



EGEE – application support and identification

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Second EGEE review

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www.eu-egee.org

INFSO-RI-508833



- Status of applications: achievements since last review
 - Deployment on the production infrastructure
 - Deployment on the PreProduction Service
 - Other achievements
- Response to comments raised at last review

Perspectives

- Short term: User forum March 1-3 2005
- Mid term: EGEE-II

Conclusion

GGCC What happened since last review

- The number of users in VOs related to NA4 activity kept growing regularly
 - from ~500 at PM9 to ~1000 at PM18
 - More than 20 applications are deployed on the production infrastructure
- The usage of the grid by pilot applications has significantly evolved
 - From data challenge to service challenge (HEP)
 - First biomedical data challenge (WISDOM)
- Several existing applications have been migrated to the new middleware by the HEP, biomedical and generic teams

Production

Enabling Grids for E-sciencE

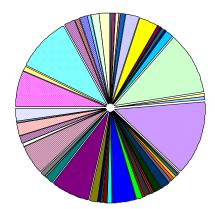
Fundamental activity in preparation of LHC start up

- Physics and detector studies
- Computing systems commissioning
- Examples:

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- LHCb: >700 CPU/years in 2005 on the EGEE infrastructure
- ATLAS: >10,000 jobs per day
 - Comprehensive analysis: see S.Campana et al., e-Science 2005, Melbourne, Australia
- A lot of activity in all involved applications (including as usual a lot of activity within non-LHC experiments like BaBar, CDF and D0)
- More details in DNA4.3.2

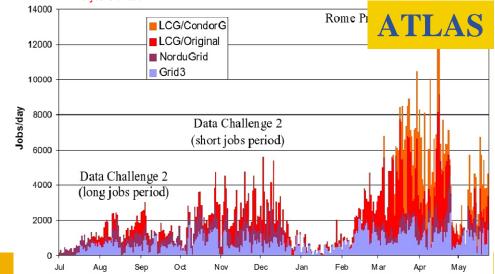
CPU used: 6,389,638 h Data Output: 77 TB



DIRAC.Barcelona.es 0.214% DIRAC.CERN.ch 0.571% DIRAC.CracowAgu.pl 0.001% DIRAC.LHCBONLINE.ch 0.779% DIRAC.PNPI.ru 0.000% DIRAC.ScotGrid.uk 3.068% DIRAC.Zurich.ch 0.756% LCG.BHAM-HEP.uk 0.705% LCG.Bari.it 1.357% I CG CERN ch 10 960% LCG.CGG.fr 0.676% LCG.CNAF.it 13.196% LCG.CPPM.fr 0.242% LCG.CY01.cy 0.103% LCG.Cambridge.uk 0.010% LCG.Durham.uk 0.476% LCG.FZK.de 1.708% I CG Eirenze it 1 047% LCG.GR-02.gr 0.226% LCG.GR-04.gr 0.056% ■ LCG.HPC2N.se 0.001% LCG.IFCA.es 0.022% LCG.IN2P3.fr 4.143% LCG.IPP.bg 0.033% LCG.Imperial.uk 0.891% LCG.JINR.ru 0.472% I CG Lancashire uk 6 796% LCG.Manchester.uk 0.285% LCG.Montreal.ca 0.069% LCG.NSC.se 0.465% LCG.Oxford.uk 1.214% LCG.PNPI.ru 0.278% LCG.Pisa.it 0.121% LCG.RAL-HEP.uk 0.938% LCG.RHUL.uk 2.168% LCG.Sheffield.uk 0.094% LCG. Toronto. ca 0.343% LCG.UCL-CCC.uk 1.455%



