eGee

NA4 Biomed Applications

Athens meeting, April 20, 2005

Johan Montagnat

www.eu-egee.org

Information Society

14:30 Biomed status (J. Montagnat)

15:00 Deploying a workflow on EGEE (T. Glatard)

15:20 P-GRADE portal to support workflow-oriented grid applications (P. Kacsuk)

15:40 GEANT4 tool for biomedical applications (P. Mendez Lorenzo)

16:00 Break

16:30 Applications report (applications developers)

17:00 gLite testing coordination

17:10 User support management

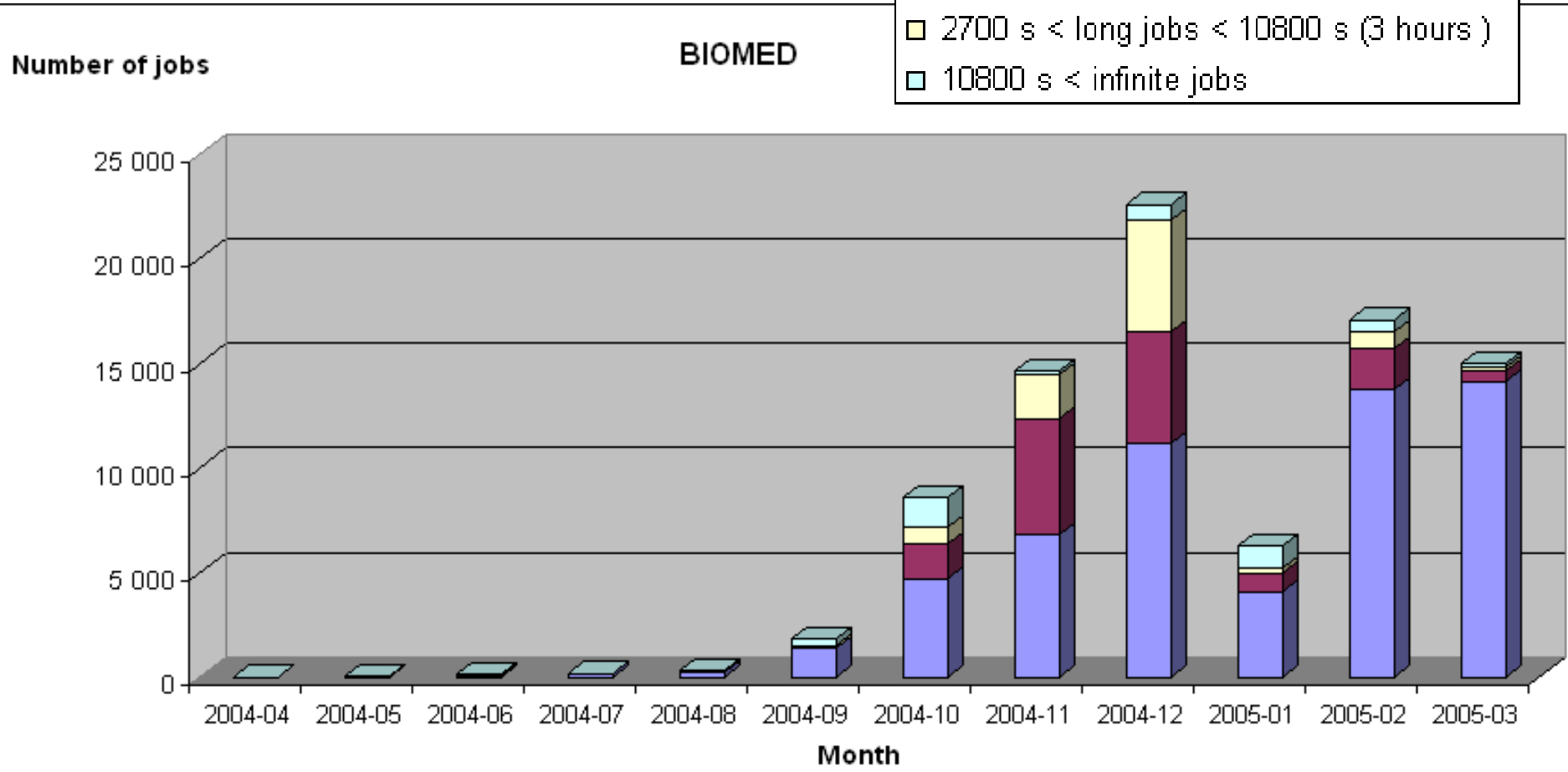**17:20 VOMS deployment status (Y. Legré, I. Blanquer)**

17:35 gLite data management testing (C. Pera, A. Llorens)

