Enabling Grids for E-sciencE

Characteristics of Grid Applications

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www.eu-egee.org

Information Society and Media

Outline

- **Status**
  - EGEE's users, applications, and virtual organizations
  - "Application Identification and Support" activity
  - Evolution: project, users, and needs

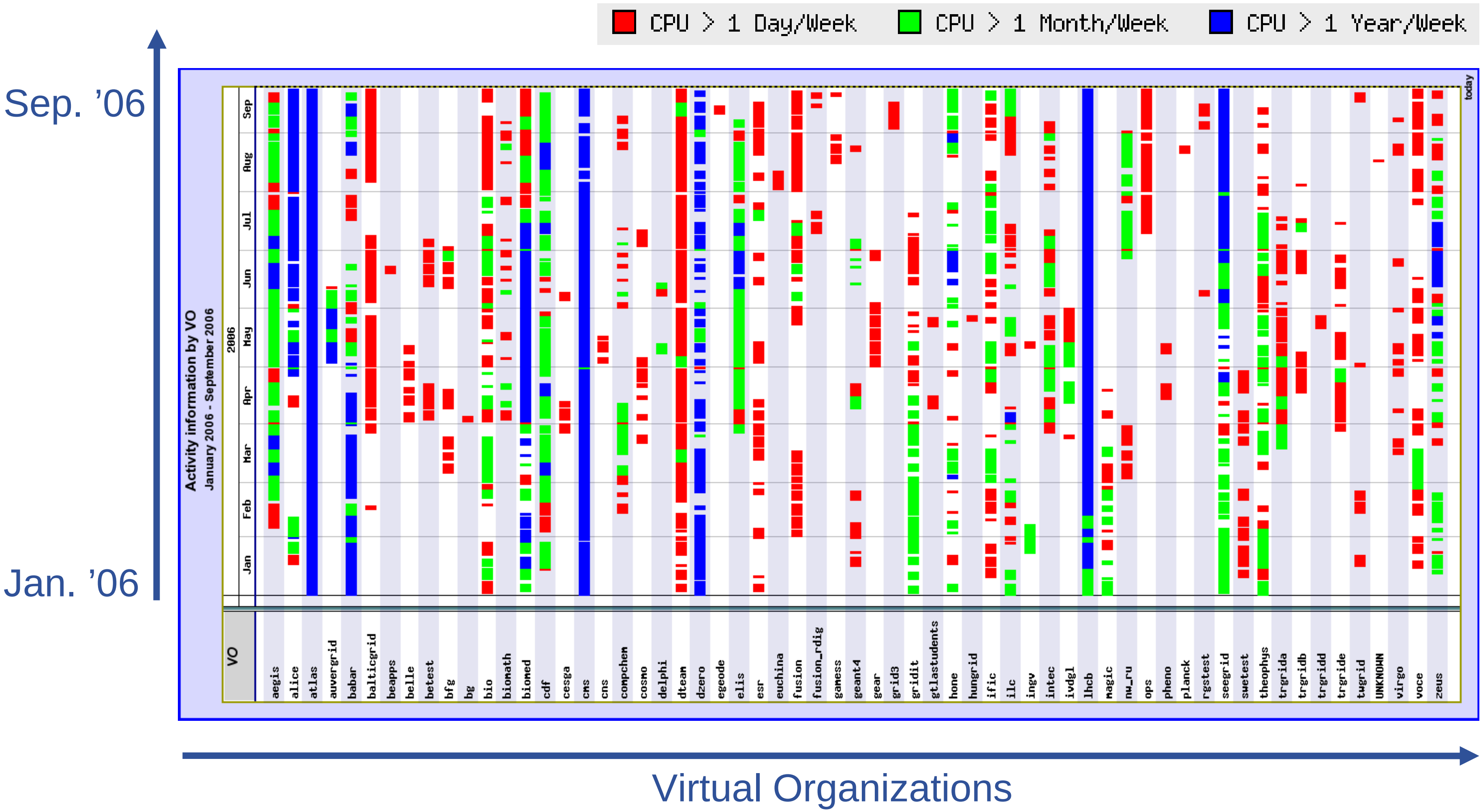
- **Grid Application "Families"**

- **Summary and Outlook**

Current Activity

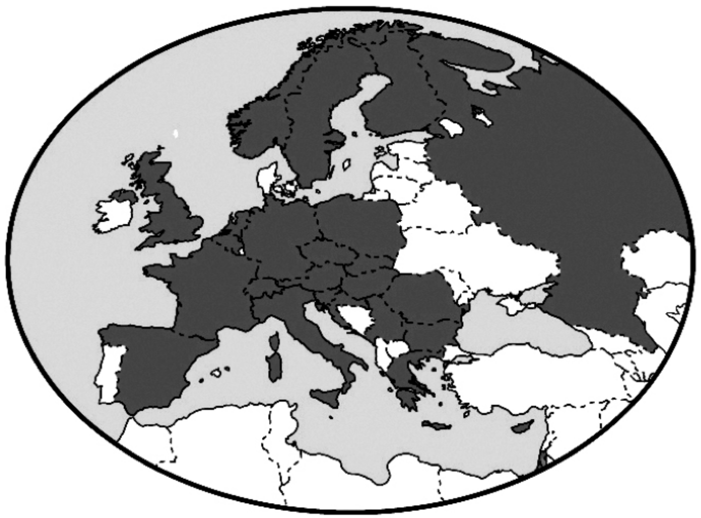
- **Routine and large-scale use of EGEE infrastructure to produce scientific results.**
- **VOs:**
  - 165+ VOs (90+ registered) using the grid
  - App. Deploy. Plan (https://edms.cern.ch/document/722131/2)
- **Domains:**
  - **High-Energy Physics**: LHC, Tevatron, HERA, …
  - **Biology**: Medical Images, Bioinformatics, Drug Discovery
  - **Earth Science**: Hydrology, Pollution, Climate, Geophysics, …
  - **Astrophysics**: Planck, MAGIC
  - **Fusion**
  - **Computational Chemistry**
  - **Related Projects**: Finance, Digital Libraries, …
  - **New areas**: nanotechnology, …

CPU Usage


Sep. '06
Jan. '06
CPU > 1 Day/Week
CPU > 1 Month/Week
CPU > 1 Year/Week
Activity information by VO
January 2006 - September 2006
2006
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
today
VO
aegis
alice
atlas
auvergrid
babar
balticgrid
beapps
belle
