Life sciences production on the EGEE grid infrastructure

CSIR

Pretoria, May 12, 2008

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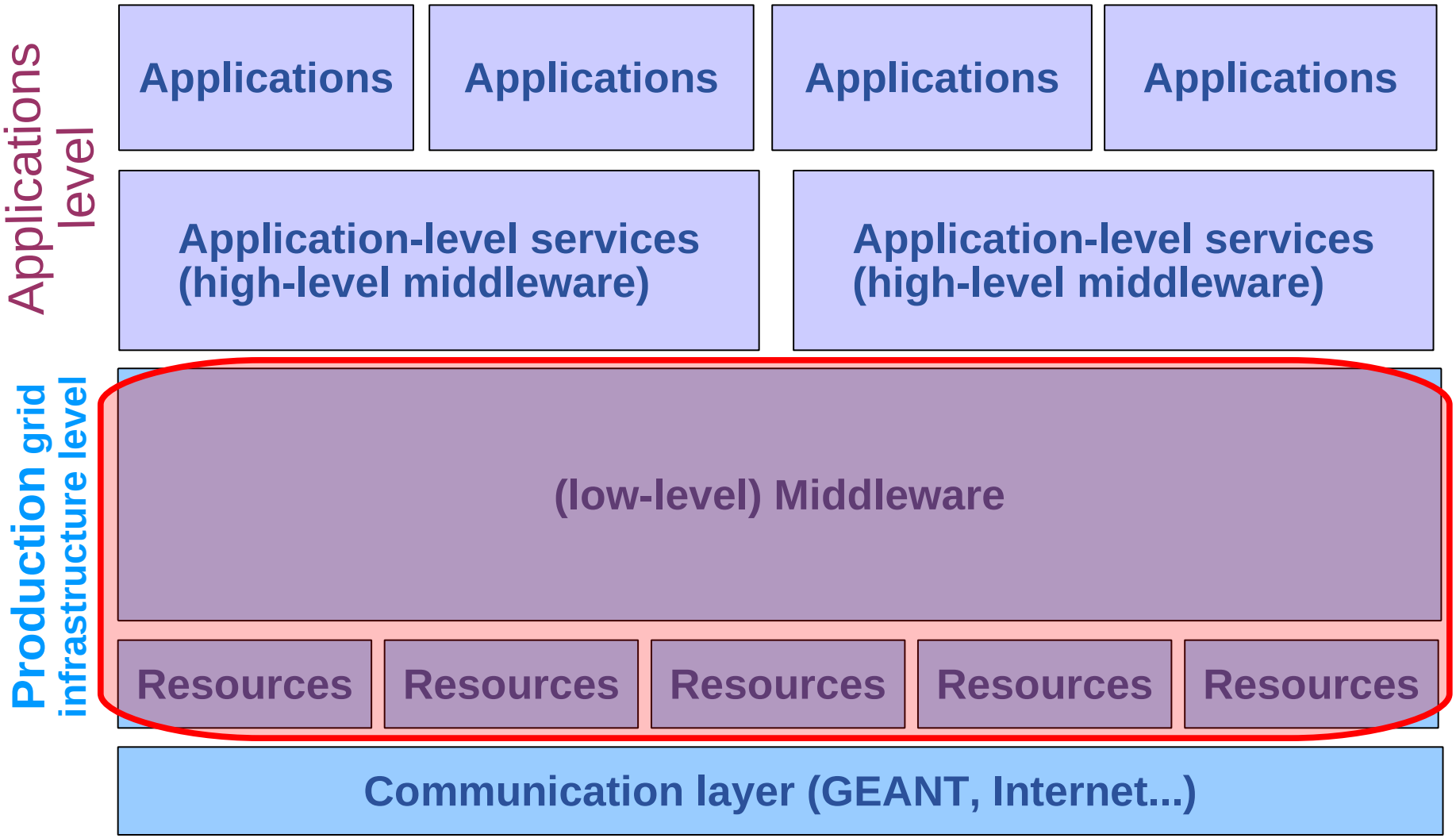
Building on Production Grids

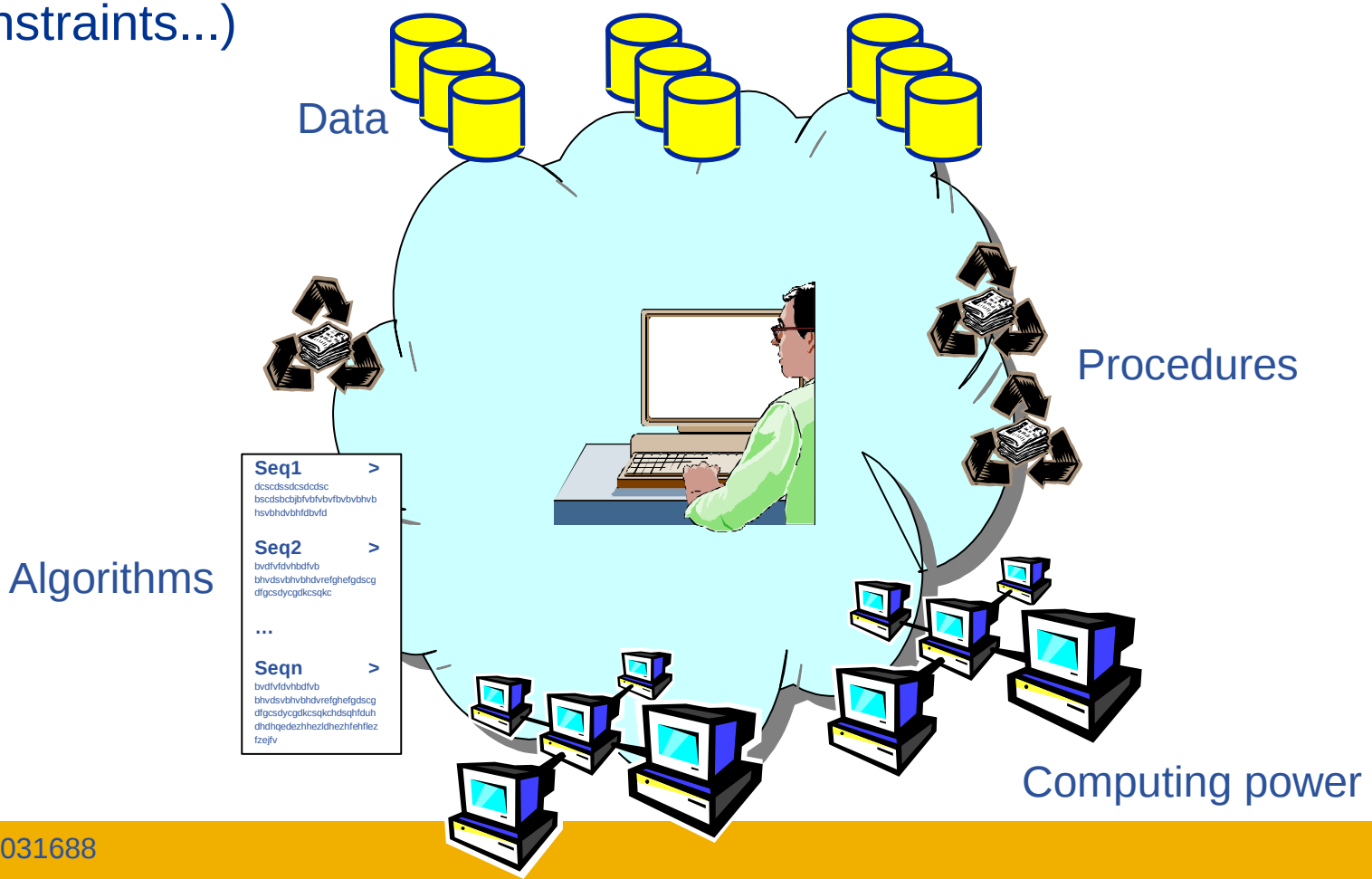


gLite middleware

- **Complex middleware stack**
  - On top of Globus Toolkit 2, VDT, CONDOR, batch schedulers...
- **Fundational services**
  - User authentication and authorization
  - Information Index: registration of Computing Elements (CEs), Storage Elements (SEs), etc.
  - Workload Management System: workload distribution over sites
  - Data Management System: virtual file hierarchy, standard (SRM) interface to storage resources
- **Batch oriented**
  - EGEE is a federation of computing centers
  - and File Servers oriented

Why grids for life sciences?

- **Sharing computing resources and algorithms**
  - Research (populations studies, models design, validation, statistics)
  - Complex analysis (compute intensive image processing, time constraints...)

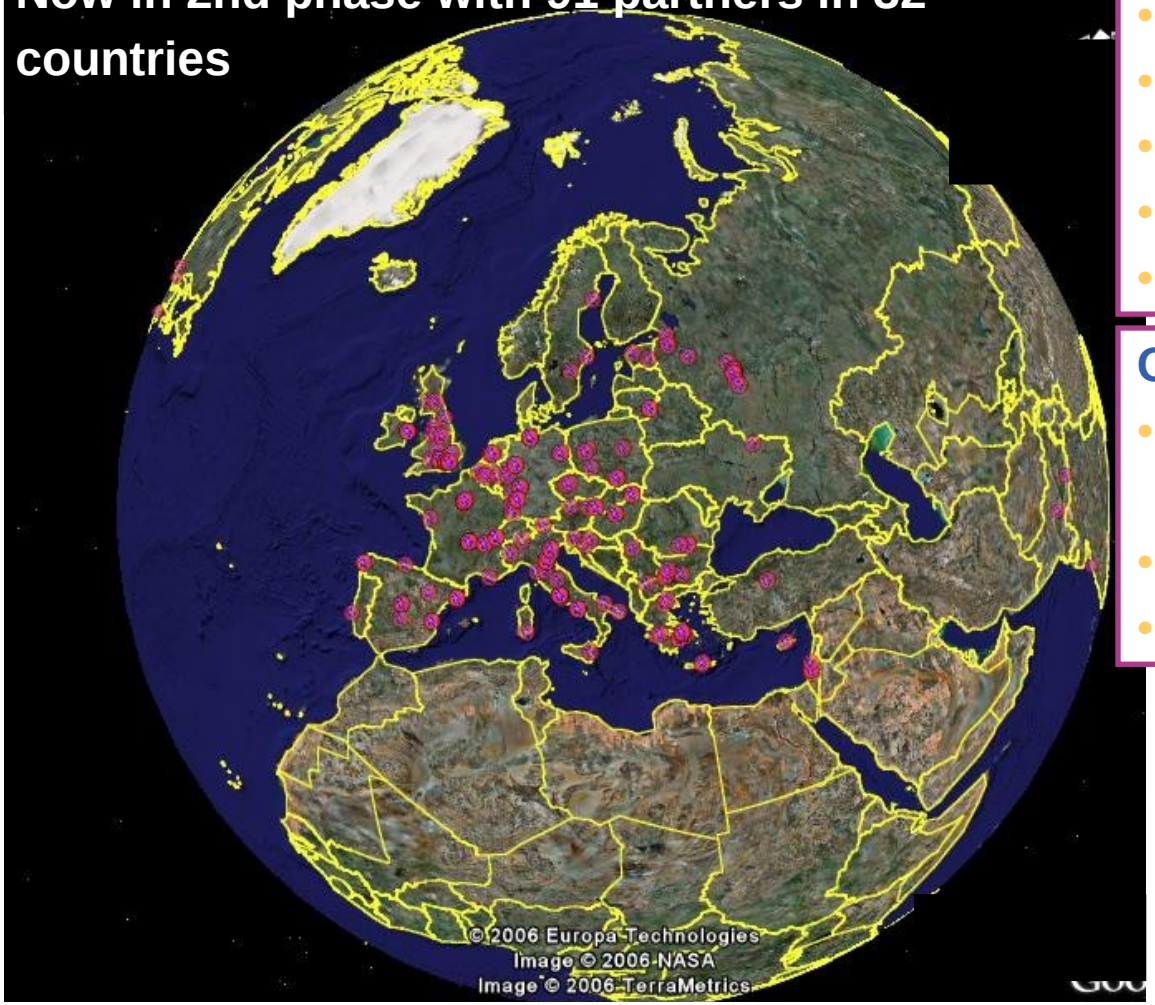


The *Biomed* Virtual Organization

- **Fostering scientific communities**
  - EGEE is an international, multi-disciplinary research infrastructure
  - Scientific communities are expanding beyond administrative boundaries
- **Virtual Organizations**
  - Authentication and Authorization management
  - Share resources (computers, data, algorithms...) inside a VO
  - Application areas identification and support unit
- **The Biomed VO now divided in 3 sectors**
  - Medical imaging
  - Bioinformatics
  - Drug discovery

