eGee

Production Demonstrations: Introduction

Marc-Elian Bégin – NA1/NA2 - CERN

EGEE 1st EU Review

09-11/02/2005

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Information Society

Enabling Grids for E-sciencE

- **Demonstration of a selection of Grid applications from different disciplines**

- **GEMS**
  - Molecular Simulator (Computational Chemistry)
  - Antonio Laganà and Osvaldo Gervasi
  - University of Perugia
- **gPTM3D**
  - Radiology Images Analysis (Biomedical / Medical Imaging)
  - Cecile Germain-Renaud and Romain Texier
  - CNRS / LRI and LAL
- **EGEODE**
  - Geophysics Application (Earth Science)
  - Dominique Thomas and Gaël Youinou
  - Compagnie Générale de Géophysique

Enabling Grids for E-sciencE

- **Setup**
  - Live usage of the Grid
  - All applications integrated with LCG-2 middleware
  - 3 demos running from a laptop accessing the Grid
    - GEMS: Through GENIUS Portal (running on GILDA)
    - EGEODE: Idem
    - gPTM3D: Directly from laptop, links to Production Service
- **They show different stages of deployment: from GILDA to the Production Service**

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Enabling Grids for E-sciencE

Show Time!!

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GEMS,
Grid Enabled Molecular Simulations

EGEE 1st EU Review – 9th to 11th February 2005

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Antonio Laganà[1], Osvaldo Gervasi[2]
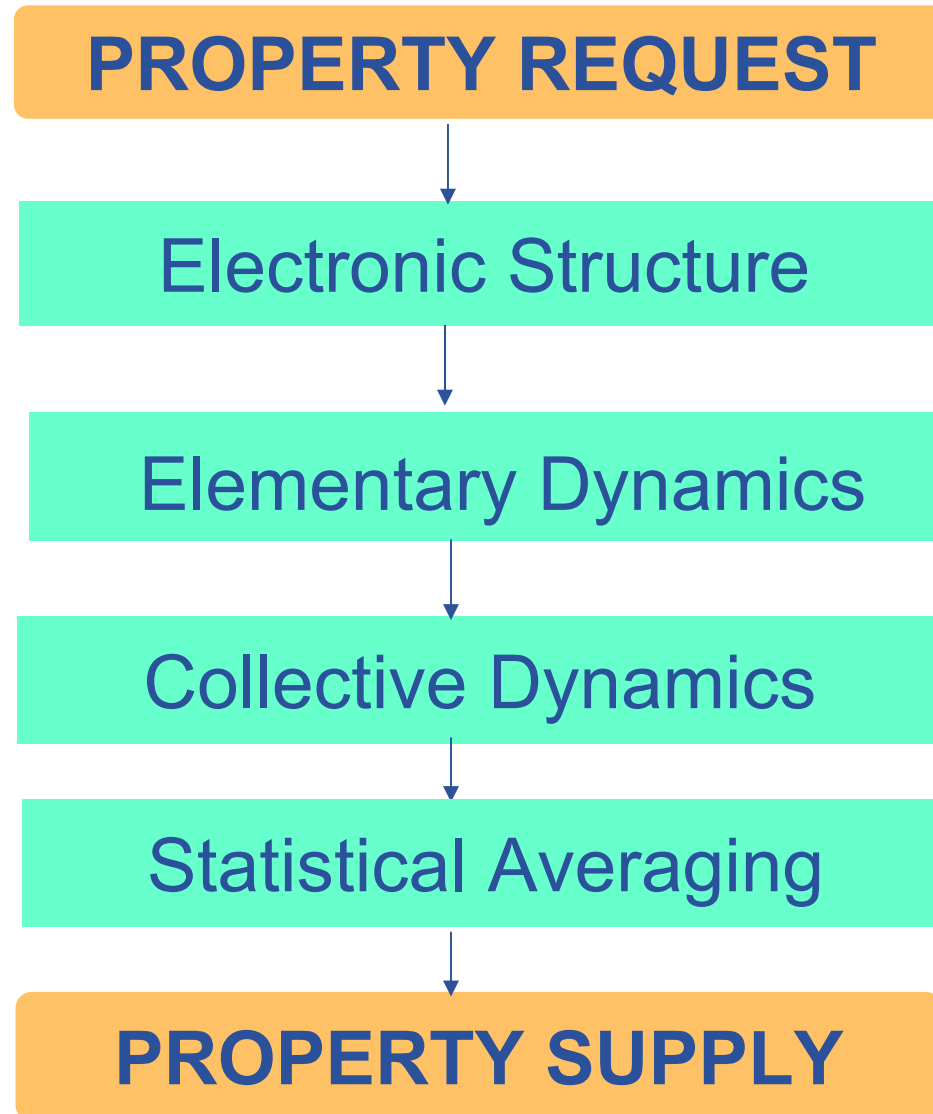
[1] Dept. of Chemistry, University of Perugia

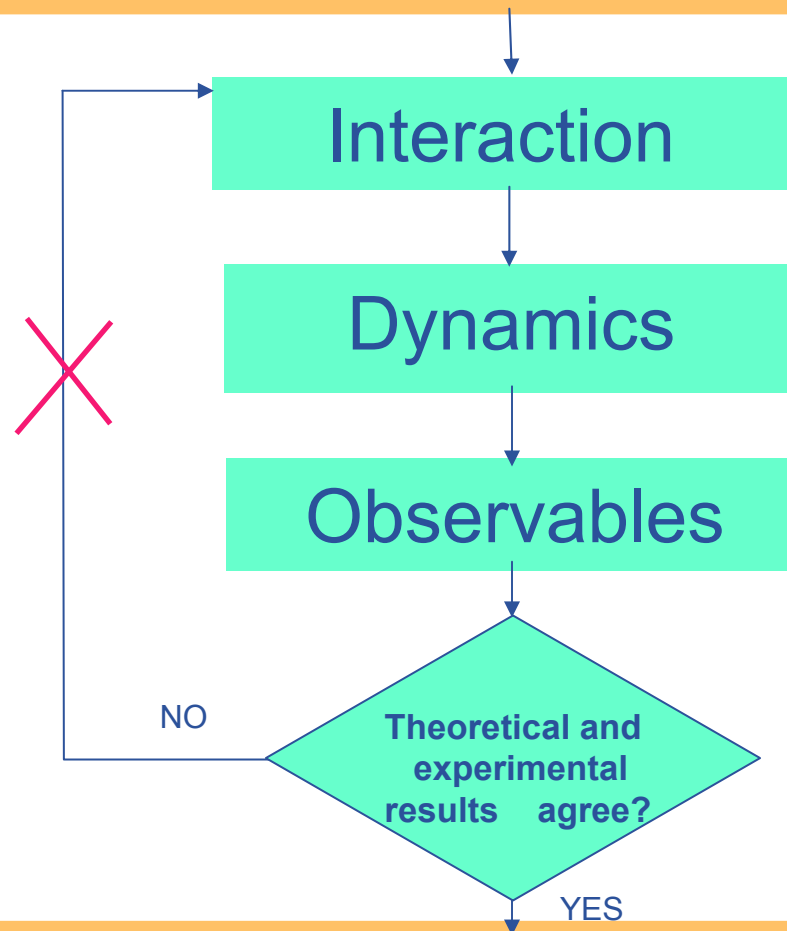*[2] Dept. of Math. & Computer Science, University of Perugia*

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- **Overview of GEMS and the prototype application**
- **Deployment layout**
- **Scale of usage**
- **Usage of LCG-2 middleware services**
- **Difficulties and workarounds**
- **Cost comparison with alternative solutions**
- **Future work and direction**
- **Challenges for full production**
- **The Chemistry and Molecular Science Community**
- **The grid added value**

PROPERTY REQUEST

Electronic Structure

Elementary Dynamics

Collective Dynamics

Statistical Averaging

PROPERTY SUPPLY

- **SPECIFIC ASSUMPTIONS OF THE GEMS.0 DEMO**

  - Focus on atom diatom systems

  - Take potential energy routine from a library

  - Adopt classical dynamics (trajectories)

