

Geant4 simulations using grid computing



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- **I : Grid architecture, the EGEE project**
 - What is a grid?
 - European grid projects, the EGEE project
 - Applications
- **II : How to distribute simulations on the grid?**
 - Installing G4 on the grid
 - The pseudorandom number generator
 - **Fiability of the pseudorandom number generator (PRNG)**
 - **Split the simulations by using non overlapping random sequences**
- **III : Jobs submissions and datasets management**
 - Security and confidentiality
 - Data services on the grid
 - Jobs submission, how to?
 - Computing time tests
- **IV: Web portal interface**
 - Functionalities

I

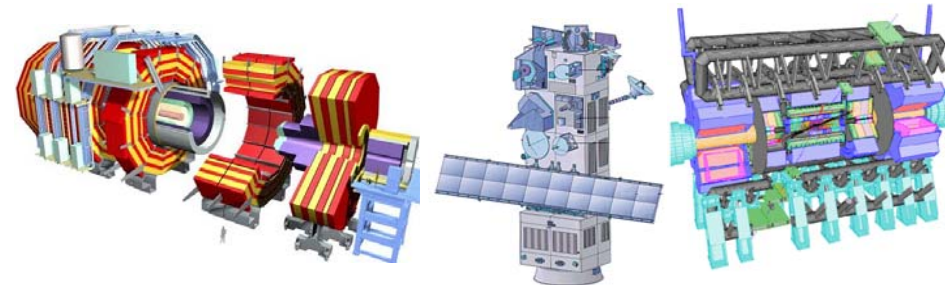
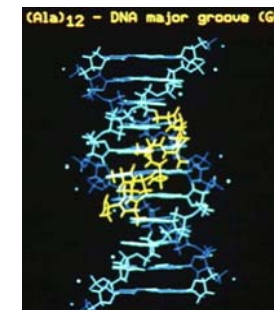
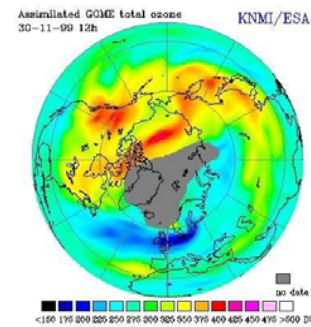
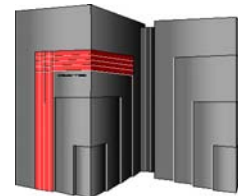
A grid architecture

I: Grid Vision

Plateforme de Calcul pour les Sciences du Vivant



Grid “Middleware”



I: Grid Vision

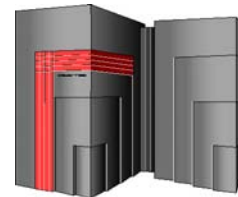
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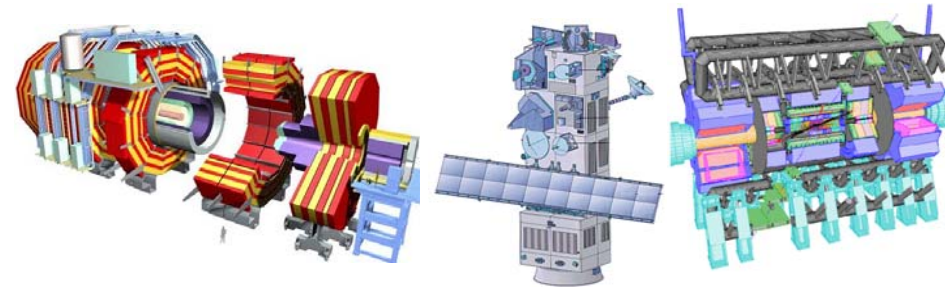
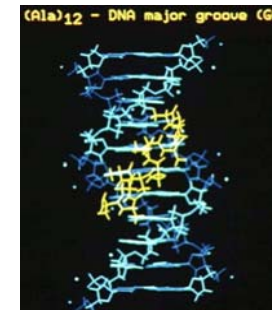
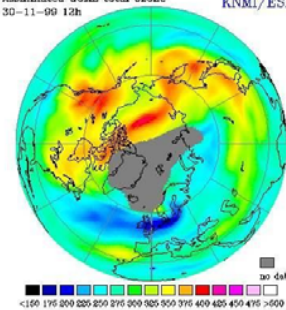
Grid technology allows scientists:

- access resources universally
- interact with colleagues
- analyse voluminous data
- share results

Grid “Middleware”

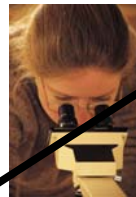


Assimilated GOME total ozone
30-11-99 12h KNMI/ESA



I: Grid Vision

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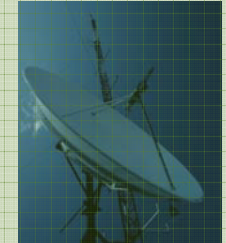
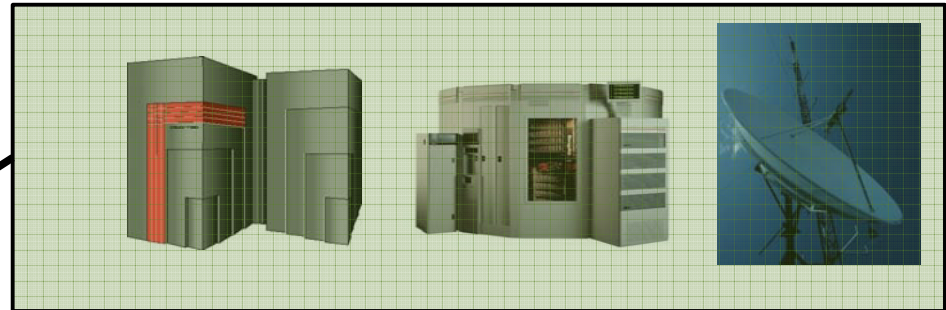
Incorporates traditional resources:

- raw compute power
- storage (disk, tape, ...)
- network connectivity

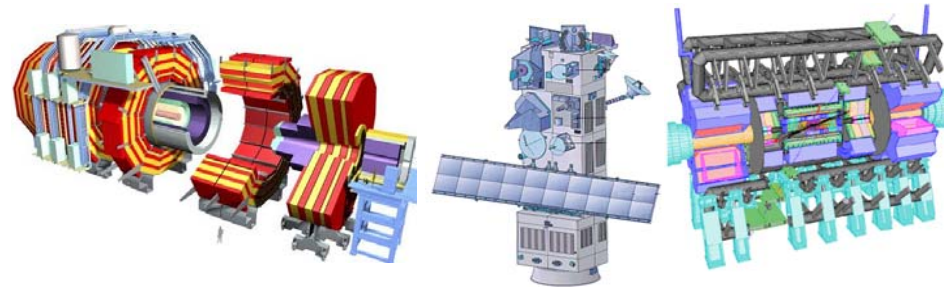
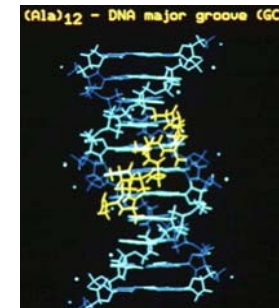
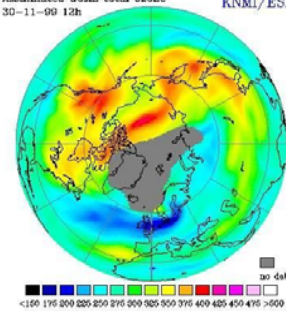
Resources are:

- heterogeneous
- dynamic

Grid “Middleware”



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I: Grid Vision

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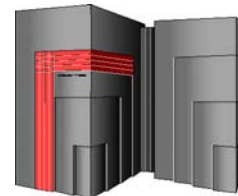


Detectors produce huge amounts of data for analysis.

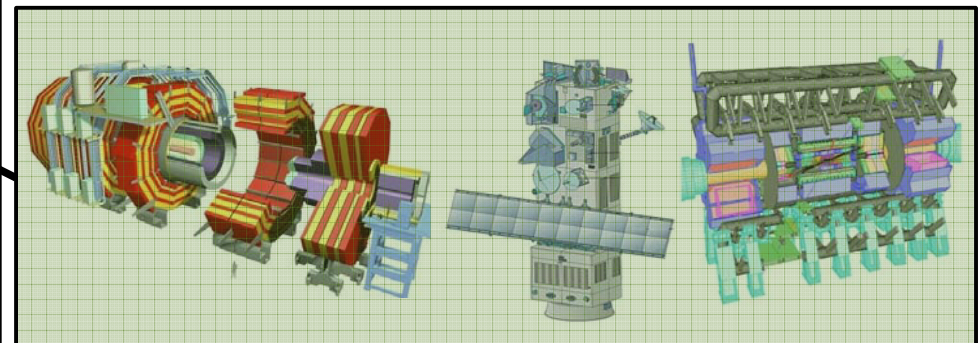
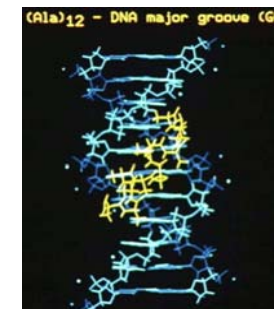
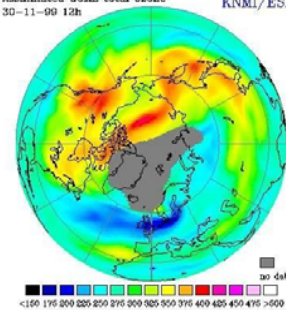
Non-traditional resources:

- **scientific instruments**
- **conferencing technologies**
 - video
 - audio
 - chat

Grid “Middleware”



