
EGEE infrastructure usage

- **Average job duration January 2005 – June 2005 for the main VOs**



EGEE pilot applications (I)

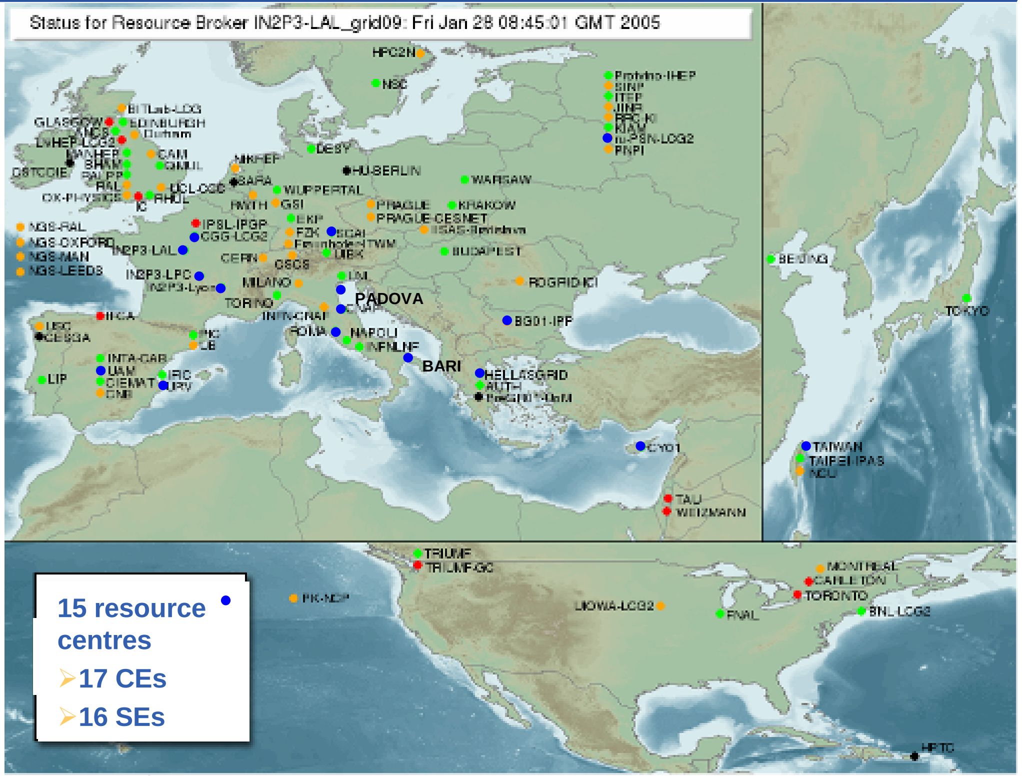
- **High-Energy Physics (HEP)**
  - Provides computing infrastructure (LCG)
  - Challenging:
    - thousands of processors world-wide
    - generating petabytes of data
    - ‘chaotic’ use of grid with individual user analysis (thousands of users interactively operating within experiment VOs)

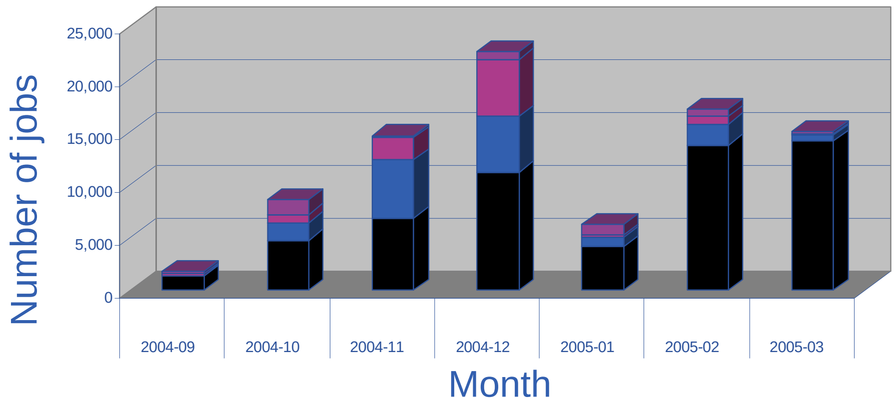


- **Biomedical Applications**
  - Similar computing and data storage requirements
  - Major additional challenge: security & privacy

BioMed Overview

- **Infrastructure**
  - ~2.000 CPUs
  - ~21 TB of disk
  - in 12 countries
- **>50 users in 7 countries working with 12 applications**
- **18 research labs**
- **~80.000 jobs launched since 04/2004**
- **~10 CPU years**