betest
bfg
bg
bio
biomath
biomed
cdf
cesga
cms
cns
compchem
cosmo
delphi
dteam
dzero
egeode
elis
esr
euchina
fusion
fusion_rdig
gamess
geant4
gear
grid3
gridit
gtlastudents
hone
hungrid
ific
ilc
ingv
intec
ivdgl
lhcb
magic
nw_ru
ops
pheno
planck
rgstest
seegrid
swetest
theophys
trgrida
trgridb
trgridd
trgride
twgrid
UNKNOWN
virgo
voce
zeus
Virtual Organizations

NA4 Activity

- **Application Identification and Support (NA4)**
  - 25 countries, 40 partners, 280+ participants, 1000s of users
- **Support the large and diverse EGEE user community:**
  - **Promote dialog**: Users' Forums & EGEE Conferences
  - **Technical Aid**: Porting code, procedural issues
  - **Liaison**: Software and operational requirements
- **Need active participation:**
  - **Feedback**: Infrastructure, configuration, and middleware
  - **Resources**: Hardware and human



Evolution

- **Evolution of Project (2001–now):**
  - European DataGrid: R&D
  - EGEE: Re-engineering & Infrastructure
  - EGEE-II: Infrastructure & Re-engineering

larger grid ↓ more apps.

- **Evolution of Grid Users:**
  - **Focus**: Grid technology ⇒ Scientific results
  - **Goal**: Grid technology ⇒ Grid as a tool
  - **Experience**: IT experts ⇒ IT "minimalists"

- **These changes are healthy, but…**
  - Rely less on IT competence of users.
  - More portable, more flexible middleware.