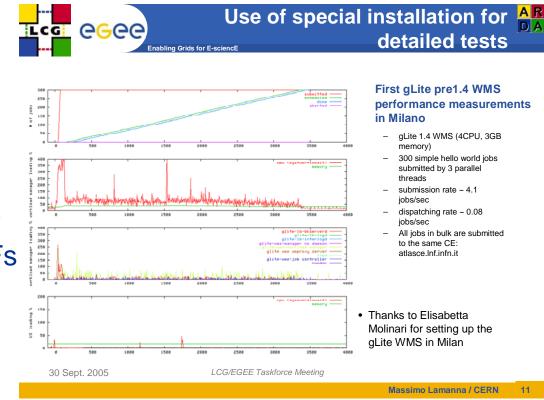
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Enabling Grids for E-science

- Task Forces
 - EGEE + experiment people. Very close and positive collaboration. Emphasis on integration onto EGEE infrastructure
- One example (direct contribution of NA4-HEP/ARDA within the ATLAS TF)
 Use of special installati
 - Detailed studies of advanced gLite feature: WMS bulk submission (ATLAS Task Force)
 - Other middleware tested in the framework of other ARDA prototypes and TFs
 - More under arda.cern.ch



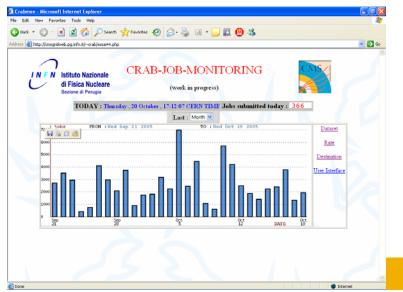
Development and integration

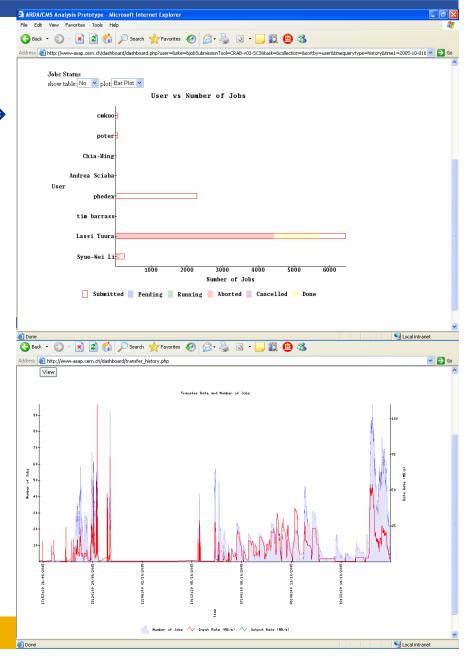
Enabling Grids for E-sciencE

 From prototypes to coherent integration (CMS)

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- NA4 HEP (ARDA/ASAP) prototype → converging on the CMS CRAB system
- SC3 activity, analysis jobs,
 productions jobs → CMS dashboard
- Clear signs of wide user activity!!!
 - ASAP and CRAB
 - ~150k jobs/month



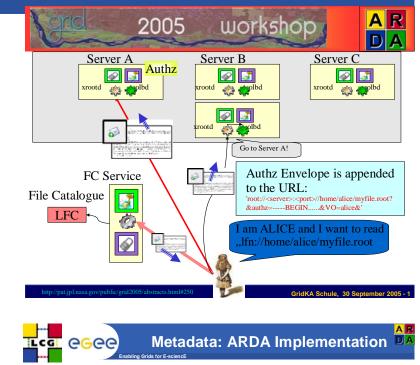


eGee

Development and integration

Enabling Grids for E-sciencE

- Other examples:
 - Efficient data access integration: File catalogue ACL and fast data access via xrootd (ALICE prototype and Task Force). Presentation at SuperComputing 2005
 - Improved user access: GANGA (ATLAS and LHCb activities). Good feedback and demo in Pisa
 - Contribution to services used also outside HEP and contributed to gLite (AMGA).
 Used in the demo of Biomed and "Generic" in Pisa EGEE Conference

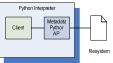


Prototype

- Validate our ideas and expose a concrete example to interested parties
- Multiple back ends
 - Currently: Oracle, PostgreSQL, SQLite, MySQL
- Dual front ends
 - TCP Streaming
 Chosen for performance
 - SOAP
 - Formal requirement of EGEE
 - Compare SOAP with TCP Streaming
- Also implemented as standalone
 Python library
 - Data stored on the file system



