Application Porting Support: UCM Applications

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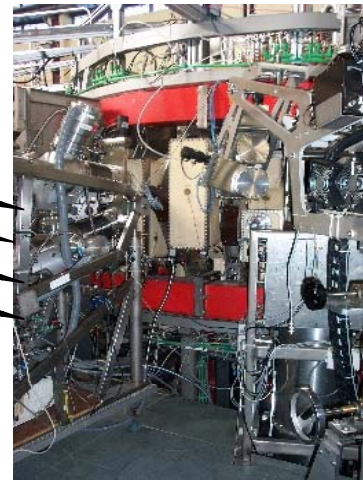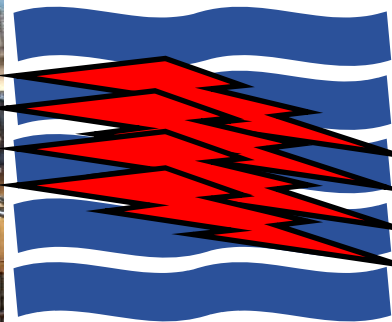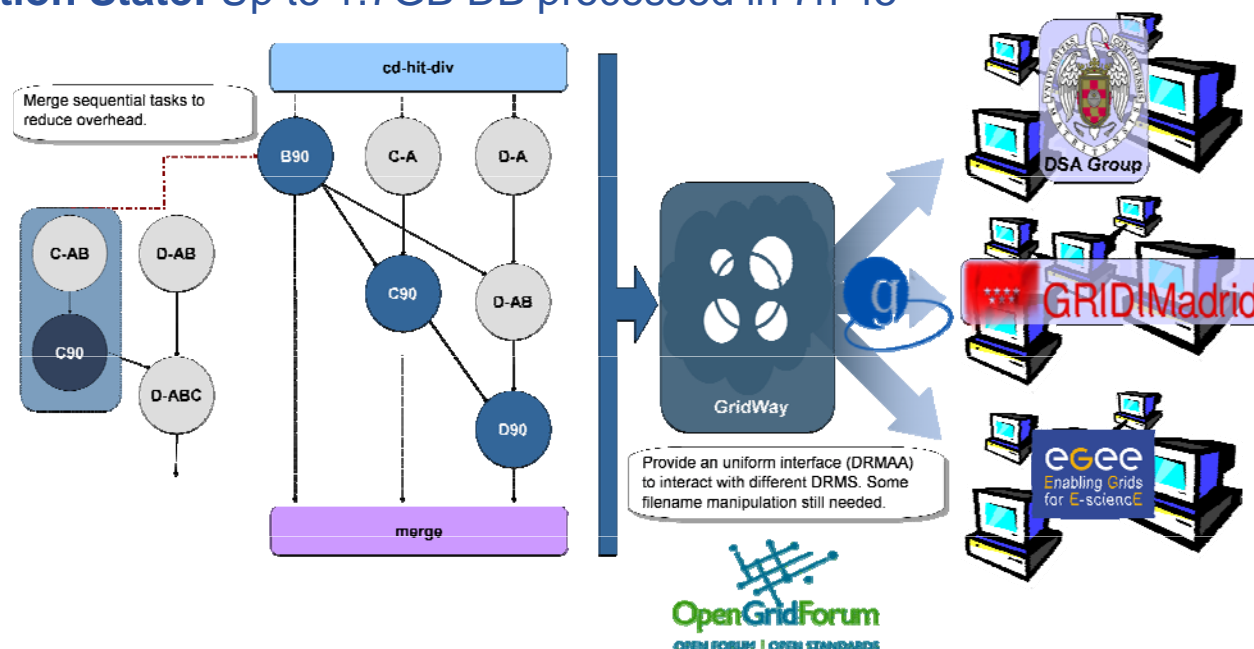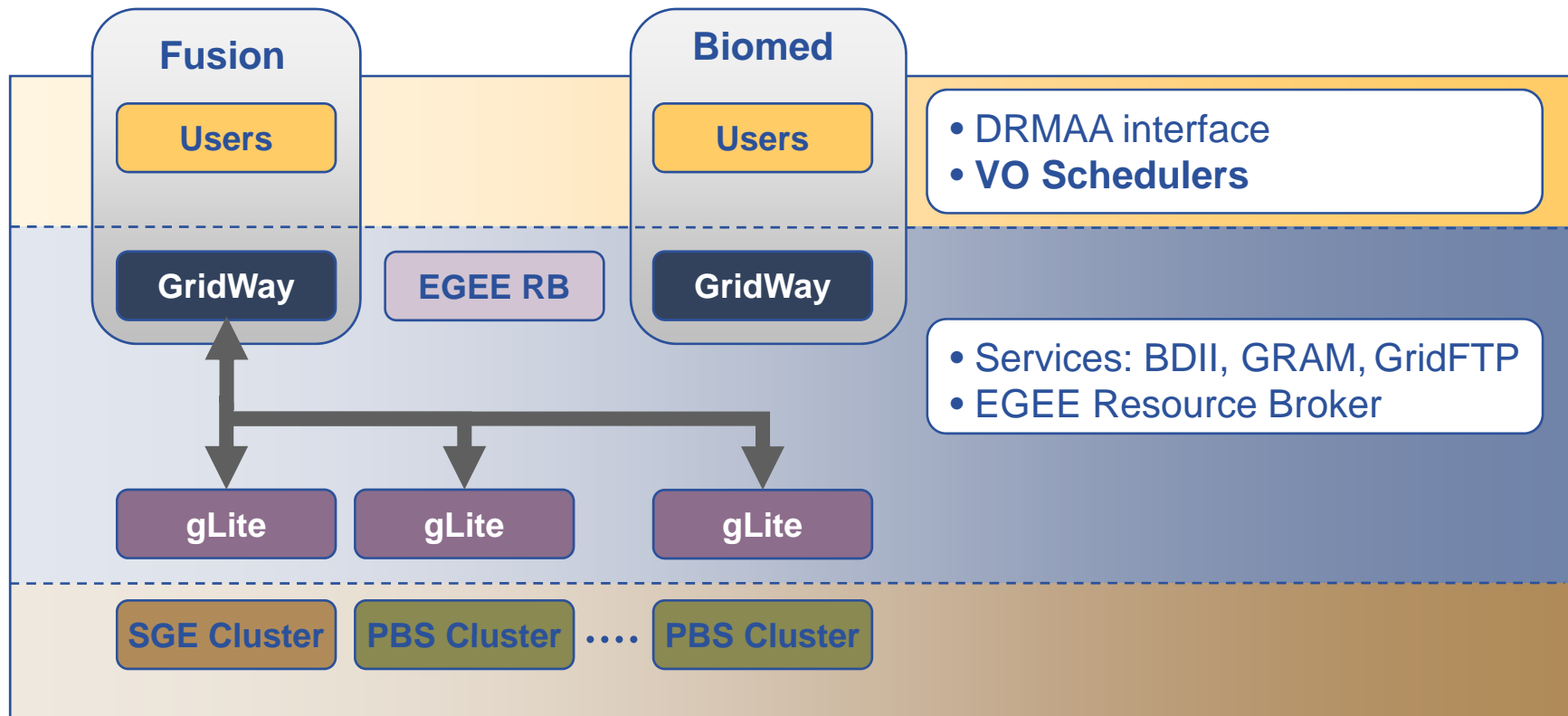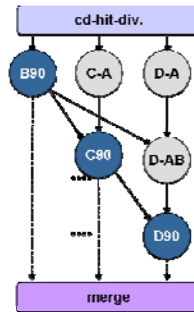**www.eu-egee.org**

Information Society and Media

- **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'

- **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'

Massive **Ra**y **Tra**cing

CD-HIT workflow

cd-hit-div.

merge

eGee
Enabling Grids
for E-sciencE

Fusion

Users

Biomed

Users

- DRMAA interface
- **VO Schedulers**

GridWay

EGEE RB

GridWay

- Services: BDII, GRAM, GridFTP
- EGEE Resource Broker

gLite

gLite

gLite

SGE Cluster

PBS Cluster •••• **PBS Cluster**

- **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

Merci!
Questions?