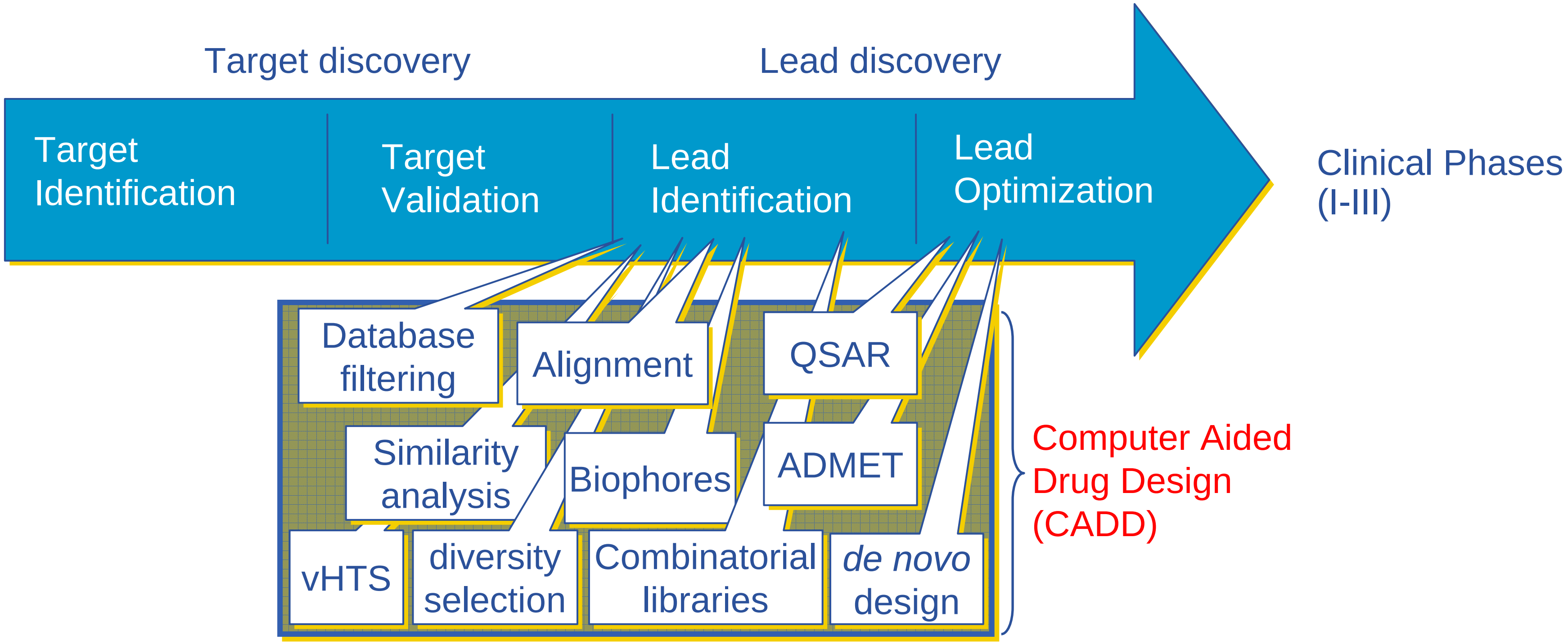
Bioinformatics

- **GPS@: Grid Protein Sequence Analysis**
  - **Gridified version of NPSA web portal**
    - Offering proteins databases and sequence analysis algorithms to the bioinformaticians (3000 hits per day)
    - Need for large databases and big number of short jobs
  - **Objective**: increased computing power
  - **Status**: 9 bioinformatic softwares gridified
  - **Grid added value**: open to a wider community with larger bioinformatic computations

- **xmipp_MLrefine**
  - **3D structure analysis of macromolecules**
    - From (very noisy) electron microscopy images
    - Maximum likelihood approach to find the optimal model
  - **Objective**: study molecule interaction and chem. properties
  - **Status**: algorithm being optimised and ported to 3D
  - **Grid added value**: parallel computation on different resources of independent jobs

