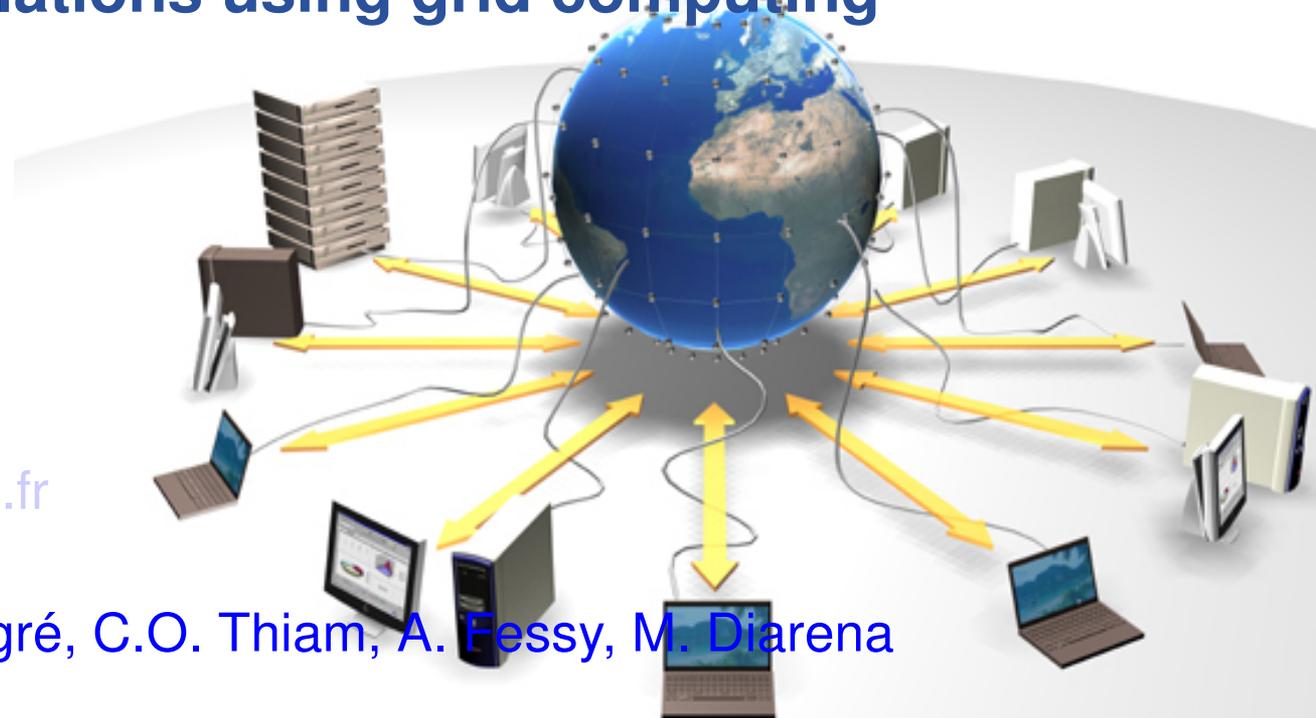




Geant4/GATE simulations using grid computing



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Clermont-Ferrand
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Crédits: V. Breton, Y. Legré, C.O. Thiam, A. Fessy, M. Diarena

- **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
 - **Split the simulations by using non overlapping random sequences**
- **III : Jobs submissions and datasets management**
 - Jobs submission, how to?
 - Computing time tests
 - Medical images in the simulations
- **IV: Web portal interface**
 - Functionalities

I

A grid architecture

I: The EGEE project

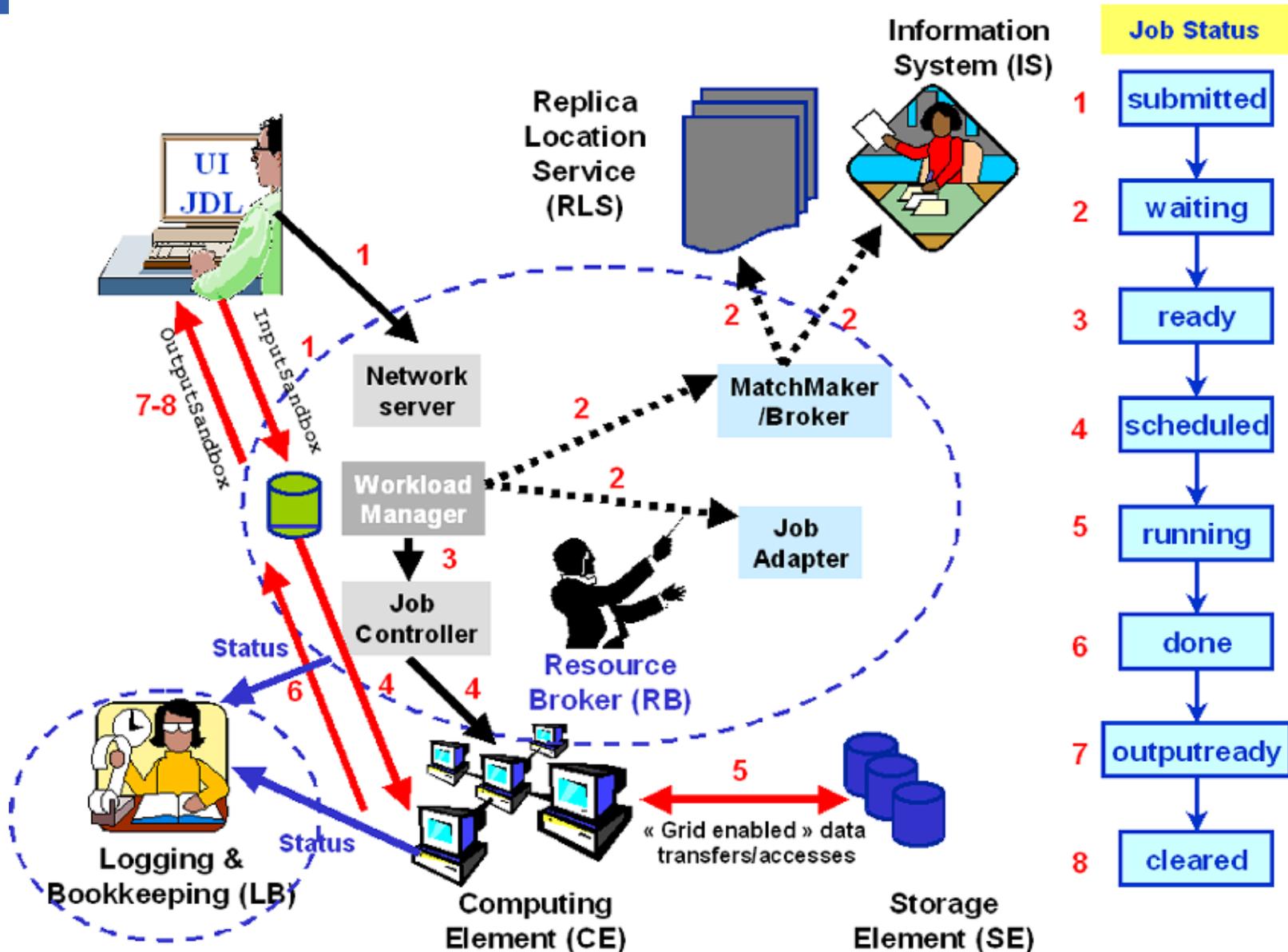
Plateforme de Calcul pour les Sciences du Vivant