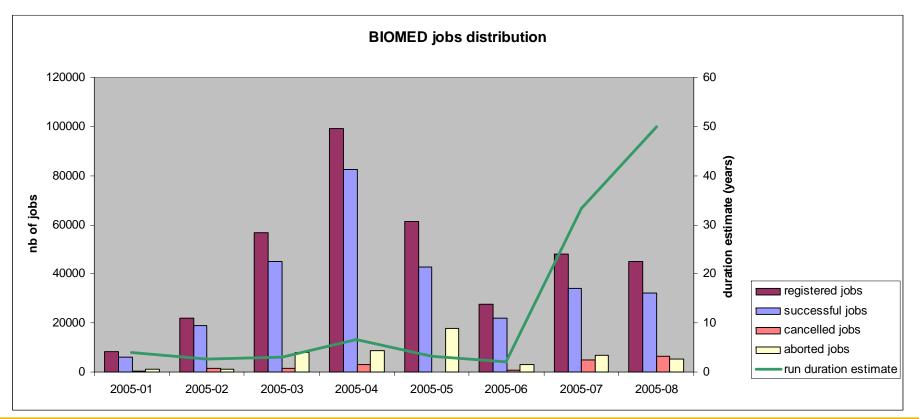
MD Serve



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- ~ 70 users, 9 countries
- > 12 Applications (medical image processing, bioinformatics)
- ~3000 CPUs, ~12 TB disk space
- ~100 CPU years, ~ 500K jobs last 6 months



First biomedical data challenge: World-wide In Silico Docking On Malaria (WISDOM)

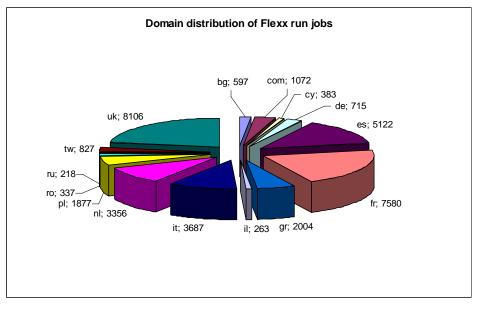
Enabling Grids for E-sciencE

Significant biological parameters

- two different molecular docking applications (Autodock and FlexX)
- about one million virtual ligands selected
- target proteins from the parasite responsible for malaria
- Significant numbers

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- Total of about 46 million ligands docked in 6 weeks
- 1TB of data produced
- Up 1000 computers in 15 countries used simultaneously corresponding to about 80 CPU years
- Average crunching factor ~600



WISDOM open day December 16th, 2005, Bonn (Germany)

Discuss Data Challenge results Prepare next steps towards a malaria Grid (EGEE-II, Embrace, Bioinfogrid) Information: http://wisdom.eu-egee.fr