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I: Grid Vision

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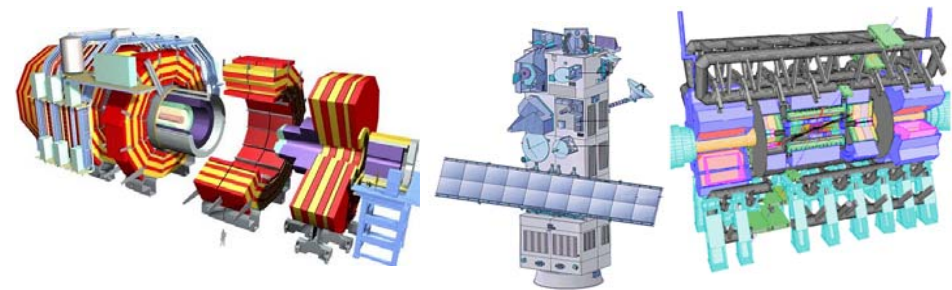
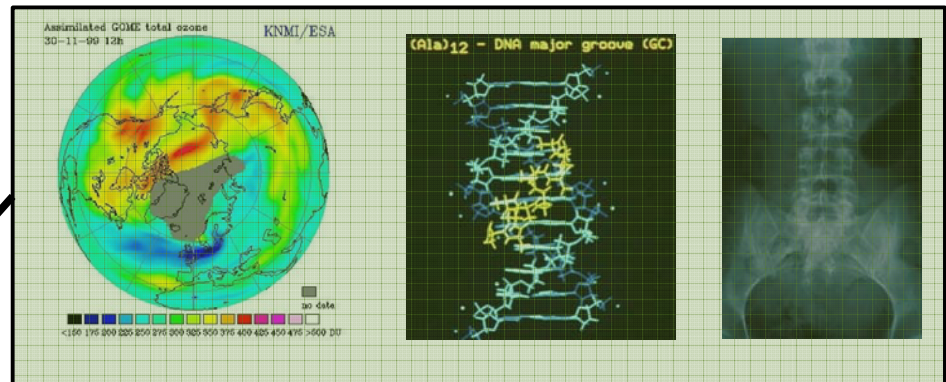
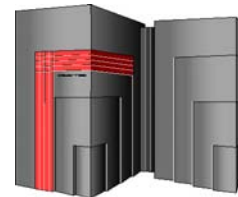
Access to data:

- data files and datasets
- databases
- replica metadata
- application metadata

Manage data:

- transfer and copy data
- locate relevant data

Grid “Middleware”

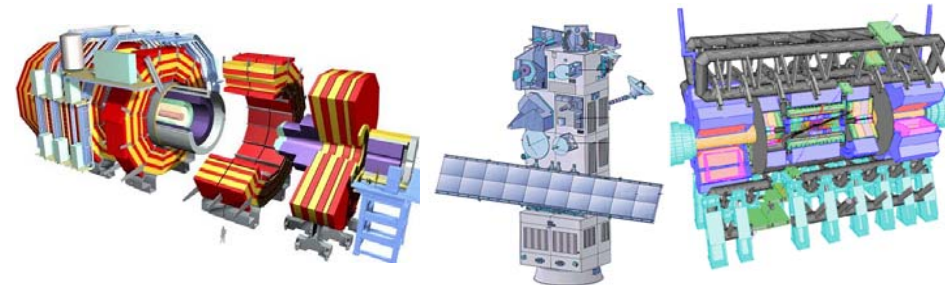
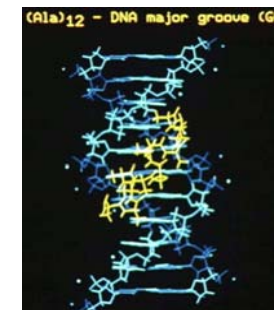
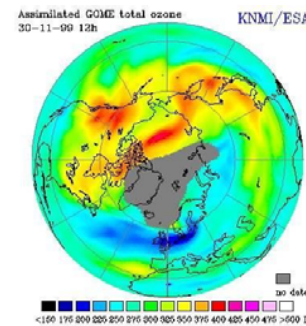
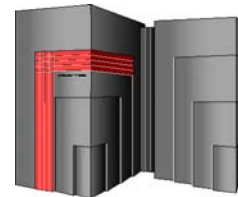




Services:

- high-level services to facilitate use of the grid
 - e.g. job brokering
- application-specific services
 - e.g. portals

Grid ‘Middleware’

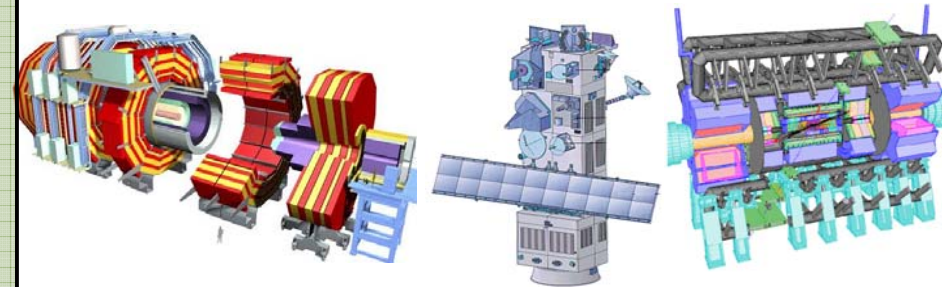
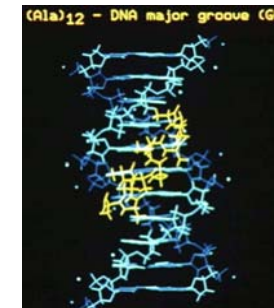
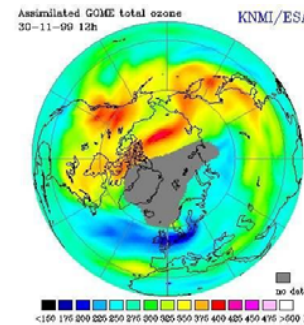
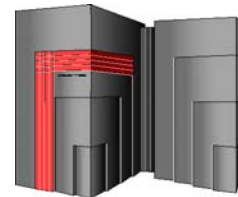




Grid “Middleware”

What is the grid?

- **Middleware:**
 - service interoperability
 - high-level services to ease use of grid
- **Resources:**
 - provided by participants
 - shared for efficient use



I: The EGEE project

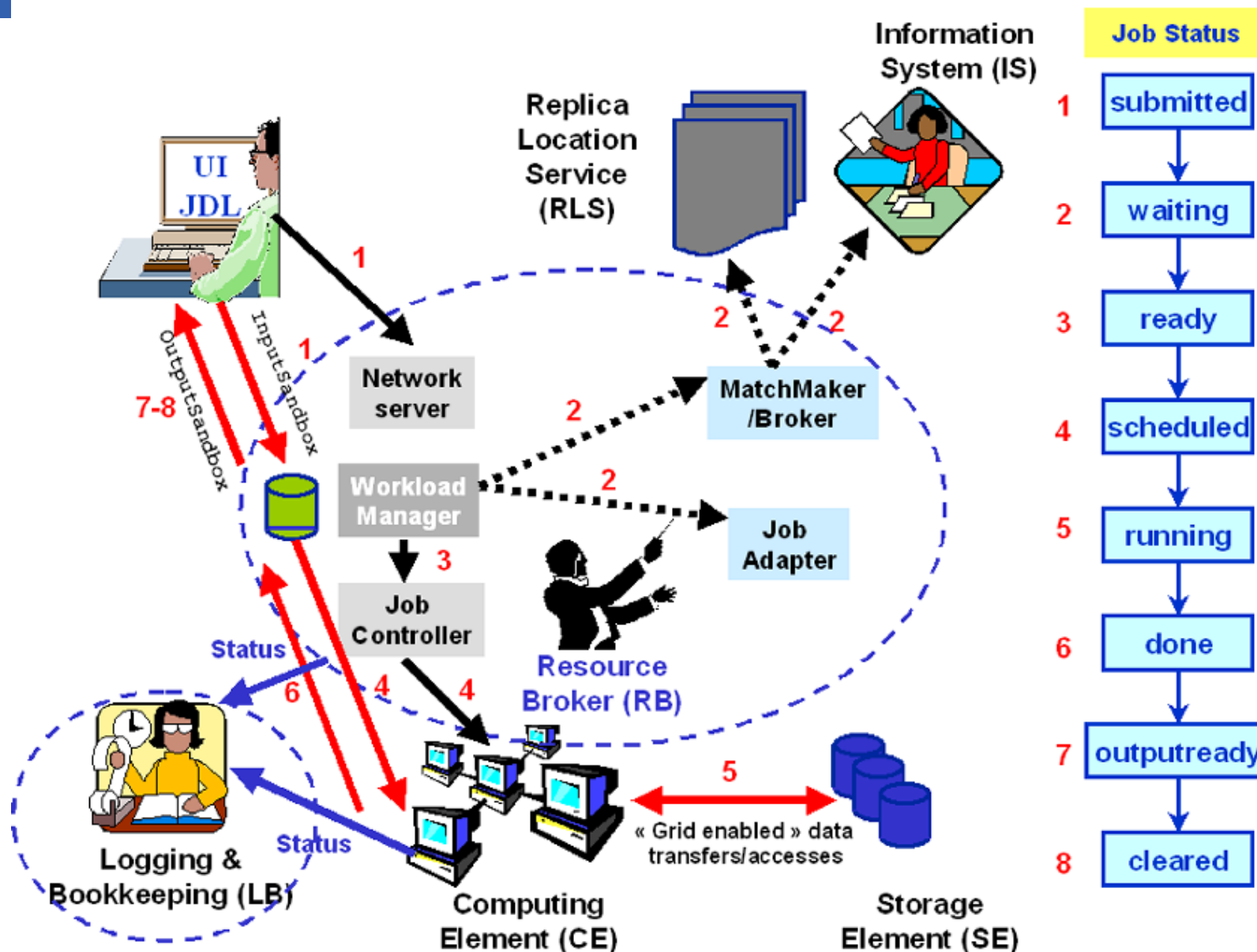
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- 4 years projects (April 2004-April 2008)
- 90 leading institutions in 32 countries, federated in regional Grids
- 32 M Euros EU funding (2004-5), O(100 M) total budget
- Aiming for a combined capacity of over 30'000 CPUs (one of the largest international Grid infrastructures ever assembled)
- 5 Petabytes of storage
- ~ 300 dedicated staff



I: What is a grid?