EGEE Grid Infrastructure

Flagship European grid infrastructure project
Now in 2nd phase with 91 partners in 32 countries

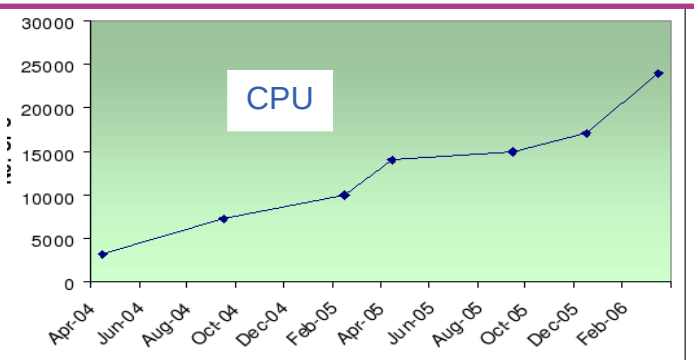


Size of the infrastructure today:

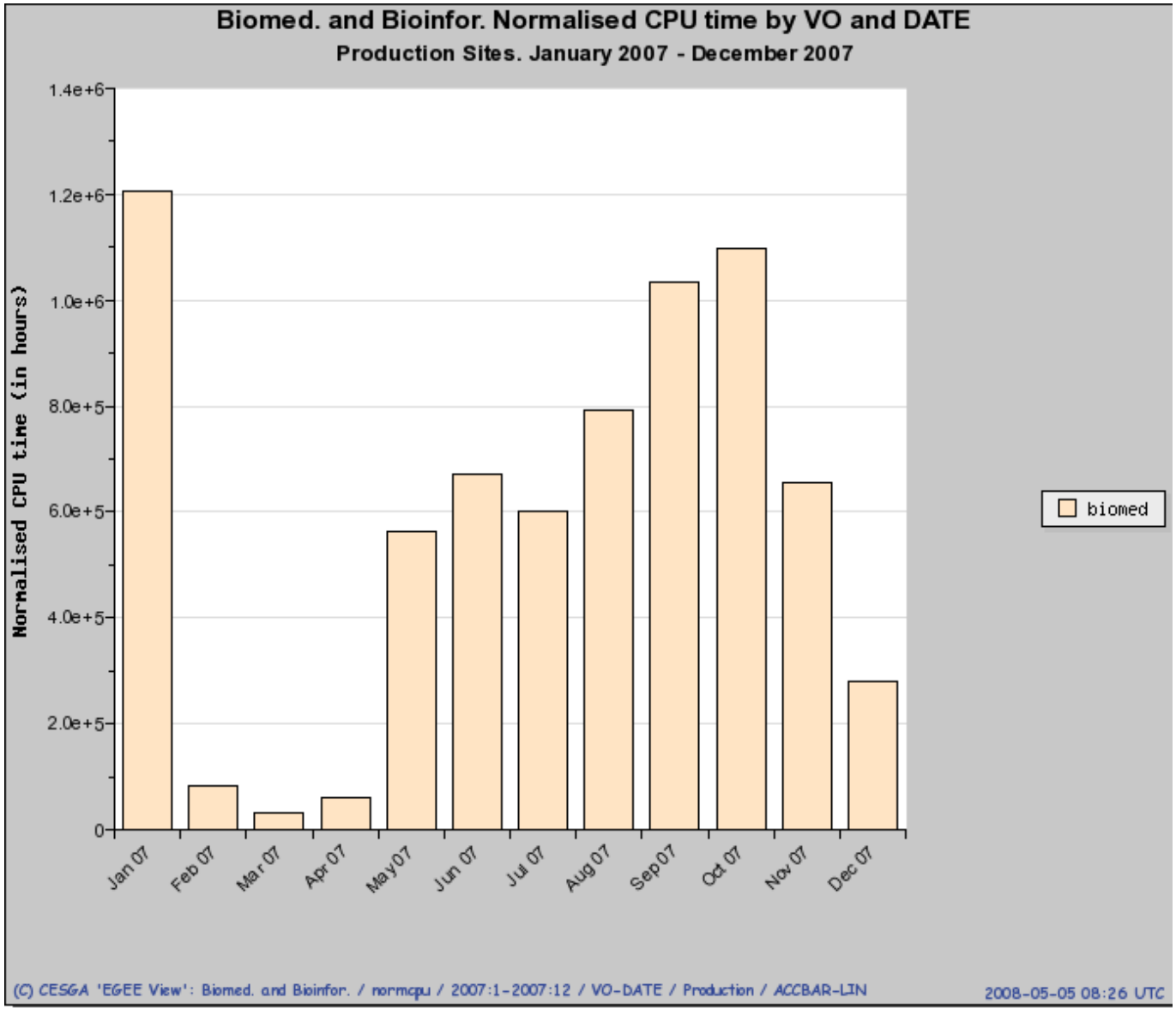
- **> 240 sites in 40 countries**
- **> 50 000 CPU**
- **~ 5 PB disk + tape MSS**
- **> 100 000 concurrent jobs/day**
- **> 8000 registered users**

Out of which, Biomed VO:

- **> 100 sites in 30 countries (170 CEs, 130 SEs)**
- **~ 17 000 CPU**
- **> 150 registered users**

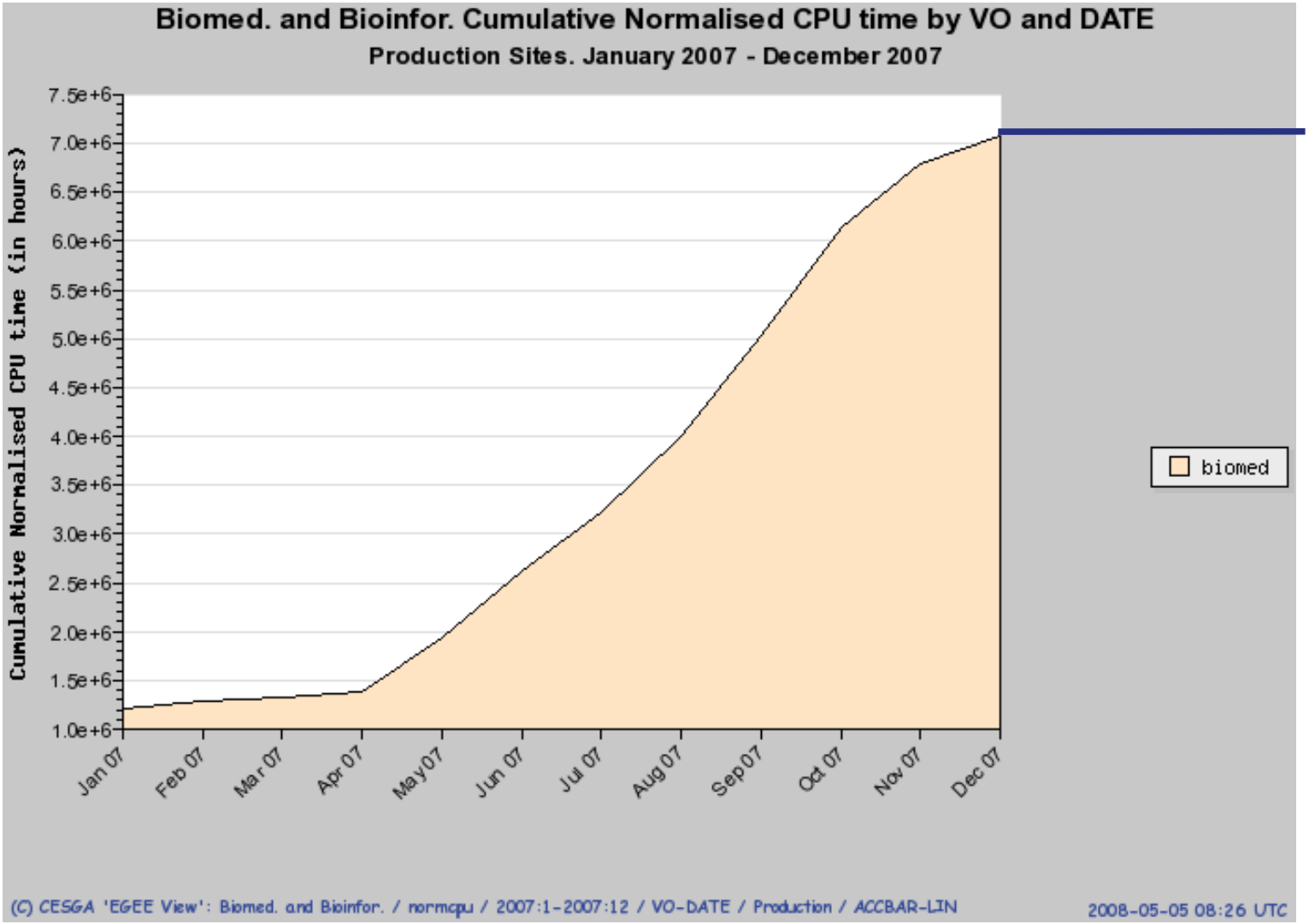


Irregular use through time



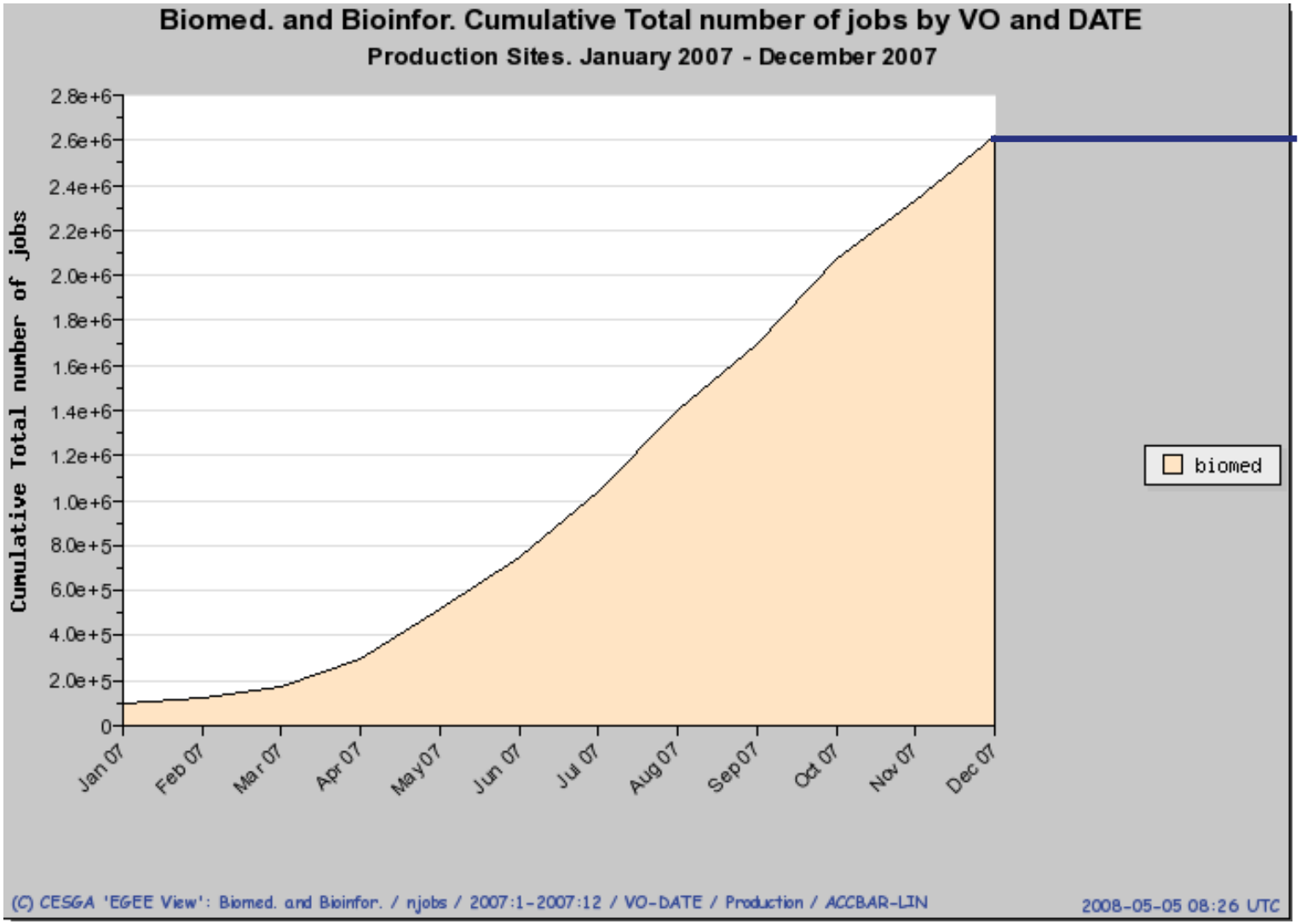
Year 2007 statistics collected per month