Drug Discovery

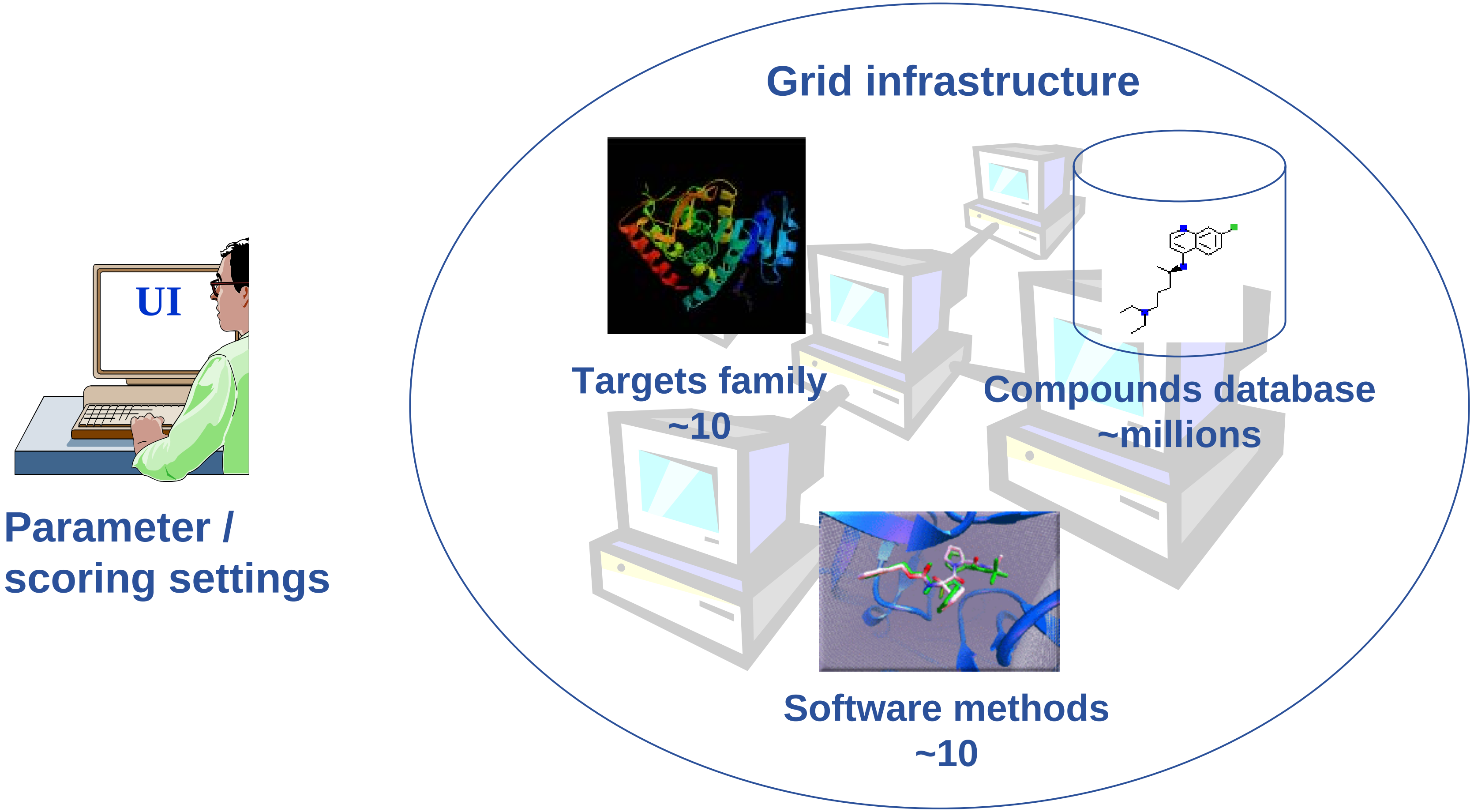
- **Demonstrate the relevance and the impact of the grid approach to address Drug Discovery for neglected diseases**



Duration: 12 – 15 years, Costs: 500 - 800 million US $

Docking platform components

- **Predict how small molecules, such as substrates or drug candidates, bind to a receptor of known 3D structure**



Drug Discovery Data Challenge

- **4 July – 26 August 2005, incl. testing**
  A. 2 weeks using commercial docking software
  B. 3 weeks using free (but slower) docking software

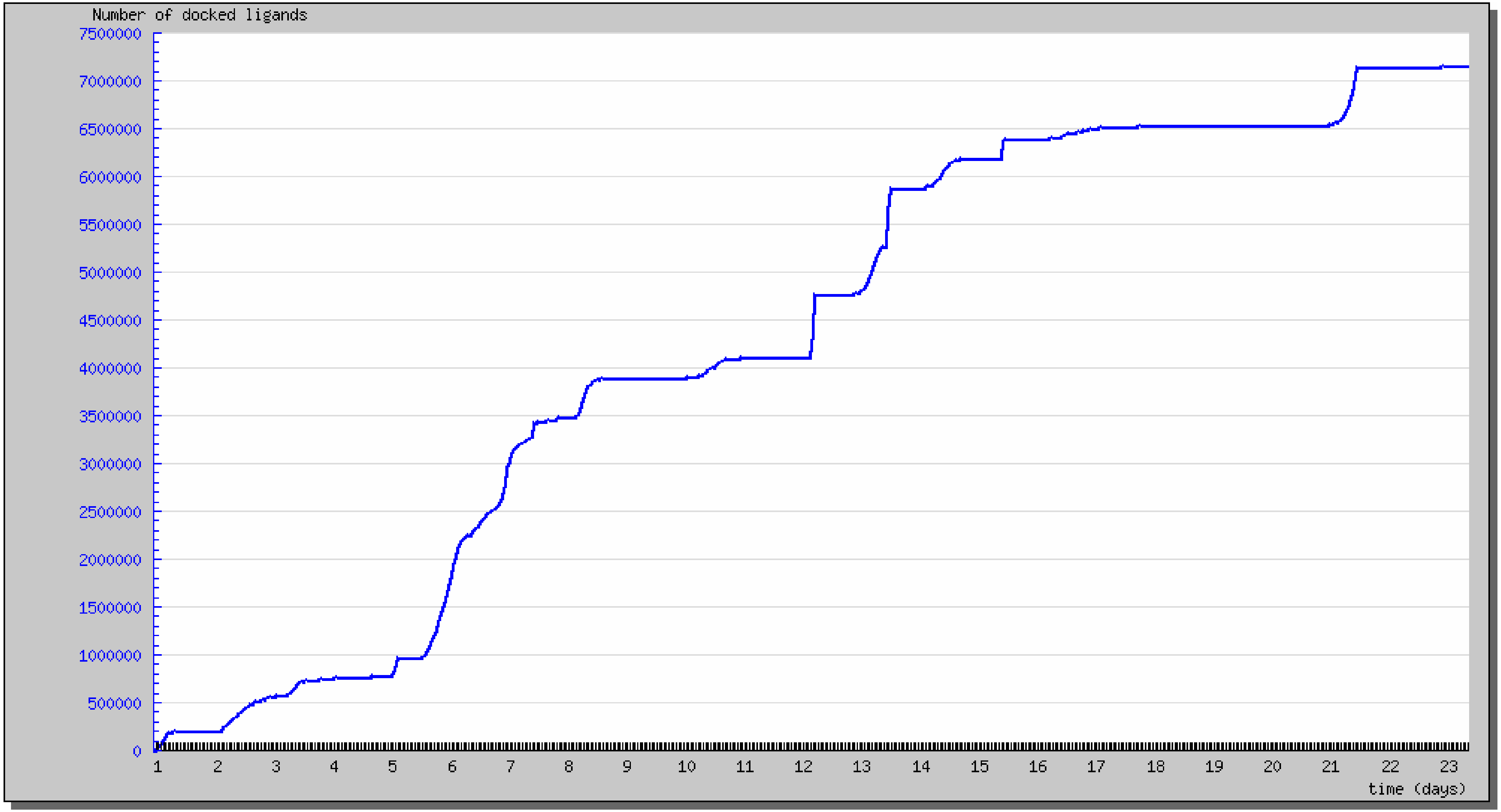
- **Phase A:**
  - 90 packets launched (~ 12900 jobs; 5 to >25 hours each)
  - **~ 20 CPU years** (800 to >1000 CPUs concurrently used)
  - 5800 correct results collected (rest are still running…)
  - file error or failures: 23% → resubmitted
  - 500 GB of data produced