- **GEMS.0 EXECUTION ON GILDA**

  - Set the demo environment

  - Input the atoms involved

  - Input energy, initial vibrational and rotational state

  - Loop on trajectories by generating randomly the other initial conditions

  - Collect results as virtual monitors (in the real application to be compared with the experiment)

$$i\hbar \frac{\partial}{\partial t} \Psi(\{W\},\{w\},t) = \hat{H}\Psi(\{W\},\{w\},t)$$
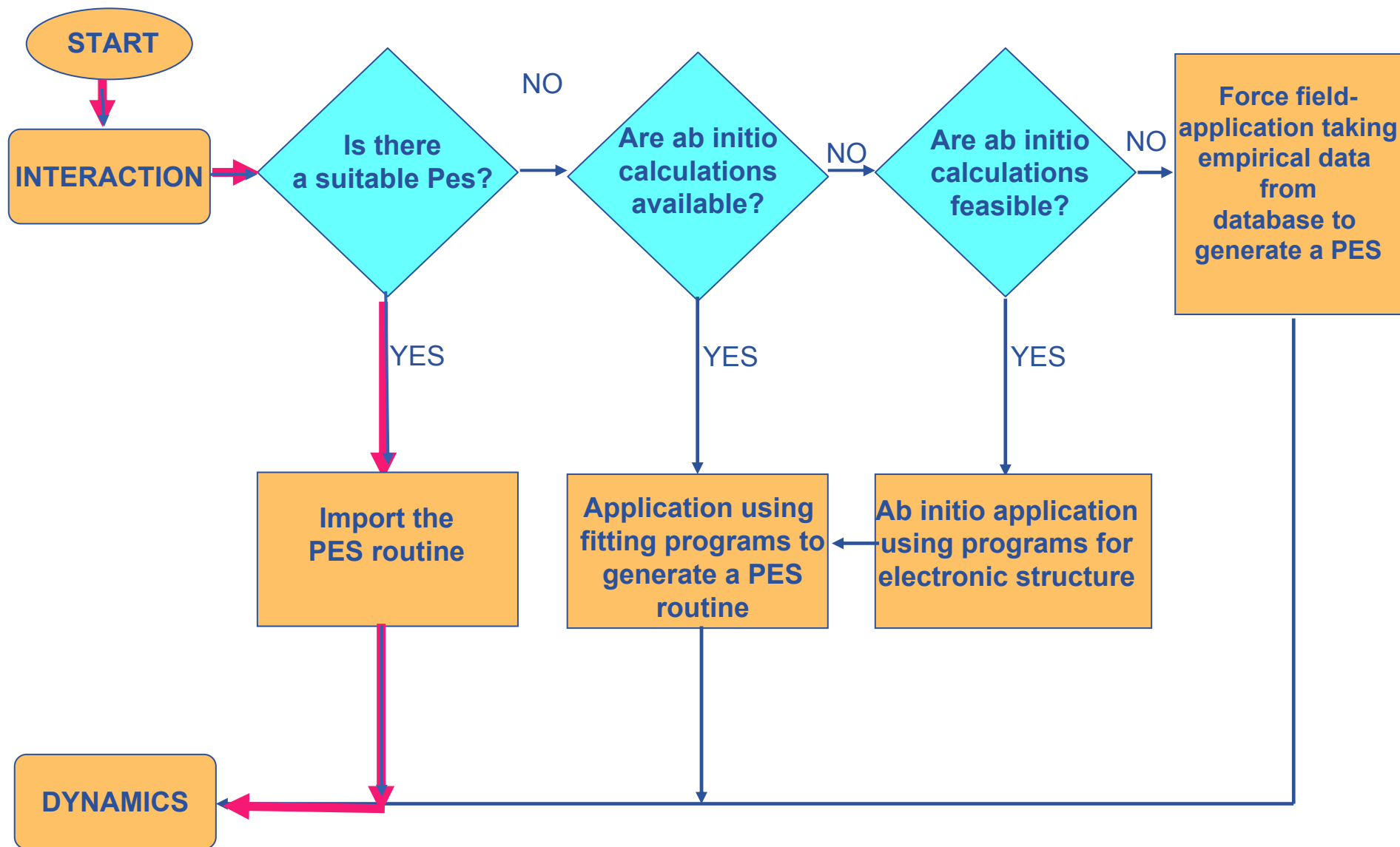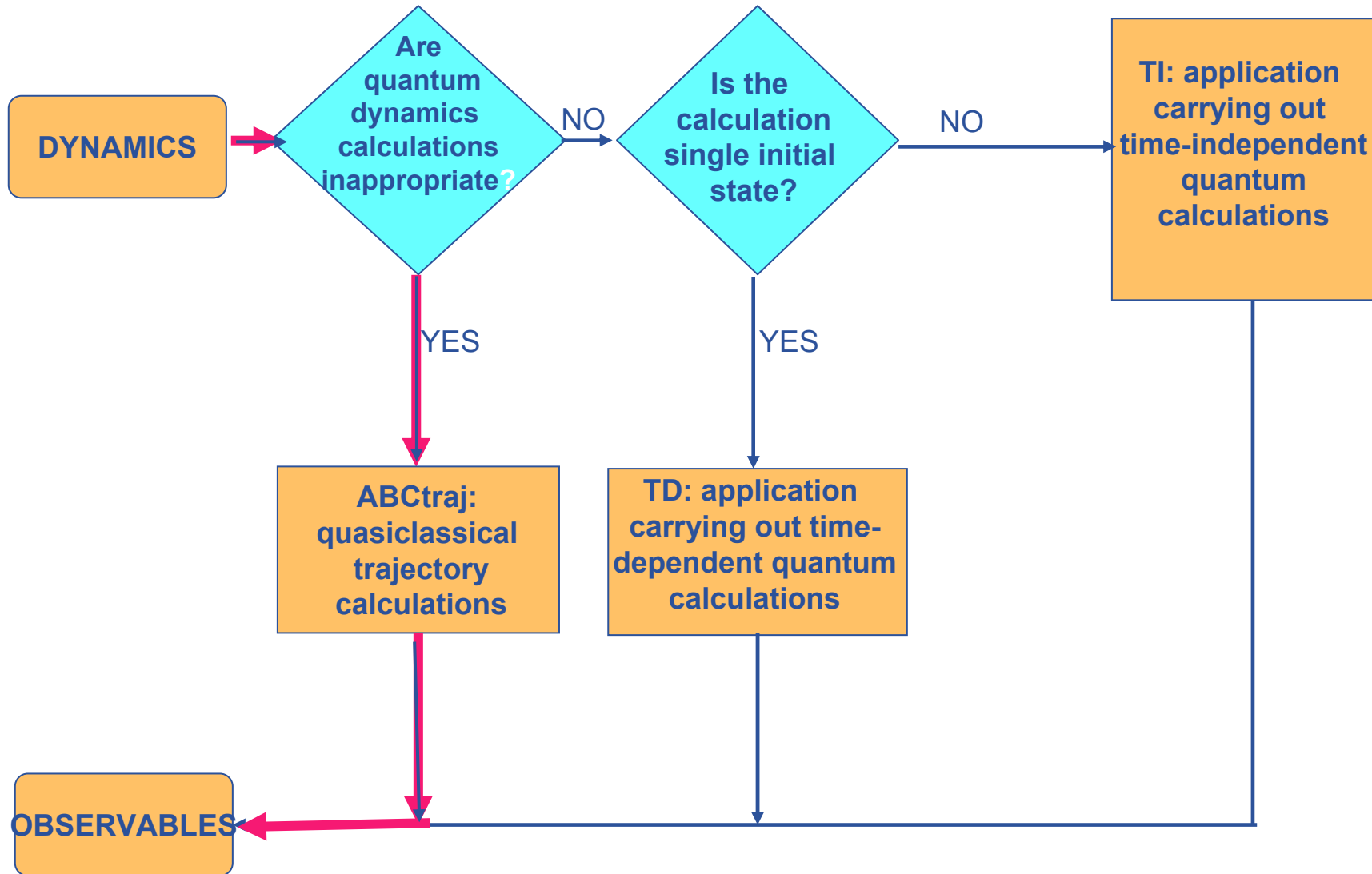
Separation of electronic and nuclear motions
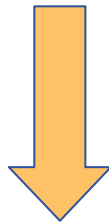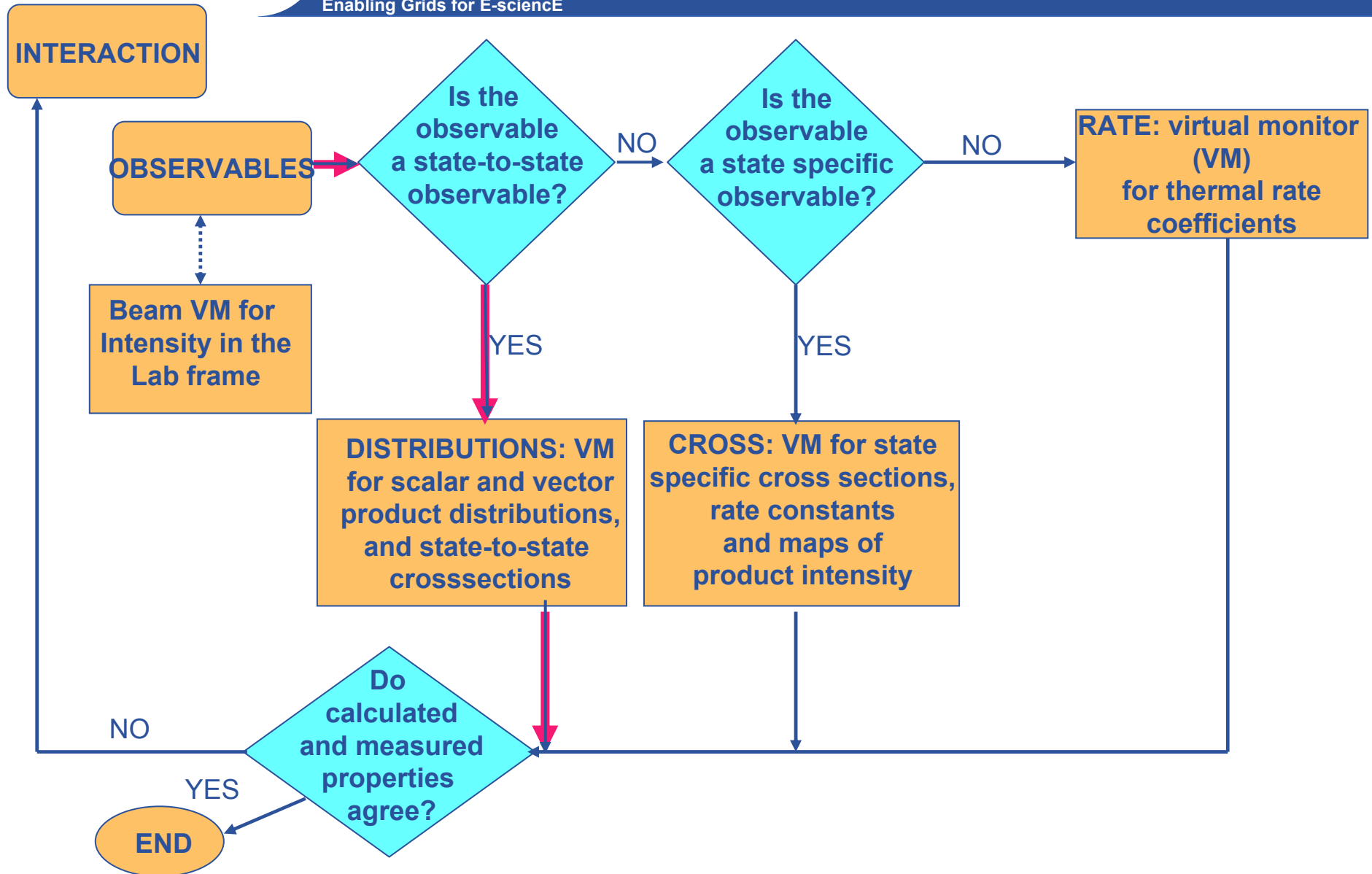
Electronic Schrödinger equation:

Nuclear Schrödinger equation:

$$\hat{H}_{elec}\Psi_n(\{w\};\{W\}) = E_n(\{W\})\Psi_n(\{w\};\{W\}) \qquad \hat{H}_n \chi_n(\{W\},t) = i\hbar \frac{\partial}{\partial t} \chi_n(\{W\},t)$$

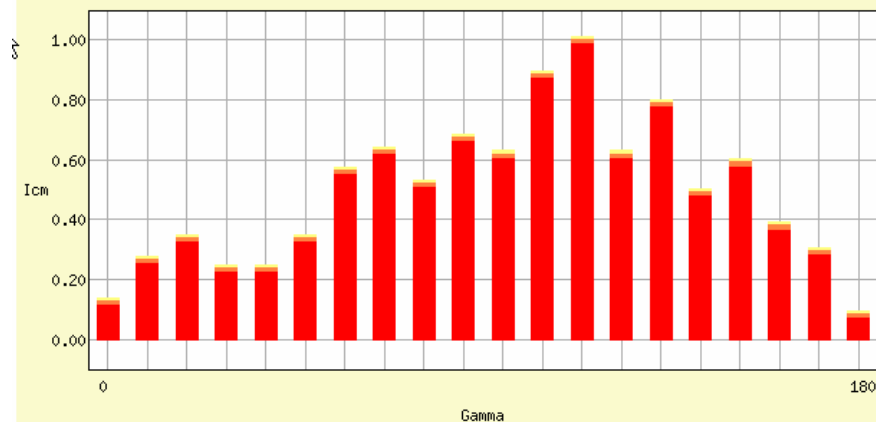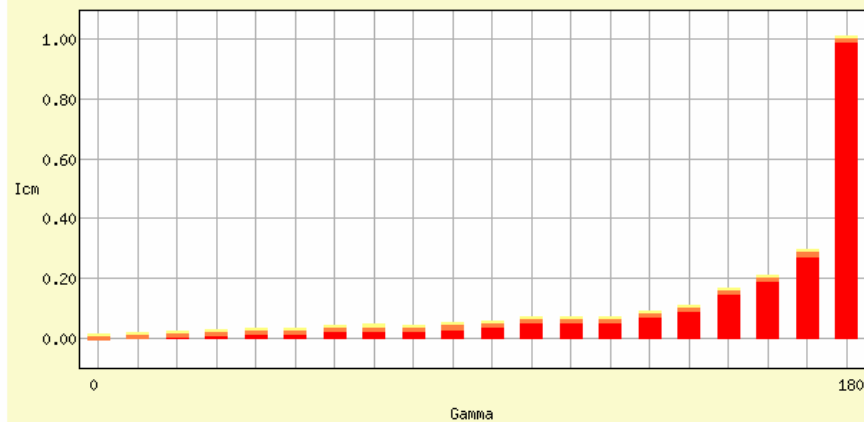## Statistical averaging for beam conditions

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START

INTERACTION

Is there a suitable Pes?

NO

Are ab initio calculations available?

NO

Are ab initio calculations feasible?

NO

Force field-application taking empirical data from database to generate a PES

YES

YES

YES

Import the PES routine

Application using fitting programs to generate a PES routine

Ab initio application using programs for electronic structure

DYNAMICS

DYNAMICS

Are quantum dynamics calculations inappropriate?

NO →

Is the calculation single initial state?

NO →

TI: application carrying out time-independent quantum calculations

YES ↓

ABCtraj: quasiclassical trajectory calculations

YES ↓

TD: application carrying out time-dependent quantum calculations

OBSERVABLES

![egee logo] Enabling Grids for E-sciencE

INTERACTION

OBSERVABLES

Beam VM for Intensity in the Lab frame

Is the observable a state-to-state observable?

NO

Is the observable a state specific observable?

NO

RATE: virtual monitor (VM) for thermal rate coefficients

YES

YES

DISTRIBUTIONS: VM for scalar and vector product distributions, and state-to-state crosssections

CROSS: VM for state specific cross sections, rate constants and maps of product intensity

Do calculated and measured properties agree?

NO

YES

END

Angular distribution: H+ICl->Cl+HI

Angular distribution: H + ICl -> H + ICl



Angular distribution: H+ICl->I+HCl
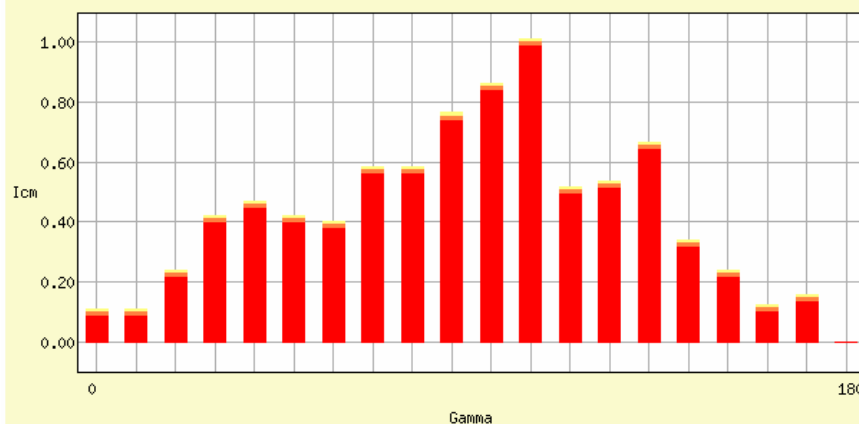
- **Sites**

  - GILDA testbed sites.

- **Key services**

  - Resource Broker: grid004.ct.infn.it

  - Computing Element: ce.grid.unipg.it

  - User Interface: grid-tutor.ct.infn.it

  - GENIUS Portal: https://genius.ct.infn.it

  - CompChem VOMS

- **Number of jobs: 10 per day**
- **Storage: 100KB – 50GB depending on the type of computational engine used and the chemical system studied:**
  - Trajectory calculations: <100KB
  - Time Dependent Quantum: 10GB
  - Time Independent Quantum: 50GB
- **RAM: 100KB – 2GB**
  - Trajectory calculations: <100K
  - Time Dependent Quantum: 1GB
  - Time Independent Quantum: 2GB
- **Success rate: 98%**
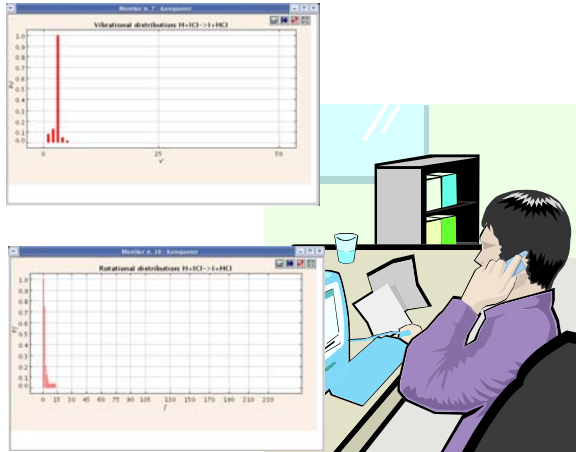
GILDA