Total production in 2007



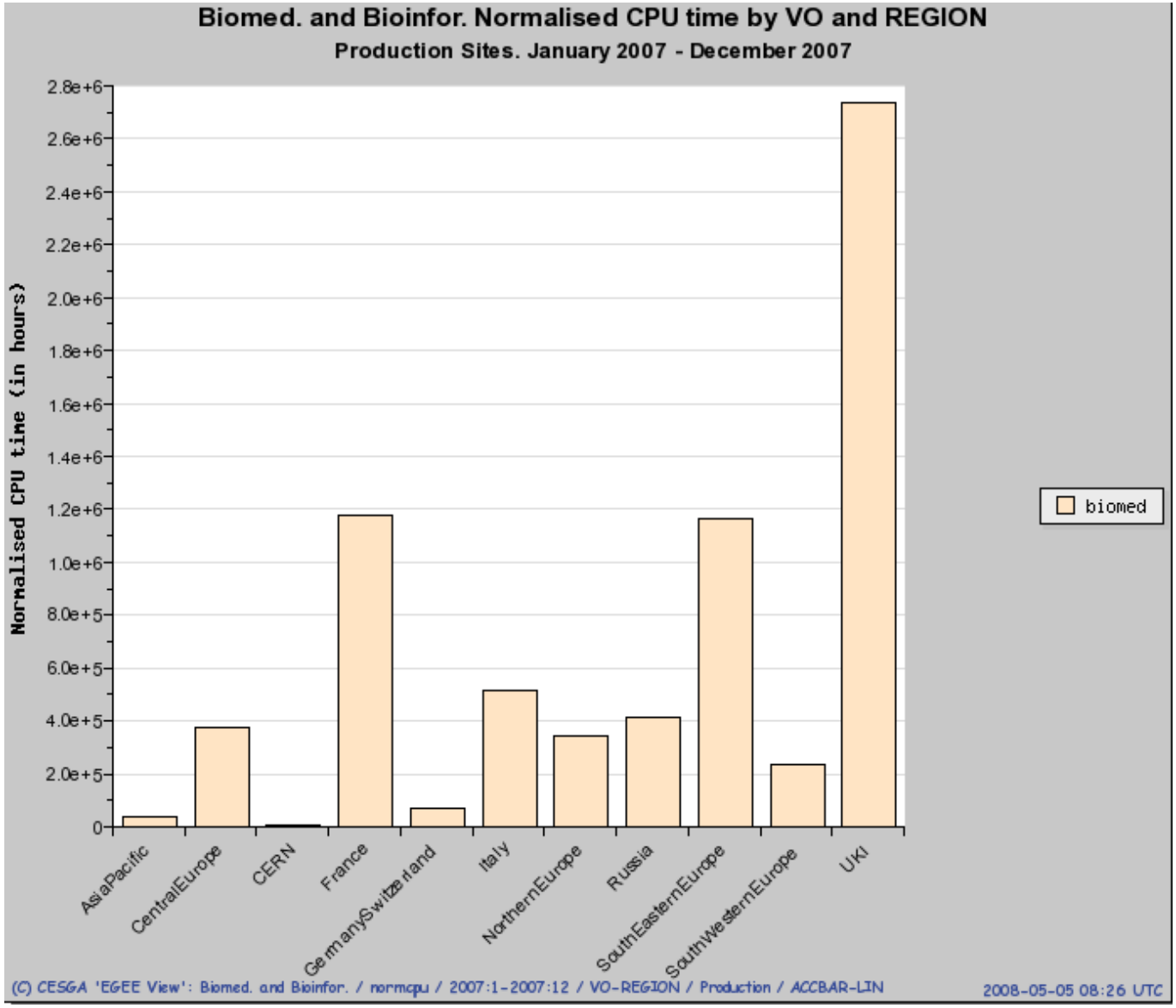
~800 CPU years
(1000 SpecInt 2000 Normalised CPU time)

Total production in 2007



~2,600,000 jobs

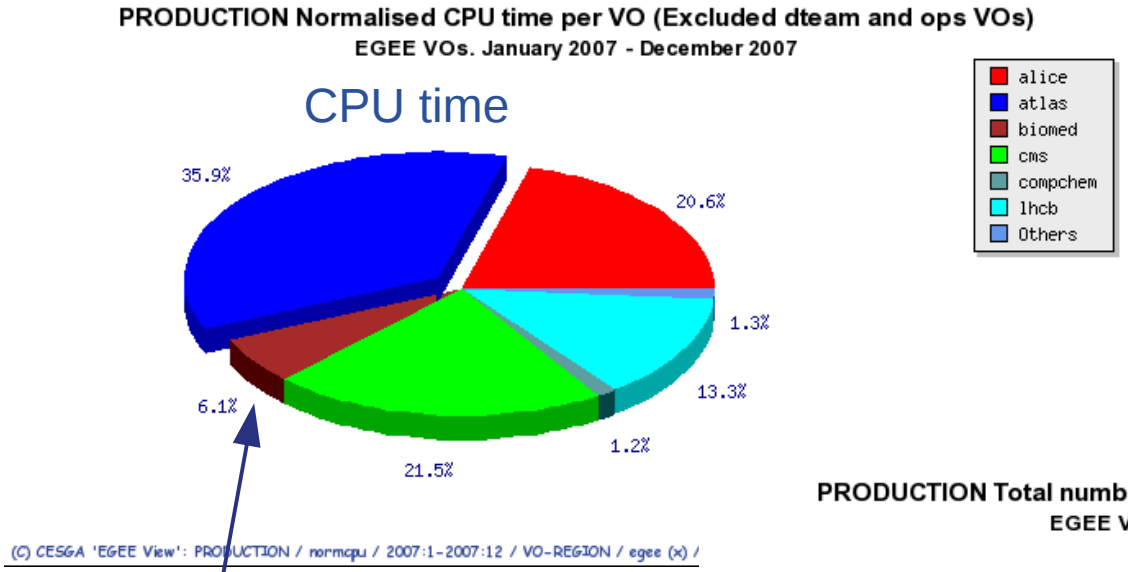
Computing resources provision



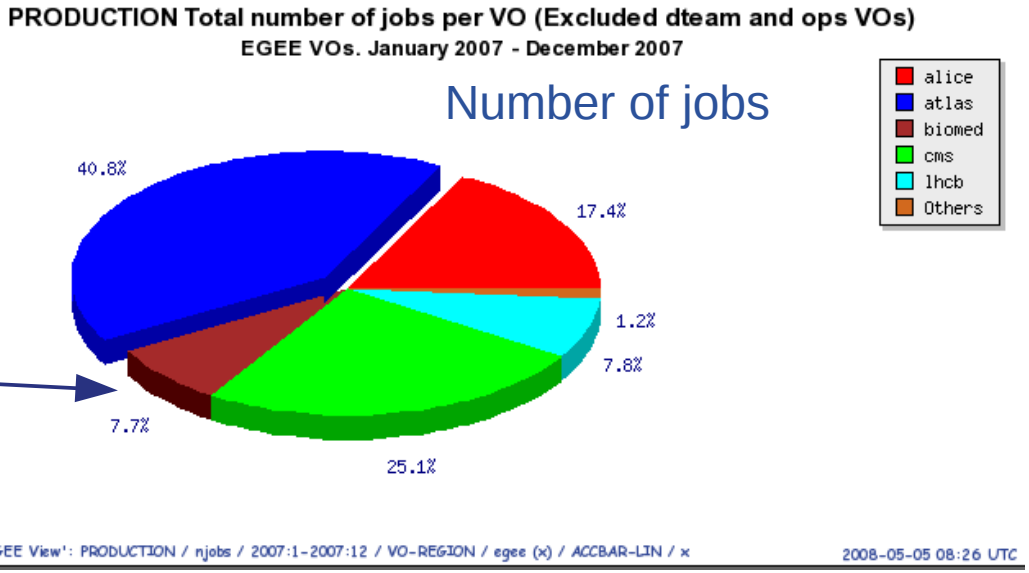
Computing hours per EGEE federation in 2007

Life sciences compared to other sciences

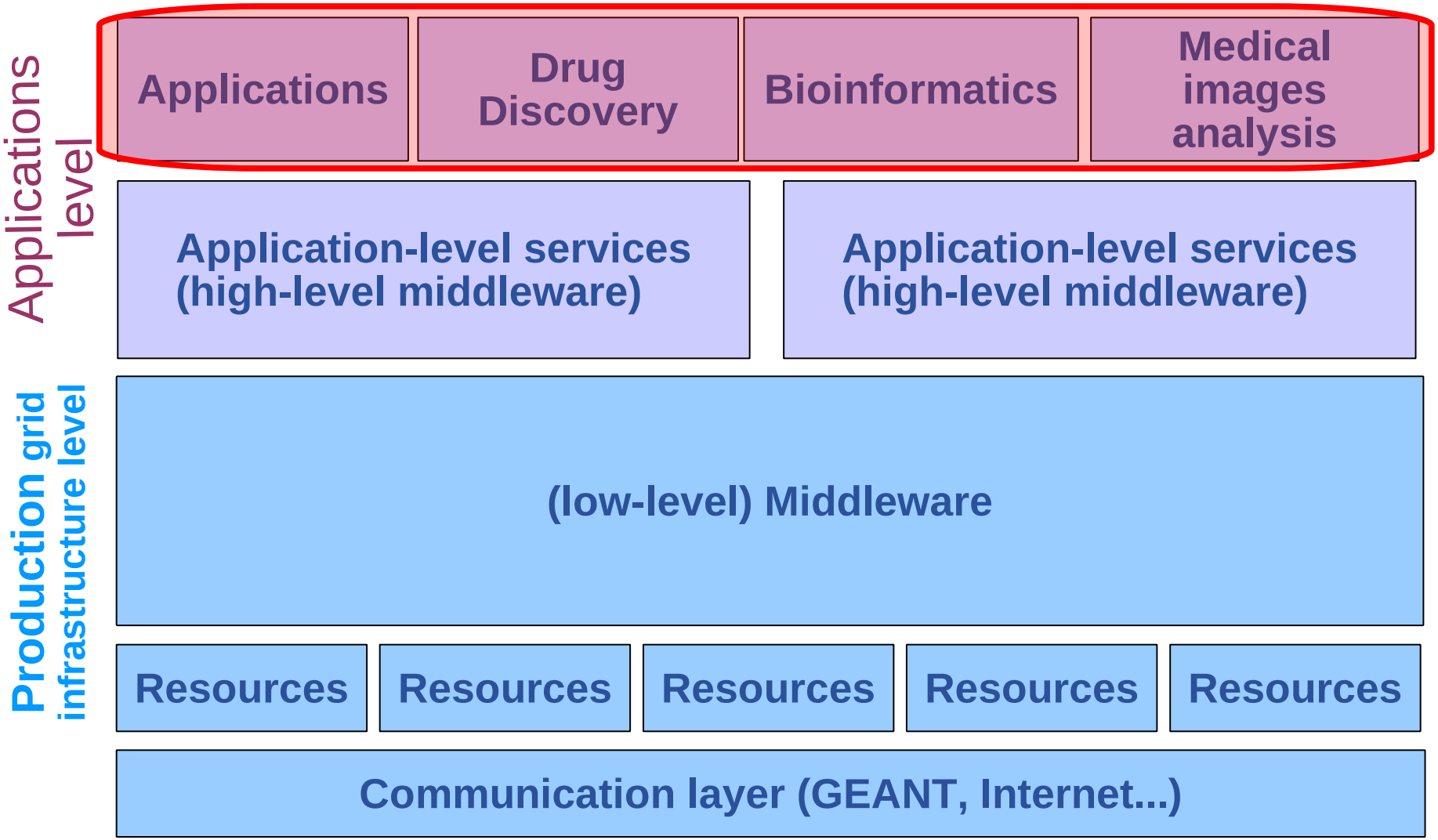
- **Biomed VO share**



Biomed VO



Building on Production Grids



WISDOM In silico Drug Discovery

- **WISDOM: http://wisdom.healthgrid.org/**
- **Goal: find new drugs for neglected and emerging diseases**
  - Neglected diseases lack R&D
  - Emerging diseases require very rapid response time
- **Need for an optimized environment**
  - To achieve production in a limited time
  - To optimize performances
- **Method: grid-enabled virtual docking**
  - Cheaper than in vitro tests
  - Faster than in vitro tests

Courtesy of V. Breton

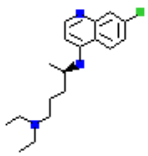
Grid-enabled virtual docking

Millions of potential drugs to test against interesting proteins!