NA4 tests on the PPS

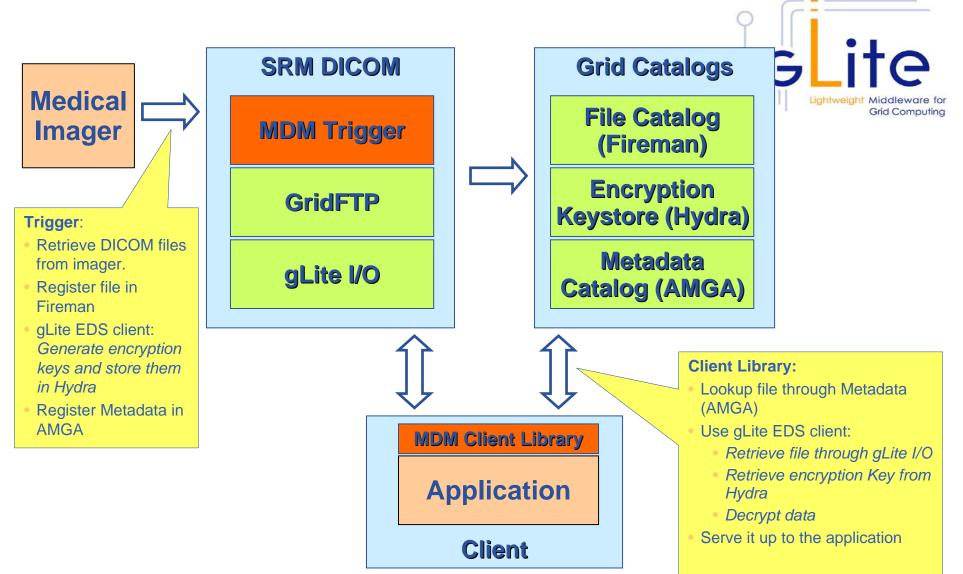
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- PPS components tested
 - Weekly testing of WMS
 - FiReMan
 - ACLs for file access
 - R-GMA
- Other gLite testing
 - Site installation (v1.0, 1.1, 1.2 and 1.3)

Enabling Grids for E-sciencE

- Advanced data management on prototype testbed
 - FiReMan, File Transfer Service
 - Metadata (AMGA)
 - File encryption
 - dCache SRM (SRM-DICOM interface)
 - Security features really needed for biomedical applications: expected on PPS soon!