- 4-year 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

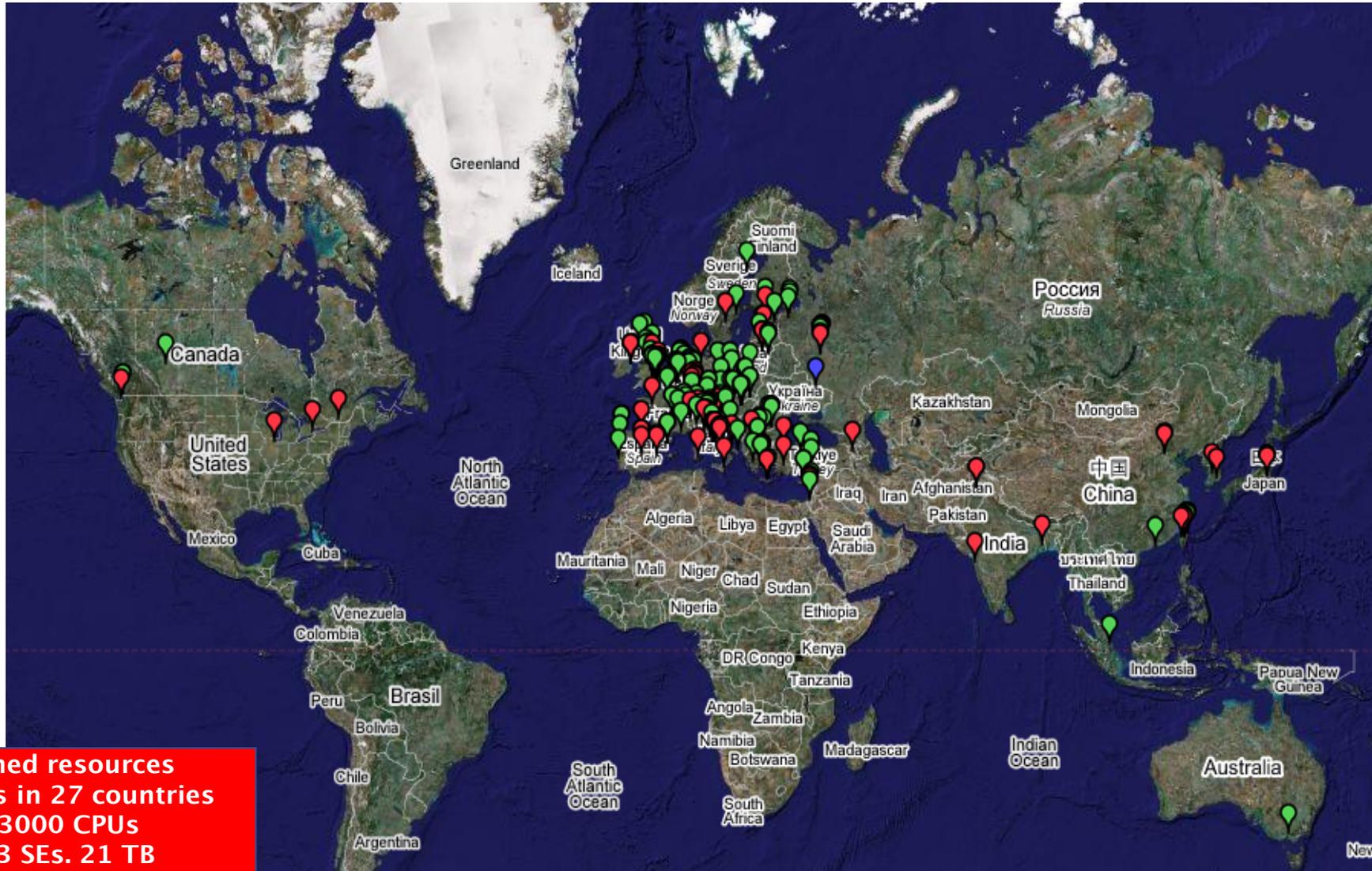
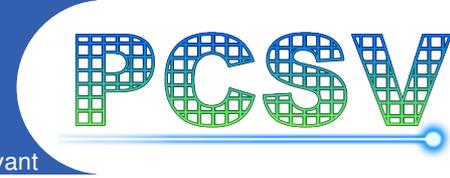


I: What is a grid?