~~High Throughput Screening ~10$/compound, several hours~~

Too costly for neglected disease!

Compounds:

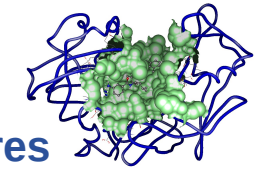


ZINC: 4.3M

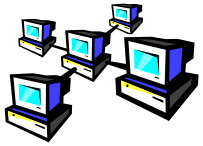
Chembridge: 500 000

Molecular docking (FlexX, Autodock)
~1 to 15 minutes

Targets:



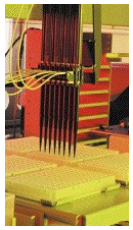
PDB: 3D structures



Data challenge on EGEE
~ 2 to 30 days on ~5000 computers

Cheap and fast!

Selection of the best hits



Hits screening using assays performed on living cells

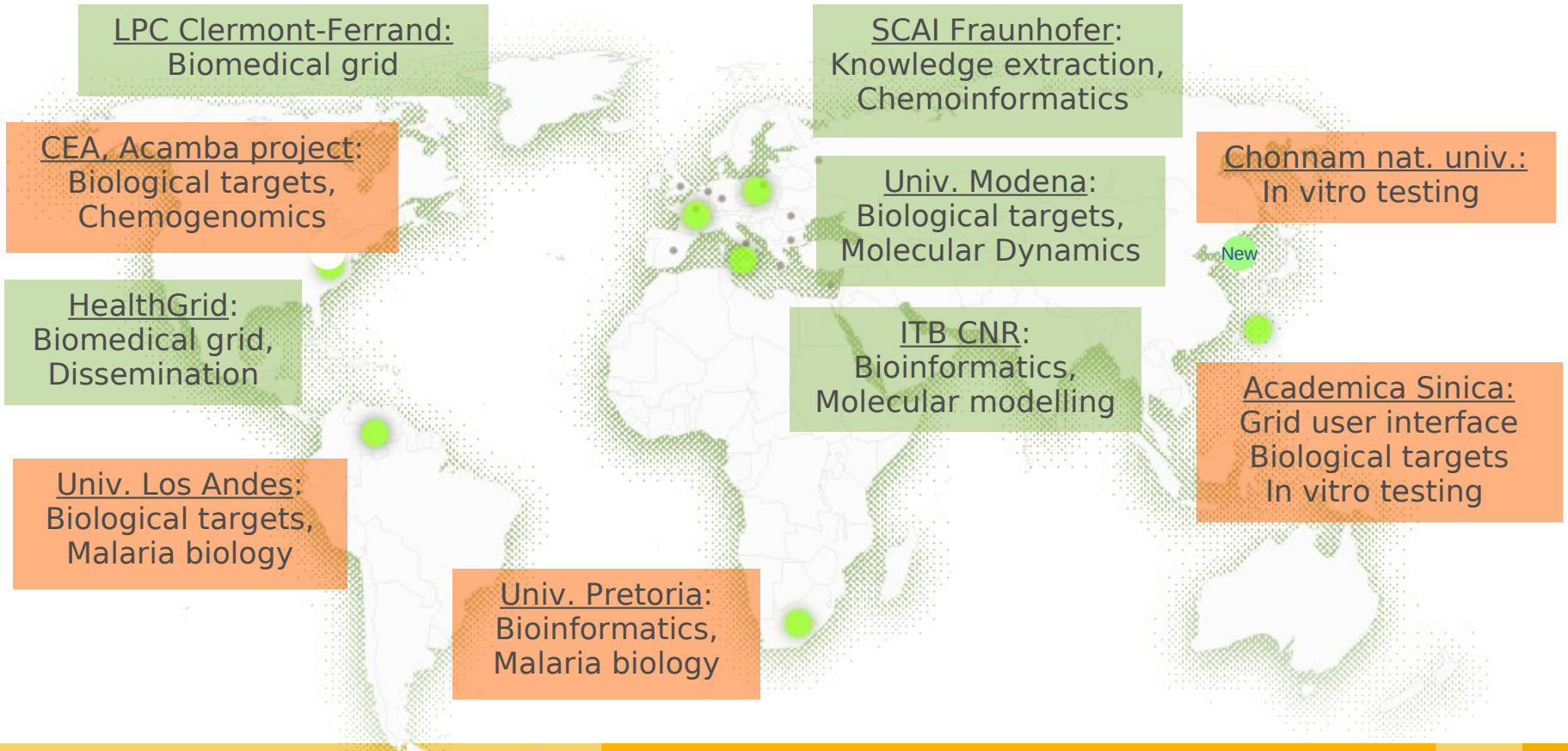
Leads

Clinical testing

Drug

The grid added value

- The grid provides the centuries of CPU cycles required on demand
- The grid provides the reliable and secure data management services to store and replicate the biochemical inputs and outputs
- The grid offers a collaborative environment for the sharing of data in the research community on avian flu and malaria

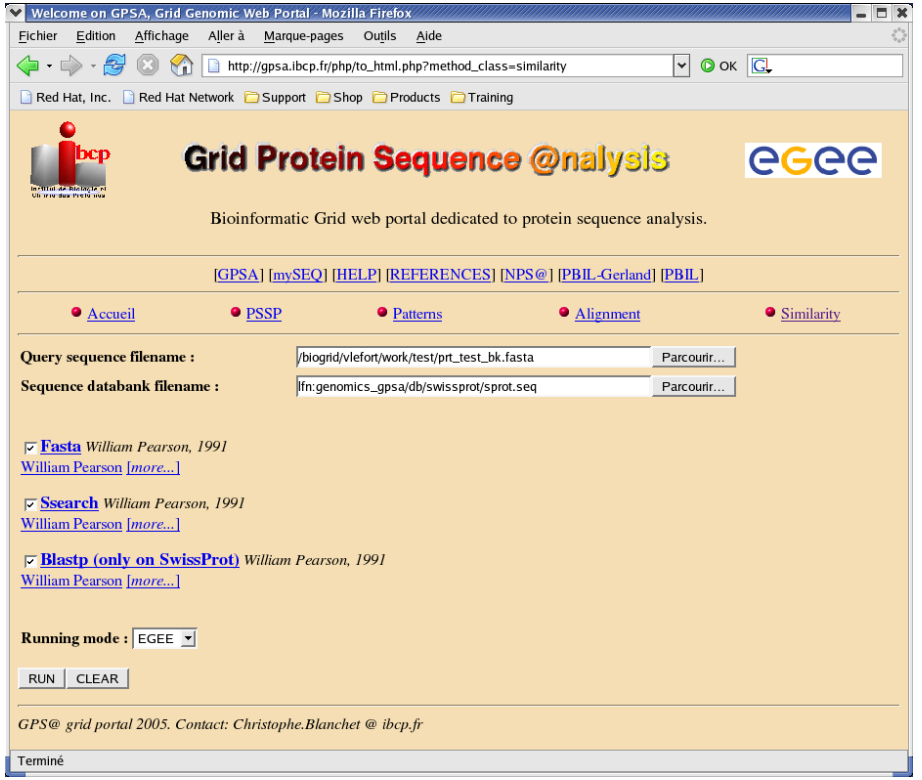


Statistics of deployment

- **First Data Challenge: July 1st - August 15th 2005**
  - Target: **malaria**
  - 80 CPU years
  - 1 TB of data produced
  - 1700 CPUs used in parallel
  - 1st large scale docking deployment world-wide on a e-infrastructure
- **Second Data Challenge: April 15th - June 30th 2006**
  - Target: **avian flu**
  - 100 CPU years
  - 800 GB of data produced
  - 1700 CPUs used in parallel
  - Collaboration initiated on March 1st: deployment preparation achieved in 45 days
- **Third Data Challenge: October 1st - 15th December 2006**
  - Target: **malaria**
  - 400 CPU years
  - 1,6 TB of data produced
  - Up to 5000 CPUs used in parallel
  - Very high docking throughput: > 100.000 compounds per hour

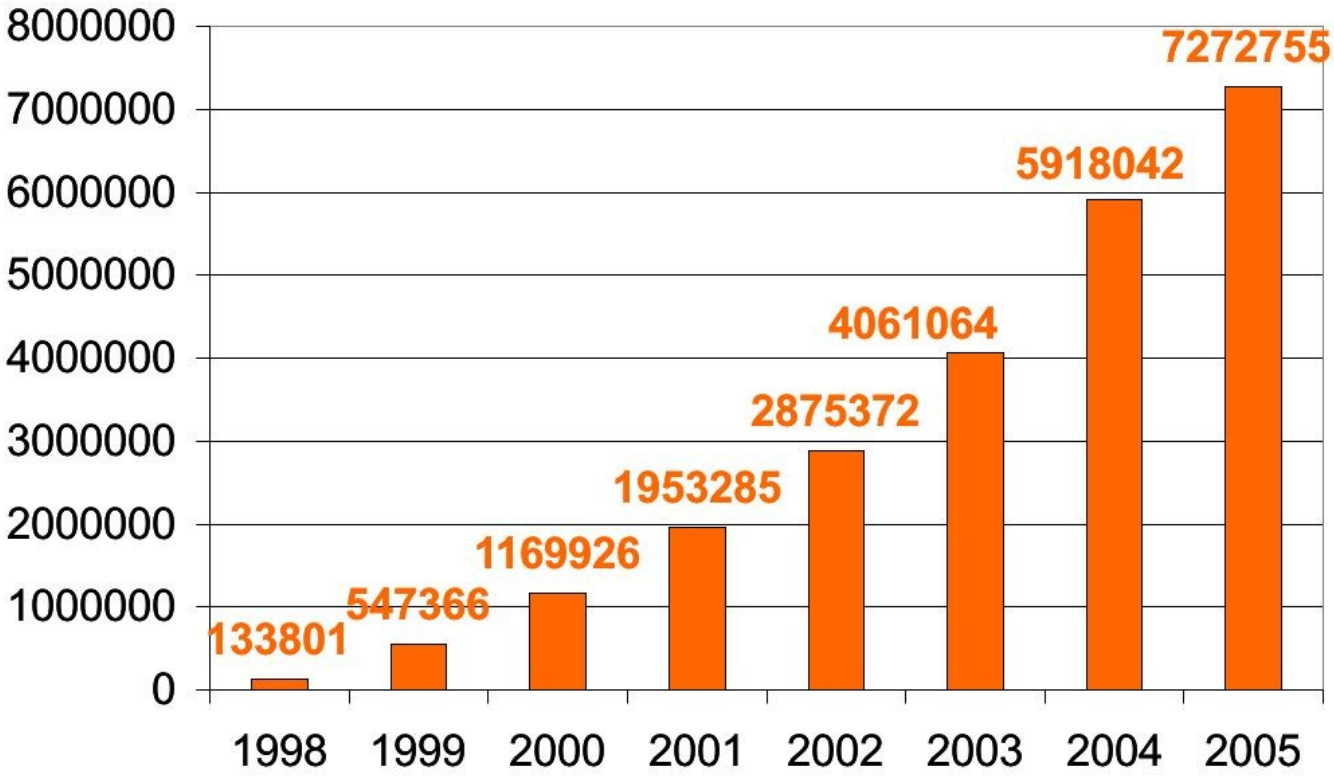
GPS@ : Grid Protein Sequence Analysis

- GPS@: bioinformatics portal
  - http://gpsa.ibcp.fr/ web portal
  - Relaces existing (but overloaded) NPSA portal
  - Tens of bioinformatics legacy code
  - Thousands of potential users
  - Large input databases