Testbed

Infrastructure

GEMS

GEMS

GEMS

GEMS

programs

GENIUS
Portal

Resource
Broker

Computing
Element

MPI
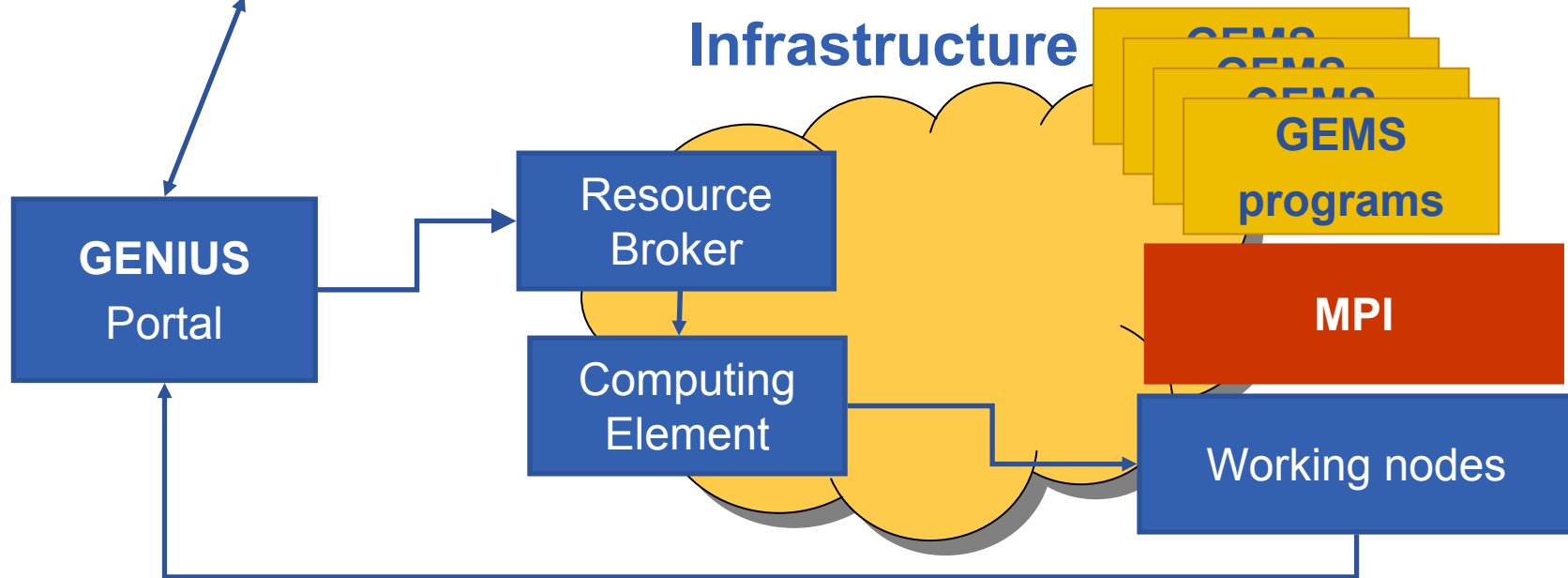
Working nodes

Outbound connectivity

- **We have encountered the following problems:**
  - Not all sites did publish the environment variables related to the outbound connectivity of the Working Nodes.
  - The job activation time is high, expecially if an high number of working nodes is requested.
  - Not all sites have enough resources (disk + RAM) for Quantum Chemistry codes.
  - In some sites MPI is not available.
  - The Firewall sometimes is misconfigured and blocks the outbound connectivity in the EGEE standard port range: 20000-25000.

- **The workarounds were**
  - Alert people involved to properly configure the environment variables.
  - Alert people to open the EGEE standard ports on the Firewall.

- **Running at weekends computers of teaching laboratories (trajectories).**

- **Making a combined use of SP4 at CINECA and CRAY T3E at Edinburgh (3D quantum).**

- **What's missing to extend the application to production**
  - Define the policy for the usage of commercial suites of programs. At present each site buys its own license and opens the access to the VO users. The commercial licence requirement for a job need to be specified in a JDL statement.
  - Credits for contributions to development and service.
  - Extend the suites of programs to other components of the molecular simulator.
  - Full deployment of the VO and consortium.
- **As Production Service, the expected usage profile is:**
  - Users: 100.
  - Sites: 30.
  - CPU consumption (per job): 100 - 1000 hours.
  - Disk Storage (per job): 10 MB - 800 GB.
  - RAM Storage (per job): 100 KB – 200 GB.

Simbex

Murqm

Dirac

Elchem

Icab

Dysts

Comovit

COMOVIT

Enabling Grids for E-sciencE
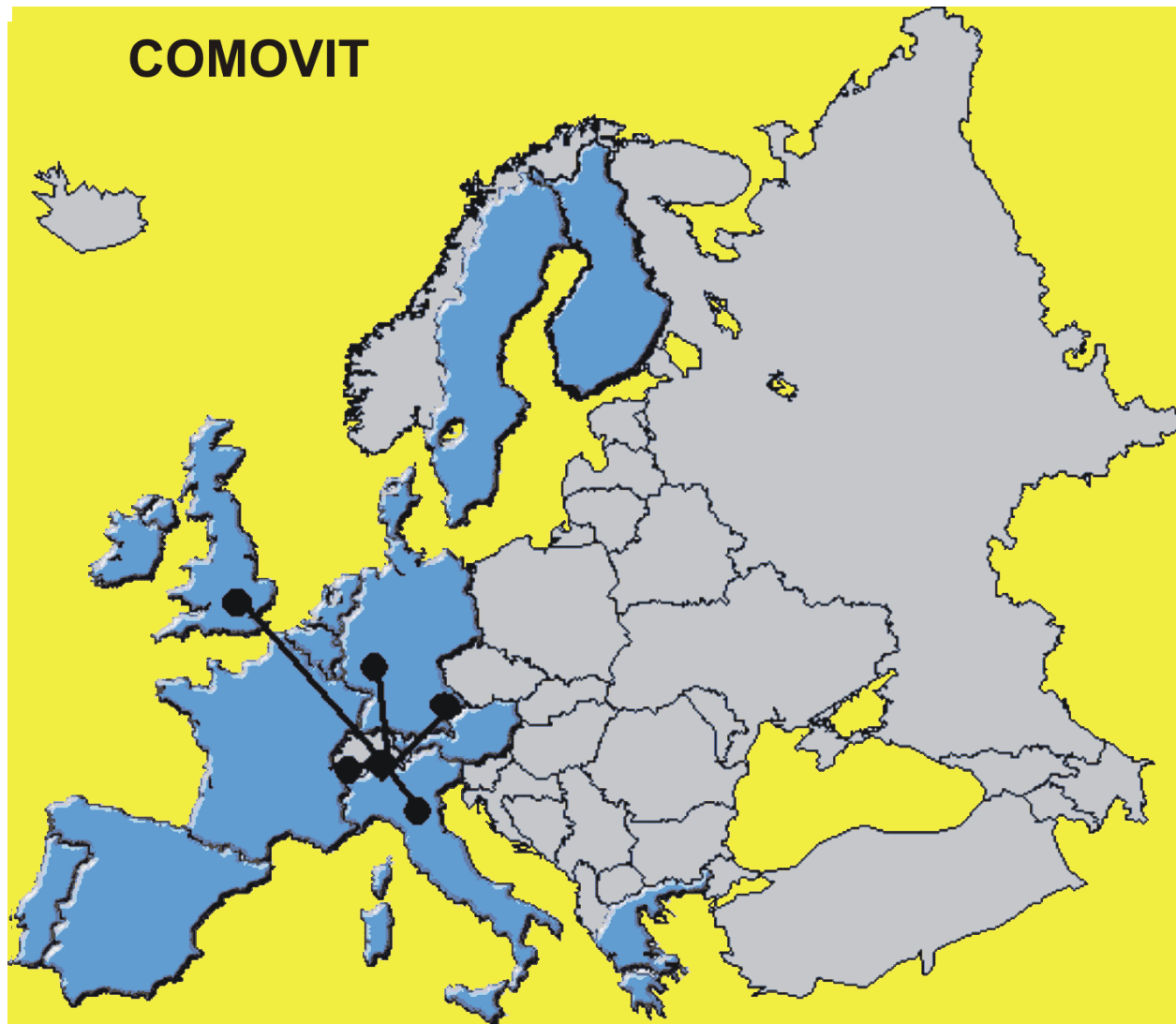
1 Isr,Pl,Sk,Nl

2 Cz,Ch, Fr, Dk, A, Sw, No

3 Hu

4 Gr

5 E

6 D, Uk,

9 I

- **3 Computer Centers**

- **New electronic structure programs (MOLCAS, DIRAC, DALTON, COLUMBUS, MR-CCSD).**

- **New Dynamics programs (AMD, TPS, KMC, condensed phase).**

- **Chemical knowledge semantic web (molecular structures, apparatuses, processes).**

- **Software integration into distributed workflows**
  - to assemble applications out of various (different or complementary) distributed competences coordinated via the grid (in the prototype electronic structure, elementary dynamics, statistical averaging, interfacing the experiment)

- **Computational Campaigns**
  - to evaluate properties depending on the fate of few out of millions, billions or more events by distributing the execution of the computations on the grid (in the prototype particular reactive events having specific energetic or steric properties)

- **Collaborative Engineering of knowledge**
  - to handle (when is the case also in a privacy protecting fashion) chemical information and knowledge including training and production of new knowledge (for the prototype the design of virtual chemical processes or laboratory experiments)

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- A consortium agreement will be signed by the new participants of CompChem VO.

- A dedicated Portal for GEMS will be implemented to run on the production environment.