I: Some grid infrastructures...



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Regional grid in Auvergne:

AuverGrid

>800 CPU

8 nodes in

(Aurillac)

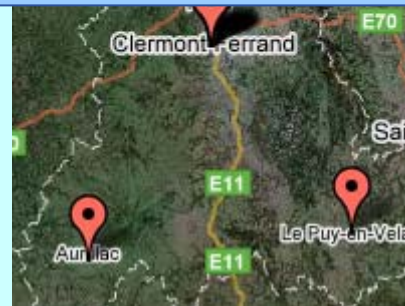


Open Science Grid

Resources partially accessible
through EGEE infrastructure



Grid of supercomputers
Middleware Unicore
5 sites: 190 Teraflops



I: Geographically distributed resources in EGEE

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Ressources biomédicales:
115 CEs dans 27 pays
~3000 CPUs
123 SEs. 21 TB disk
30 RBs

- **Bioinformatics:**

- WISDOM

- Speed up the research of drug discovery against malaria with the in silico docking approach

- **Medical imaging:**

- SiMRI3D

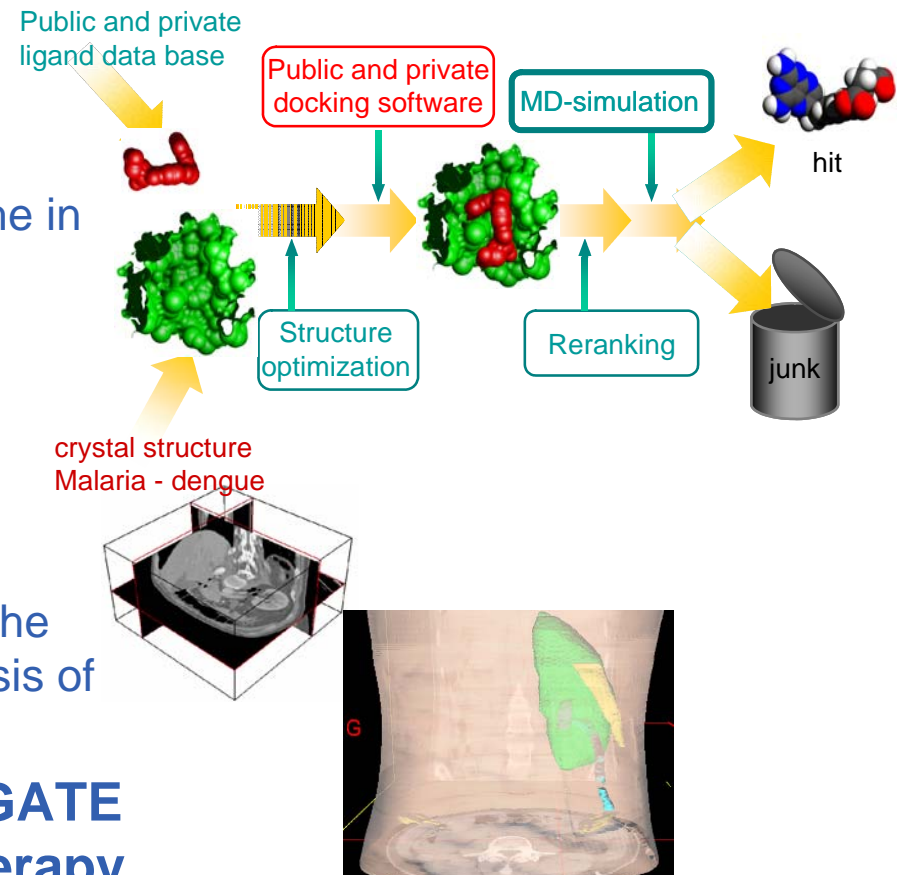
- Simulation of 3D MRI images

- gPTM3D

- Help to diagnostic of cancer by the collection, production and analysis of 3D images of organs

- **Monte Carlo simulations using GATE for nuclear imaging and radiotherapy**

- Computing time reduction
 - Utilization of medical images (scans) for voxelized fantoms in simulations



II

Distribute simulations on the grid The PRNG

II: Installing G4 software

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- **RPMs installation**
 - Build rpms for each installation if necessary for:
 - The G4 software
 - The CLHEP software, needed for the generation of pseudorandom numbers in the
 - The data analysis softwares such as ROOT, AIDA, etc...
- **Register installation packages (rpms) on grid SE**
- **Send an installation job as « super user » biosgm on each biomed site**
- **Install job goal:**
 - Copy installation packages from SE to CE in the VO_BIOMED_SW_DIR path
 - Install packages
 - Test the installation
- **Update of the environment variable**
 - Example for GATE installation: VO-biomed-GATE-3.0.0

II: Pseudorandom number generator (PRNG)

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- We choose to work with **F.James' algorithm**:
 - HEPJamesRandom in CLHEP libraries
 - Very long period: 2^{144}
 - Creation of 900 millions of sub-sequences having a length of $\sim 10^{30}$
 - Combination of a Fibonacci sequence and an arithmetic sequence
 - Fibonacci sequence:
 - Each number is equal to the sum of the 2 previous numbers
 - Improvement: Each number is the result of an arithmetic or logical operation between 2 numbers drew earlier in the sequence..

$$s_i = \left(s_{i-p} \quad s_{i-q} \right) \bmod m$$

- Pseudorandom number sequences are generated depending of the initialization of the PRNG.
 - => Each simulation must use a non correlated pseudorandom numbers.

II: Using a PRNG in G4 simulation

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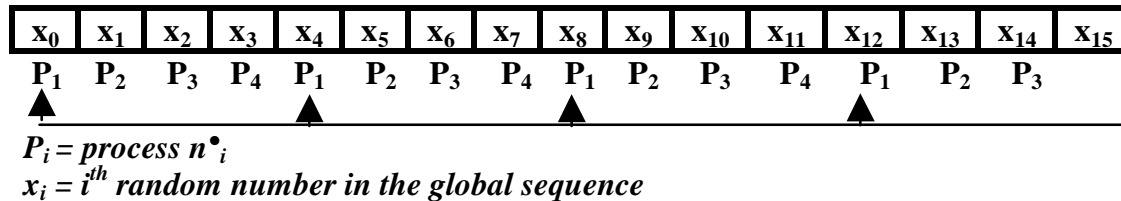
- 1) Set up of an internal table, containing a large number of seeds (~between 10 and a few hundreds), and the values of a few indices (typically two, i and j) pointing to seeds in the table, are also initialized.
 - 2) The generation of pseudorandom number by combining only those seeds corresponding to the current values of the indices.
 - 3) The update of the seeds just used and the pseudorandom generation of new indices to point to other seeds.
- **Sequences of random numbers:**
 - defined by a state (e.g seed and table) that contains all that is needed to initialize a recurrence formula which enables the generation of the random sequence.

II: 3 methods to get pseudorandom numbers sequences

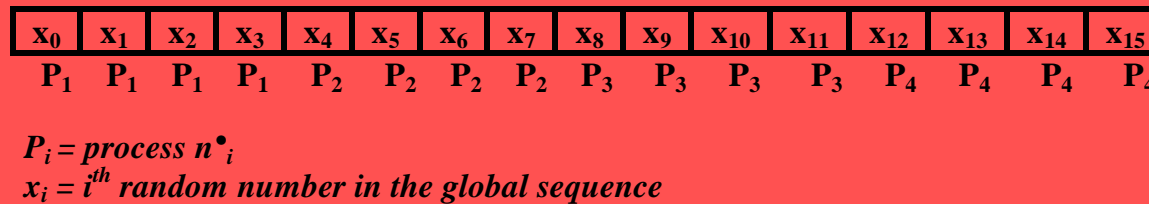
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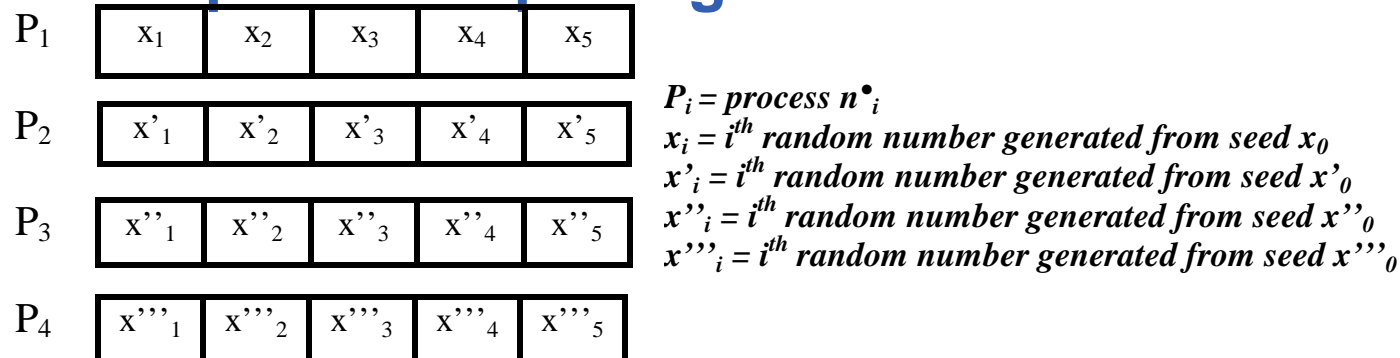
- Leap Frog Method