I: Geographically distributed resources in EGEE

Plateforme de Calcul pour les Sciences du Vivant



Biomed resources
115 CEs in 27 countries
~3000 CPUs
123 SEs, 21 TB
30 RBs

II

Distribute simulations on the grid The PRNG

- 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 SEs
- 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

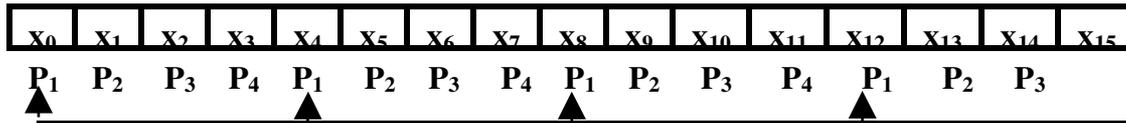
- We choose to work with **F.James' algorithm**:
 - HEPJamesRandom in CLHEP libraries
 - **Very long period: 2^{144}**
 - **Creation of 900 millions of sub-sequences having a length of $\sim 10^{30}$**
 - **Combination of a Fibonacci sequence and an arithmetic sequence**
 - Fibonacci sequence:
 - *Each 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..*

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

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

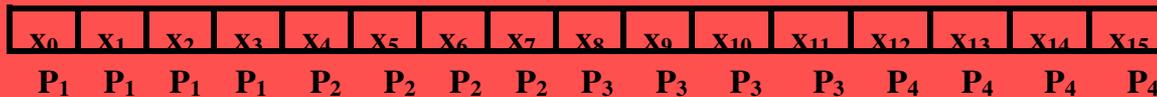
II: 3 methods to get pseudorandom numbers sequences

- Leap Frog Method**



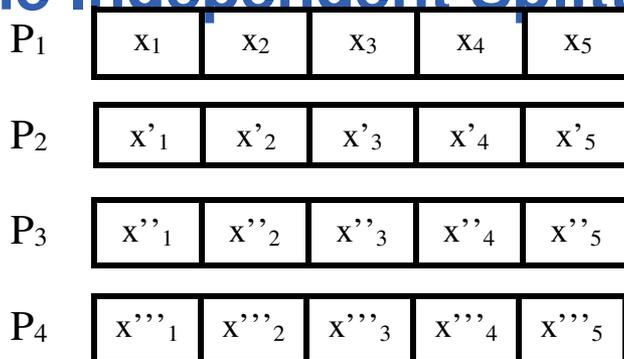
$P_i = \text{process } n^{\circ}_i$
 $x_i = i^{\text{th}}$ random number in the global sequence

- The Sequence Splitting Method**



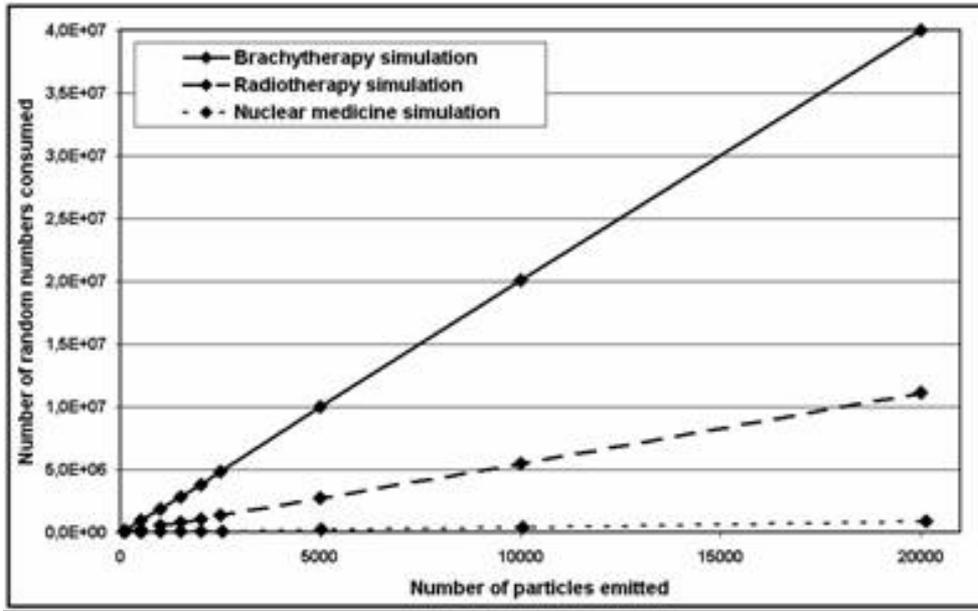
$P_i = \text{process } n^{\circ}_i$
 $x_i = i^{\text{th}}$ random number in the global sequence

- The Independent Splitting**



$P_i = \text{process } n^{\circ}_i$
 $x_i = i^{\text{th}}$ random number generated from seed x_0
 $x'_i = i^{\text{th}}$ random number generated from seed x'_0
 $x''_i = i^{\text{th}}$ random number generated from seed x''_0
 $x'''_i = i^{\text{th}}$ random number generated from seed x'''_0