- Various computational engines will be implemented in order to offer grid services based on the a priori simulation of molecular systems.

- Molecular Virtual Reality components will be combined with Human-size Virtual Reality to offer multiscale realistic representations of material structures and processes.

- Design appropriate cost models for supporting research, project and service activities.

gPTM3D : Grid-Enabling Interactive Medical Analysis

EGEE 1st EU Review – 9th to 11th February 2005

CERN

Cécile Germain, Romain Texier et al.

LAL & LRI – CNRS

NA4 Biomed

- **Goal: Grid-enable PTM3D**
  - PTM3D (Poste de Travail Médical 3D) is
    - A medical images analysis software developed at LIMSI (CNRS)
    - With clinical usage: CHU Tenon, Sainte Anne, FMP,…, InfoRad RSNA *Certificates of Merit* (2002, 2003, 2004)
  - Step1 (this demo): interactive response time for CPU-intensive volume reconstruction
  - Next steps: interactive response time for all components
- **Contexts**
  - Computational steering
  - Medical research and clinical requirements: IMAGE'04 report
- **EGEE status**
  - NA4 internal application
  - On a production grid
  - Collaborations: CNRS STIC labs, French research programmes

- **One data set is**
  - DICOM files: 100MB – 1GB
  - One radiological image: 20MB – 500MB
- **Complex interface: optimized graphics and medically-oriented interactions**
- **Physician interaction is required at and inside all steps**

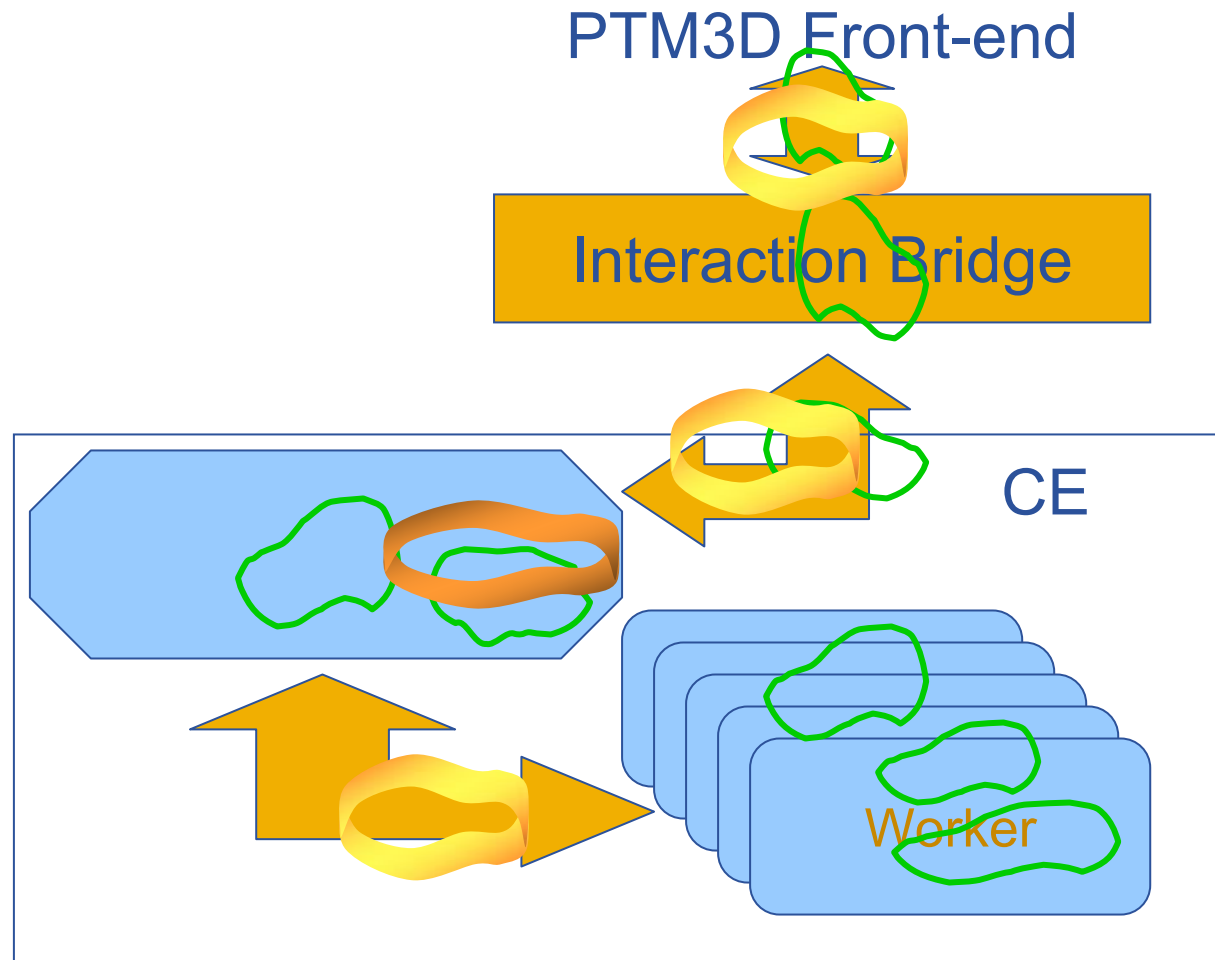 Poorly discriminant data, pathologies, medical windowing

