



Enabling Grids for E-sciencE

Application Porting using DRMAA and Globus GridWay on the EGEE Infrastructure

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EGEE08 (Istambul)

www.eu-egee.org

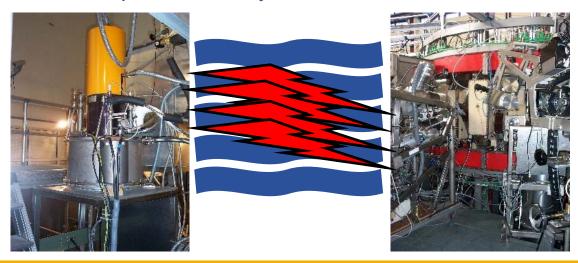






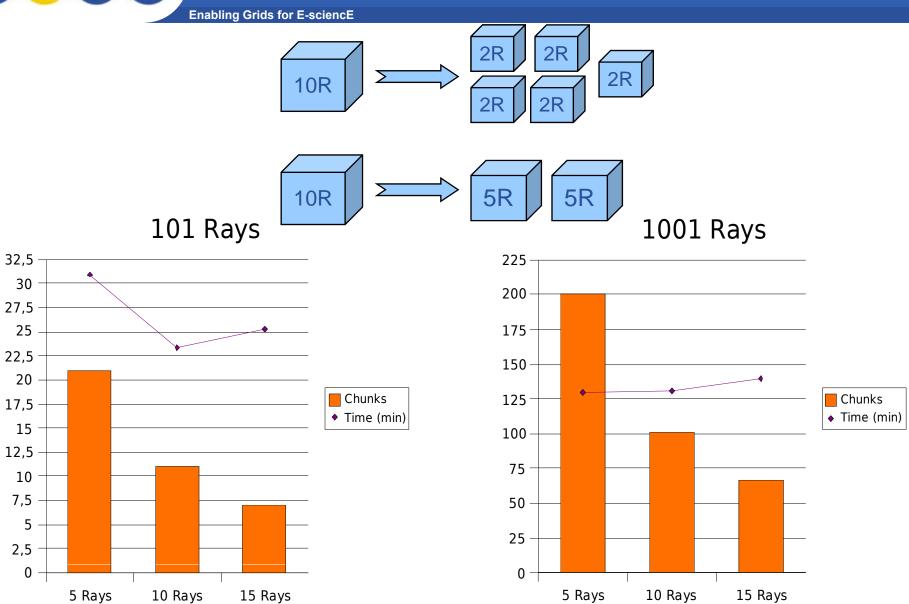
MaRaTra

- Massive Ray Tracing in Fusion Plasmas
 - Traces each ray contained in a microwave beam which heats fusion plasma
 - Finds best "shooting" position
 - Needs to be executed as much as possible in less time
- Fusion Physics (Fusion VO) Proposed by CIEMAT (Spain)
- Parameter Sweep (with pre and postprocess)
- 1 ray = 1 job = 9' on a Pentium 4
 - Upgrade: Using chunks reduces transfer and queue overhead
- CLI developed using OGF DRMAA C API provided by GridWay
 - lcg2.1.69 User Interface C++ API was tested at the beginning (couldn't handle big collections of jobs)
- Production Status: up to 1001 Rays in 2h 10'