- 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 Mersenne Twister

High level statistical properties for the Mersenne Twister PRNG

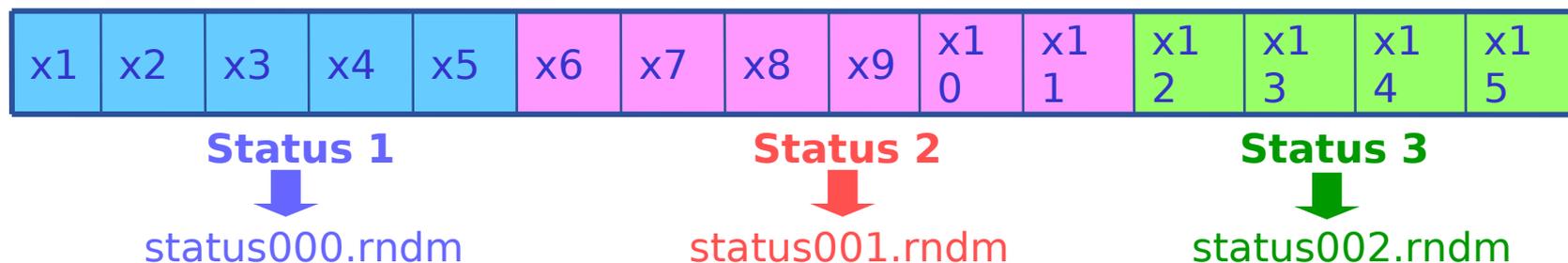
(period = 2^{19320})



Need to test the PRNG on the physics

II: Status of PRNGs

- 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 $3 \cdot 10^{10}$

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

III

Jobs submissions and Datasets management

**Example: GATE/G4 for
medical applications**

III: Submission on the grid



Scanner slices:
DICOM
DICOMR
T format

Concatenation

Image:
text file

Binary file:
Image.raw
Size 19M

Submission of jdl's to the CEs

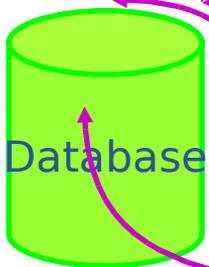
Copy the medical image from the SE to the CE

Retrieving of output files from CEs



User interface

Anonymisation



Database

GATE

GATE

GATE

GATE



Computing Element



Computing Element



Computing Element



Computing Element



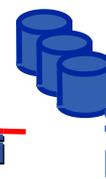
Storage Element



Storage Element



Storage Element



Storage Element

Site1

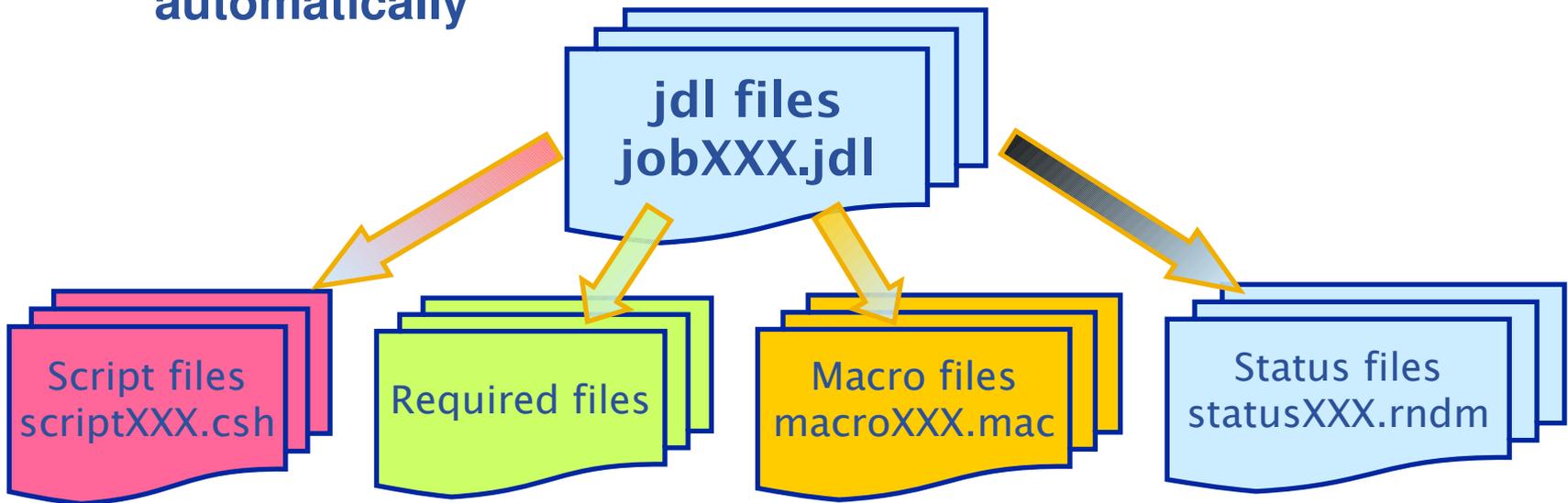
Site2

Site3

Site4

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



• 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.",
    "/home/user/GATEJOB/macro0.",
    "/home/user/GATEJOB/stat",
    "/home/user/GATEJOB/G",
    "/home/user/GATEJOB/ery_gate.mac",
    "/home/user/GATEJOB/Batr",
    "/home/user/GATEJOB/PROFIL_LATClass0.C",
    "/home/user/GATEJOB/PROFIL_LATClass0.h"
  };

  requirements = (Member("VO-biomed-GATE-3.0.0-1" other.GlueHostApplicationSoftwareRunTimeEn
&&(other.GlueCEPolicyMaxCPUTime>102));
  Rank = (other.GlueCEStateWaitingJobs == 0 ? other.GlueCEStateFreeCPUs : -other.GlueCEState
]
```

▪ **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

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
```