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Enabling Grids for E-sciencE
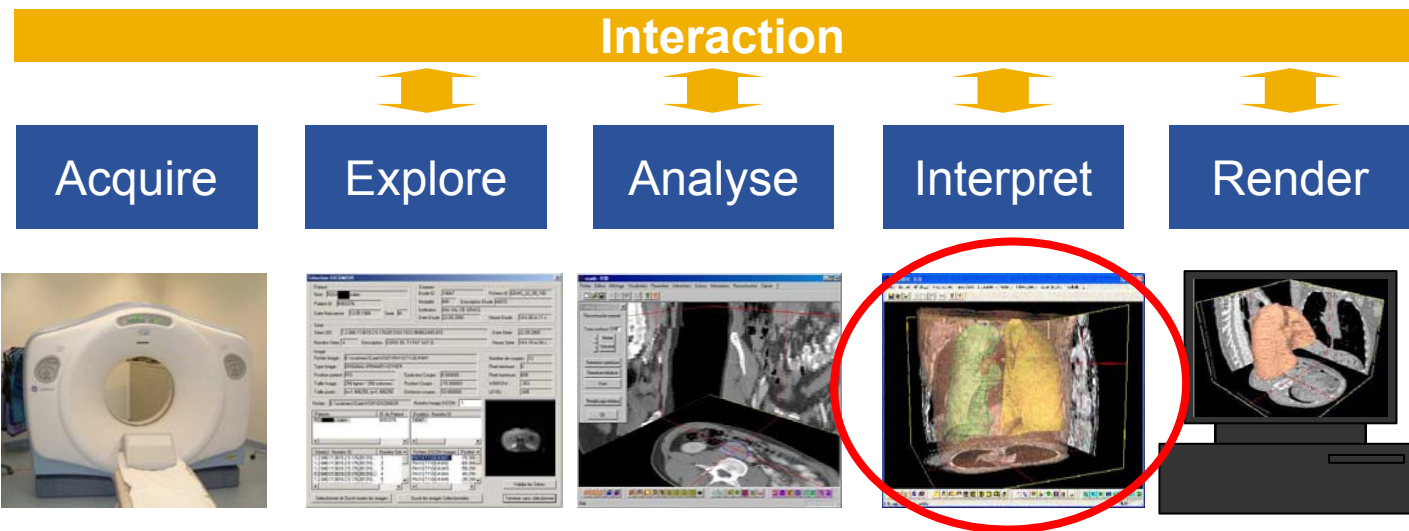
	Dataset	Input data	Output data	Tasks	Standalone Execution	EGEE Execution 14 procs.
Small body	87MB	3MB 18KB/slice	6MB 106KB/slice	169	5min15s *1min54s*	37s *18s*
Medium body	210MB	9.6 MB 25KB/slice	57MB 151KB/slice	378	33min *11min5s*	2min30s *1min15s*
Lungs	87MB	410KB 4KB/slice	2.3MB 24KB/slice	95	36s	24s
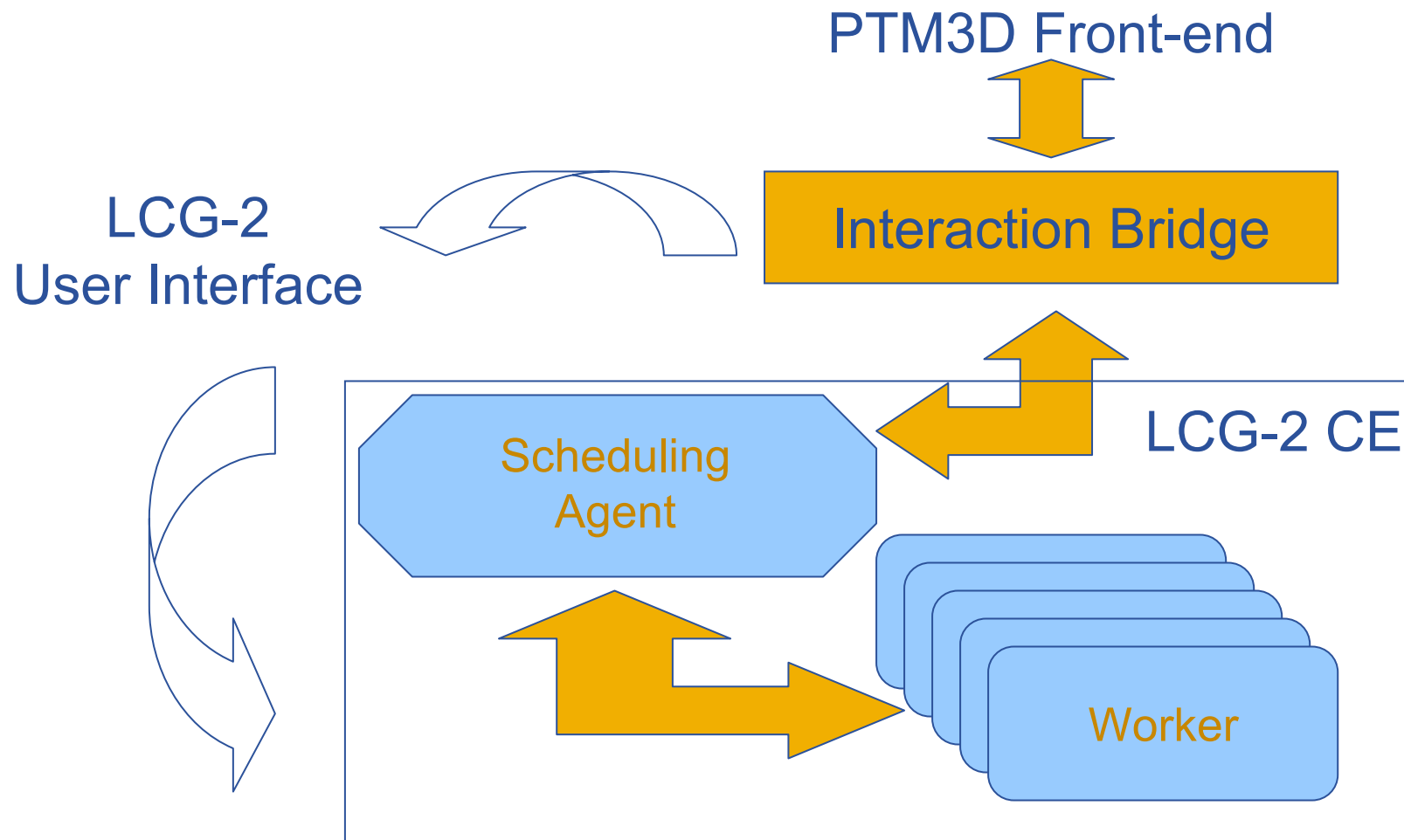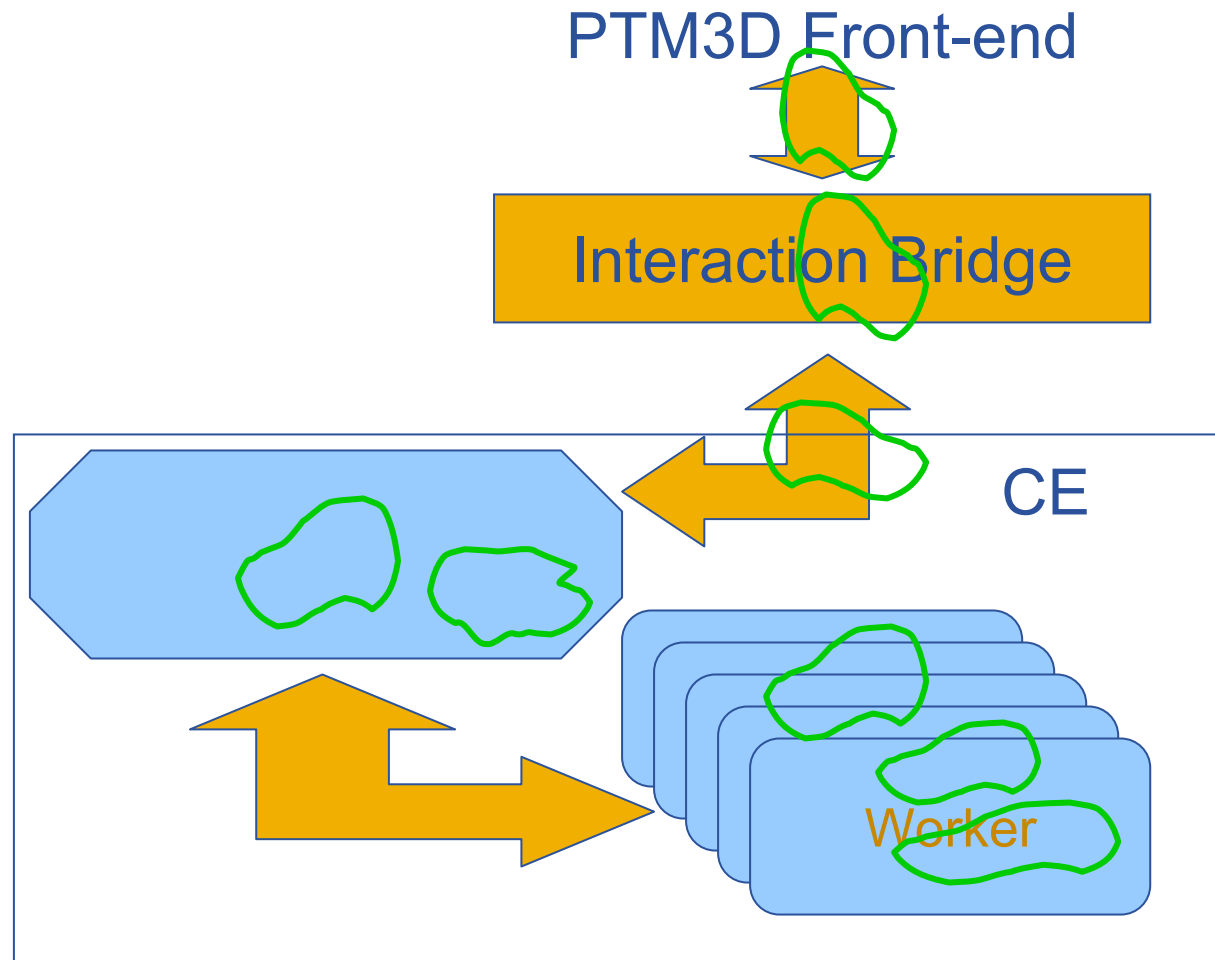
Enabling Grids for E-sciencE

PTM3D Front-end

LCG-2
User Interface

Interaction Bridge

LCG-2 CE

Scheduling
Agent

Worker

PTM3D Front-end

Interaction Bridge

CE

- Stage data
- Pull model: workers pull contours at their own pace

Worker

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Enabling Grids for E-sciencE

PTM3D Front-end

Interaction Bridge

CE

- Stage data
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Worker

Enabling Grids for E-sciencE

PTM3D Front-end

Interaction Bridge

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Enabling Grids for E-sciencE