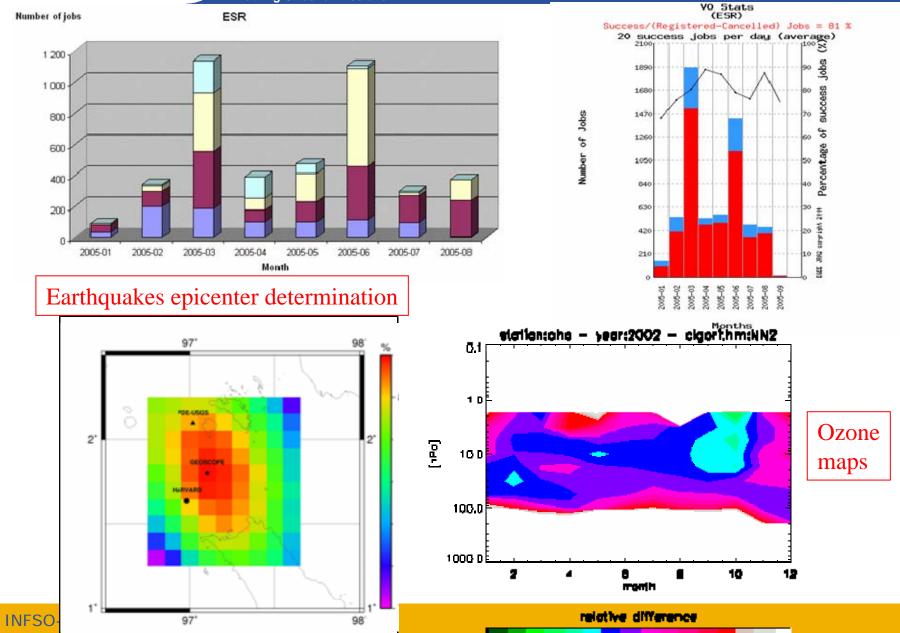


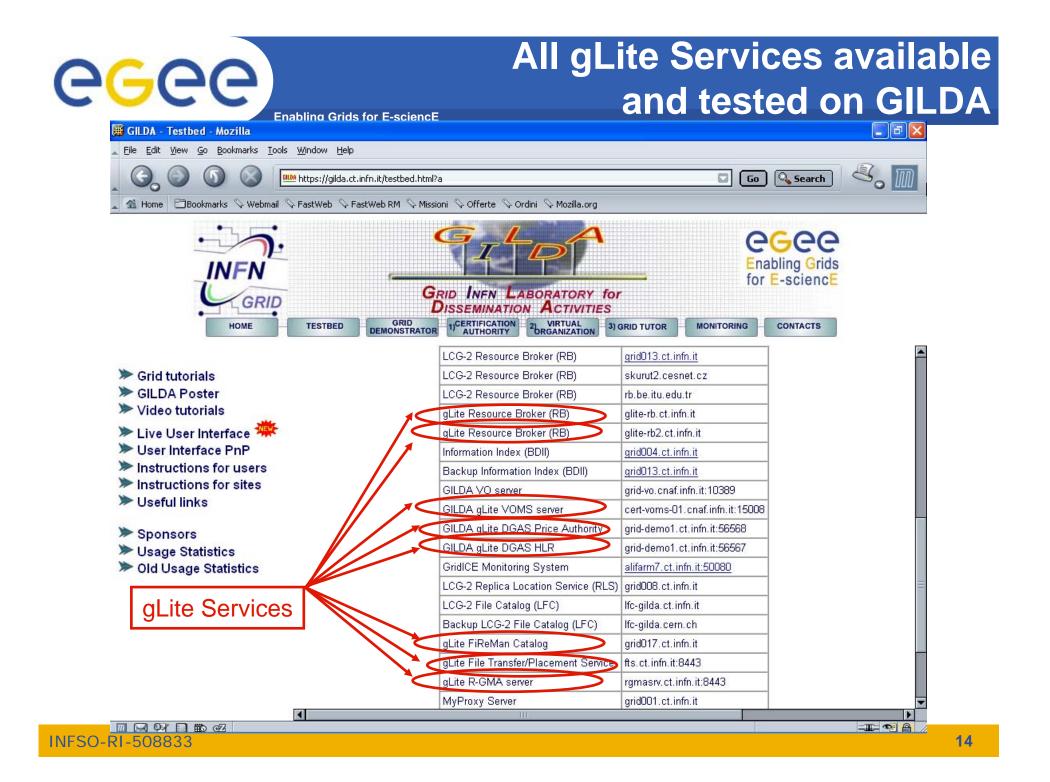
- Applications accepted by Project Executive Board
 - Earth Science Research (Earth Observation, Hydrology, Climate)
 - Geophysics (Industry)
 - Computational Chemistry
 - Astrophysics (MAGIC and Planck collaborations)
 - Finance (EGRID)
- New Applications recommended to PEB by EGEE Generic Applications Advisory Panel (EGAAP)
 - Fusion (ITER)
 - Archaeology
 - EC projects (EELA, EUMEDGRID, EUCHINAGRID, BIOINFOGRID)

Generic Applications' use of EGEE

Enabling Grids for E-sciencE

eGee







- Demonstrated scientific benefits of the EGEE grid
- Capture of requirements and assessment of middleware
- Improved process to select new application areas
- Migration to gLite



Demonstrated scientific benefits of the EGEE grid

- Demonstrated added value in terms of deployment scale
 - Heavy production of simulated data for LHC Computing Grid
 - Essential for the commissioning of the experiments
- Demonstrated added value in terms of response time
 - Computation of seism epicenter
 - Search for new drugs: large scale in silico docking (WISDOM)
- Demonstrated added value in terms of data distribution
 - Distribution of LHC data on the grid and sizeable users activity (~150k jobs/month in the CMS case)
- Coming:
 - medical data management



capture of requirements and assessment of middleware

- Status at PM18
 - A database of requirements has been setup by the Project Technical Forum
 - This database includes already >400 requirements
 - This database is populated by the scientific communities deploying applications on EGEE and by FP6 projects (eg Diligent, Seegrid,...)
- capture of requirements from FP5 projects
 - Several FP5 projects were granted access to the database (Grace Mammogrid)
 - But it generally turnt out to be difficult to collect explicitly requirements
 - No formalization of requirements
 - Projects finished
 - Requirements are mostly collected through the scientific communities (Crossgrid, Datagrid)