- The Sequence Splitting Method



- The Independent Splitting

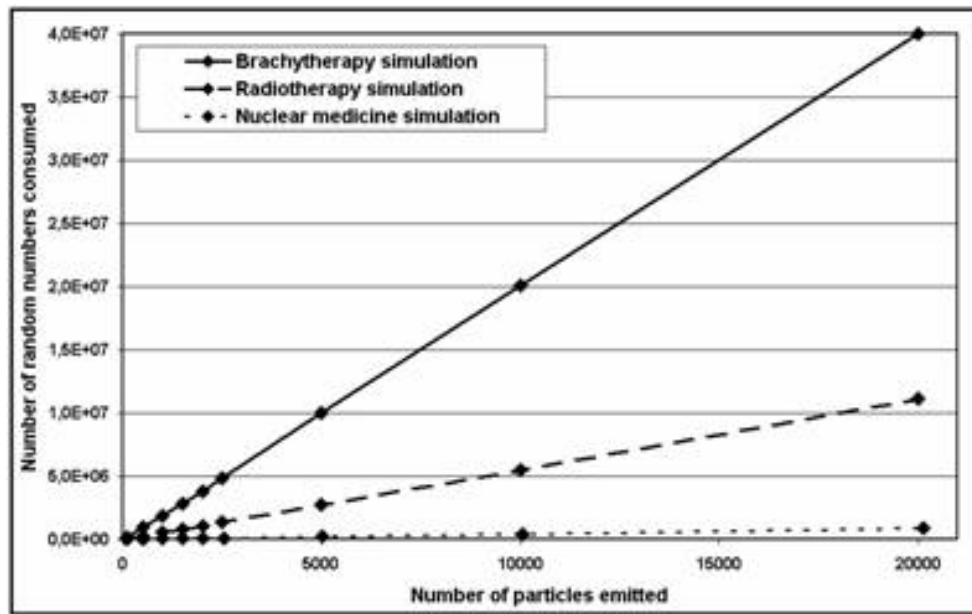


II: Consumption in random numbers

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- Testing the consumption in pseudo random numbers



Comparison between different use cases

GOAL: Evaluate the length of the PRN sequences

RESULT: High level consumption for brachytherapy simulations (ionisations)

- Testing the pseudorandom number generator (PRNG)

- Statistical tests of comparison between PRNG

- 122 statistical tests suggested by Lecuyer

- 36/122 success with the algorithm James Random used by GATE

- 120/122 success with the algorithm Merseur Twister

High level statistical properties for the Merseur Twister PRNG

(period = 2^{19320})

➡ **Need to test the PRNG on the physics**

- The random numbers generator (RNG) in MC simulations

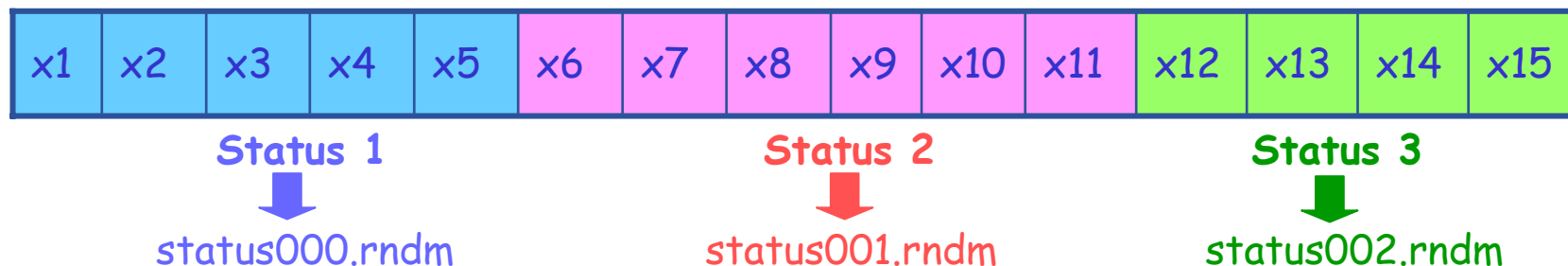
- Based on deterministic algorithm

- Characteristics: (example for HEPJamesRandom: the GATE RNG)

- Very long period RNG: 2^{144}
 - Creation of 900 million sub-sequences non overlapping with a length of 10^{30}

- Pre-generation of random numbers

- The Sequence Splitting Method



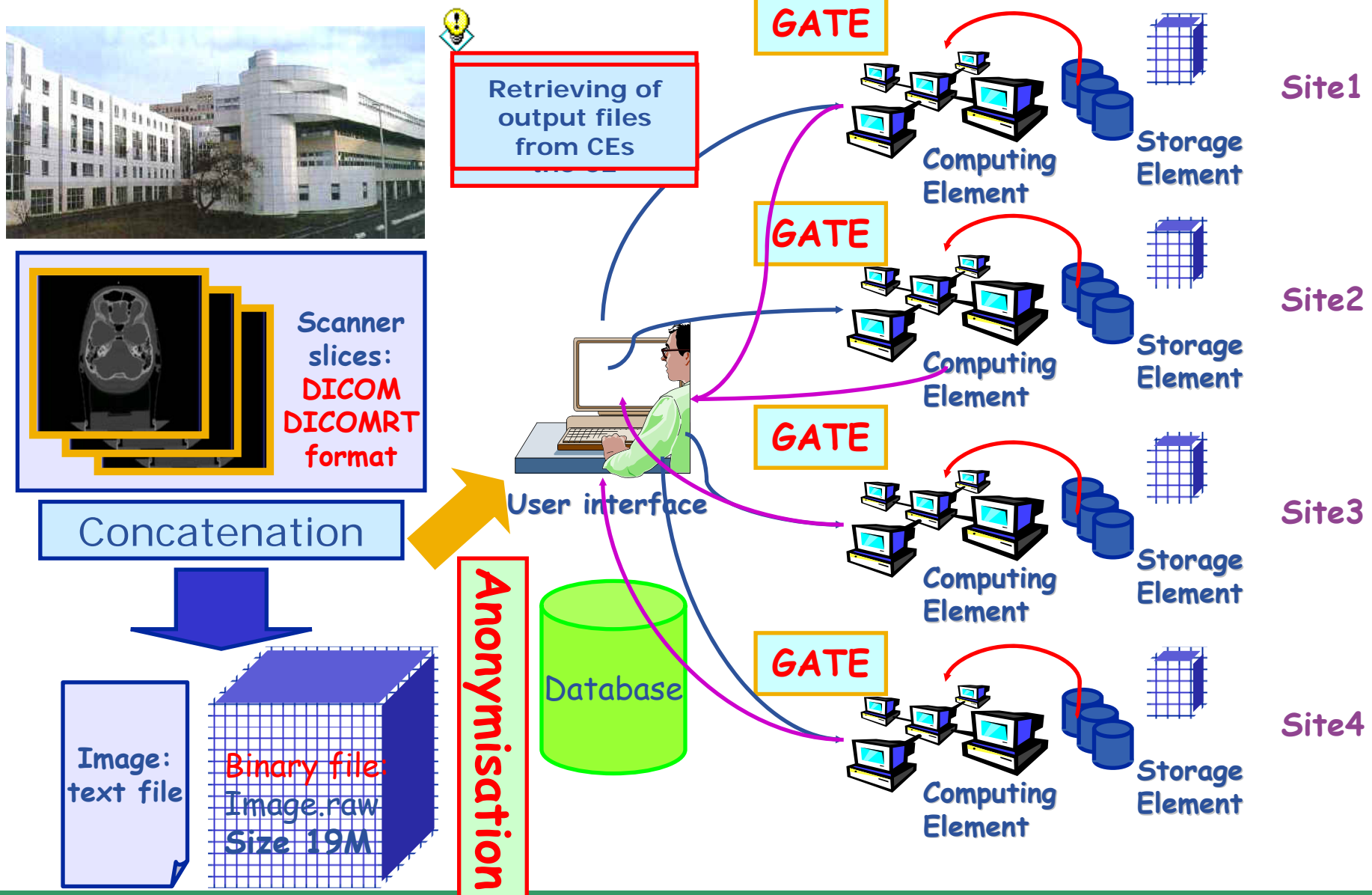
- Until now, 2 000 status files generated with a length of 3.10^{10}

Each status file is sent on the grid with a G4/GATE simulation

III

Jobs submissions and Datasets management

III: Submission on the grid



III: Access permission and authentication

- To use the grid in a secure way, you must:



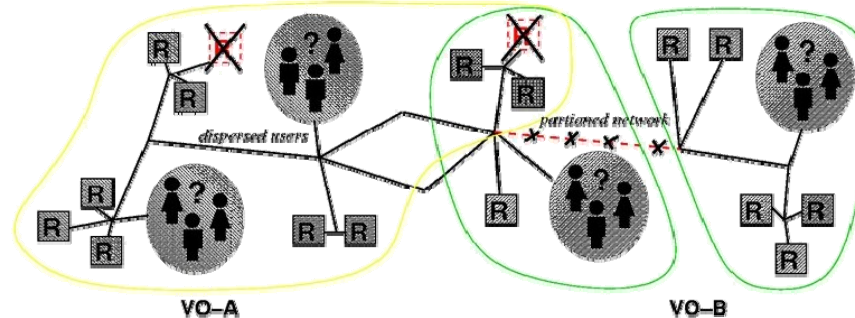
- Obtain X509 personal certificate by CA ➡ Who are you?

- 2 keys: public (certificate) and private with password (on your computer)
- 1 year of validity



- Be part of a Virtual Organization (VO) ➡ What are your rights?

- Organize people and resources through scientific experience
- Ex: Biomed, Earth observation, HEP VOs: Alice, Atlas, D0, LHCb....



- VOMS (Virtual Organization Membership Service) service:

- Allows confidentiality between members of the same VO
- Members hierarchy: simple user, software manager, etc...