PTM3D Front-end

Interaction Bridge

CE

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Worker

PTM3D Front-end

Interaction Bridge

CE
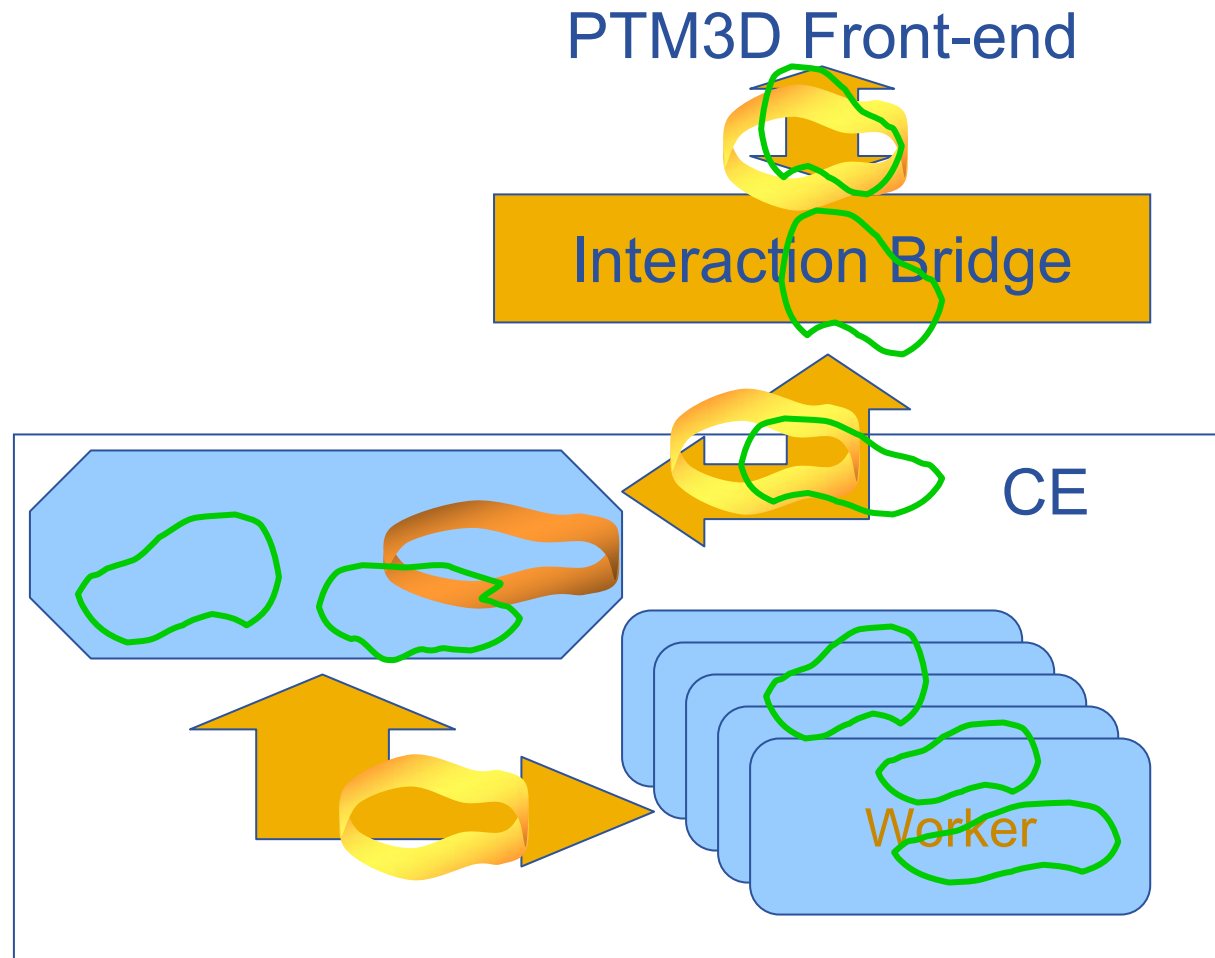
- Stage data
- Pull model: workers pull contours at their own pace
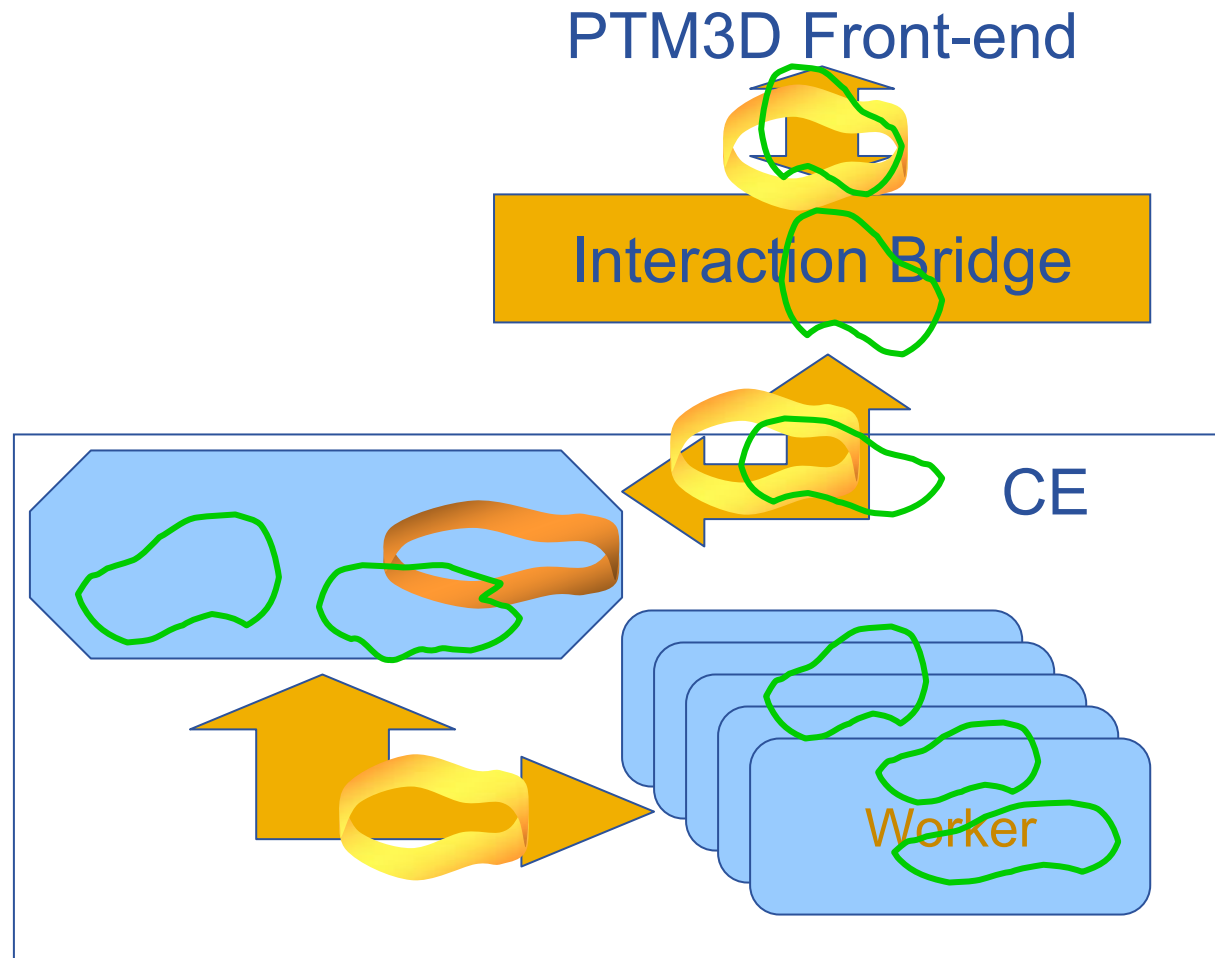
Worker

Enabling Grids for E-sciencE
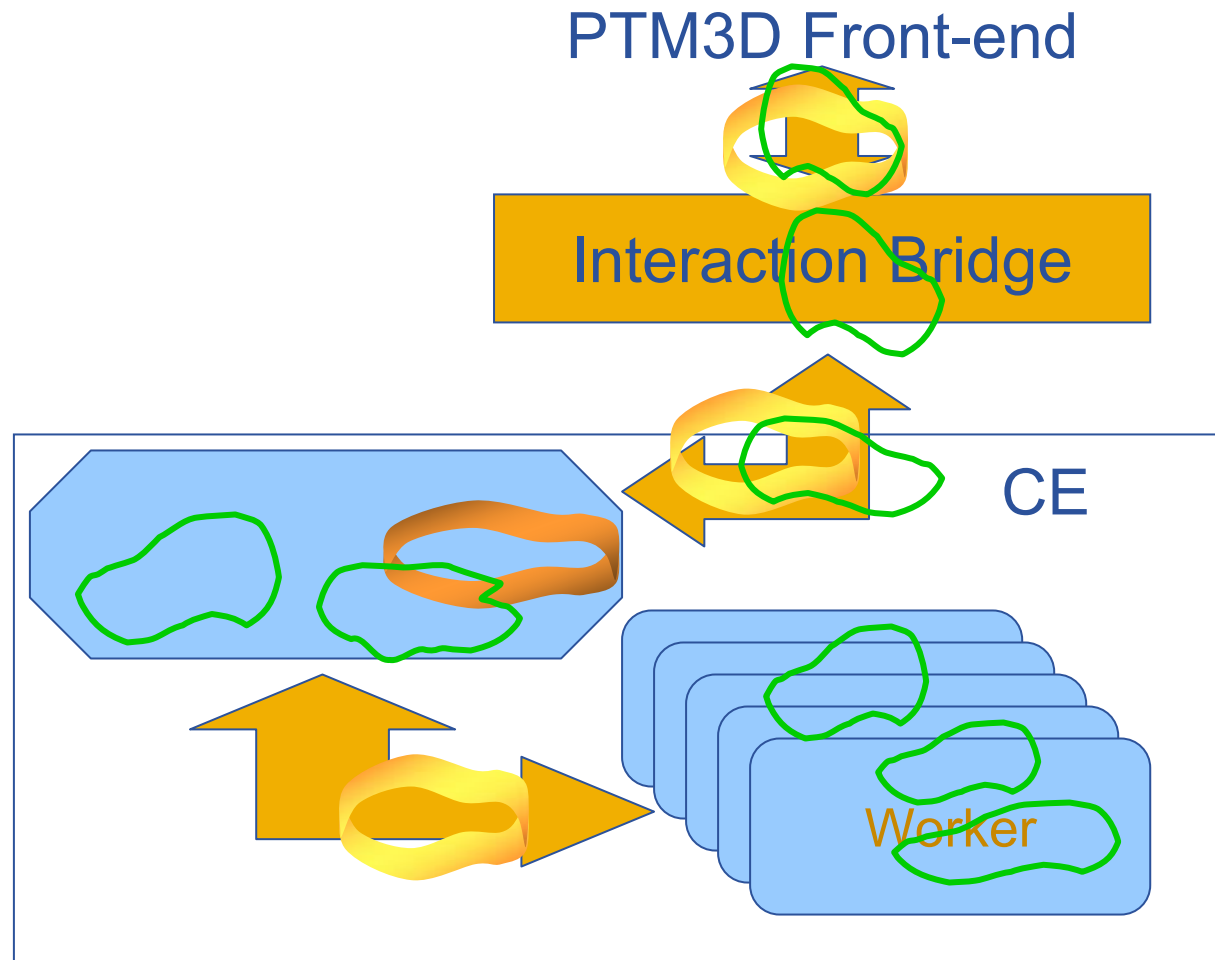
- **Technical**
  - Convergence with other EGEE applications : AliEn, DiRac
  - Port to gLite
  - Scheduling policy: Time-sharing and QoS across the scheduling stack
    - GGF GRAAP and GSA
    - Admission control from sensors
  - Interact with *remote* data
    - Clinical research: evaluate registration algorithms on large existing databases – ACI AGIR

