Experience and plans using gLite (Biomed)

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Contents

- **The Biomed Applications**
- **Requirements and Needs from the Biomed Applications**
- **Experience in the Use of gLite**
  - Installation
  - Security
  - Job Submission
  - Data Access
  - Programming and Documentation
- **Usage of the gLite-Based Infrastructure**
- **Development Plans**
  - CDSS
  - Other
- **Conclusions**

The Biomed in EGEE and Interest on the Grid.

- **gps@: Grid Protein Sequence Analysis.**
  - High-Throughput Computing of Short Jobs Through a Web Portal.
- **CDSS: Clinical Decision Support System.**
  - Resource Discovering and High-Throughput Computing of Short Jobs Through Web Services.
- **GATE: Geant4 Application for Tomography Emission.**
  - High-Performance / High-Throughput Computing.
- **gPTM3D: Medical Imaging on the Grid.**
  - High Performance Computing in Interactive Time.
- **GridGRAMM and GROCK : Molecular Docking**
  - High-Throughput Computing.
- **xmipp_ml_multirefine: Molecular Imaging**
  - High-Throughput Computing of Medium/Large Jobs.

Requirements and Needs from the Biomed Applications

- User interface installation and portability
- User Interface configuration
- Application Programming Interface
- Group/anonymous login (portals)
- Parallel jobs execution
- Short jobs execution
- Prioritised jobs execution
- Multiple data jobs
- Compound jobs execution (pipelining)
- Interactive jobs
- Job access to data
- Simple job submission
- Job execution control
- Job killing
- Resources reservation
- Scalability
- File names translation
- File access interface
- Fine grain control of access rights
- Group of files
- Metadata associated to files
- Access rights delegation
- Data updates and versioning
- File name changes
- Data replication control
- Data registration, retrieval, and deletion
- Data access cost estimation
- Partial file access
- File browsing
- Scalability
- Jobs information and status notification
- Top level information system index
- Resource brokers index
- Grid resource browsing
- On-disk encryption
- Interface to new storage systems
- Hook on data privacy manager
- Communications encryption
- Outbound connectivity
- Guaranteed and configurable bandwidth
- VO creation
- User control
- User login
- Software package publication
- Robustness
- Multiple VOs registration
- NA4 Metrics and QoS
- NA4 Metrics requirement - Abort codes classification and recording
- NA4 Metrics: Network usage
- Licensed software management
- JRA2 - Job statistics

Experience in the Use of gLite

- Installation
- Security
- Job Submission
- Data Access
- Programming and Documentation

Installation

- **The Autonomous Installation of Current Prototype is Complex.**
  - Lack of Documentation.
  - Many Requirements.
    - ant-contrib, ares, axis, bbftp, bcprov-jdk14, boost, cgsi-gsoap, checkstyle, classads, clover, commons-cli, commons-collection, commons-dbcp, commons-logging, commons-pool, condor, cpanplus, cpptasks, cppunit, cyrus_sasl, db, edg-java-security, egee-ant-ext, expat, globus, gridsite, gsoap, hsqldb, jabberd, jalopy, javacc, jclassads, jglobus, jug, junit, libiconv, libidn, log4cpp, log4j, mm-mysql, mockdoclet, mockobjects, myproxy, mysql, openldap, oracle-jdbc, oracle-sqlj, perl, pyanttasks, pyxml, swig, texdoclet, tomcat, util-concurrent, wsdl4j, wsi-test-tools, xalan-c, xdoclet, xerces2-j, xerces-c.
- **Requirements Makes the Selection of the Basic Operative System Difficult, Although Multiplatform is Forecasted (Even Ms-Windows).**
  - When Will This be Supported?
- **Low Requirements on the Worker Node is Really a Good New.**
- **R0001, R0002 Requirements**
  - User interface installation and portability.
  - User Interface configuration.