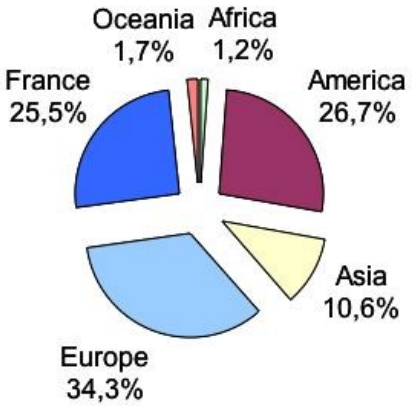


Courtesy of C. Blanchet

NPS@ Hits (from 1998)



- **> 7.000.000 analyses**
- **> 5000 analyses/day**

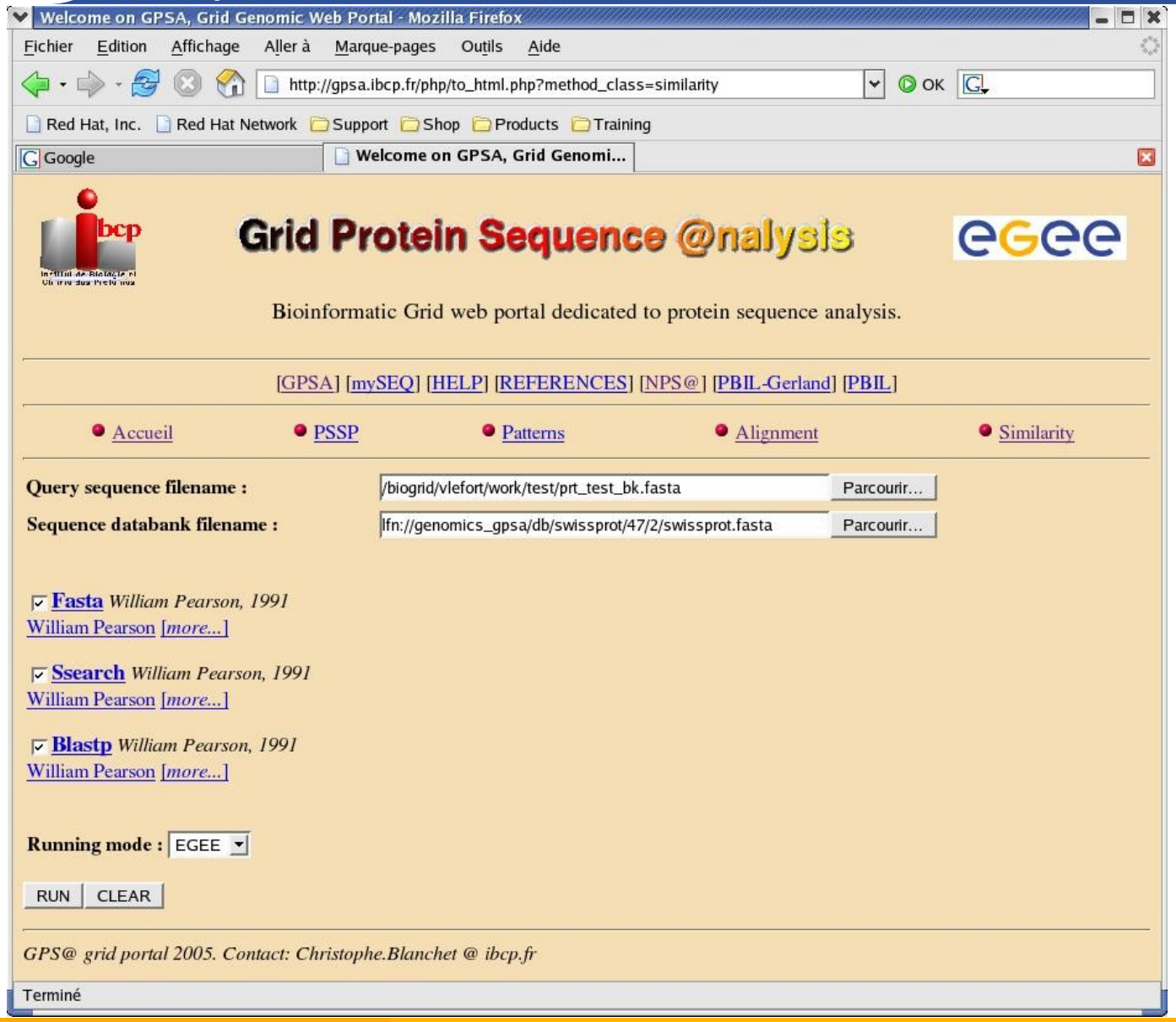


Courtesy of C. Combet

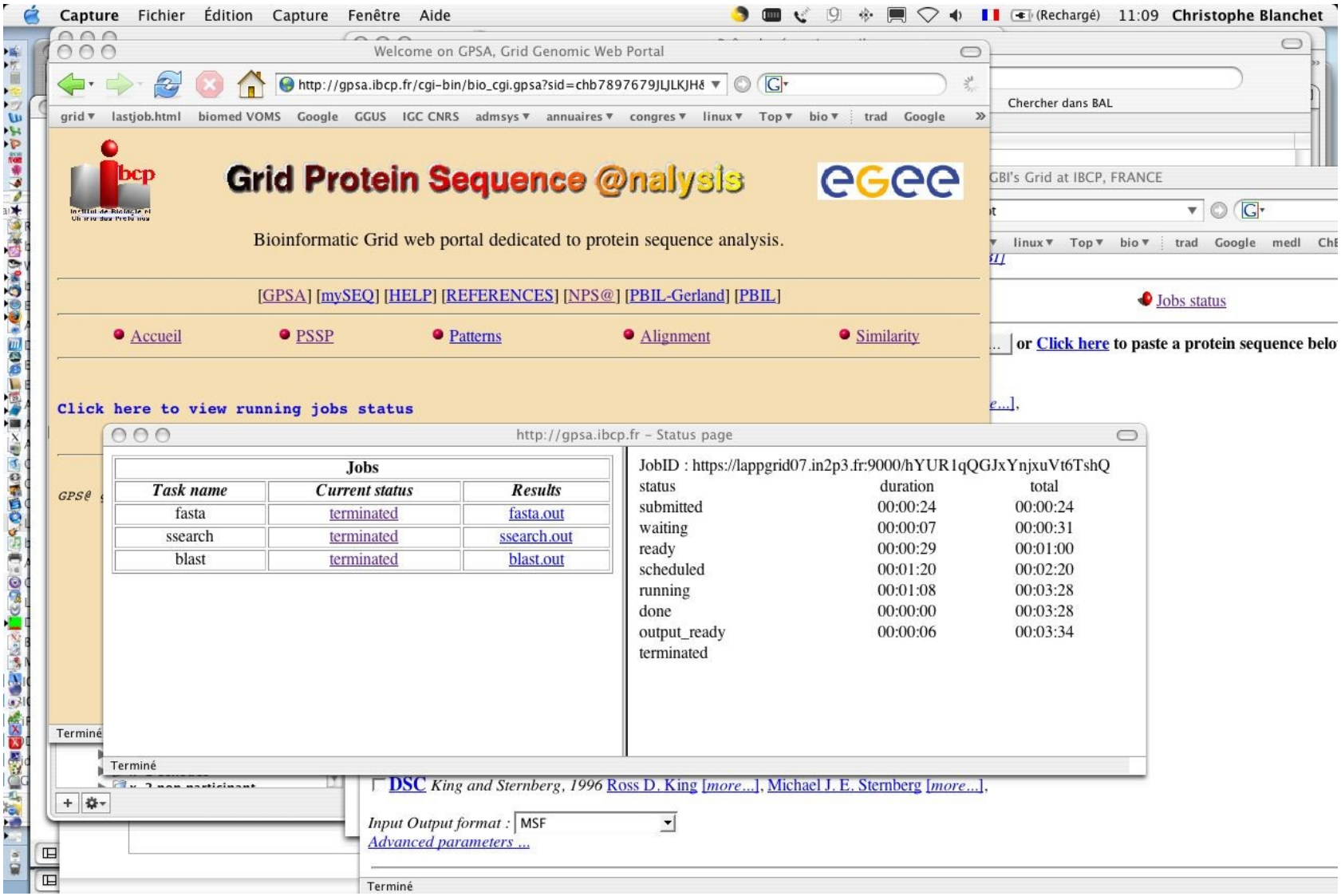
GPS@ services

- **Protein analysis methods**
  - Sequence similarity: BLAST, SSEARCH, FASTA
  - Multiple Alignment: ClustalW, MultAlin
  - Protein site/signatures: PattInProt
  - Secondary Struct. Pred: Predator, Gor4, Simpa96
- **Biological data (clear and encrypted)**
  - Sequence Bank: SWISSPROT, TrEMBL
  - Pattern/Profile bank: PROSITE

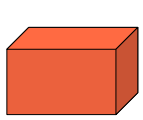
GPS@ Web Portal



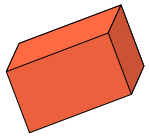
GPS@ Web Portal



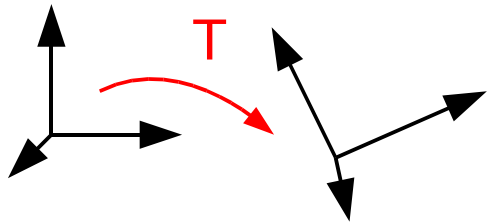
Application to rigid registration algorithms evaluation