- **Phase B:**
  - 60 packets launched (~30000 jobs; 10 to >25 hours each)
  - **~ 40 CPU years**
  - 1 TB will be produced

- **Final data production: 1,5 TB**

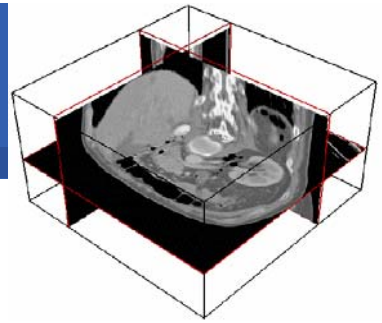
Drug Discovery Data Challenge (II)

- **Number of docked ligands vs. time**



Status 25 July 2005

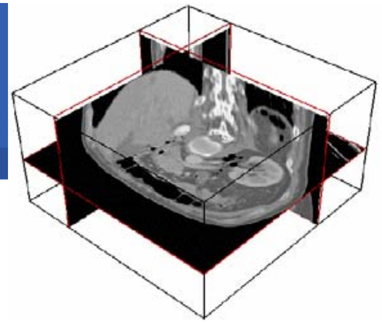
Medical imaging



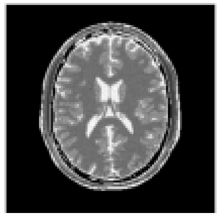
- **GATE**
  - **Radiotherapy planning**
    - Improvement of precision by Monte Carlo simulation
    - Processing of DICOM medical images
  - **Objective**: very short computation time compatible with clinical practice
  - **Status**: development and performance testing
  - **Grid Added Value**: parallelisation reduces computing time

- **CDSS**
  - **Clinical Decision Support System**
    - Assembling knowledge databases
    - Using image classification engines
  - **Objective:** access to knowledge databases from hospitals
  - **Status**: from development to deployment, some medical end users
  - **Grid Added Value**: ubiquitous, managed access to distributed databases and engines

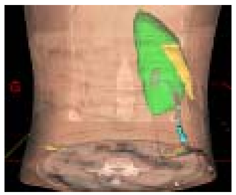
Medical imaging



- **SiMRI3D**
  - **3D Magnetic Resonance Image Simulator**
    - MRI physics simulation, parallel implementation
    - Very compute intensive



  - **Objective**: offering an image simulator service to the research community
  - **Status**: parallelised and now running on EGEE resources
  - **Grid Added Value**: enables simulation of high-res images
- **gPTM3D**
  - **Interactive tool to segment and analyse medical images**
    - A non gridified version is distributed in several hospitals
    - Need for very fast scheduling of interactive tasks



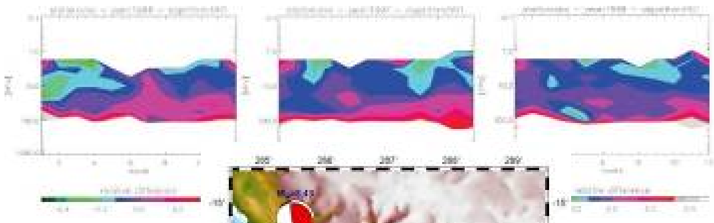
  - **Objectives**: shorten computation time using the grid
    - Interactive reconstruction time: < 2min and scalable
  - **Status**: development of the gridified version being finalized
  - **Grid Added Value**: permanent availability of resources