Security

- **Security on the Users**
  - Is Spanish CA Certificate Updated?
  - Integration of Certificates with Web Browser Certificates.
    - Applications Through Web browsers must be used to Deal with the Problems of Operative System and User-Friendliness.
    - Automatic Usage of Web Browser Certificates will be a Very Effective way to Create proxys.
    - It will Skip the Requirement of Creating Longer-Term proxies Through MyProxy or Similar Approaches.
    - It will Reduce the Need of Having Portal-Based Certificates (Although it will still be Important for Large User Groups Occasionally using the Grid).

Security

- **Security on the Storage of the Data**
  - Data Results are Visible by All Users in a VO.
  - Access Control Lists ACL at Which Level (group, user, file, directory)?
    - Fine Control of Access Rights is R0019.
  - VO Management.
  - Data Encrypted Storage (R0035, On Disk Encryption) Mentioned in the Design.
- **Group/anonymous login:**
  - R0004 Requirements Web-portal Certification. Already Solved with the Open Possibility in EGEE.

Job Submission

- **Random Execution Time.**
  - The Time Consumed in Each Stage of the Job is not the Same Even if the Job, the Target Computer and the Workload are the Same (Big Difference).
  - Latency in Submission seems to be Very Long.
  - Would it be much Different in Production?
- **Random Output Retrieval Time.**
  - From Job Termination Until the Availability of the Output Files (stderr, stdout and Other Files) there is an Arbitrary Long Waiting Time.
- **Split**
  - Very Interesting Attribute.
  - Examples for the Different Type of “split” Behaviours (file, directory, event, userdefined) will be Important.
  - Split on only several arguments (not all) would be desirable.
- **Input Files and Executable Must be on the Same Directory.**
  - Otherwise, Although gLite Does not Generally Issue Any Error, Processes Remain Indefinitely in the Started stag.

Job Submission

- Although the Execution was Correct, a CONDOR error Appears at the End of the Process Sometimes.

001 1095160093 [state]: Job 4636 inserted from iblanquer@lxplus018.cern.ch

002 1095160126 [state]: Job state transition from INSERTING to WAITING

003 1095160130 [state]: Job state transition to QUEUED |=| procinfotime: 1095160130 site: EGEE::CERN::CONDOR

004 1095160155 [state]: Job state transition to STARTED |=| procinfotime: 1095160155 site: EGEE::CERN::CONDOR started: 1095160155 node: lxb1435.cern.ch

005 1095160164 [state]: Job state transition from STARTED to RUNNING |=| procinfotime: 1095160164 site: EGEE::CERN::CONDOR started: 1095160164 spyurl: lxb1435.cern.ch:8087 node: lxb1435.cern.ch

006 1095160164 [state]: Job state transition from RUNNING to SAVING |=| procinfotime: 1095160164 site: EGEE::CERN::CONDOR

007 1095160239 [state]: Job state transition to DONE |=| procinfotime: 1095160239 site: EGEE::CERN::CONDOR error: spyurl: finished: 1095160239

Requirements Stated

- **Short Jobs Execution (R0006)**
  - Could it be solved Directly Configuring Dedicated Resources in Short-Job Queues?
- **Prioritised (R0007) and Interactive (R0010) Jobs.**
- **Parallel Computing Jobs (R0005) .**
  - Is it Supported in gLite?
- **Licensed Software Management (R0051).**
  - Use of R-GMA.