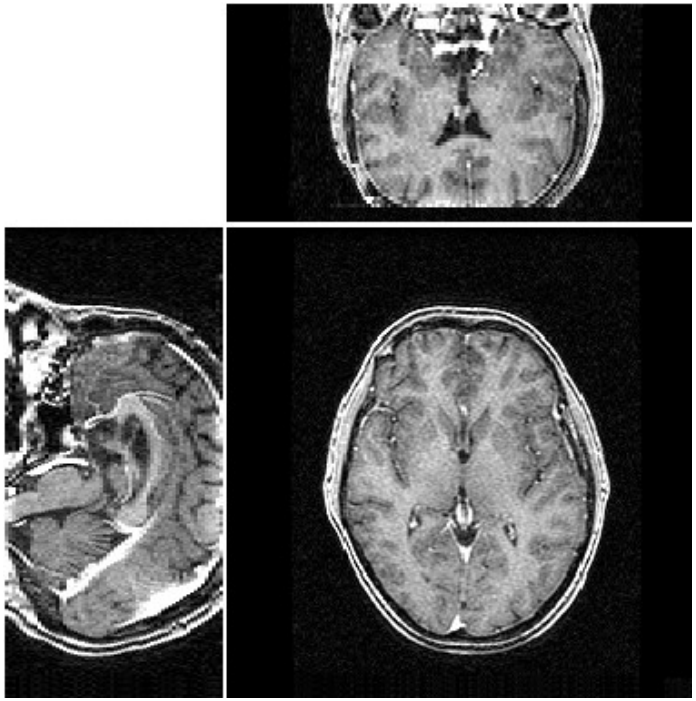


O_1

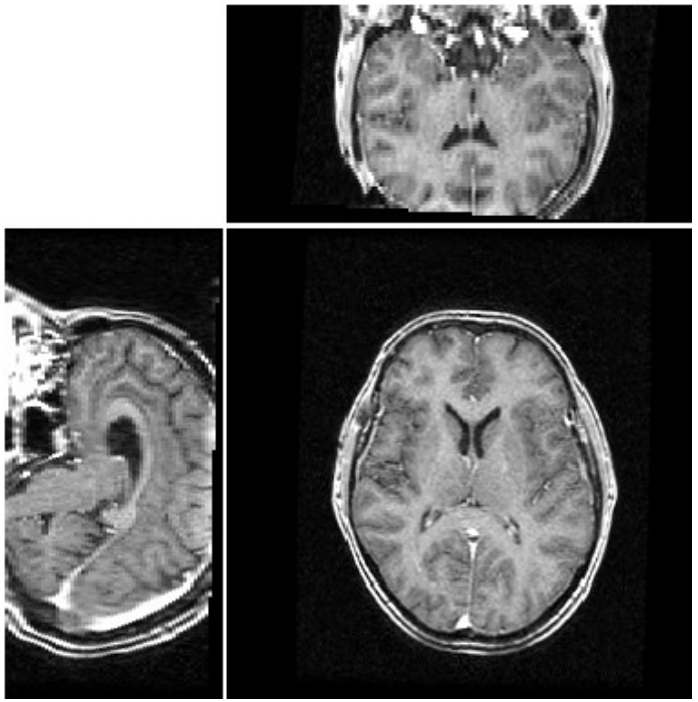


O_2





Unregistered

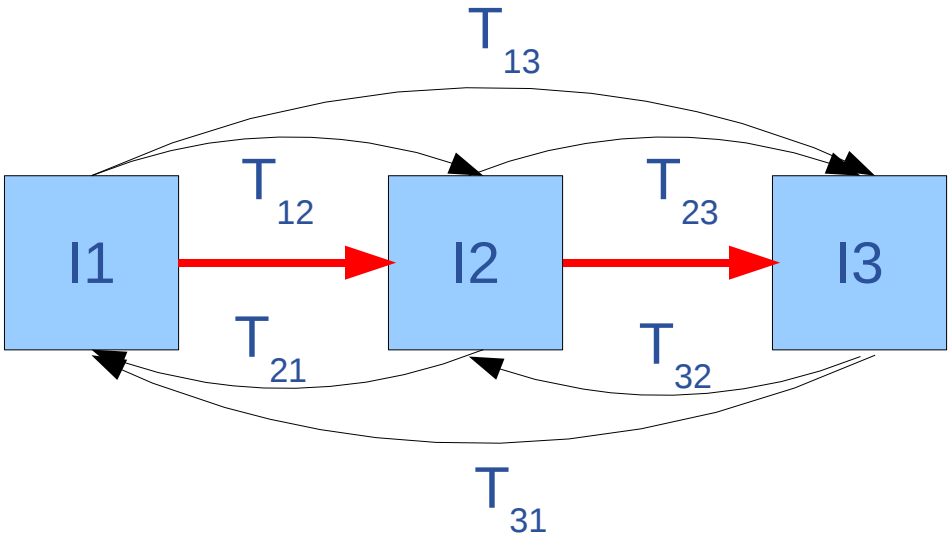


Registered

Bronze standard estimation

- **N images, m algorithms**
- **N.(N-1).m transformations measured**
- **N-1 transformations to estimate**

} Redundancy



- **Exploit redundancy to compute**
  - Mean transformations $\overline{T}_{ij}$ (Bronze standard)
  - Variances on the transformations (Accuracy)

Bronze standard workflow

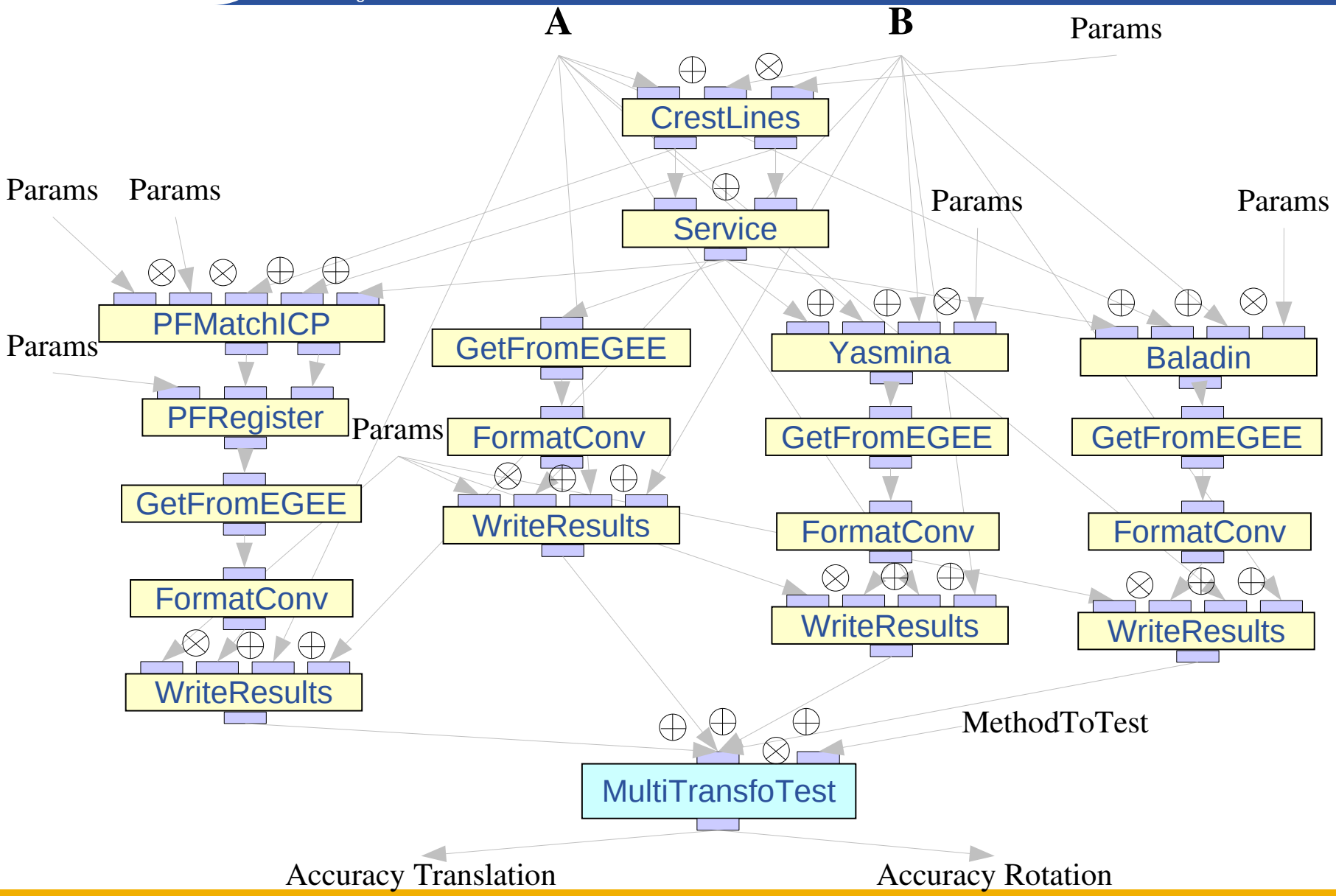
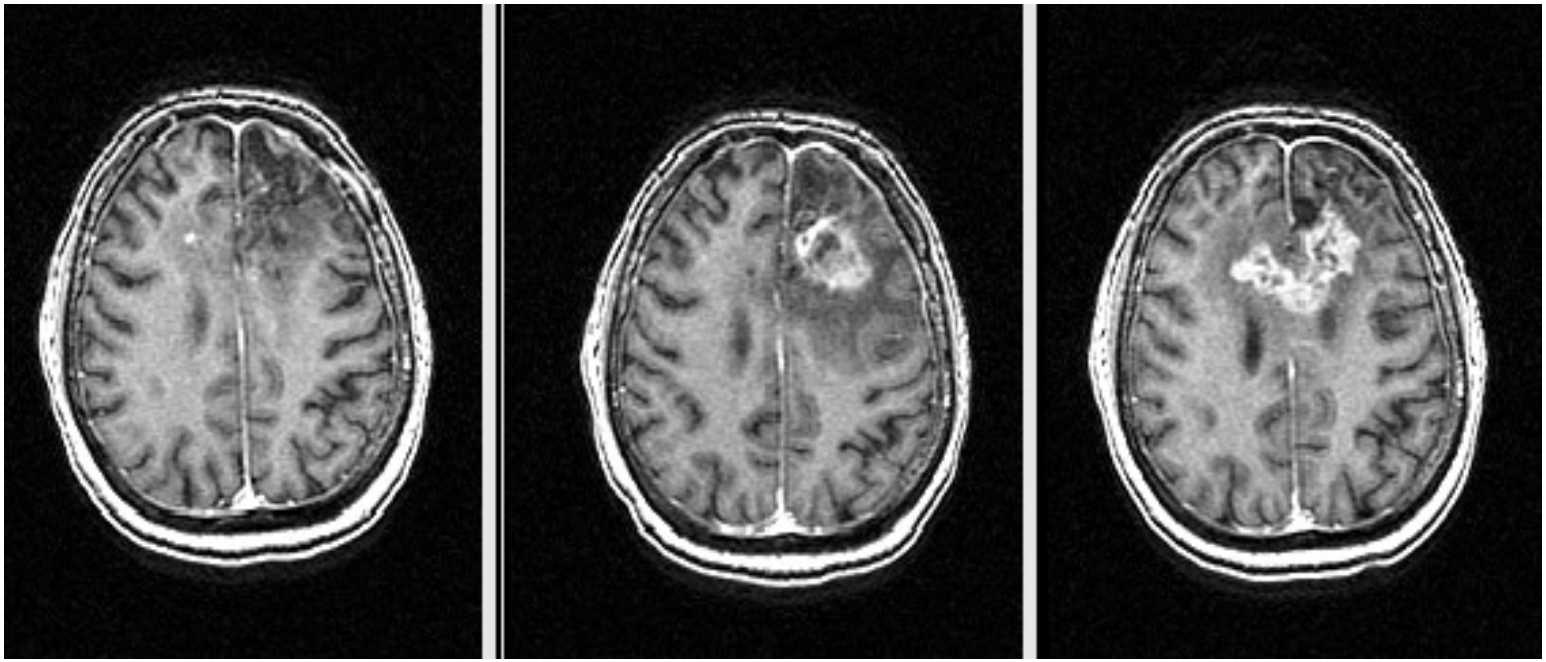


Image database

- 29 patients
- 2 time points minimum
- Gadolinium injected T1 MRIs
- Example for one patient (3 time points):