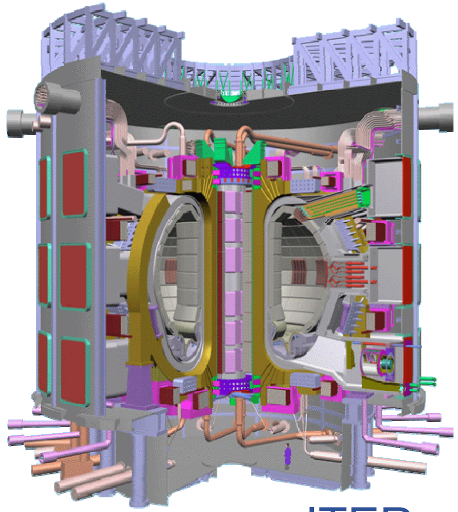
Application Families

- Simulation
- Bulk Processing
- Responsive Apps.
- Workflow
- Parallel Jobs
- Legacy Applications

Simulation

- **Examples**
  - LHC Monte Carlo simulation
  - Fusion
  - WISDOM—malaria/avian flu
- **Characteristics**
  - Jobs are CPU-intensive
  - Large number of independent jobs
  - Run by few (expert) users
  - Small input; large output
- **Needs**
  - Batch-system services
  - Minimal data management for storage of results

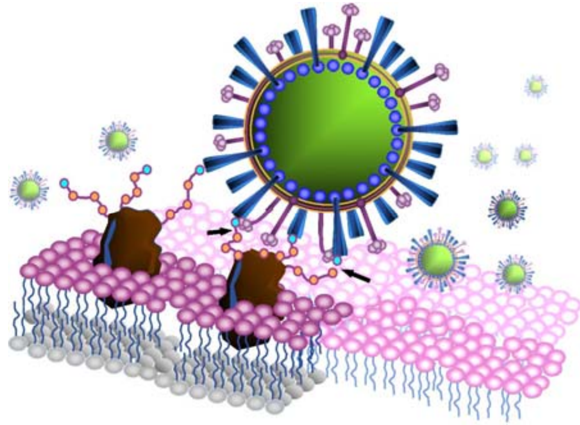
ATLAS



ITER

Drug Discovery

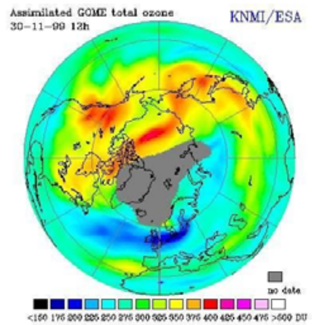
- **WISDOM focuses on in silico drug discovery for neglected and emerging diseases.**



- **Malaria — Summer 2005**
  - 46 million ligands docked
  - 1 million selected
  - 1TB data produced; 80 CPU-years used in 6 weeks
- **Avian Flu — Spring 2006**
  - H5N1 neuraminidase
  - Impact of selected point mutations on eff. of existing drugs
  - Identification of new potential drugs acting on mutated N1
- **Fall 2006**
  - Extension to other neglected diseases

Bulk Processing

- **Examples**
  - HEP processing of raw data, analysis
  - Earth observation data processing
- **Characteristics**
  - Widely-distributed input data
  - Significant amount of input and output data



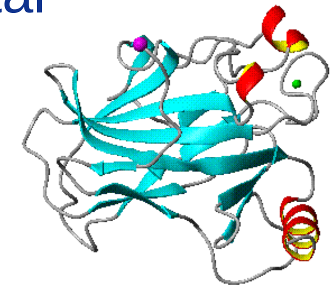
- **Needs**
  - Job management tools (workload management)
  - Meta-data services
  - More sophisticated data management

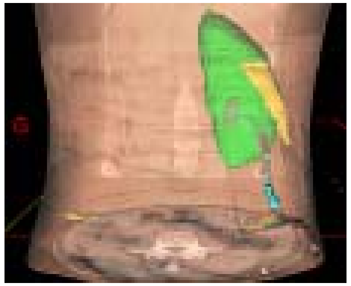
Responsive Apps. (I)

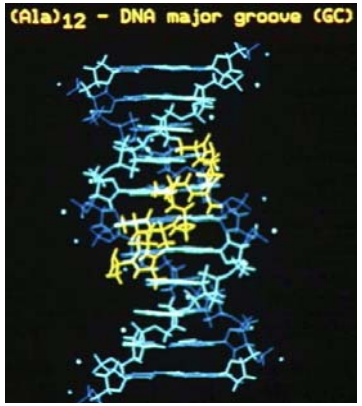
- **Examples**
  - Prototyping new applications
  - Monitoring grid operations
  - Direct interactivity
- **Characteristics**
  - Small amounts of input and output data
  - Not CPU-intensive
  - Short response time (few minutes)
- **Needs**
  - Configuration which allows “immediate” execution (QoS)
  - Services must treat jobs with minimum latency