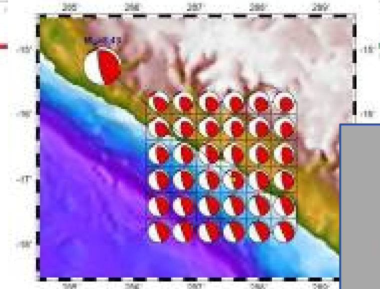
Generic Applications

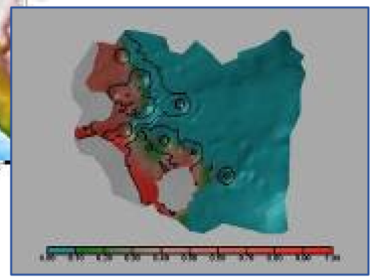
- **EGEE Generic Applications Advisory Panel (EGAAP)**
  - UNIQUE entry point for “external” applications
  - Reviews proposals and make recommendations to EGEE management
    - Deals with “scientific” aspects, not with technical details
    - Generic Applications group in charge of introducing selected applications to the EGEE infrastructure
  - 6 applications selected so far:
    - Earth sciences (earth observation, geophysics, hydrology, seismology)
    - MAGIC (astrophysics)
    - Computational Chemistry
    - PLANCK (astrophysics and cosmology)
    - Drug Discovery
    - E-GRID (e-finance and e-business)
    - GRACE (grid search engine, ended Feb 2005)

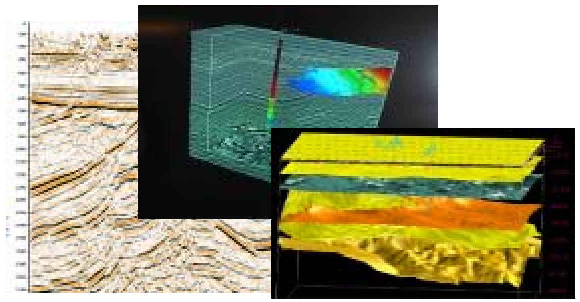
Earth sciences applications

- **Earth Observations by Satellite**
  - Ozone profiles
- **Solid Earth Physics**
  - Fast Determination of mechanisms of important earthquakes
- **Hydrology**
  - Management of water resources in Mediterranean area (SWIMED)
- **Geology**
  - Geocluster: R&D initiative of the Compagnie Générale de Géophysique





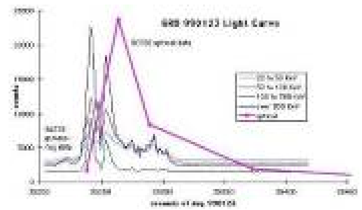


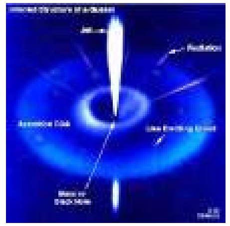


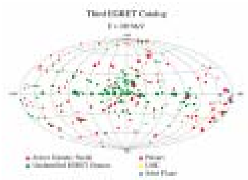
- **A large variety of applications ported on EGEE which incites new users**
- **Interactive Collaboration of the teams around a project**

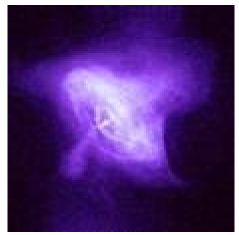
MAGIC

- **Ground based Air Cerenkov Telescope 17 m diameter**
- **Physics Goals:**
  – Origin of VHE Gamma rays
  – Active Galactic Nuclei
  – Supernova Remnants
  – Unidentified EGRET sources
  – Gamma Ray Burst
- **MAGIC II will come 2007**
- **Grid added value**
  – Enable "(e-)scientific" collaboration between partners
  – Enable the cooperation between different experiments
  – Enable the participation on Virtual Observatories