- Obtain an account on a User Interface (UI)

III: Scope of data services on the grid



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- **Simply, DMS provides all operation that all of us are used to performing**
 - **Uploading /downloading files**
 - **Creating file /directories**
 - **Renaming file /directories**
 - **Deleting file /directories**
 - **Moving file /directories**
 - **Listing directories**
 - **Creating symbolic links**
- **Note: Files are write-once, read-many**
 - Files cannot be changed unless remove or replaced
 - No intention of providing a global file management system

III: Data Issues and Grid Solutions



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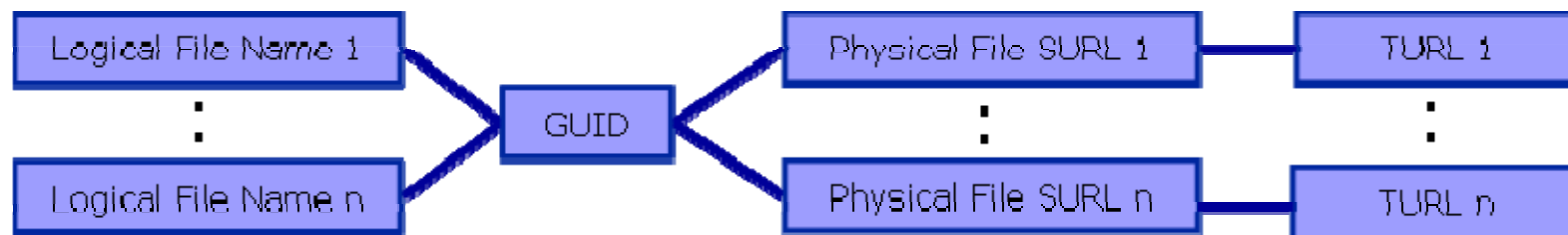
- **Resource centers need meet growing demand for storage**
 - **Storage Element** capable to manage **multiple disk pools**
 - **Disk Pool Manager (DPM), dCache, CASTOR**
- **Data is stored on different storage systems technologies**
 - **Common interface** required to **hide** underlying complexity
 - **Storage Resource Manager (SRM)** – storage management protocol
 - **GridFTP** – secure file transfer
- **Data is stored at different locations with separate namespace**
 - **File catalogue** to provide **uniform view** of Grid data
 - **LCG File Catalog (LFC)**

III: Name conventions



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- **Logical File Name (LFN)**
 - An alias created by a user to refer to some item of data, e.g.
“lfn:/grid/cms/20030203/run2/track1”
- **Globally Unique Identifier (GUID)**
 - A non-human-readable unique identifier for an item of data, e.g.
“guid:f81d4fae-7dec-11d0-a765-00a0c91e6bf6”
- **Storage URL (SURL) or Physical File Name (PFN)**
 - The location of an actual piece of data on a storage system, e.g.
“srm://pcrd24.cern.ch/flatfiles/cms/output10_1” (SRM)
“sfn://lxshare0209.cern.ch/data/alice/ntuples.dat” (Classic SE)
- **Transport URL (TURL)**
 - Temporary locator of a replica + access protocol: understood by a SE, e.g.
“rfio://lxshare0209.cern.ch//data/alice/ntuples.dat”



III: Summary of lcg-utils commands



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Replica Management

lcg-cp	Copies a grid file to a local destination
lcg-cr	Copies a file to a SE and registers the file in the catalog
lcg-del	Delete one file
lcg-rep	Replication between SEs and registration of the replica
lcg-gt	Gets the TURL for a given SURL and transfer protocol
lcg-sd	Sets file status to “Done” for a given SURL in a SRM request

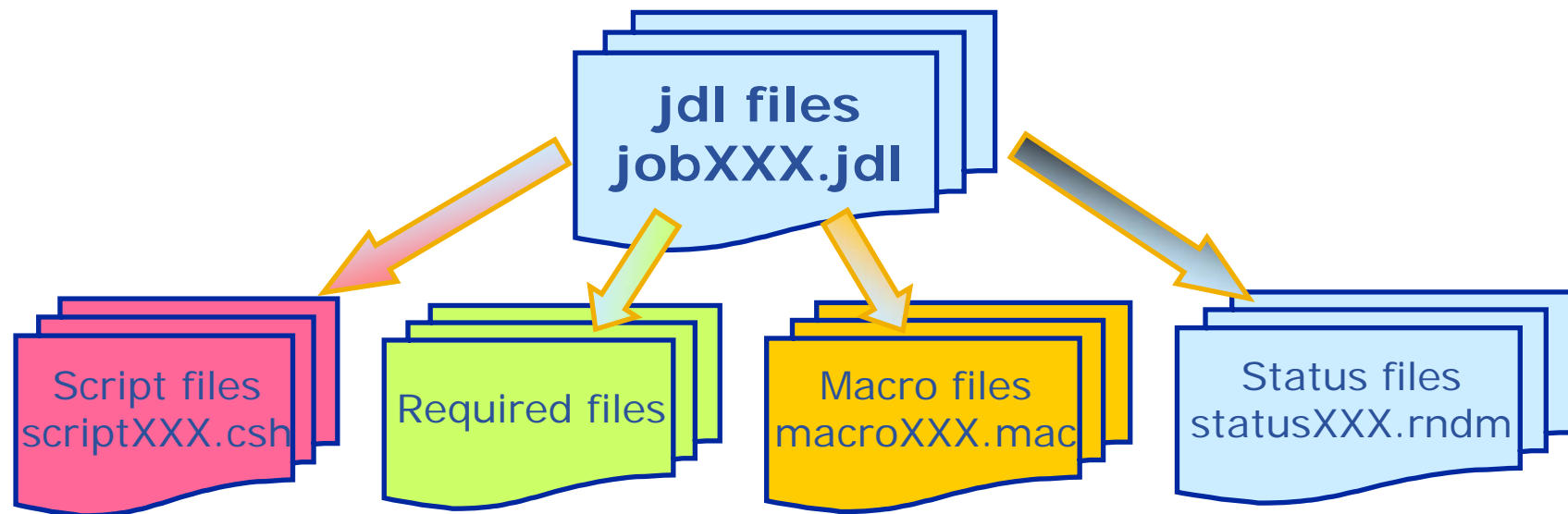
III: Files submitted



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Splitting a Monte Carlo GATE simulation of 10 M of events as follow:

- ◆ 10 simulations generating 1M de particles
 - ◆ 20 simulations generating 500 000 particles
 - ◆ 50 simulations generating 200 000 particles
- Other files necessary to launch simulations are produced automatically



III: JDL files characteristics



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• Job characteristics

```
[
  Executable = "/bin/sh";
  Arguments = "./script0.sh";
  StdOutput = "std0.out";
  StdError = "std0.err";
  OutputData = { [
    OutputFile = "result0.root" ;
    StorageElement = "grid002.ics.forth.gr" ;
    LogicalFileName = "lfn:/grid/biomed/ROOT" ; ]};
  RetryCount = 3;
  JobType = "normal";
  Type = "Job";
  InputData = "lfn:Scan_patientDUPOND"
  InputSandbox = {
    "/home/user/GATEJOB/script0.sh",
    "/home/user/GATEJOB/macro0.mac",
    "/home/user/GATEJOB/status0.x",
    "/home/user/GATEJOB/GateM...s.db",
    "/home/user/GATEJOB/pr...aGat...mac",
    "/home/user/GATEJOBatch0.c",
    "/home/user/GATEJOB/PROFILATClass0.C",
    "/home/user/GATEJOB/PROFILATClass0.h"
  };
  requirements = (Member("VO-biomed-GATE-3.0.0-1",other.GlueHostApplicationSoftwareRunTimeEnvironment)
&&(other.GlueCEPolicyMaxCPUTime>102));
  Rank = (other.GlueCEStateWaitingJobs == 0 ? other.GlueCEStateFreeCPUs : -other.GlueCEStateWaitingJobs);
]
```

▪Requirements:

- GATE, G4 software TAG

- MaxCPUTime

▪RANK:

- the site with none waiting jobs, if it's not the case,
- the sites with the largest number of free CPUs

If more that one resource matches, then the rank is used to determine which is the most desirable resource.

III: Script files characteristics



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Bash shell
Files readable from any node
tcsh also accepted

▪Source of the environment file:
▪update of necessary variables

```
#!/bin/sh
#Script Launching on EGEE
# Cheick Thiam
#CE_node :
#####
###                GATE Environment                ###
#####
#list content of PWD
ls -l $PWD
echo " GATE Env Configuration "
source ${VO_BIOMED_SW_DIR}/gate_env_main.sh
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$VO_BIOMED_SW_DIR/gate/lib/root
echo " GATE Run "
#####
# Launching a simulation #
#####
${VO_BIOMED_SW_DIR}/gate/bin/Linux-g++/Gate macro0.mac
ls -l
echo " ROOT ANALYZE "
echo " ===== "
root -b Batch0.C
ls -l
echo " TEST COPY : test lcg-cr -v -d "
lcg-cr -v -d grid002.ics.forth.gr -l lfn:/grid/biomed/ROOT/result0.root --vo biomed file: $PWD/result0.root
```