• assessment of middleware w.r.t requirements

On-going work with JRA1 within the framework of PTF and TCG



- Situation at PM18
 - No new call for applications since EGEE review
 - New application communities (finance, archeology, fusion) asked for access to infrastructure
 - EC funded projects are also asking for collaboration with EGEE
- Improved process under design
 - Creation of lightweight recognized VOs vs supported VOs
 - Only supported VOs would be asked to write a Memorandum of Understanding
 - Decentralized integration vs centralized EGAAP like approach
 - Initial deployment at regional level
- Improved Memorandum of Understanding between EGEE and the scientific communities

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Other achievements:MoUs almost finalized

Enabling Grids for E-sciencE

Actions	Comp Chem	Magic	Planck	Drug Discovery	Egeode	ESR
MoU filled by applications	ОК	ОК	ОК	ОК	Waiting feedback	OK
SA1 questionnaire	ОК	ОК	ОК	ОК	ОК	ОК
SA1	ОК	ОК	ОК	ОК	-	ок
SA2	ОК	ОК	ОК	ОК	-	OK
NA3	ОК	ОК	ОК	ОК	-	OK



Migration to gLite

- Status at PM18
 - gLite offers unprecedented functionalities for user communities
 - The migration of several existing applications to gLite is achieved (see demos)
 - ARDA prototypes for HEP
 - Several biomed applications (Pharmacokinetics, CDSS, ...)
 - gLite available for early deployment on GILDA
 - gLite brought to 100s during EGEE tutorials with GILDA

Issues

 The availability of gLite software on the pre-production and production services



EGEE first User Forum

- Enabling Grids for E-sciencE
- Dates: March 1-3 2006
- Location: CERN, Switzerland
- Target attendance: 150 participants
- Goals
 - Get a consistent understanding across the EGEE related projects of expectation, present status and possible evolution
 - Promote cross-application fertilisation
 - Prepare EGEE-II
- Participation open to external projects and EGEE members
- Format: 3-day workshop
 - Presentations by thematic areas selected by invitation and through a call for contributions
 - EGEE presentations (integration of new applications, access to resources, status of middleware,...)
 - With a lot of time for discussion
- URL:
 - http://egee-intranet.web.cern.ch/egee-intranet/User-Forum/index.html



NA4 in EGEE-II

- Ongoing support to 2 pilot areas (High Energy Physics, Biomedicine) with established user communities and large scale applications
- **On-going support to GILDA, the virtual grid laboratory**
- Increased support to 4 scientific disciplines (Astrophysics, Computational Chemistry, Earth Sciences, Fusion), 3 of them coming out of EGEE generic applications •
- Increased effort to foster a cohesive application community at NA4 management level •
- Increased complexity from the wider regional distribution and the associated projects

Goal	Resource allocation in PM	Fraction
Support teams to help with consulting and porting of applications	1005	51%
Evolution of pilot applications with evolving middleware services	215	11%
Validation of the efficient production and continuous availability of data for the scientific communities	282	14%
Grid laboratory to attract and expose new applications to grid computing	192	10%
Management of the large and diverse set of application and institutes involved in NA4	269	14%
	Support teams to help with consulting and porting of applications Evolution of pilot applications with evolving middleware services Validation of the efficient production and continuous availability of data for the scientific communities Grid laboratory to attract and expose new applications to grid computing Management of the large and diverse set of application and institutes	allocation in PMSupport teams to help with consulting and porting of applications1005Evolution of pilot applications with evolving middleware services215Validation of the efficient production and continuous availability of data for the scientific communities282Grid laboratory to attract and expose new applications to grid computing192Management of the large and diverse set of application and institutes269



- Achievements
 - The number of users in VOs related to NA4 activity has doubled
 - The usage of the grid by pilot applications has significantly evolved
 - The migration of several existing applications to gLite is achieved

Issues

- The availability of gLite software on the pre-production and production services;
- The amount of effort required by the VOs in order to obtain useful results from the use of the grid
- The availability, accessibility and quality of user documentation
- Perspectives: User Forum, EGEE-II