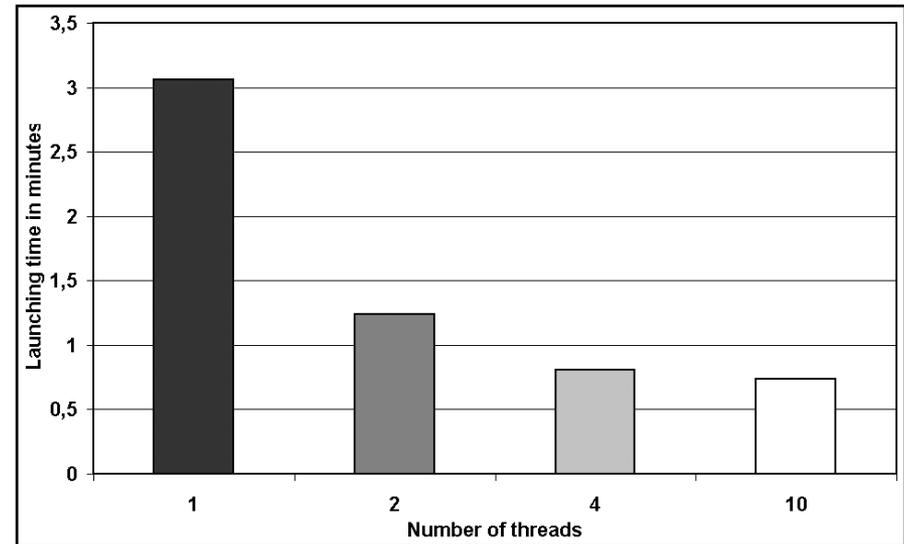
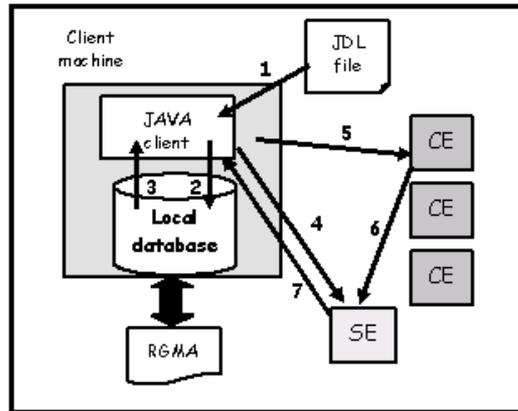
▪ **Executable**
▪ **Macro file in parameter**

▪ **Execution of a Root analysis after the G4 simulation**

▪ **Copy of results on SE with creation of an lfn**

- **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**

– The running time

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

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

– The waiting time

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

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

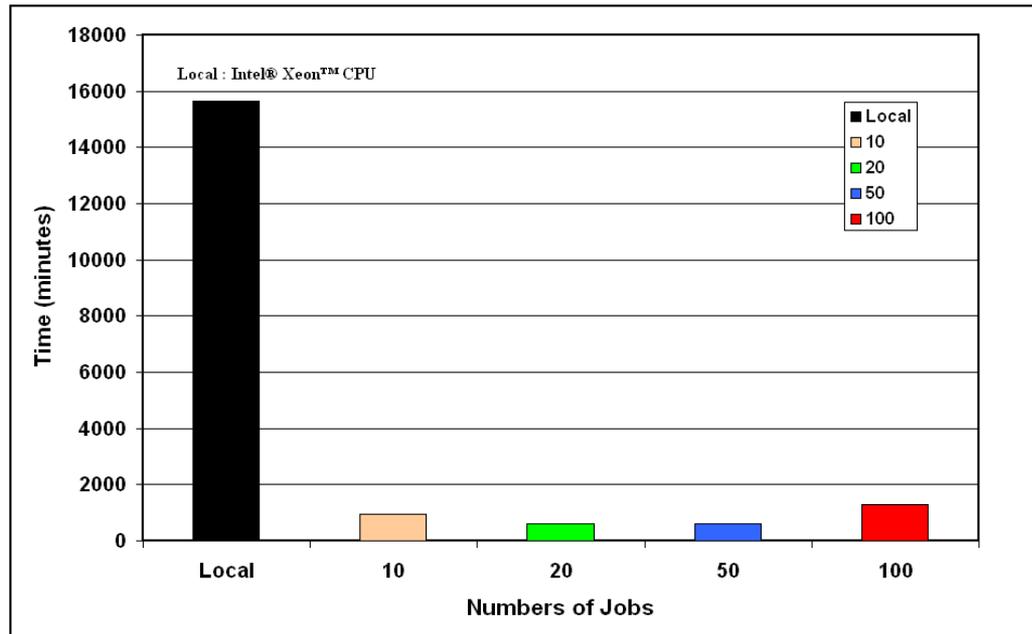
– The arrival time

- **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**

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**

- **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

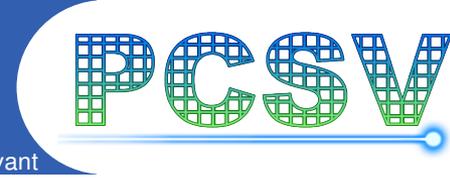


GAIN 26 for 50 jobs submitted

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

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

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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:

➤ Database access service for Grid applications which allows user jobs running on the Grid to access databases.