17:50 Conclusions and AoB

- **GATE:** Geant4 Application for Tomographic Emission (LPC)
- **Docking platform for tropical diseases:** grid-enabled docking platform for in sillico drug discovery (LPC)
- **CDSS:** Clinical Decision Support System (UPV)
- **GPS@:** Grid genomic web portal (IBCP)
- **SiMRI 3D:** Magnetic Resonance Image simulator (CREATIS)
- **gPTM 3D:** Interactive radiological image visualization and processing tool (LRI)
- **xmipp_ML_refine:** Macromolecular 3D structure analysis (CNB)
- **xmipp_multiple_CTFs :** Electronmicroscopic images CTF calculation (CNB)
- **GridGRAMM:** Molecular Docking web (CNB)
- **GROCK:** Mass screenings of molecular interaction (CNB
- **Mammogrid:** Mammograms analysis (EU project)
- **SPLATCHE:** Genome evolution modeling (U. Berne/WHO)

- **SPLATCHE**
  - first application being migrated from GILDA to biomed VO
- **Pharmacokinetics in MRI (UPV)**
  - MRI registration for contrast agent diffusion study
- **Some progress on biological sequences analysis (M. Lexa)**
- **...**

- **JRA2 statistics**
  - ~15Kjobs per month

BIOMED

Legend:
- short jobs < 300 secondes (5 min)
- 300 s < medium jobs < 2700 s (45 min)
- 2700 s < long jobs < 10800 s (3 hours)
- 10800 s < infinite jobs
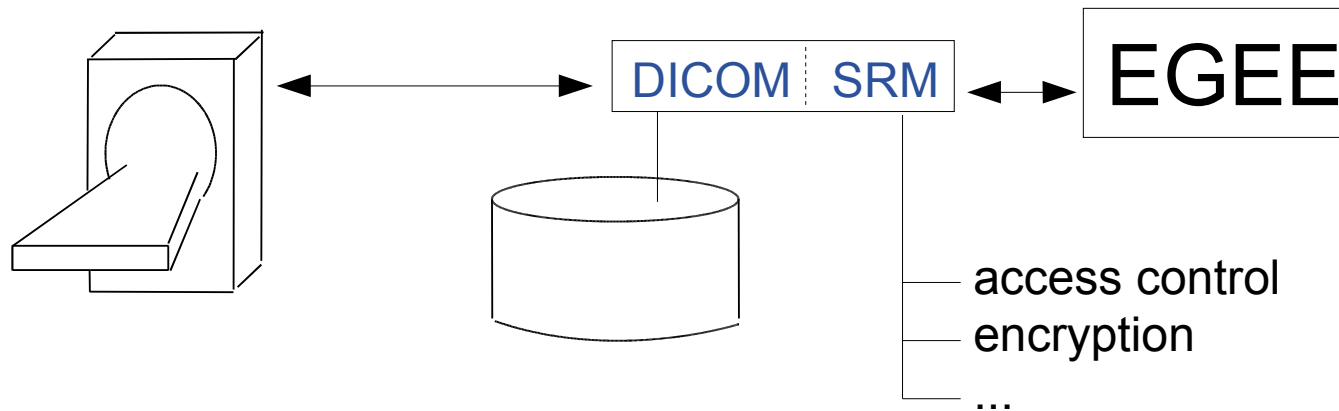
Number of jobs

Month

- **Focus on demonstration of grid interest for applications**
  - Contact taken with the decrypthon project
  - Nicolas Jacq proposal for a data challenge organisation
  - **Focus on scientific content of applications**

- **A data challenge in biomed this summer**

	Done		Challenge
Number of targets **Number of drug candidates**	1 10^5	1 10^6	5 $3.3\ 10^6$
Total CPU time **Gain of time**	188 days 149	5 years? ?	80 years? ?

- **Need for input for response to EU review**
  - JRA2 statistics
  - Application gains

- **gLite**
  - Lot of testing activity inside biomed
  - Release 1.0 available
  - pre-production service expected to bring much more robustness
- **Tutorial from ARDA experts**
  - to be organized end of May
  - in Lyon?
  - in conjunction with next biomed meeting?
- **Non-application specific work initiated in the biomed activity**
  - Workflows
  - DICOM-SRM interface

- **Direct Grid access to medical servers**

- **Developed at LAL (Daniel Jouvenot, Cal Loomis...)**

- **DICOM/SRM interface**
  - prototype including basic functionalities being finalized
  - on top of existing SRM implementation (dCache)/DCMTK (DICOM Toolkit)
  - Many functionalities still to be implemented