Data Access

- **Several Stability Problems**
  - Registration Failed Several Times.
  - Registration through an URL was Much More Stable. Very Interesting Feature to Ease External Storage (R0036 - Interface to new storage systems).
  - Unpredictable Response Time.
- **Problems with the Replicas**
  - Can the Precise Replica (Resource) be Specified in the get Command?
- **Syntax**
  - 'lcg-' commands have a different syntax for specifying local files than in gLite (gLite uses one additional '\' after the ':').
- **Metadata Cataloguing**
  - Good According to the Requirements of Biomed.
- **Requirements**
  - R0023 (Data Updates and Versioning)
  - R0028 (Partial File Access)
  - R0037 (Hook on data privacy manager)

Programming and Documentation

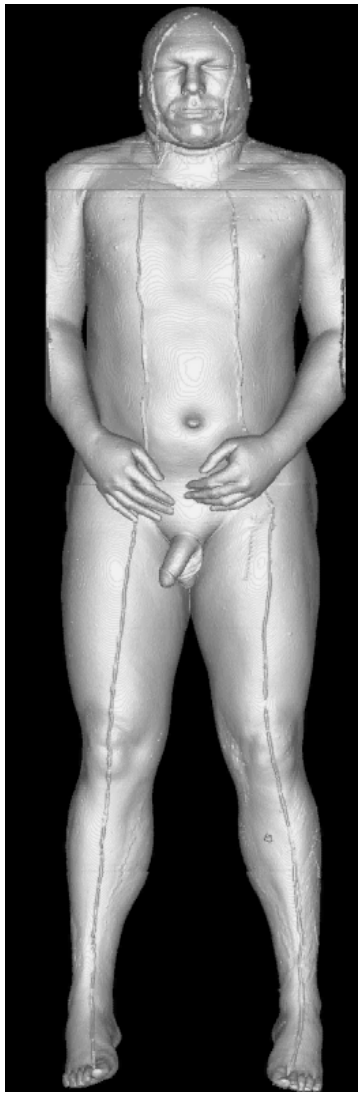
- **APIs**
  - Need for Programmable (non CLI-based) Interface (R0003, Application Programming Interface).
  - When Will it be Released and Documented?
- **Problems Clearly Being Faced**
  - Lack of Updated Documentation.
  - Lack of Contact Points for Support.
  - Documentation has Broken Links (Section c of JDL syntax).
    - There is a Link on Further Information on “packages” Which Does Not Exist.
    - In the Split Section There is a Link That Does Not Exist.
- **Problems Regarding Usability**
  - Scripts Must be Executed From Outside of the gLite Console.
  - No Editing Facilities within the gLite Console.
  - Monitoring Tools will be Welcome.

Usage of the gLite-Based Infrastructure

- **No Personal Installation.**
  - UPV
    - Usage of CERN's lxplus UI.
    - Runs of up to 10 simultaneous jobs.
    - Data Storage Usage of about 10 Megabytes.
    - About one hundred executions for testing.
  - CNRS
    - Usage of CERN's lxplus UI.
    - Small Tests for Training and Got Used.
    - Starting defining tests to validate the quality of the system.
  - OTHERS
    - MAMMOGRID migrated the prototype P1 from Alien to gLite.