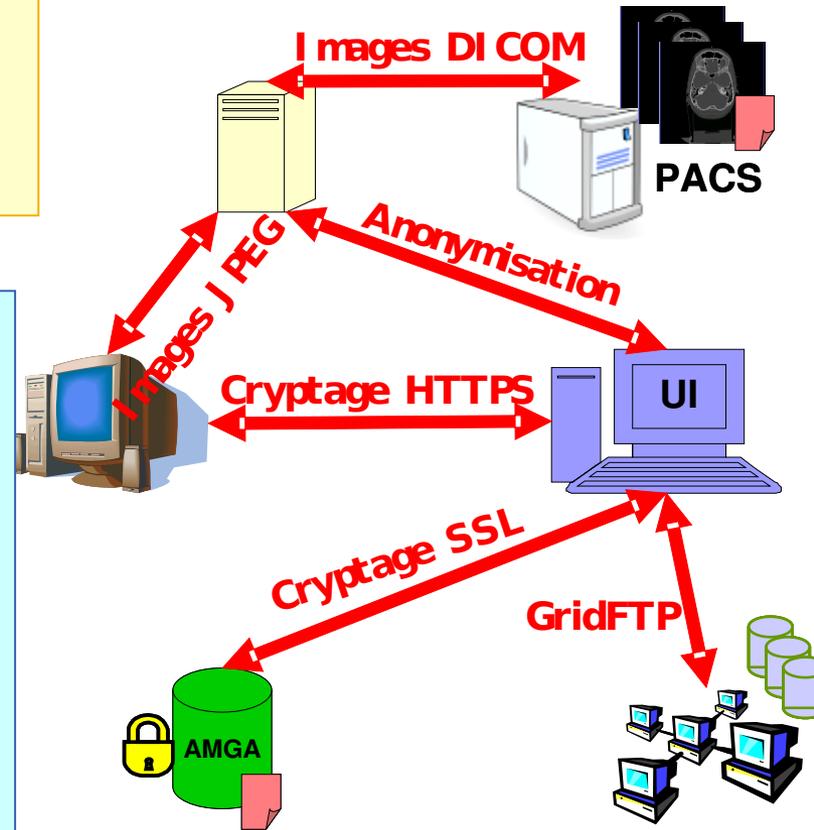
➤ AMGA intends to provide a replication layer which makes databases locally available to user jobs and replicate the changes between the different participating databases.

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

Registration and management of medical images

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

Jobs submissions and management

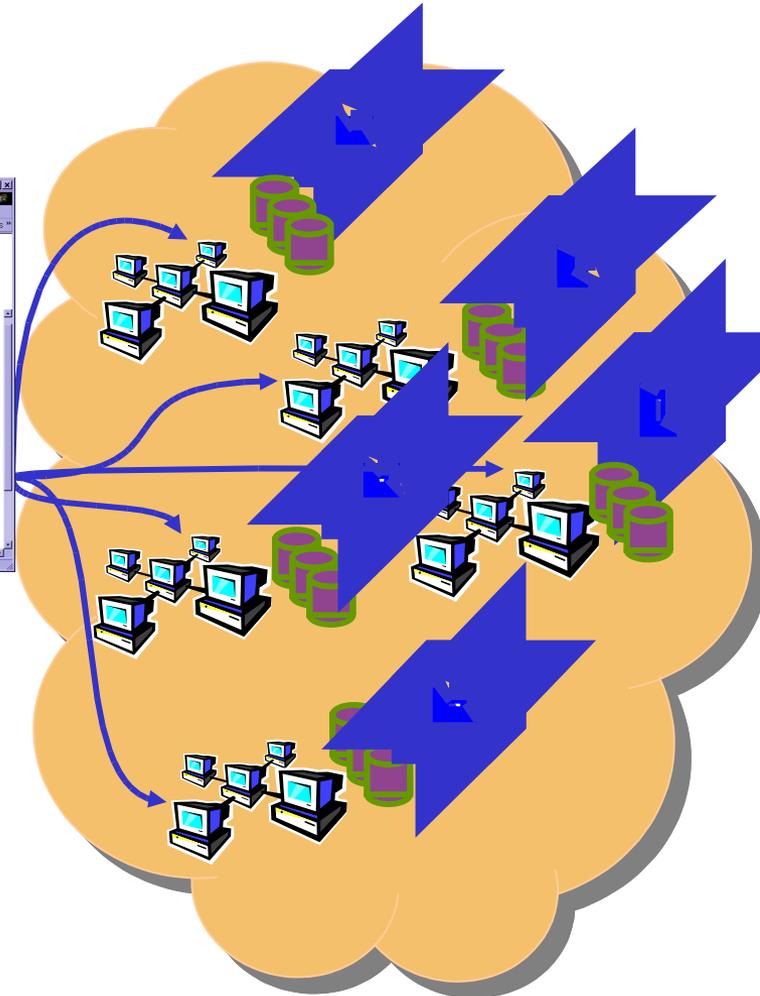
- **User secured authentication**
- **Splitting of simulations**
- **Automatic files creation** submitted to the grid
- **Jobs submission**
- **Jobs management**
- **Automatic data retrieving** (spectrum, isodoses...)



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 [Home](#)
[Resource Broker: biomed](#)
[Virtual Organization: biomed](#)
[Catalog Type: fireman](#)
[Catalog Server: gilda](#)
[Your Data](#)
[Logout](#)

Welcome to GENIUS and Biomedical GATE Application Portal

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

This portal is best viewed with Mozilla 1.7.12 or higher.
 Netscape (4.79, 4.80, 0 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 M: 10:53



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)

InputData lfn:
 macro (.mac)

Number of Partitions

Status Files (=Number of Partitions)

Jobs Settings

- up
- ▶ 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

- 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	
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