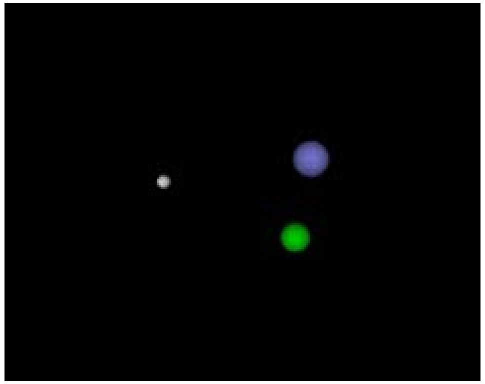


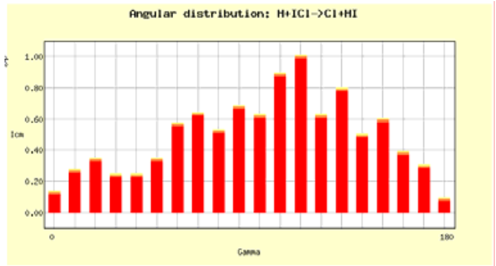


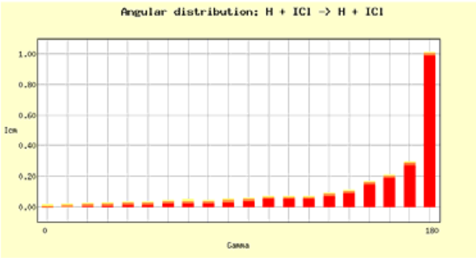


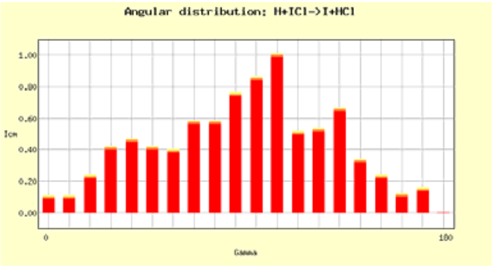
Computational Chemistry

- **The Grid Enabled Molecular Simulator (GEMS)**
  – Motivation:
    - Modern computer simulations of biomolecular systems produce an abundance of data, which could be reused several times by different researchers.
      → data must be catalogued and searchable
  – GEMS database and toolkit:
    - autonomous storage resources
    - metadata specification
    - automatic storage allocation and replication policies
    - interface for distributed computation