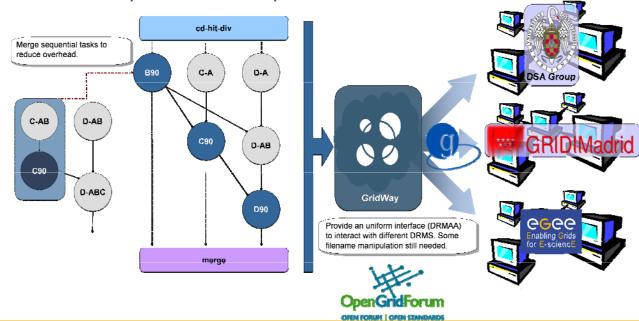
MaRaTra





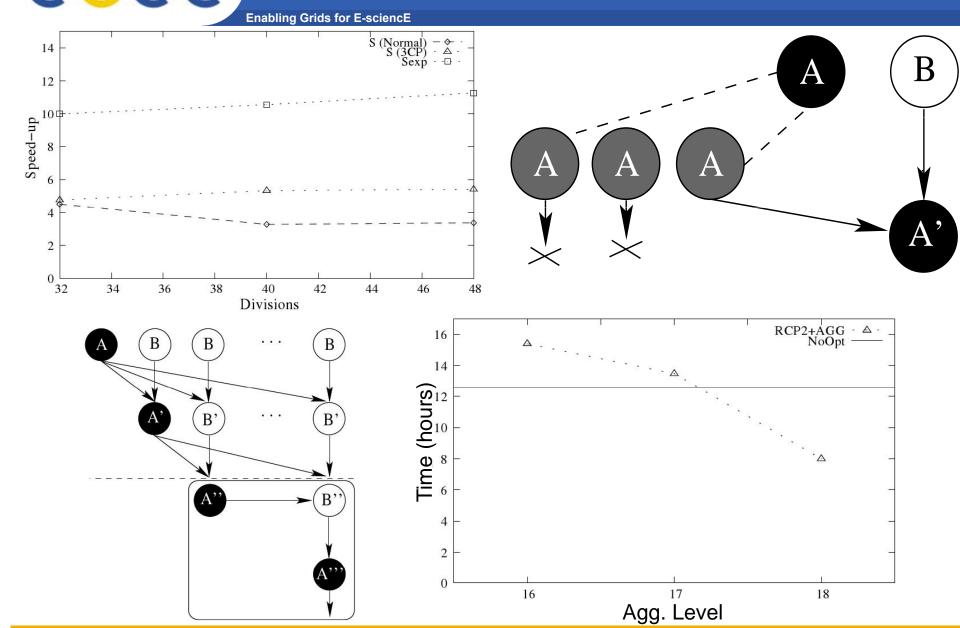
CD-HIT Grid

- CD-HIT: Cluster Database at High Identity with Tolerance
 - Compares protein DB entries and eliminates redundancies
 - Example: UniRef data sets generated by UniProt
 - Infeasible to be executed on a single machine (memory requirements and total execution time)
- Bioinformatics (BioMed VO) Proposed by CNIO (Spain)
- Intree Workflow (with pre and postprocess)
 - Grain can be adjusted
 - Upgrade: optimization heuristics for efficient execution have been added
- CLI developed using OGF DRMAA C API provided by GridWay
- Production State: Up to 1.7GB DB processed in 7h 45'



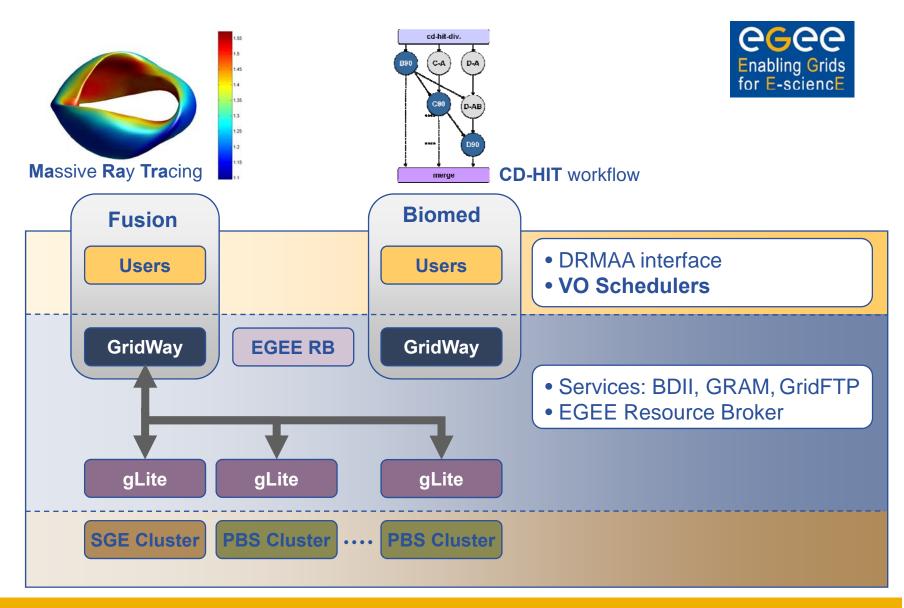
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CD-HIT Grid