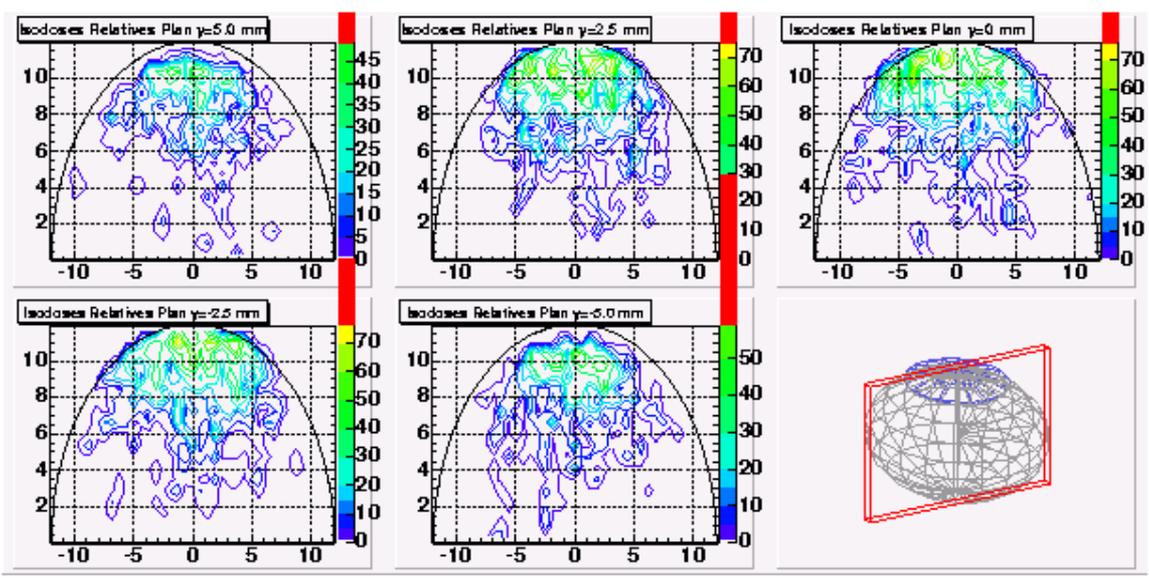
Job execution completed, analysing data.....
 Merging of Root files done.....creating graphical output
 All jobs output have been retrieved in `/home/maigne/GATE/outputs/gate_job_list_20041112_143643`. If the production was less than 3 days ago, you can also inspect the output from its copy on the spooler directory [gate_job_list_20041112_143643](#)



Grid Enabled web eNvironment for site Independent User job Submission

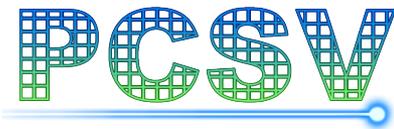
- Jobs Services
- up
- Jobs Settings
- Jobs Submission
- Jobs Queue
- GATE job data

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



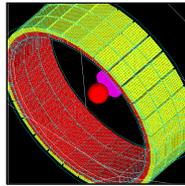
IV: Functionalities of a web portal for simulations in medical physics

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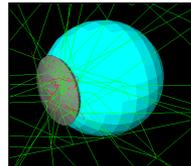


Projects using web services
(Sept 2007 - Sept 2008)

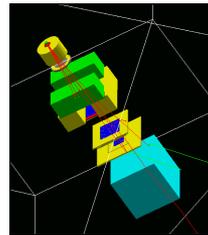
Simulations Monte Carlo



Camera TEP

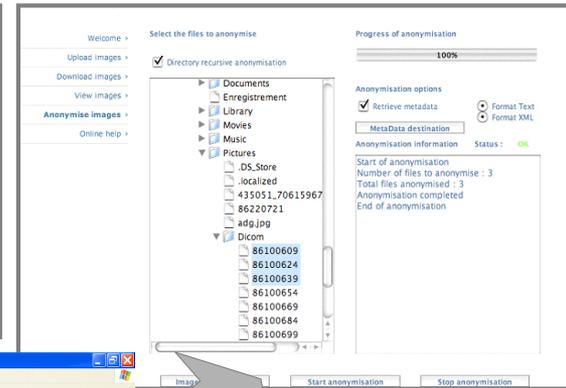
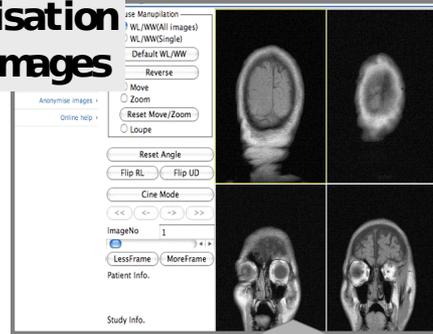


