Enabling Grids for E-science in Europe

All Activities Meeting
September 13, 2004

LCG2 compliant Biomedical Applications

Johan Montagnat

Biomedical applications

Enabling Grids for E-science in Europe

- Applications description page
  - http://egee-na4.ct.infn.it/biomed/applications.html
- Three types of application
  - **Pilots**: LCG2 compliant applications at day 0
  - **Internal**: from project partners, to be deployed on EGEE
  - **External**: from other projects, to go through a selection procedure
- Applications available today
  - **Pilots**: GATE, GPS@, CDSS
  - **Internal**: SiMRI3D, PTM3D, xmipp_MLrefine
  - **External**: Mammogrid

GATE

- Contact
  - Lydia Maigne, maigne@clermont.in2p3.fr
- Description
  - Monte Carlo simulation for radiotherapy planning
  - Demonstrated for the 3rd EDG review
- Deployment and status
  - Installed at CC-IN2P3
  - GENIUS interface
- Users
  - developers only
  - sets of 5 to 10 jobs, 4 minutes each, for testing
- Plans
  - to install on LPC (Clermont-Ferrand) and CNB (Madrid) clusters
  - larger scale tests when deployed on more nodes available
- Problems
  - too long waiting time (up to 30 minutes) for short jobs

GPS@

- Contact
  - Christophe Blanchet, christophe.blanchet@ibcp.fr
- Description
  - Web portal for bioinformatics
- Deployment and status
  - NPSA is a production web portal hosting proteins databases and algorithms
  - GPS@ is the grid version under development deployed on LCG2
- Users
  - NPSA serves hundreds of bioinformaticians daily (about 3000 jobs/day) but limited resources (4 CPUs)
- Plans
  - to replace NPSA with GPS@ when showing similar robustness
- Problems
  - too long waiting time for short jobs
  - no service certificate for the portal
  - no RLS service for data management

CDSS

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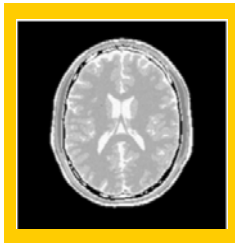
- Contact
  - Ignacio Blanquer, iblanque@dsic.upv.es
- Description
  - Clinical Decision Support System: expert system for medicine
- Deployment and status
  - Original developed under serviced-based approach, now ported to LCG2
- Users
  - About 10 medical users from 5 organizations
  - About 10 runs per day (1 hour each)
- Plans
  - Migrate from current in-site LCG2 installation to EGEE infrastructure
  - Enlarge the user community when more resources become accesible
- Problems
  - None reported



SiMRI3D

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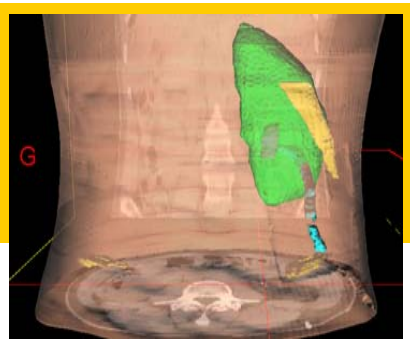
- Contact
  - Fabrice Bellet, fabrice.bellet@creatis.insa-lyon.fr
- Description
  - Magnetic Resonance Images parallel simulator
- Deployment and status
  - MPI simulator implemented
  - Some performance study lead on local cluster
  - Tests on CINES supercomputers
- Users
  - Developers (5 users)
  - 1000 to 2000 jobs this year, minutes to weeks per job
- Plans
  - Very large potential community
  - To open the simulator as soon as gridification is achieved
- Problems
  - No MPI-enabled resources available on EGEE infrastructure



gPTM3D

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- Contact
  - Cécile Germain-Renaud, germain@lal.in2p3.fr
- Description
  - Radiological data interactive segmentation and analysis
- Deployment and status
  - Application ported to LCG2 on top of the interactive job submission service
  - Deployed on Orsay resources
- Users
  - Developers
  - Potential medical users
- Problems
  - Interactivity made difficult due to bypass-based communication performance limitations

xmipp_MLrefine

- Contact
  - Angel Merino, AJ.Merino@cnb.uam.es
- Description
  - Macromolecular 3D structure analysis
- Deployment and status
  - Recently ported to LCG2 and tested both on Clermont and Madrid clusters
- Users
  - Developers
  - One experiment corresponds to about 500 jobs and one week of computations on Madrid site
- Plans
  - To shorten experiments time by using more resources
- Problems
  - Resource shortage

Show stoppers and planning

- Limitations induced by infrastructure
  - Limited VO acceptance (CNAF RB)
  - No RLS service for biomedical VO
    - CC-IN2P3 proposal to host the service, under study in September
    - INFN proposal to temporarily set up a RLS service meanwhile
  - No MPI-enabled resources available for parallel applications
    - INFN reported that an MPI-enabled cluster exists on INFN-Grid
  - Lack of service redundancies
    - High sensitivity to CNAF RB health
- Future plans
  - to focus more on applications and less on infrastructure deployment
  - to set up a communication channels
    - to notify users of SA1 maintainance operations and problems
    - to provide feedback to SA1 on problems encountered
  - to set up a new community integration procedure with SA1 including:
    - VO creation
    - RB registration
    - RLS provision