t1 t2 t3

Accuracy results

- **Mean error on the transformations:**

$$\sigma_r = 0.130\ deg\ ;\ \sigma_\tau = 0.345\ mm$$

- **Error on the bronze standard:**

$$\sigma_r = 0.05\ deg\ ;\ \sigma_\tau = 0.148\ mm$$

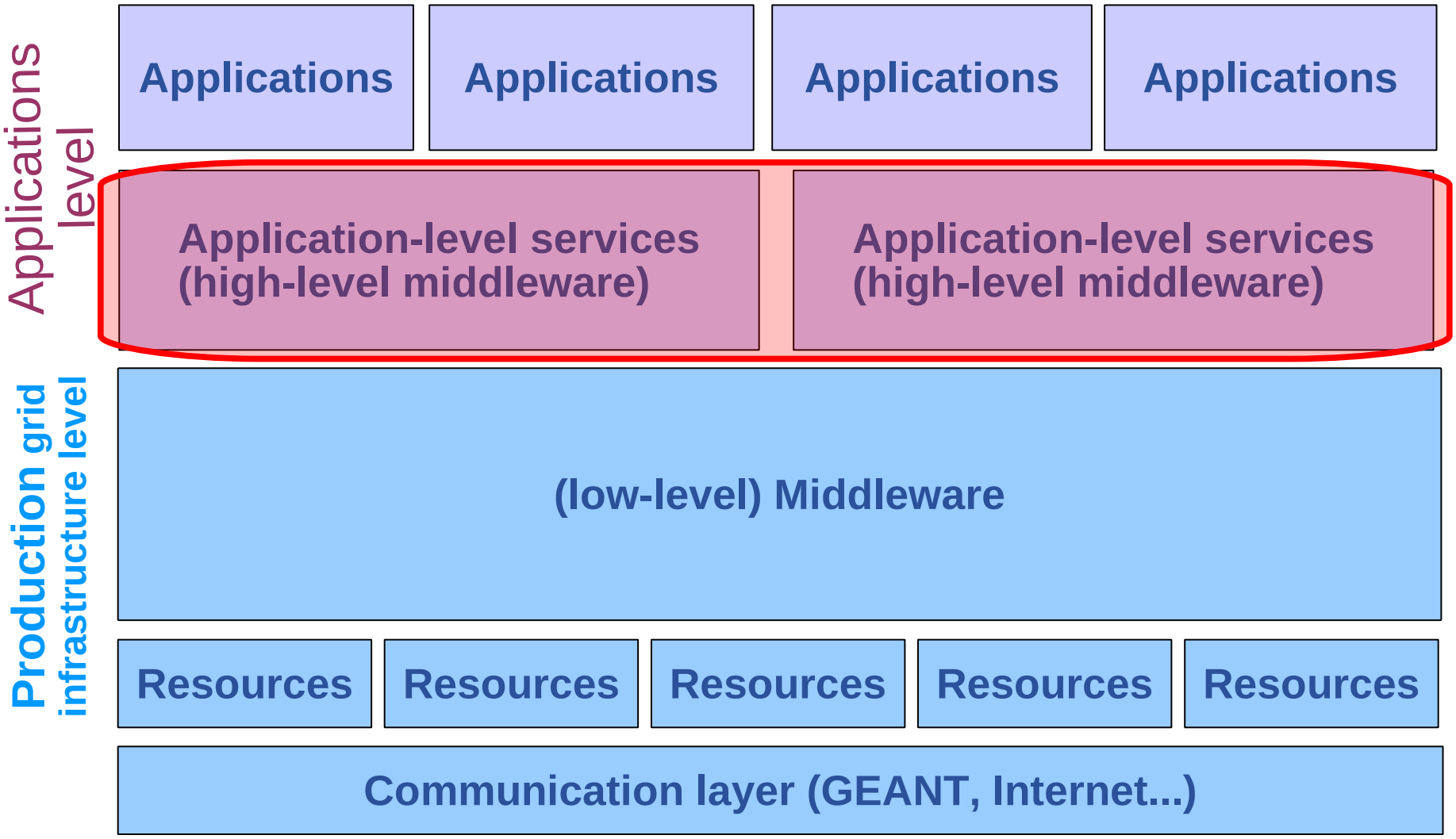
- **Accuracy of the algorithms:**

Algorithm	$\sigma_r (deg)$	$\sigma_t (mm)$
CrestMatch	0.150	0.424
PFRegister	0.180	0.416
Baladin	0.139	0.395
Yasmina	0.137	0.445

Application specific requirements

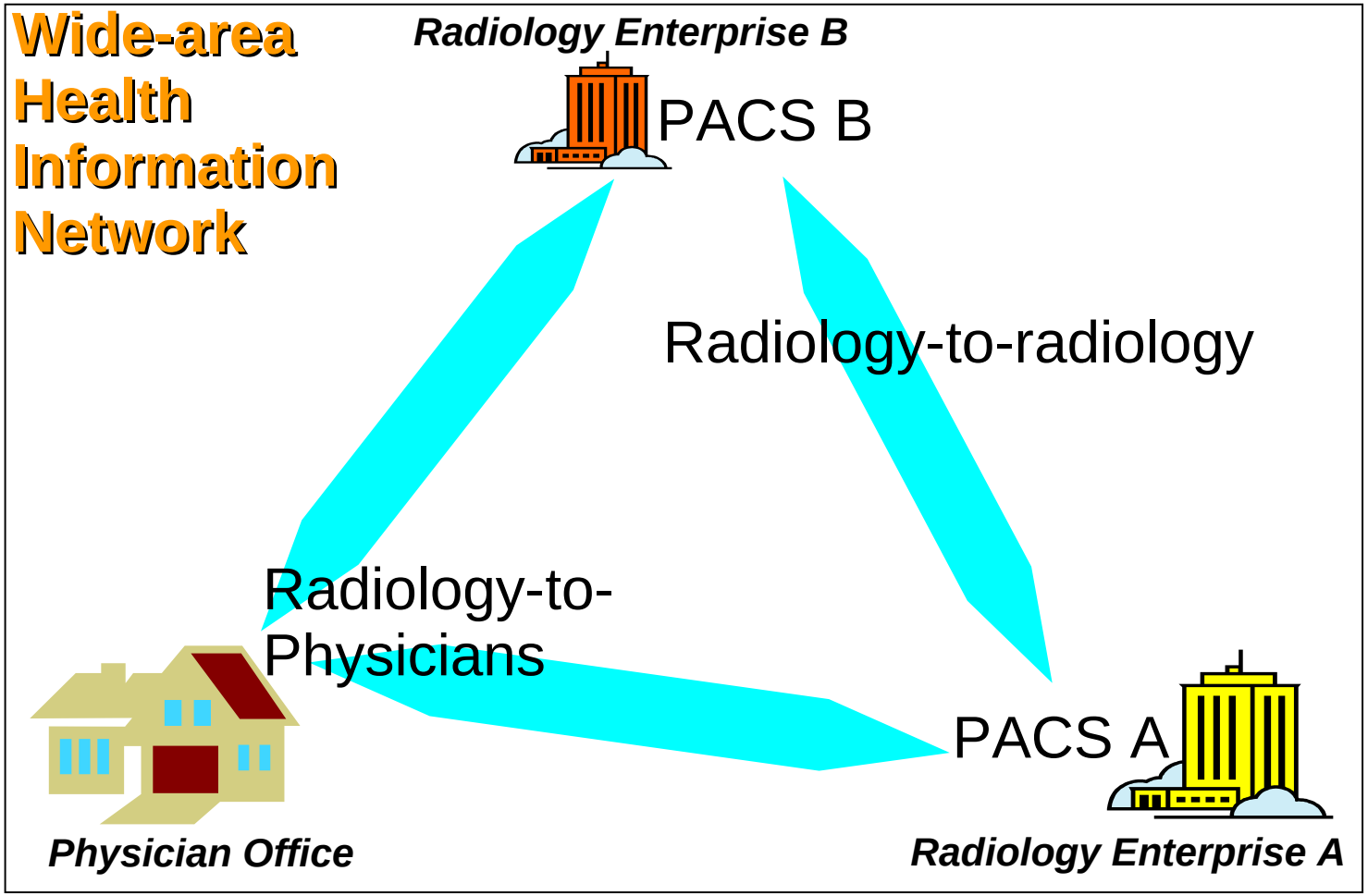
- “Embarassingly” parallel problem
- Fast turn over of short jobs
- Data confidentiality
- Interactivity
- Fine grain parallelism (MPI)
- Workflow-based
- Portals / user interface