▪Executable
▪Macro file in parameter

▪Execution of a Root analysis
after the G4 simulation

▪Copy of results on SE with
creation of an lfn

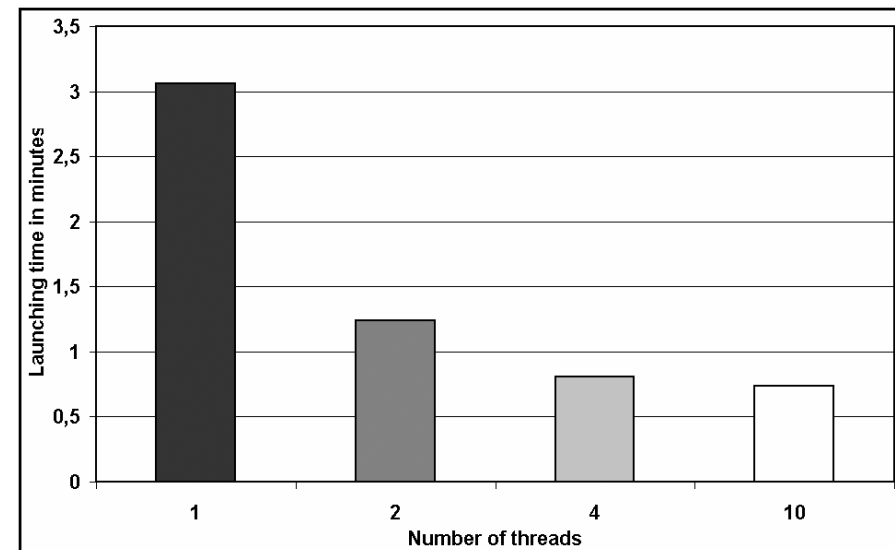
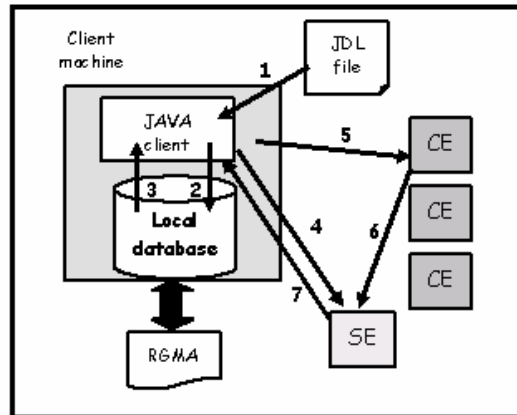
III: Submission of the simulations on the grid, 2 approaches

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- **Multiple threading**

- By using a Java application that doesn't take into account the RB bottleneck, the more the threads are important, the lower the launching time is ➡ **Gain in computing time**



- By using the RB

- Impossible to increase the multithreading as much as we want
- Sequential acceptance of the jobs from the RB (3s/job treated)

➡ **A good knowledge of the grid RBs is necessary for an optimal submission**

III: Submission of the simulations



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- Workload analysis:** the analysis of the cluster workload is essential to find the best scheduling policies for the users' needs

Queue	Max CPU (H:M:S)	Max Wall (H:M:S)	Max Jobs
Test	0:05:00	0:15:00	130
Short	0:20:00	1:30:00	130
Long	8:00:00	24:00:00	130
Day	24:00:00	36:00:00	130
Infinite	48:00:00	72:00:00	130

Queue configuration at LPC site

– The running time

Queue	Mean	Standard deviation	CV
Test	31.0	373.6	12
Short	149.5	1230.5	8.2
Long	2943.2	11881.2	4.0
Day	6634.8	25489.2	3.8
Infinite	10062.2	30824.5	3.0

- Maximum CPU time: unadapted variable to describe the length of a job
- Look at short jobs

– The waiting time

Queue	Mean	Standard deviation	CV	Number of jobs
Test	33335.9	148326.4	4.4	45760
Short	1249.7	27621.8	22.1	81963
Long	535.1	5338.8	9.9	32879
Day	466.8	8170.7	17.5	19275
Infinite	1753.9	24439.8	13.9	49060

- Launch not too short jobs compared to their waiting factor
- Do not send jobs very often in order that they all wait together in a queue.
- Execution of long jobs delayed by the scheduler to run shorter jobs

– The arrival time

Group	Mean (seconds)	Standard deviation	CV
Biomed	223.6	5194.5	23.22
Dteam	256.2	2385.4	9.31
LHCb	2474.6	39460.5	15.94
Atlas	2824.1	60789.4	21.52
Dzero	5018.7	50996.6	10.16

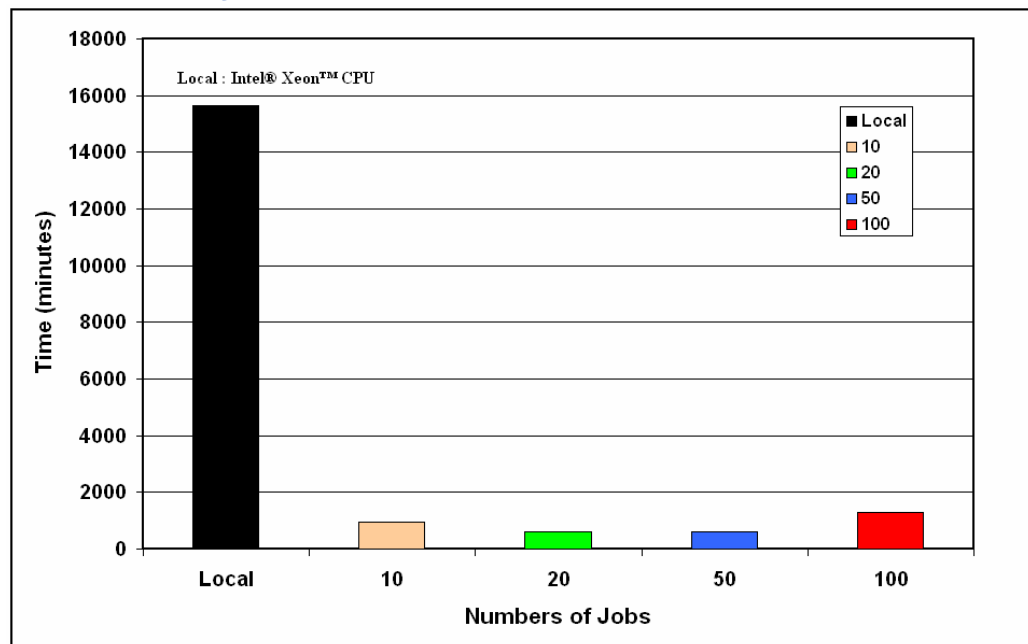
- activity peak around midday, 2pm and 4pm
- Moments of interarrival time for each group of users are very irregularly, distributed and do not correspond to Poisson processes

III: Installation status and computing tests



Plateforme de Calcul pour les Sciences du Vivant

- **Installations**
 - Biomed resources: 115 CEs, 3500 CPUs, 120 TB, 75 users
 - Gate.3.0.0 installed on each biomed CE
- **Radiotherapy simulation:**



Local computing:
260 hours on 3GHz processor

Grid computing:
10 hours for 50 partitions



GAIN 26 for 50 jobs submitted

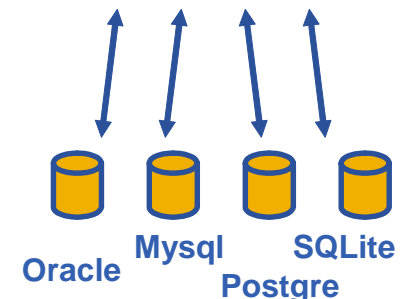
- **SPECT simulation:**
 - 1813 Jobs, 24h/job
 - **Gain=800**
(907 days with a 3 GHz CPU)
 - Results in 3 days

III: Datasets with metadata: the AMGA server

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AMGA server



- AMGA is a metadata service for the Grid.
 - ***Describe file, locate files based on their contents and simplifies the need of structured data required by some applications***AMGA currently supports 4 different database backends via ODBC drivers.
- It is a database access service for Grid applications which allows user jobs running on the Grid to access databases.
- It provides a Grid style authentication as well as an opaque layer which hides the differences of the different underlying database systems from the user.
- AMGA is a service sitting between the RDBMS and the user's client application.
- AMGA intends to provide a replication layer which makes databases locally available to user jobs and replicate the changes between the different participating databases.

III: Example: secure management of medical images on the grid

Plateforme de Calcul pour les Sciences du Vivant

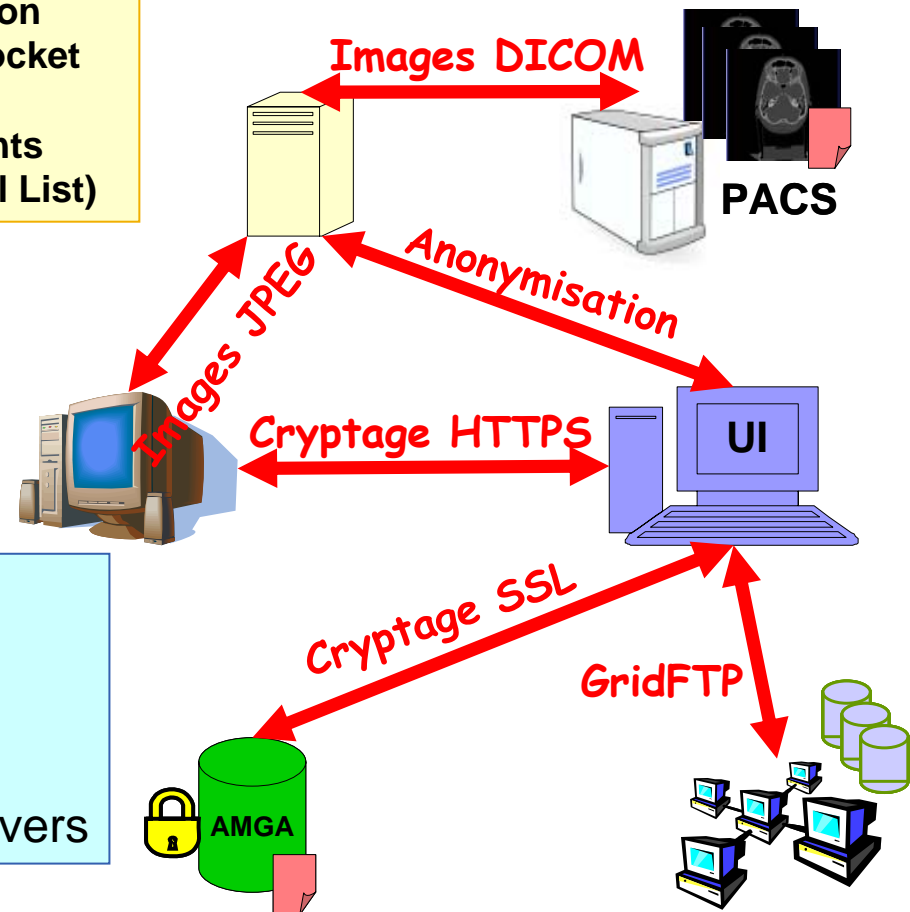


Medical images access on the grid

FTP like transfers: GridFTP secured protocol

Metadata access:

Proxy authentication and VOMS authorization
Secured connections using SSL (Secure Socket Layer):
cryptographic systems to transfer documents
Authorization using ACLs (Access Control List)



The AMGA server:

Langages based on SQL

Hierarchical organization of metadata (tree)

Dynamic schemas: add, delete, modify fields

Replication of metadata on other AMGA servers

IV

Web portal interface to access the grid

IV: Overview

Plateforme de Calcul pour les Sciences du Vivant

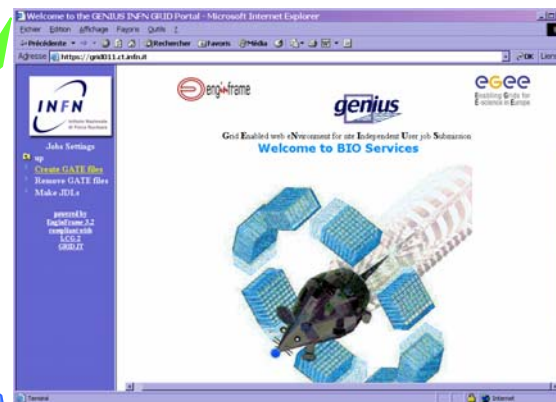


Registration and management of medical images

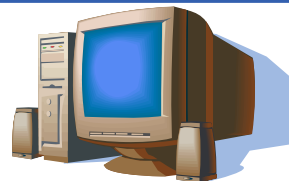
- Registration and replication anonym medical images
- One logical file name corresponding to multiple physical images
- Automatic adding and suppression of images

Jobs submissions and management

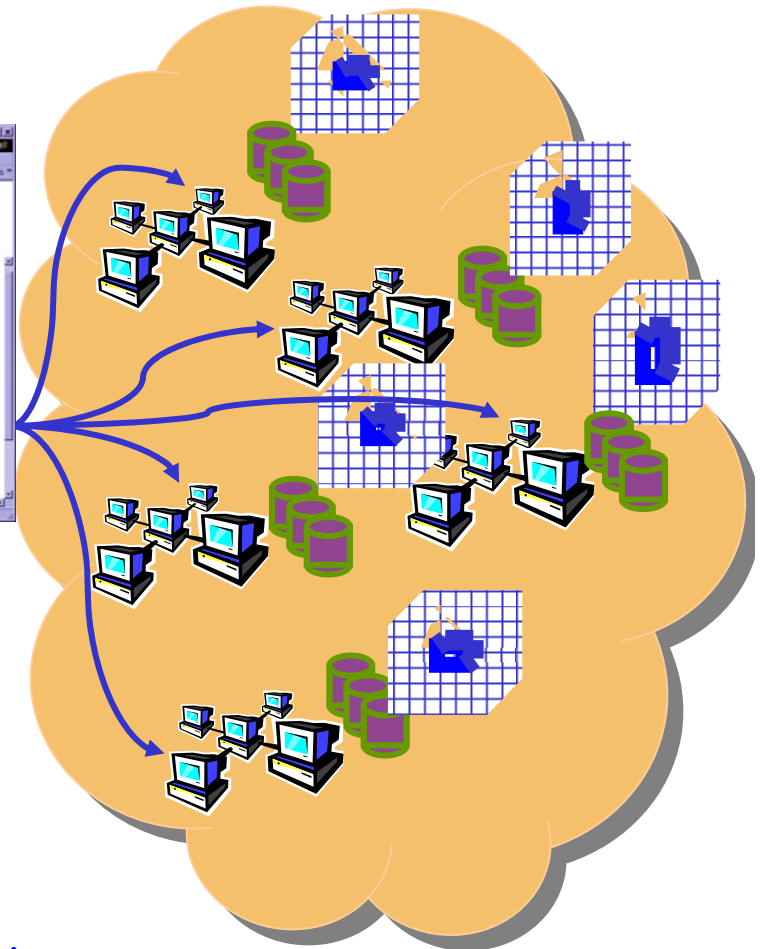
- User secured authentication
- Splitting of simulations
- Automatic files creation submitted to the grid
- Jobs submission
- Jobs management
- Automatic data retrieving (spectrum, isodoses...)



Internet connexion



Working station
Starting of the installation at
Centre Jean Perrin







Welcome to the GENIUS Grid Portal - Mozilla

File Edit View Go Bookmarks Tools Window Help

Back Forward Reload Stop <https://clrpcsv12.in2p3.fr/> Search Print

Home Bookmarks Scientific Linux Distros










Welcome thiam Resource Broker: biomed Virtual Organization: biomed Catalog Type: fireman Catalog Server: gilda Your Data Logout

Genius Services


- BIOMED GATE APPLICATION
 - GATE SUBMIT SERVICES
 - Create GATE files
 - Remove GATE files
 - Make JDLs
 - Submit GATE Jobs
 - Jobs Status
 - MEDICAL IMAGE SERVICES
 - File or sngle Image Upload
 - Copy on Grid (SE)
 - Replicate data/file
 - Delete data/file
 - Download a grid file
 - Images Upload
 - Images Anonymization
 - Images Viewer
- File
- Security
- Job
- Data
- Info
- Monitoring
- Interactive
- Preferences

Welcome to GENIUS and Biomedical GATE Application Portal


ver. 3.0
compliant with [gLite-1](#) and [LCG-2](#) middlewares
[Credits](#)

This portal is best viewed with Mozilla 1.7.12 or higher.
Netscape (4.79, 4.80, 8 or higher) and Internet Explorer (5 or higher) can also be used.
The use of any other web browsers could induce some visualization mismatches and is not currently suggested.

powered by


Last update: Fri 03 February 2006

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Tue Mi 10:53



Jobs Settings



- Create GATE files
- Remove GATE files
- Make JDLs

powered by
[EnginFrame 3.2](#)
compliant with
[LCG-2](#)
[GRID.IT](#)



Grid Enabled web eNvironment for site Independent User job Submission

RB: gilda

VO: gilda

RLS: GILDA

Your Data

Logout

Create GATE files

With this service it will be created/checked your GATE Repository and Settings. If you choose to perform Root Analysis, please read these few [instruction](#) for your root class files.

Repository Name

Root Analysis

☒ Yes☐ No

InputSandbox Files (3 files)

Select...

Clean

InputData lfn:

macro (.mac)

Select...

Number of Partitions

Status Files (=Number of Partitions)

Select...



Internet



Jobs Services

- up
- Jobs Settings
- Jobs Submission
- Jobs Queue
- GATE job data

powered by
[EnginFrame 3.2](#)
 compliant with
[LCG-2](#)
[GRID.IT](#)



Grid Enabled web eNvironment for site Independent User job Submission

RB: gilda		VO: gilda		RLS: GILDA		Your Data	Logout
No	Job ID	Last update	Destination	Status			
4	https://grid004.ct.infn.it:9000/qdCL6HCv4AMG9QFqn645kw	Fri Nov 12 13:38:01 2004	grid010.ct.infn.it:2119/jobmanager-lcgpbs-infinite	Scheduled			
3	https://grid004.ct.infn.it:9000/moI2CgILw9k5Dik4eJ682w	Fri Nov 12 13:40:47 2004	grid010.ct.infn.it:2119/jobmanager-lcgpbs-infinite	Running			
2	https://grid004.ct.infn.it:9000/epYl_-EMrNzeyyFJ7ulEzQ	Fri Nov 12 13:40:48 2004	grid010.ct.infn.it:2119/jobmanager-lcgpbs-infinite	Running			
1	https://grid004.ct.infn.it:9000/DuNF0S0k9m3PonYf-rTizA	Fri Nov 12 13:40:48 2004	grid010.ct.infn.it:2119/jobmanager-lcgpbs-infinite	Running			



Grid Enabled web eNvironment for site Independent User job Submission

Jobs Services

up

Jobs Settings

Jobs Submission

Jobs Queue

[GATE job data](#)

powered by
EnginFrame 3.2
compliant with
LCG-2
GRID.IT

RB: gilda VO: gilda RLS: GILDA Your Data Logout

The Job output of <https://grid004.ct.infn.it:9000/qdCL6HCv4AMG9QFqn645kw> has been successfully retrieved in your HOME

No	Job ID	Last update	Destination	Status
4	https://grid004.ct.infn.it:9000/qdCL6HCv4AMG9QFqn645kw	Fri Nov 12 14:12:58 2004	grid010.ct.infn.it:2119/jobmanager-lcgpbs-infinite	Done

Job execution completed, analysing data now.....