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- **gLite testing activities within biomed**
  - gLite installation:
    - VOMS (Yannick)
    - Most services (Ignacio)
  - gLite usage:
    - Generic testing (Adelyne)
    - Data (Antoine) and metadata (Christophe P.) management
  - application porting
    - CDSS (Ignacio)
- **...and beyond (see Tuesday's talk from Massimo)**
  - ARDA (ARDA workshops as a source of information)
  - NA4 test team
  - JRA1 and SA1 testing
  - ...
- **Pre-production service announced (in early may?)**

- **Checklist**
  - documentation known by testers
    - lot of documentation released recently -> **Comments welcome!**
    - may be scattered
  - other testing activities known
    - refer to Massimo's talk
  - features to test understood
  - efficient testing procedure
    - I need feedback
    - Testing may involve periodical checks, etc
  - feedback channels known

- **Future of biomed testing**
  - new functionalities, specific services
  - scale and performance testing
  - from testing to application porting
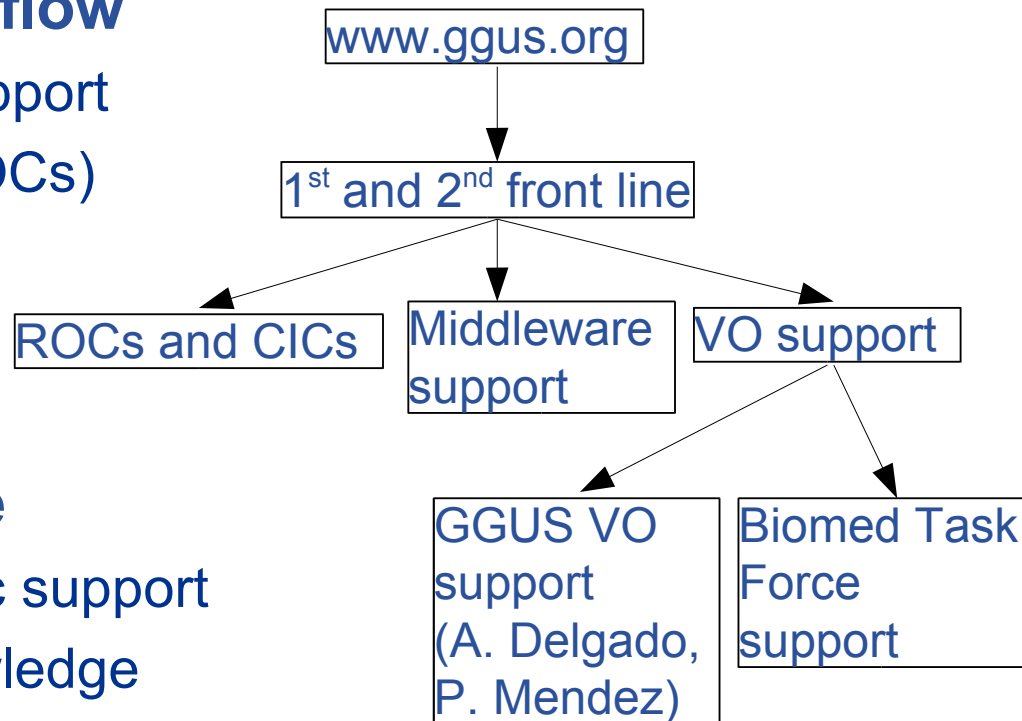
- **Experts and GGUS ticket flow**
  - First and second line of support
  - Site problems (CIC and ROCs)
  - Generic problems
  - VO support
  - Middleware developers
- **Role of biomed task force**
  - Provide application-specific support
  - Participate to the grid knowledge acquisition of biomed users
- **Current organization**
  - Tickets sent to technical team mailing list and assigned to 'biomed VO'
  - Christophe Pera to assign messages to experts
  - Use the GGUS portal to follow on tickets

www.ggus.org

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1st and 2nd front line

ROCs and CICs   Middleware support   VO support

GGUS VO support (A. Delgado, P. Mendez)   Biomed Task Force support

- **We have to learn**
  - Biomed experts to register as 'ticket administrators' and learn the GGUS ticket management tool
  - Christophe to identify the correct targets
  - People to whom tickets are assigned to should be reactive
  - Need for a rollback procedure (expect redirection errors at least in the first phasis)
  - Need to check that all tickets are followed on

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- **Catch up with the growing rate of the biomedical community**
  - Organise gLite knowledge acquisition and testing
  - Organise biomed user support
- **Focus on scientific results and demonstration of the benefit of the grid**
  - Need for quantitative numbers on biomed applications activity (**this week**!)
- **Important milestones**
  - data challenge
  - gLite migrations
- **gLite tutorial to be organised in may**
- **Aob?**