Responsive Apps. (II)

- **Grid as a backend infrastructure:**
  - gPTM3D: interactive analysis of medical images
  - GPS@: bioinformatics via web portal
  - GATE: radiotherapy planning
  - DILIGENT: digital libraries
  - Volcano sonification

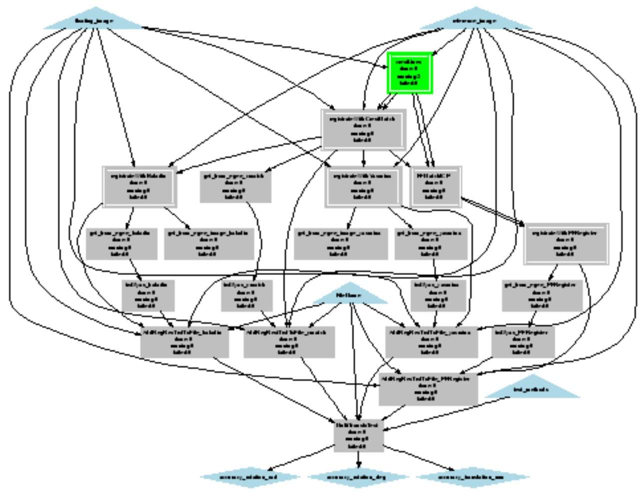






- **Characteristics**
  - Rapid response: a human waiting for the result!
  - Many small but CPU-intensive tasks
  - User is not aware of “grid”!
- **Needs**
  - Interfacing (data & computing) with non-grid application or portal
  - User and rights management between front-end and grid

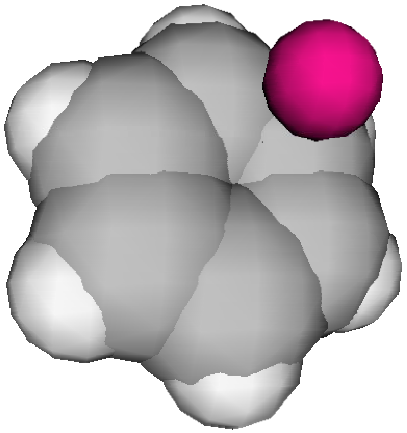
Workflow



- **Examples**
  - “Bronze Standard”: image registration
  - Flood prediction

- **Characteristics**
  - Use of grid and non-grid services
  - Complex set of algorithms for the analysis
  - Complex dependencies between individual tasks
- **Needs**
  - Tools for managing the workflow itself
  - Standard interfaces for services (I.e. web-services)

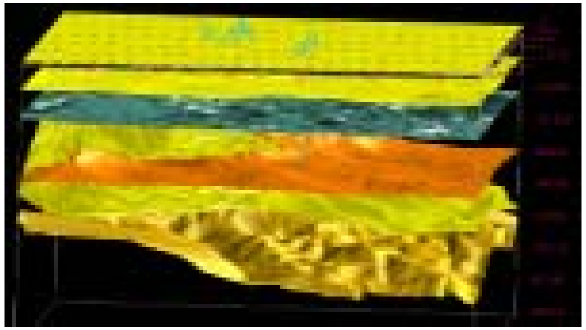
Parallel Jobs



- **Examples**
  - Climate modeling
  - Earthquake analysis
  - Computational chemistry
- **Characteristics**
  - Many interdependent, communicating tasks
  - Many CPUs needed simultaneously
  - Use of MPI libraries
- **Needs**
  - Configuration of resources for flexible use of MPI
  - Pre-installation of optimized MPI libraries

Legacy Applications

- **Examples**
  - Commercial or closed source binaries
  - Geocluster: geophysical analysis software
  - FlexX: molecular docking software
  - Matlab, Mathematics, …



- **Characteristics**
  - Licenses: control access to software on the grid
  - No recompilation ⇒ no direct use of grid APIs!
- **Needs**
  - License server and grid deployment model
  - Transparent access to data on the grid