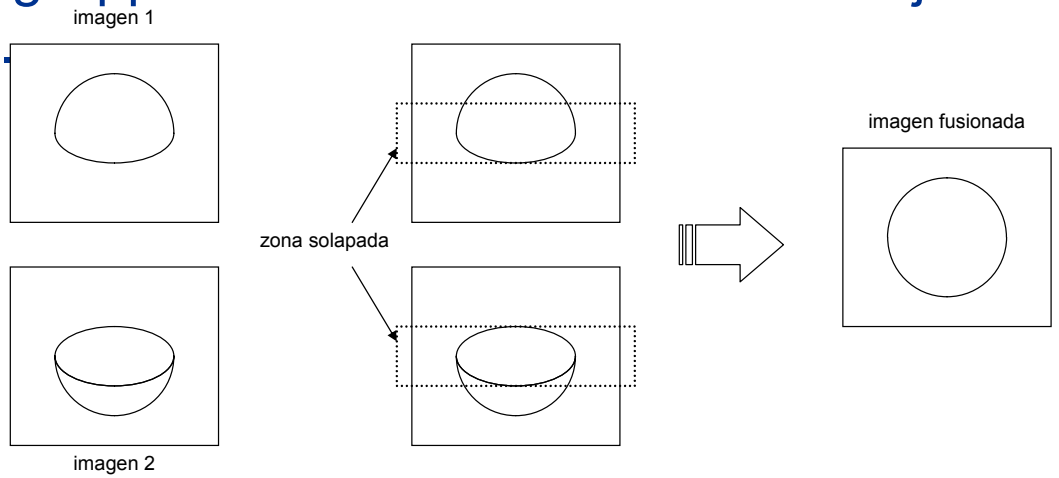
Application Tested

- **Migration of a LCG-2 Application for Volume Rendering on the gLITE Environment.**
  - Volume Rendering of Large Datasets (The Visible Human Project, 512x512x1500x2 bytes).
  - Aimed at Sharing Computing and Memory Resources.
  - Sequential Version Cannot be Executed in a Single Standard Computer due to the High Need of RAM (About 4Gbytes).
  - It Generates Videos with a Rotation Around any Axis.
  - No clear community behind the test: Relevant for IT and Medical Training



Architecture

- **The Volumetric Projection is Divided into Blocks which are Submitted as Individual Jobs.**
  - It Reduces the Memory Requirements.
  - It Implements an Intrinsic Parallelism.
- **The Grid Application is Divided into Two Parts.**
  - A Control Application Splits the Volume, and Retrieves and Postprocesses the Results.
  - A Computing Application that Processes the Projection of Each Subvolume.



Migration to gLite

- **A Shell Script Executes Individual gLite Commands.**
- **Steps**
  - Splits the Volume Into ‘n’ Parts.
  - Register the Data Files in gLITE.
  - Creates a JDL file with the Appropriate Input for Each Part.
  - Submits each JDL.
  - Waits for the Completion of All Tasks (Polling the Output Directory).
  - Creates a JDL for the Postprocessing.
  - Submits the Postprocessing Job.
  - Retrieves the Final Output (Bitmap Files Containing the Frames).

Development Plans

- **CDSS**
  - The Application was Originally Designed to work in a Service-Oriented Basis.
  - Batch-like LCG Services were Embedded on Services to Enable the use of EGEE in the Application.
  - Once gLite is Available, Direct Usage of the Web Services will be Performed.
  - Migration will Start As Stable Prototypes are Released.

Development Plans

- **Other Applications**
  - The UPV is Implementing on the frame of Other Collaboration a Virtual Workbench for Medical Image Processing.
    - Based on GT3 but Aiming at a Stable Web-Service Platform.
    - With the Collaboration of the Spanish Society for Medical Radiology.
    - Oriented to the Training of Novel Radiologists.
  - gPTM3D biomed Application is also Planning to Migrate to gLite.

Development Plans

- **MAMMOGRID**
  - Prototype P1.5 Architecture delivered and deployed
    - P1.5 already present in CERN, Oxford, Cambridge & Udine hospitals
    - 2004-2005 testing phase
    - Need feedback from clinicians
  - Deployment of P1.5 grid services
  - P2 Architecture under development
    - New services to provide
      - *enhanced security and confidentiality*
      - *further image and non-image handling services*
      - *enhanced query services*
    - MammoGrid Meta-Data Database
      - *to facilitate schema discovery*
    - EGEE/GLite prototype testing and adaptation

Conclusions

- **Expectancy is High on the Release of a Stable gLite Middleware.**
  - Improved Documentation
  - Predictable Response Time and Resource Consume.
  - Robustness (Especially on the Data Storage).
- **The Consideration of The Most Important Requirements of Biomed Applications in the Design of the Architecture is Very Positive.**
- **Improved Autonomous Installation is Very Important.**
- **Robustness is Low but it is Understandable since it is a Testbed.**
- **Production in Biomed will not be Produced until Applications are Migrated to gLite and the Infrastructure Provides a Degree of Reliability.**