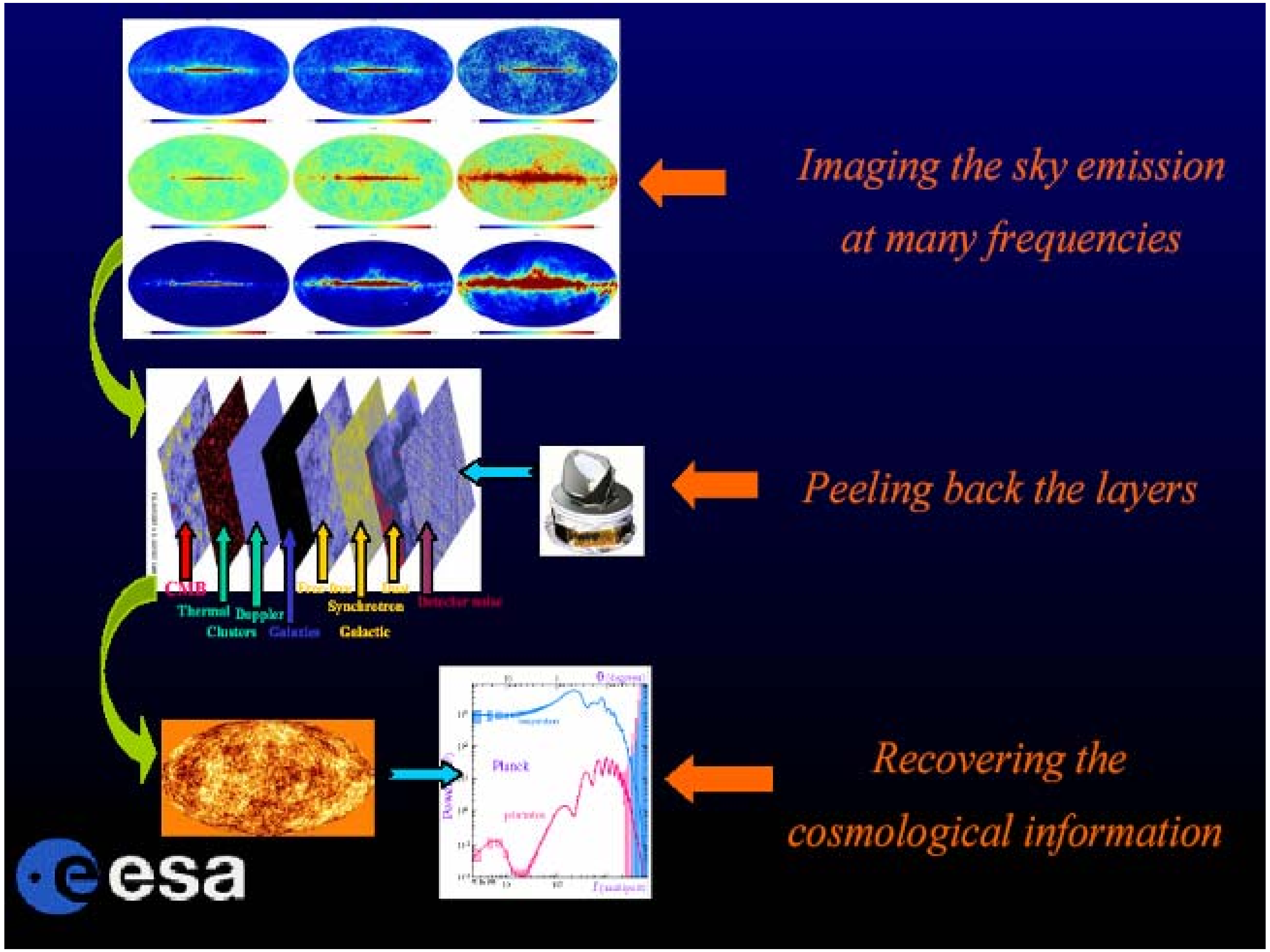






Planck

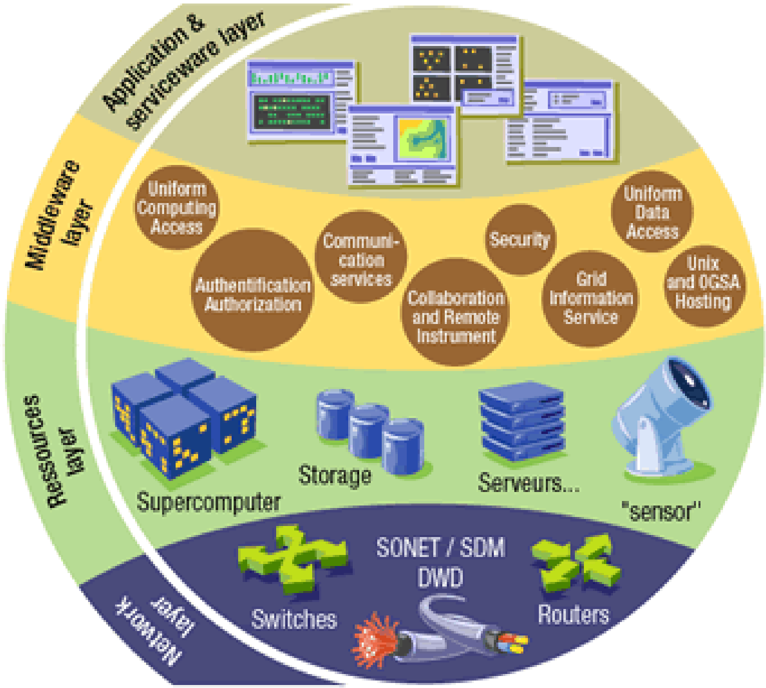
- **On the Grid:**
  - > 12 time faster
  - (but ~5% failures)
- **Complex data structure**
  - → data handling important
- **The Grid as**
  - collaboration tool
  - common user-interface
  - flexible environment
  - new approach to data and S/W sharing



Grid middleware

- **The Grid relies on advanced software, called middleware, which interfaces between resources and the applications**

- **The GRID middleware:**
  - Finds convenient places for the application to be run
  - Optimises use of resources
  - Organises efficient access to data
  - Deals with authentication to the different sites that are used
  - Runs the job & monitors progress
  - Recovers from problems
  - Transfers the result back to the scientist

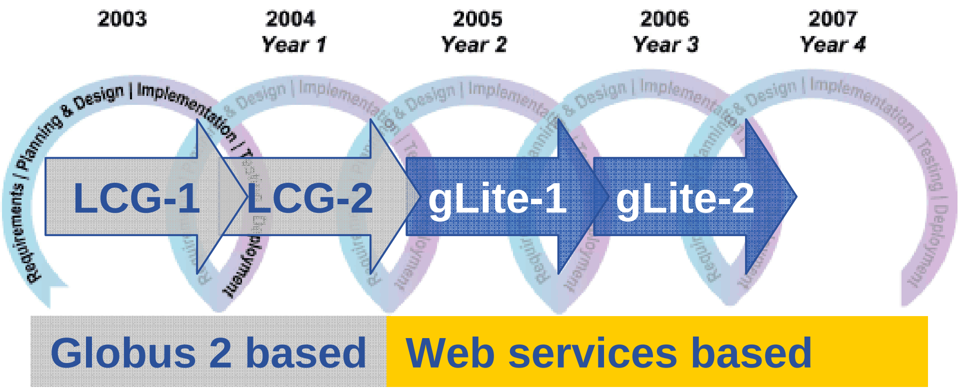


EGEE Middleware gLite

- **First release of gLite end of March 2005**
  - Focus on providing users early access to prototype
  - Release 1.1 in May 05
  - Release 1.2 in July 05
  - see www.gLite.org
- **Interoperability & Co-existence with deployed infrastructure**
- **Robust: Performance & Fault Tolerance**
- **Service oriented approach**
- **Open source license**

EGEE Middleware

- Intended to replace present middleware with production quality services
- Developed from existing components
- Aims to address present shortcomings and advanced needs from applications
- Prototyping short development cycles for fast user feedback
- Initial web-services based prototypes being tested



Application requirements http://egee-na4.ct.infn.it/requirements/

Architecture & Design

- **Design team includes**
  - Representatives from middleware providers (AliEn, Condor, EDG, Globus,…)
  - Colleagues from the Operations activity
  - Partners from related projects (e.g. OSG)
- **gLite development takes into account input and experiences from applications, operations, related projects**
  - Effective exchange of ideas, requirements, solutions and technologies
  - Coordinated development of new capabilities
  - Open communication channels
  - Joint deployment and testing of middleware
  - Early detection of differences and disagreements

gLite is not "just" a software stack, it is a "new" framework for international collaborative middleware development

User information & support

- **More than 140 training events across many countries**
  - >2000 people trained
    induction; application developer; advanced; retreats
  - Material archive online with >200 presentations

- **Public and technical websites constantly evolving to expand information available and keep it up to date**

- **3 conferences organized**
  ~ 300 @ Cork
  ~ 400 @ Den Haag
  ~ 450 @ Athens

- **Pisa: 4th project conference 24-28 October ’05**

Collaborations

- **EGEE closely collaborates with other projects, e.g.**
- **Flooding Crisis (CrossGrid) demonstrated at 3rd EGEE conference in Athens**
  - Simulation of flooding scenarios
  - Display in Virtual Reality
  - Optimize data transport