Traitement de curiethérapie oculaire



Radiothérapie

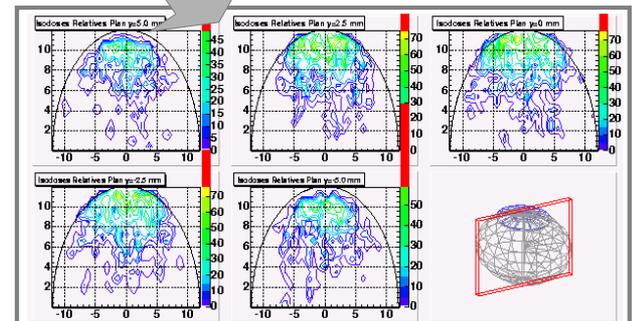
Visualisation des images



Anonymisation des images



La visualisation des résultats



AppletViewer: amga.Amgainterface.class

Select Dicom metadata you want to register

<input checked="" type="checkbox"/> Modality	<input checked="" type="checkbox"/> Study ID	<input checked="" type="checkbox"/> Image number
<input checked="" type="checkbox"/> Patient name	<input checked="" type="checkbox"/> Study description	<input checked="" type="checkbox"/> Image type
<input checked="" type="checkbox"/> Patient ID	<input checked="" type="checkbox"/> Study date	<input checked="" type="checkbox"/> Image date
<input checked="" type="checkbox"/> Patient sex	<input checked="" type="checkbox"/> Study time	<input checked="" type="checkbox"/> Image time
<input checked="" type="checkbox"/> Patient weight	<input checked="" type="checkbox"/> Acquisition number	<input checked="" type="checkbox"/> Sequence name
<input checked="" type="checkbox"/> Patient birth date	<input checked="" type="checkbox"/> MR acquisition type	<input checked="" type="checkbox"/> Scanning sequence
<input checked="" type="checkbox"/> Patient age	<input checked="" type="checkbox"/> Acquisition date	<input checked="" type="checkbox"/> Sequence variant
<input checked="" type="checkbox"/> Patient position	<input checked="" type="checkbox"/> Acquisition time	<input checked="" type="checkbox"/> Slice thickness
<input checked="" type="checkbox"/> Physician name	<input checked="" type="checkbox"/> Series number	<input checked="" type="checkbox"/> Slice location
<input checked="" type="checkbox"/> Institution name	<input checked="" type="checkbox"/> Series description	<input checked="" type="checkbox"/> Imaging frequency
<input checked="" type="checkbox"/> Institution address	<input checked="" type="checkbox"/> Series date	
<input checked="" type="checkbox"/> Station name	<input checked="" type="checkbox"/> Series time	
<input checked="" type="checkbox"/> Manufacturer model		
<input checked="" type="checkbox"/> Manufacturer		

Select Dicom images to register

Directory recursive Amga registration

Progress of Amga registration: 0%

Amga registration information

Start Amga registration

Number of files to register : 1

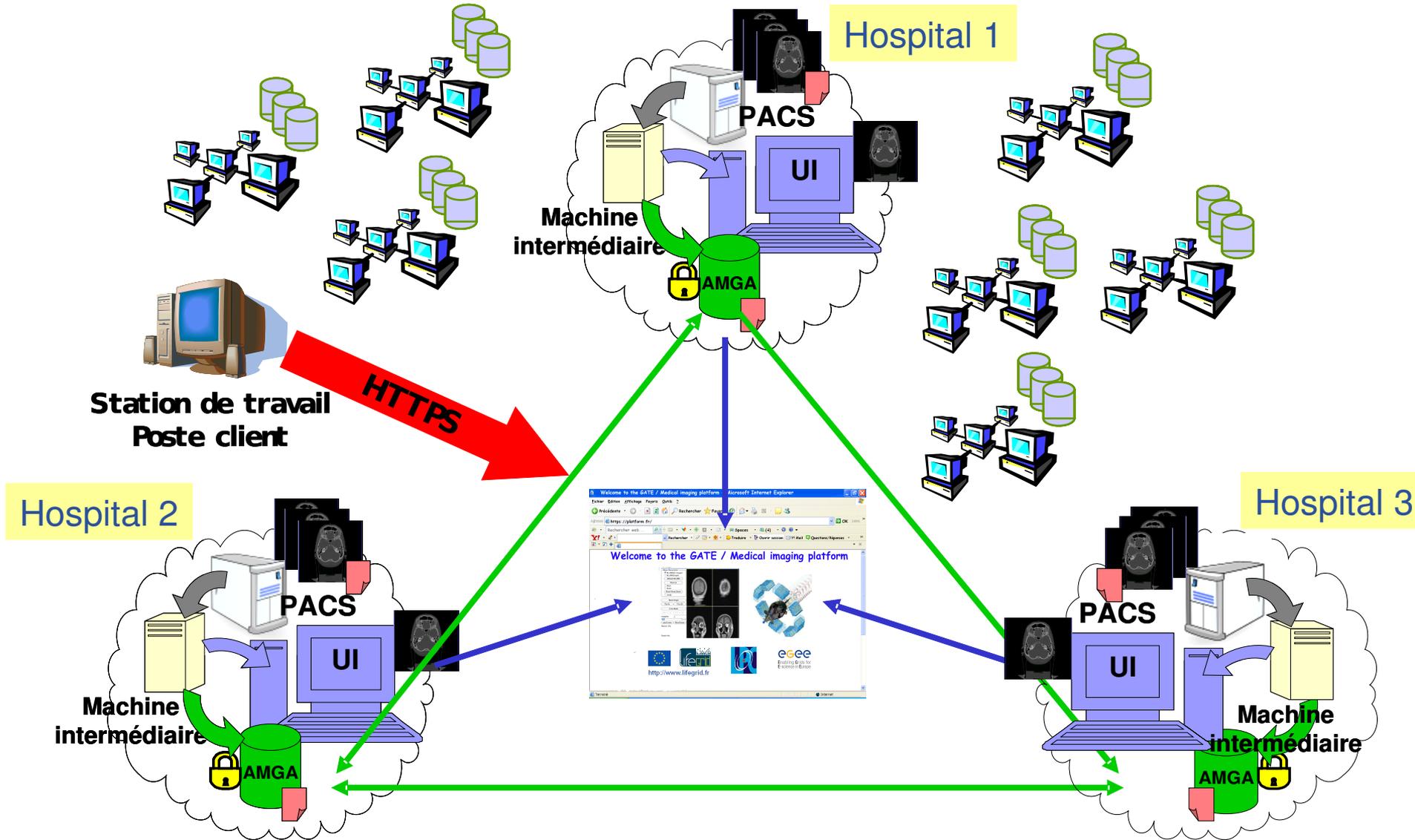
Disabled Dicom fields :

- > Modality
- > Patient name
- > Patient ID
- > Patient sex
- > Patient birth date

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 (not current but still useful)**
 - <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/>
to submit incidents for a VO, a site, etc.