Merging of Root files done.....creating graphical output

All jobs output have been retrieved in `/home/maigne/GATE/outputs/gate_job_list_20041112_143643`. If the production was less than 3 days ago, you can also inspect the output from its copy on the spooler directory [gate_job_list_20041112_143643](#)



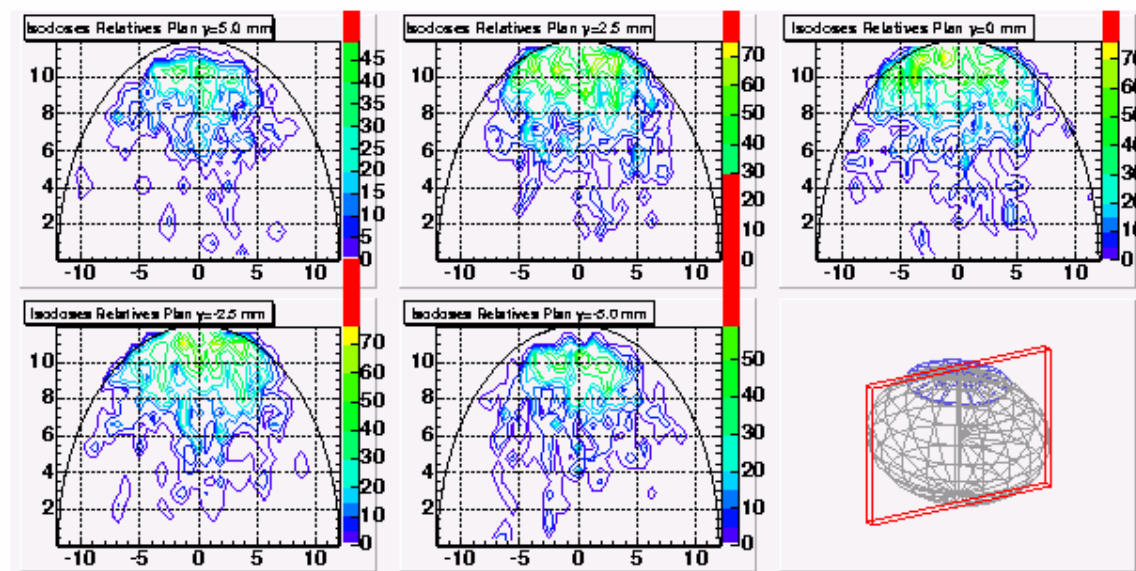
Jobs Services

- up
- Jobs Settings
- Jobs Submission
- Jobs Queue
- GATE job data

powered by
EnginFrame 3.2
compliant with
LCG-2
GRID.IT



Grid Enabled web eNvironment for site Independent User job Submission



IV: Functionalities of a web portal for simulations in medical physics

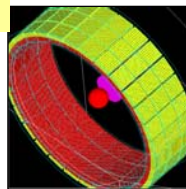
Plateforme de Calcul pour les Sciences du Vivant



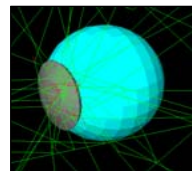
Développements
utilisant des
services web
(Sept2007-
Sept2008)

Visualisation
des images

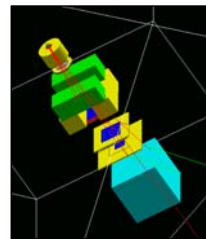
Simulations
Monte Carlo



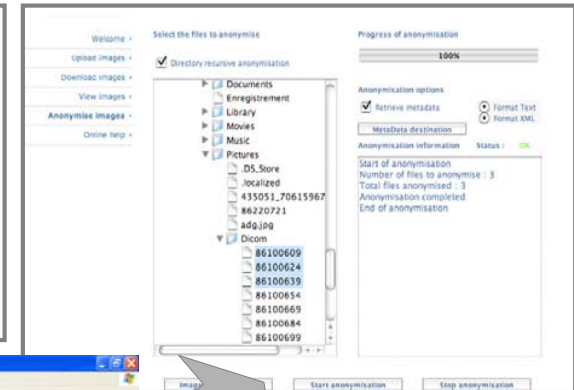
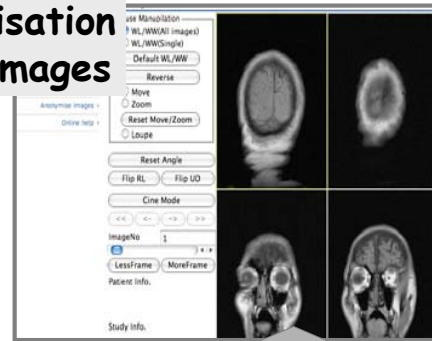
Camera TEP



Traitement de
curiethérapie
oculaire



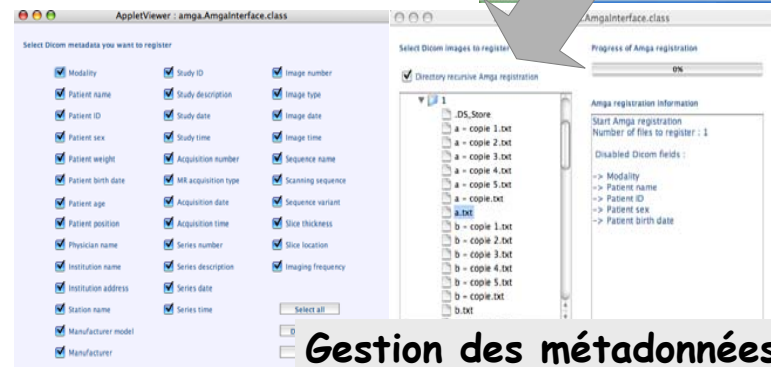
Radiothérapie



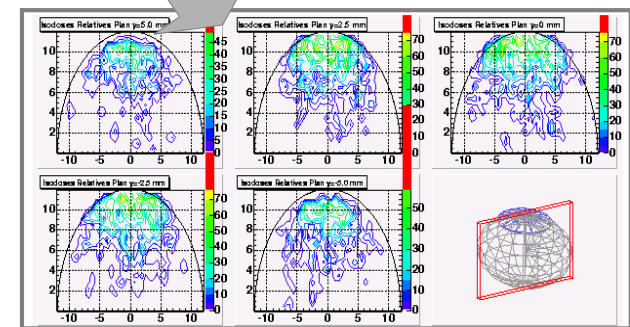
Anonymisation
des images



La visualisation
des résultats

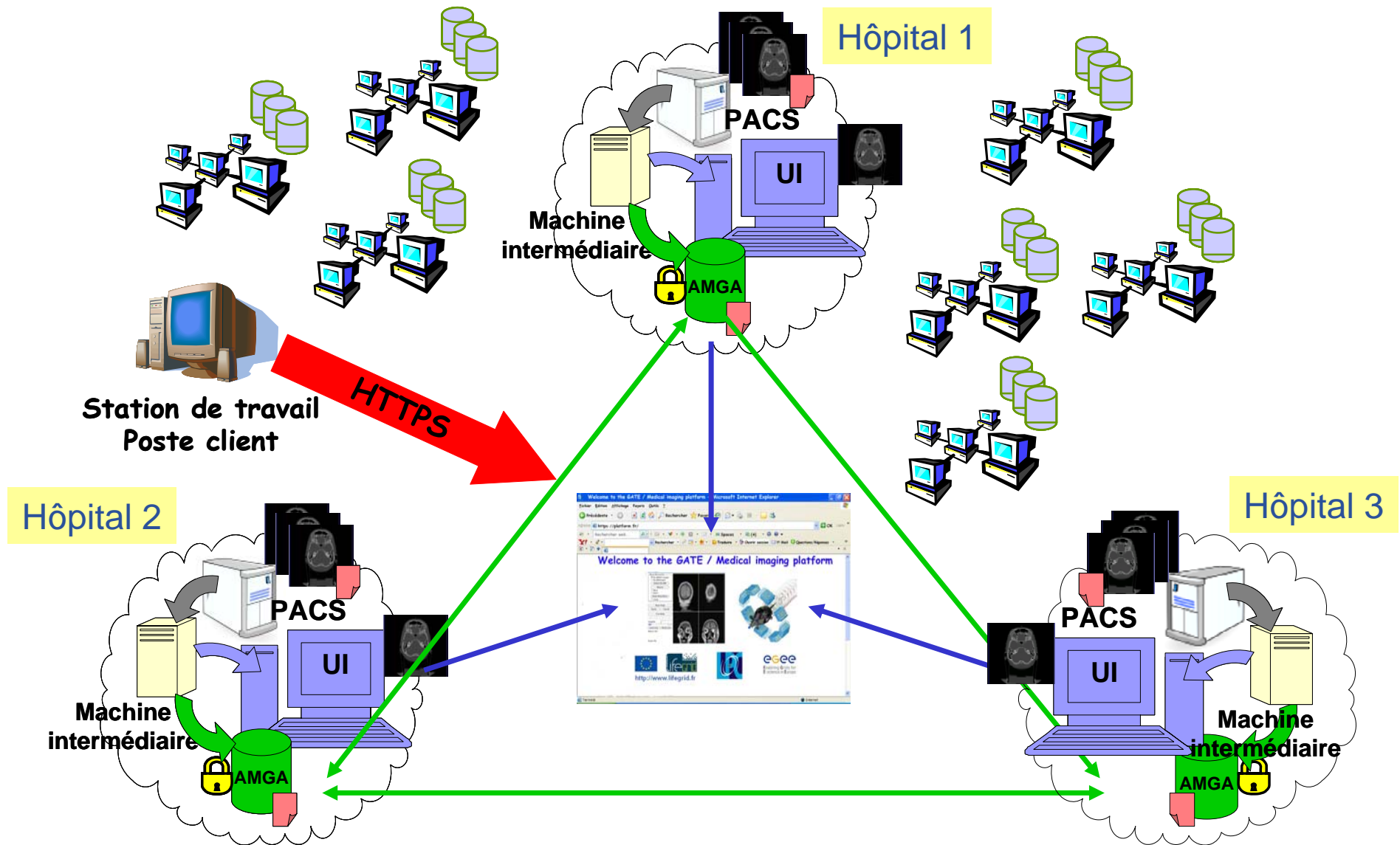


Gestion des métadonnées



IV: How to use it for connections between hospitals

Plateforme de Calcul pour les Sciences du Vivant



- **European grid project**
 - <http://www.eu-egee.org>
- **Regional grid project: AUVERGRID**
 - <http://www.auvergrid.fr>
- **Information system for life sciences on grid: LifeGrid**
 - <http://www.lifegrid.fr>
- **Tutorial on EGEE**
 - <http://www.eu-egee.org/try-the-grid>
- **LCG user**
 - <http://lcg.web.cern.ch/LCG/users/users.html>
- **LCG User Guide**
 - <https://edms.cern.ch/file/454439//LCG-2-UserGuide.html>
- **LCG FAQ (pas à jour mais ça aide quand même)**
 - <https://edms.cern.ch/file/495216/1/LCG-Faq.html>
- **Docs on the grid**
 - <https://gus.fzk.de/pages/docu.php>
- **User Support**
 - <http://www.ggus.org/>
pour soumettre des incidents pour la VO, pour un site...