Building on Production Grids



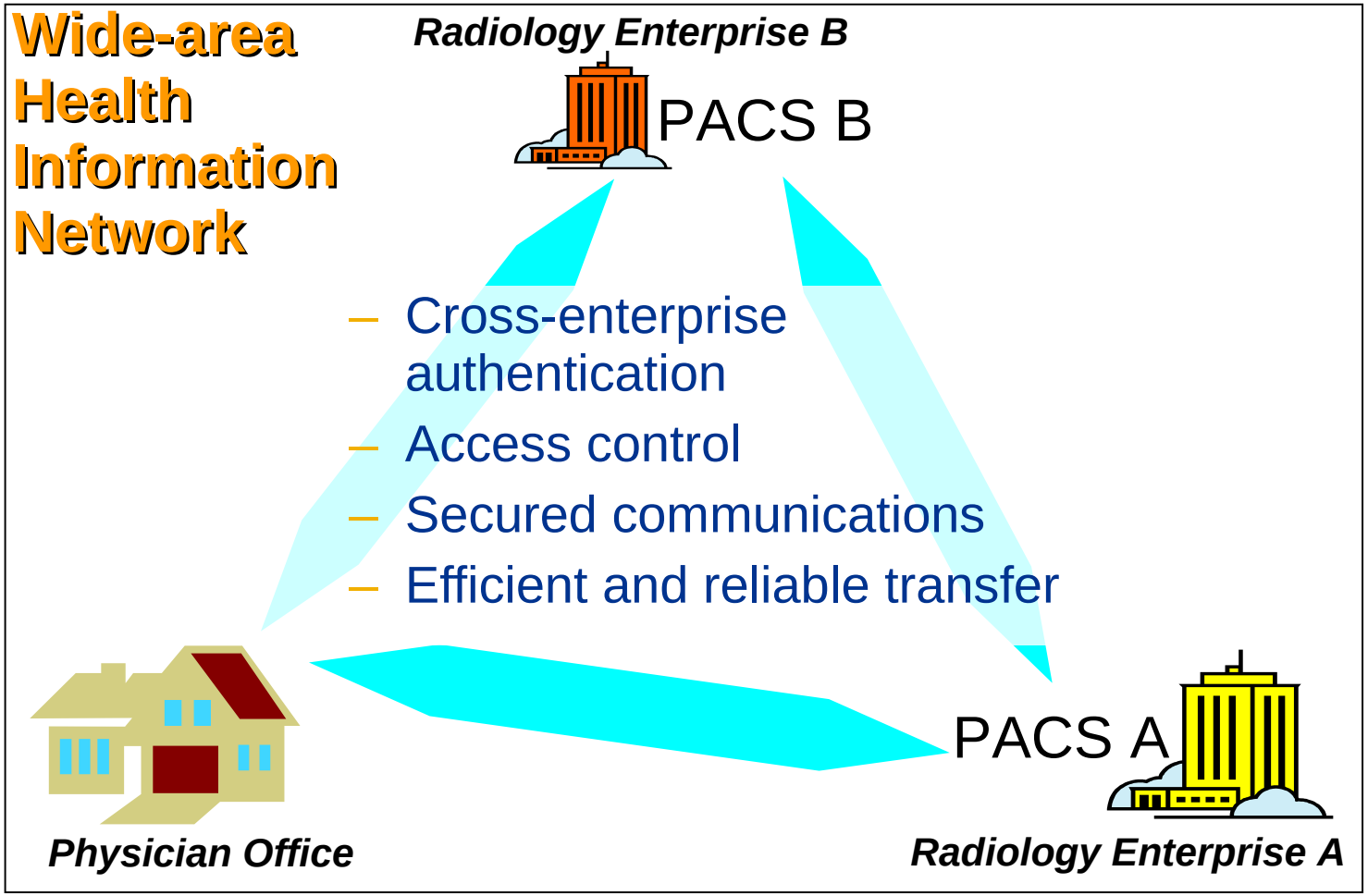
WAN medical image exchange

- **Cross-enterprise exchange of radiology reports and images**



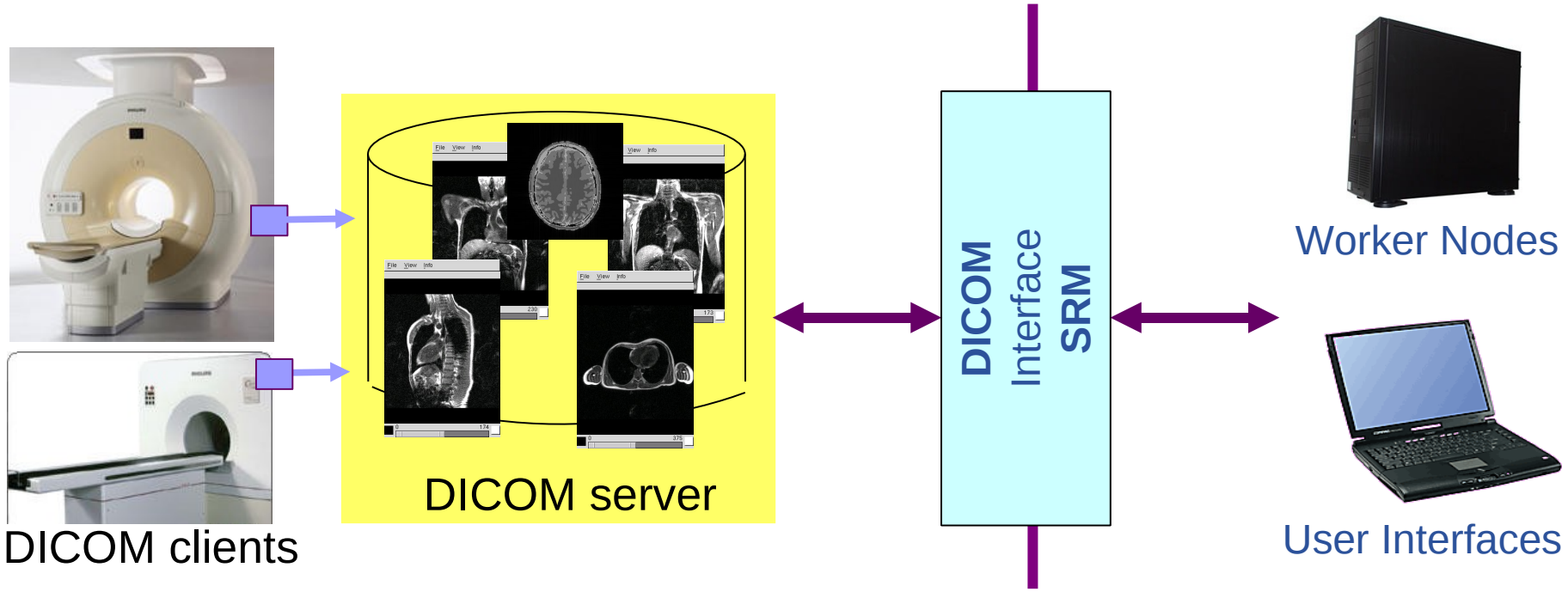
WAN medical image exchange

- **Grid technologies**



Medical Data Manager

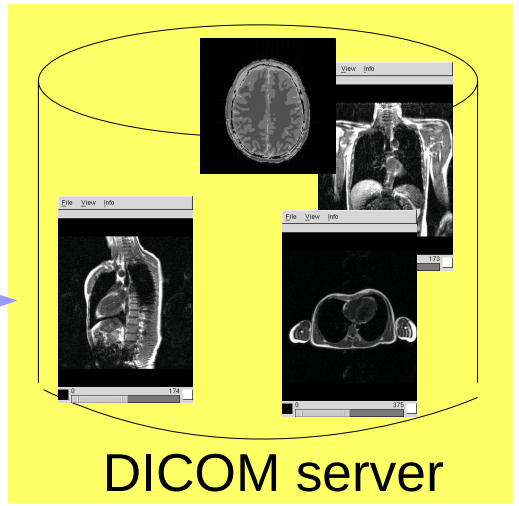
- **Objectives**
  - Expose a **standard grid interface** (SRM) for **medical image servers** (DICOM)
  - Use native DICOM storage format
  - Fulfill medical applications security requirements
  - Do not interfere with clinical practice



Medical Data Registration

1. Image is acquired

2. Image is stored in DICOM server



3. lcg client

GFAL
API

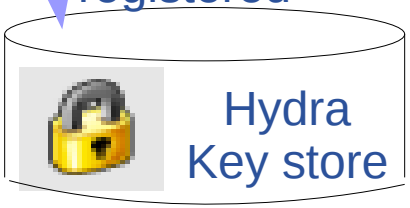
3a. Image is registered (a GUID is associated)

LCG File Catalog

4. image metadata are registered

AMGA Metadata

3b. Image key is produced and registered



Medical Data Retrieval

Worker Node

User Interface

1. get GUID from metadata

AMGA Metadata

Metadata ACL control

2. lcg client

LCG File Catalog

File ACL control

GFAL API

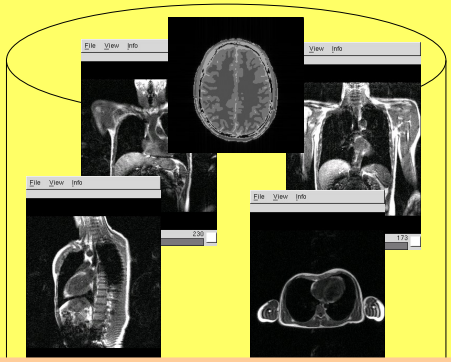
3. get SURL from GUID

4. request file

6. on-the-fly encryption and anonimyzation return encrypted file

7. get file key and decrypt file locally

SRM-DICOM interface



Anonimization & encryption

DICOM server

Key ACL control

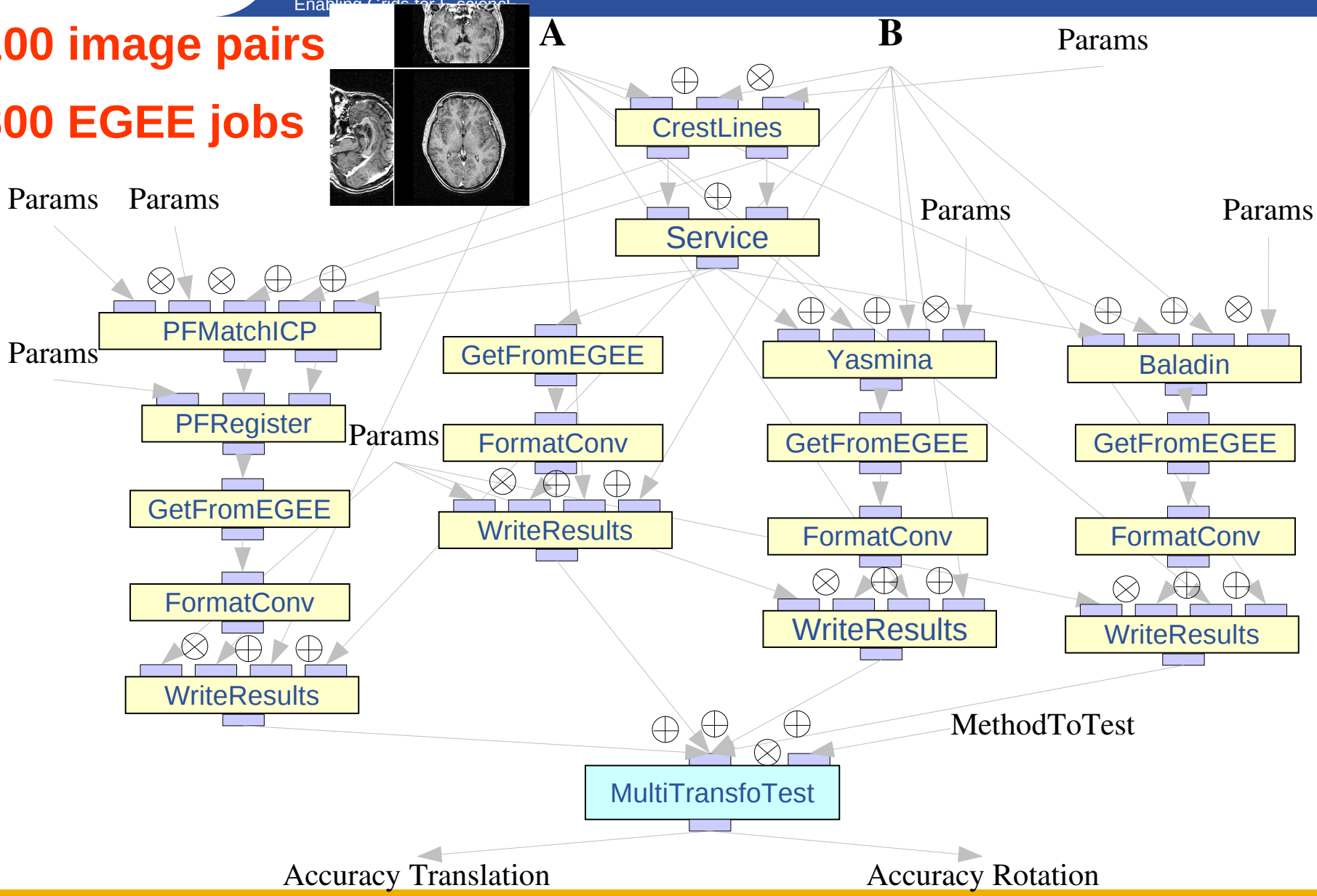
Hydra Key store

5. get file key

Image analysis pipeline

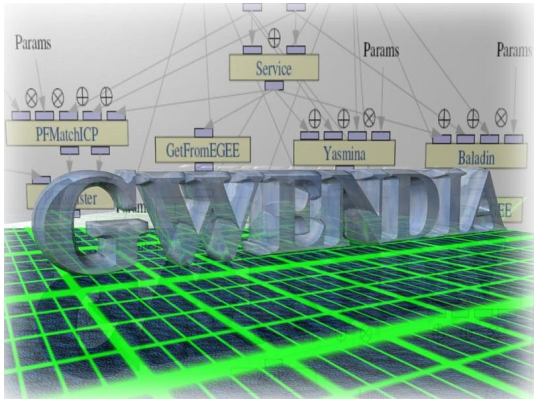
~100 image pairs

~800 EGEE jobs



Workflow management

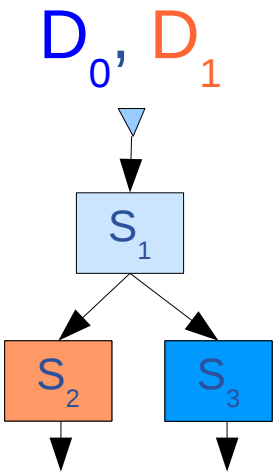
- **MOTEUR, I3S laboratory, CNRS**
  - http://egee1.unice.fr/MOTEUR
- **High level interface**
  - Hides grid complexity to the user
- **Service-based approach**
  - Legacy code service wrapper
- **Scufl language (myGrid / Taverna)**
  - Pure data flow approach
- **Grid submission interfaces**
  - EGEE (LCG2, gLite)
  - Grid5000 (OAR, DIET)
- **Transparent parallelism exploitation**
  - Code and data parallelism



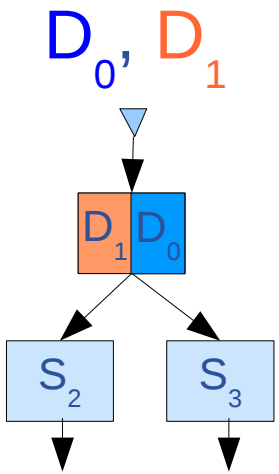
Efficient parallel execution

- A workflow naturally provides application parallelization
- MOTEUR transparently exploits 3 kinds of parallelism

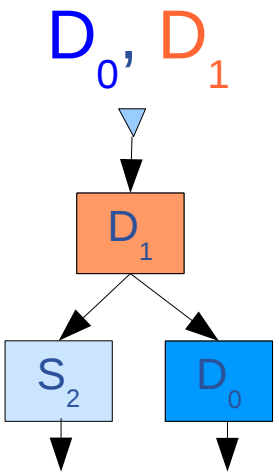
Workflow parallelism



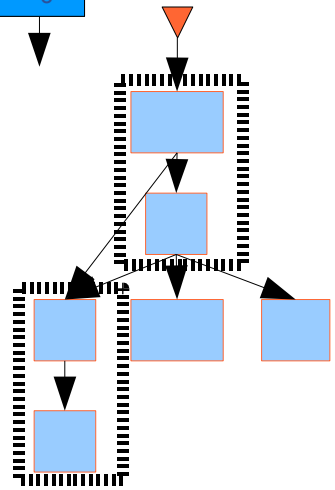
Data parallelism



Service parallelism



- Jobs grouping strategy in sequential branches in order to reduce grid latency



http://egee1.unice.fr/MOTEUR

Short Deadline Jobs

- **Torque + MAUI batch scheduler**
  - Used in most EGEE sites
  - specific configuration (virtual processors allocation)
  - Does not interfere with normal batch scheduling (shared processor time)
  - Enables efficient processing of short tasks on the production infrastructure
  - Alternative to jobs prioritization
- **Special submission queues**
  - Three SDJ queues deployed on biomed-compliant sites
  - Time-limited queues
- **Submit-or-reject paradigm**
  - Jobs are immediately executed or rejected if a too high number of short jobs are already executing.

Conclusions

- **Grid used for sustained production in life sciences**
  - Regular usage in drug discovery, bioinformatics and medical imaging community
  - Closer to non computing-specialized end-users
    - RSNA'08 demonstration (EGEE-MEDICUS)
    - Bioinformatics web portal
    - ...

- **Application-domain high level services being developed**
  - Data protection
  - Data semantics
  - User interfaces
- **Demonstrated direct interest for uses community**
  - Computing power... but not only computing power
  - Data, algorithms and procedures federation