Universal Needs

- **Security**
  - Ability to control access to services and to data
    - Fine-grained access control lists
    - Encryption & logging for more demanding disciplines
    - Access control consistently implemented over all services
- **VO Management**
  - Management of users, groups, and roles
  - Changing the priority of jobs for different users, groups, roles
  - Quota management for users, groups, roles
  - Definition and access to special resources
    - Application-level services
    - Responsive queues (guaranteed, low-latency execution)

Grid Middleware

- **Services exist for many of the application needs and plans exist to fix existing deficiencies or holes.**

- **No longer "one-size-fits-all" world:**
  - Works for low-level services (CPU, storage).
  - Higher-level services imply trade-offs:
    - E.g. latency vs. bulk response of meta-schedulers
    - E.g. security vs. speed for data access
  - Commonalities allow "one-size-fits-many" solutions.
- **Future evolution:**
  - Standards more important than ever: plug-and-play services.
  - Diversification of higher-level services is healthy and inevitable.
  - Integration of third-party tools an absolute necessity.

Summary

- **Observe routine and large-scale use of the EGEE infrastructure by numerous, diverse set of users.**
- **EGEE provides backbone services which support wide range of different grid application families.**
  - Simulation, Bulk Processing, Responsive Apps., Workflow, Parallel Jobs, Legacy Applications
- **Third-party tools are becoming increasingly important for providing specialized (but flexible) services to particular groups of applications.**

Participation

- **Related projects:**
  - DEGREE
  - DILIGENT
  - EGRID
  - EU ChinaGRID
  - EU MedGRID
  - GRIDCC
  - many more…
- **Other collaborations:**
  - Geant4
  - ITU
  - ProActive
  - many more…

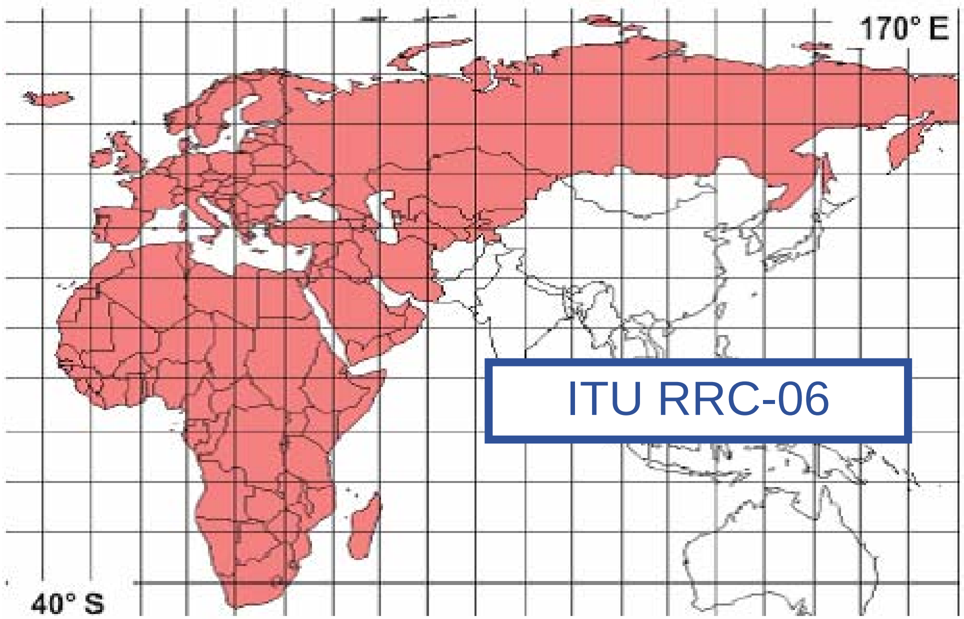


Figure 1
The extent of the planning area for the RRC-06

Participate

- **EGEE Conferences and Users' Forums**
  - Share your expertise, learn from other users.
  - Be open to collaboration with others.

- **Do (or don't) like something, speak up!**
  - VO issues, needs ⇒ VO Managers' Group
  - Resource, proc. problems ⇒ Operations Advisory Group (OAG)
  - Talk with NA4 steering committee
- **Report problems:**
  - Don't be afraid to use GGUS.
  - Report middleware annoyances ⇒ someone else is annoyed too!

- **NA4 website (http://egeena4.lal.in2p3.fr/)**