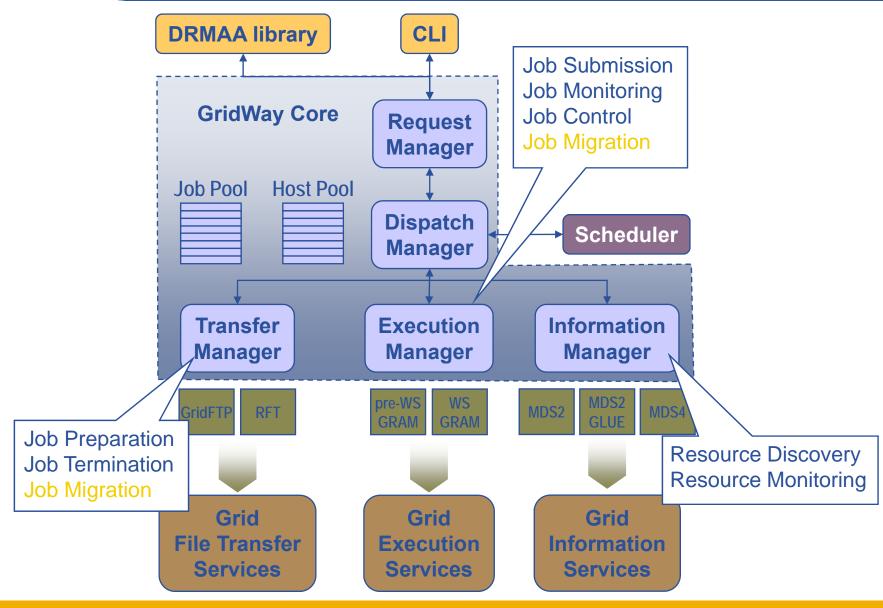


Grid Execution Architecture





The GridWay Metascheduler





The GridWay Metascheduler

OPEN FORUM | OPEN STANDARDS

Enabling Grids for E-sciencE

What is DRMAA?

- Distributed Resource Management Application API
 - http://www.drmaa.org/
- Open Grid Forum Standard
- Homogeneous interface to different Distributed Resource Managers (DRM):
 - SGE
 - Condor
 - PBS/Torque
 - GridWay
 - C
 - JAVA
 - Perl
 - Ruby
 - Python





The GridWay Metascheduler

Enabling Grids for E-science

Development Process

- Community Open Source Project. Globus Development Philosophy
- **Development Infrastructure** (thanks to Globus Project!)
 - Mailing Lists
 - Bugzilla
 - CVS
- You are very welcome to contribute:
 - Reporting Bugs (gridway-user@globus.org)
 - Making feature requests for the next GridWay release (gridway-user@globus.org)
 - Contributing your own developments (bug fixes, new features, documentation)
- Detailed Roadmap:
 - GridWay Campaigns at bugzilla.mcs.anl.gov/globus/query.cgi
 - www-unix.mcs.anl.gov/~bacon/cgi-bin/big-roadmap.cgi#Gridway



Supported Application Porting

- Chemistry
 - GAMESS and GAUSSIAN at group QCyCAR (UCLM)
 - Chemical Reactor Design in BE14 ("New Product & Process Development") of BEinGRID project
- Life Sciences
 - Dynamic BLAST at UABGrid
 - Multi-Resolution Docking at Centro de Investigaciones Biológicas (CSIC)
 - Verification and Optimization of Radiotherapy Treatments in BE25 ("BEinEIMRT: Business Experiment in Enhanced IMRT planning using Grid services on demand with SLAs") of BEinGRID project
- Astronomy
 - XMM-Newton Data Processing at ESAC (ESA)
 - Use of Special Hardware for N-Body Dynamics in Galactic Nuclei at AstroGrid-D
- Climate
 - Global Atmospheric Climate Simulations at EELA
 - Weather Research and Forecasting at LAGrid
- Geology
 - Petroleum Reservoir Simulations at TIGRE



Teşekkür ederim! Questions?