→ **won prize for "best demo"**

Collaboration with Slowak Academy of Sciences

EGEE as partner

- **Ongoing collaborations**
  - **with non-EU partners: US, Israel, Russia, Korea, Taiwan…**
    - **MoU with the Chonnam–Kangnung–Sejong–Collaboration project (CKSC)**
    - **Strong relationship KISTI (Korea Institute of Science and Technology Information), developing into partnership for EGEE II**
  - **with other European projects, in particular:**
    - **GÉANT**
    - **DEISA**
    - **SEE-GRID**
  - **with non-European projects:**
    - **OSG: OpenScienceGrid (USA)**
    - **NAREGI (Japan)**
    - **International Grid Trust Federation**
      - ***EU-GridPMA joining with Asia-Pacific and American counterparts***

Distributed European Infrastructure for Supercomputing Applications

- **EGEE as incubator**
  - **18 recently submitted EU proposals supported**
  - **More proposals in next calls and national funding programmes**

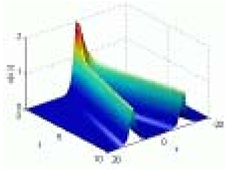
Related projects under negotiation

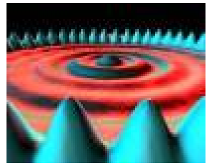
Name	*Description*	*Common partners with EGEE*
BalticGrid	EGEE extension to Estonia, Latvia, Lithuania	KTH – PSNC – CERN
EELA	EGEE extension to Brazil, Chile, Cuba, Mexico, Argentina	CSIC – UPV – INFN – CERN – LIP – RED.ES
EUChinaGRID	EGEE extension to China	INFN – CERN – DANTE – GARR – GRNET
EUMedGRID	EGEE extension to Malta, Algeria, Morocco, Egypt, Syria, Tunisia, Turkey	INFN – CERN – DANTE – GARR – GRNET – RED.ES
ISSeG	Site security	CERN – CSSI – FZK – CCLRC
eIRGSP	Policies	CERN – GRNET
ETICS	Repository, Testing	CERN – INFN – UWM
ICEAGE	Repository for Training & Education, Schools on Grid Computing	UEDIN – CERN – KTH – SZTAKI
BELIEF	Digital Library of Grid documentation, organisation of workshops, conferences	UWM
BIOINFOGRID	Biomedical	INFN – CNRS
Health-e-Child	Biomedical – Integration of heterogeneous biomedical information for improved healthcare	CERN

Exact budget and partner roles to be confirmed during negotiation

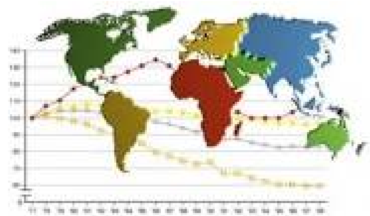
From Phase I to II

- **From 1st EGEE EU Review in February 2005:**
  - “The reviewers found the overall performance of the project very good.”
  - “… remarkable achievement to set up this consortium, to realize appropriate structures to provide the necessary leadership, and to cope with changing requirements.”

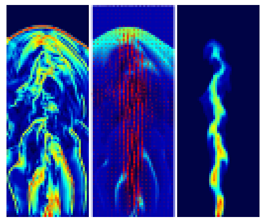


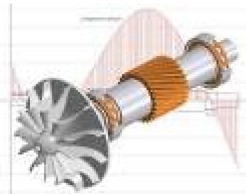


- **EGEE I**
  - Large scale deployment of EGEE infrastructure to deliver production level Grid services with selected number of applications



- **EGEE II**
  - Natural continuation of the project’s first phase
  - Emphasis on providing an infrastructure for e-Science
    - → increased support for applications
    - → increased multidisciplinary Grid infrastructure
    - → more involvement from Industry
  - **Extending the Grid infrastructure world-wide**
    - → **increased international collaboration**
      (Asia-Pacific is already a partner!)





Conclusions I

- Grids are a powerful new tool for science – as well as other fields
- Grid computing has been chosen by CERN and HEP as the most cost effective computing model
- Several other applications are already benefiting from Grid technologies (biomedical is a good example)
- Investments in grid projects are growing world-wide
- Europe is strong in the development of Grids also thanks to the success of EGEE and related projects

Conclusions II

- **Collaboration across national and international programmes is very important:**
  - Grids are above all about collaboration at a large scale
  - Science is international and therefore requires an international computing infrastructure
- **EGEE I and II are always open to further collaboration**
- **The Asia-Pacific region is very important for EGEE and the EU**
  - CKSC is a partner in EGEE, and along with KISTI will form the Korean Federation in EGEE II
- **EGEE is interested in discussing possible future new collaborations**

Contacts

- **EGEE Website**

  http://www.eu-egee.org

- **How to join**

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

- **EGEE Project Office**

  project-eu-egee-po@cern.ch

Thanks for the opportunity to present EGEE to all of you and for your kind attention!