- **Dissemination: demonstrations at**
    - HealthGrid 2005
    - Journées de la Société Française de Radiologie 2005
    - InfoRad-RSNA 2005

Planning percutaneous nephrolithotomy

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PTM3D Front-end

Interaction Bridge

CE

Application Level Scheduler

Worker
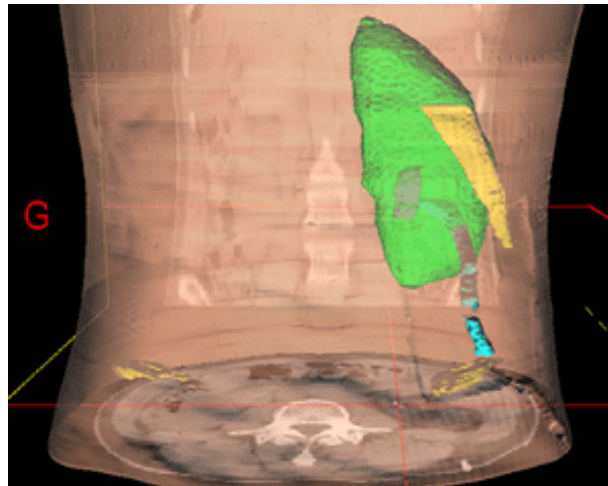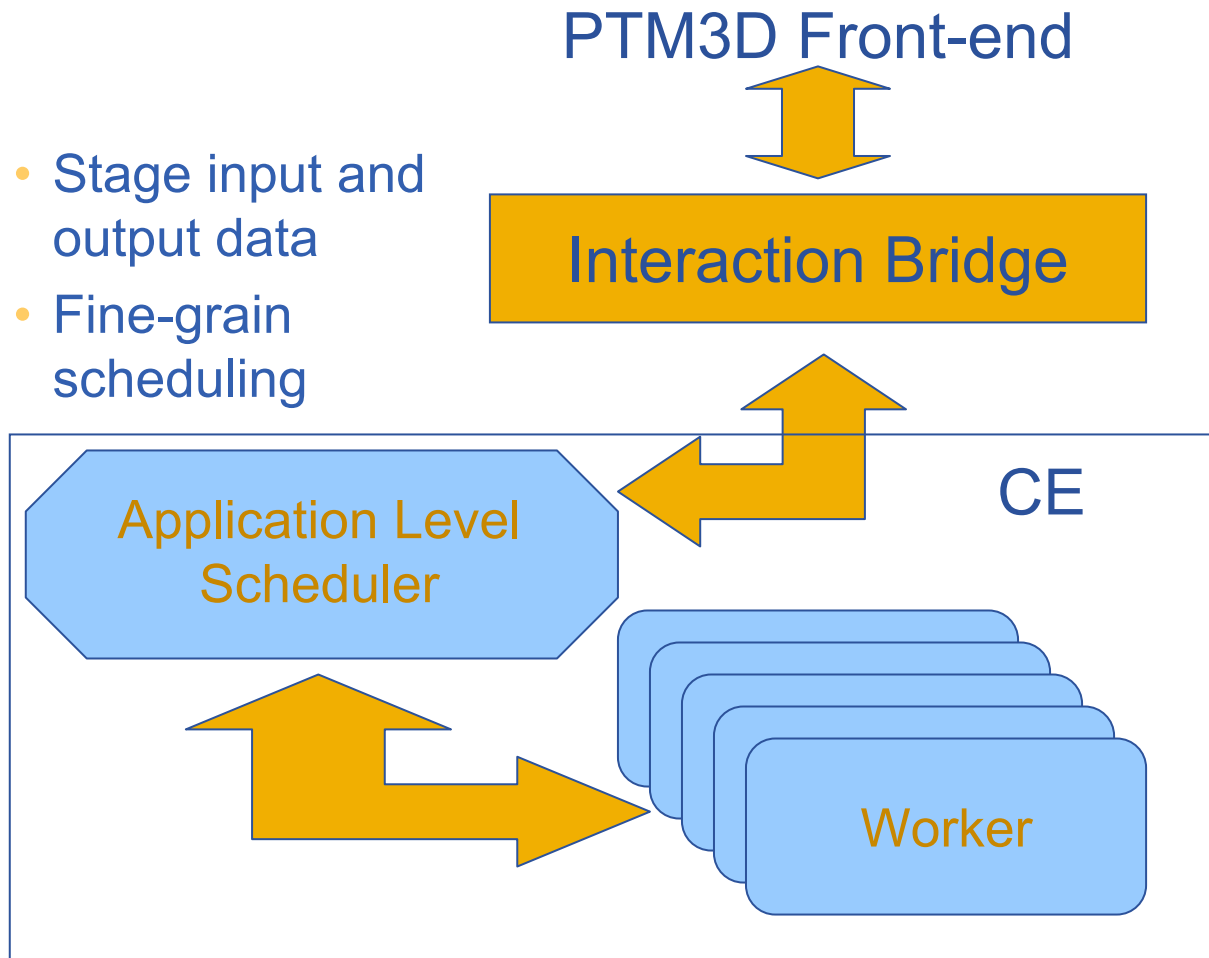
- Stage input and output data
- Fine-grain scheduling

- Stage input and output data
- Negotiate for interactive vs batch
- Admission control
- Schedule interactive jobs
  - No reservation
  - Soft real-time scheduling

Earth Sciences: EGEODE

《 Expanding Geosciences On Demand 》

EGEE 1st EU Review – 9th to 11th February 2005
CERN
Dominique Thomas; Gaël Youinou
Compagnie Générale de Géophysique (CGG, France)
R&D

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Enabling Grids for E-sciencE

- **Geocluster, the *seismic processing* generic platform from CGG**
  - Being ported to EGEE for *Industry* and Academia
  - The main focus of EGEODE Virtual Organization

- **Close collaboration with ESR « Earth Sciences Research » VO.**
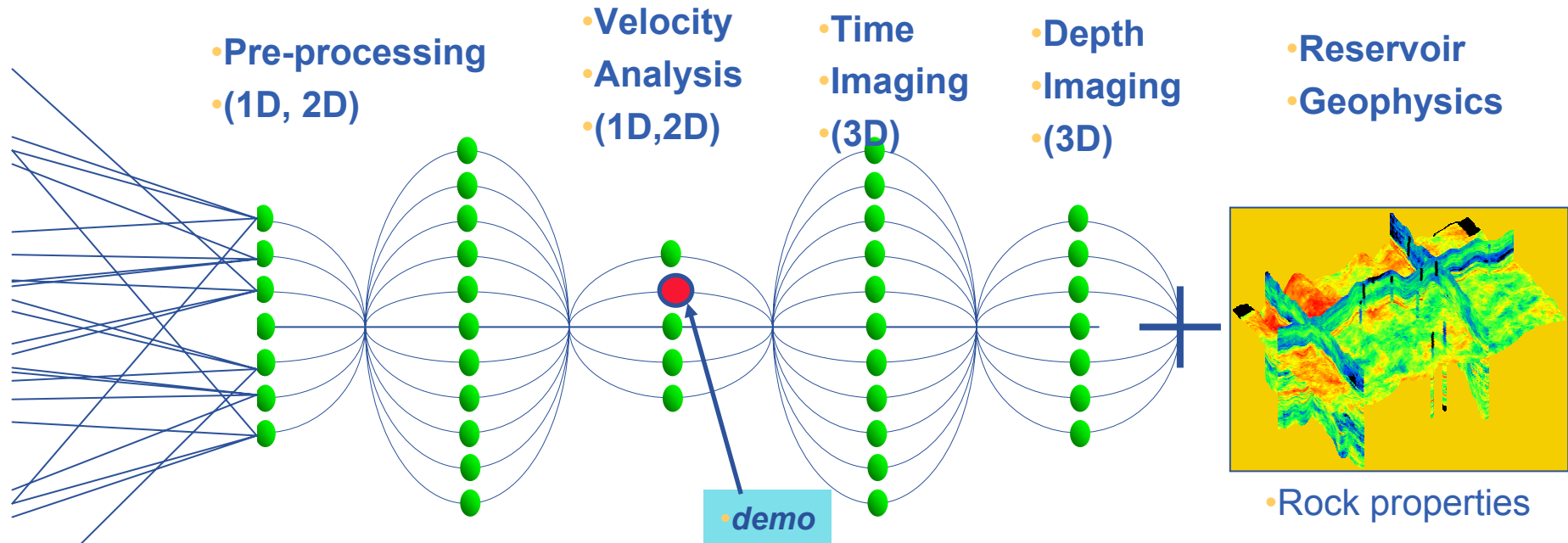 (Earth Observation, Climate, Hydrology, Solid Earth Geophysics)

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Enabling Grids for E-sciencE
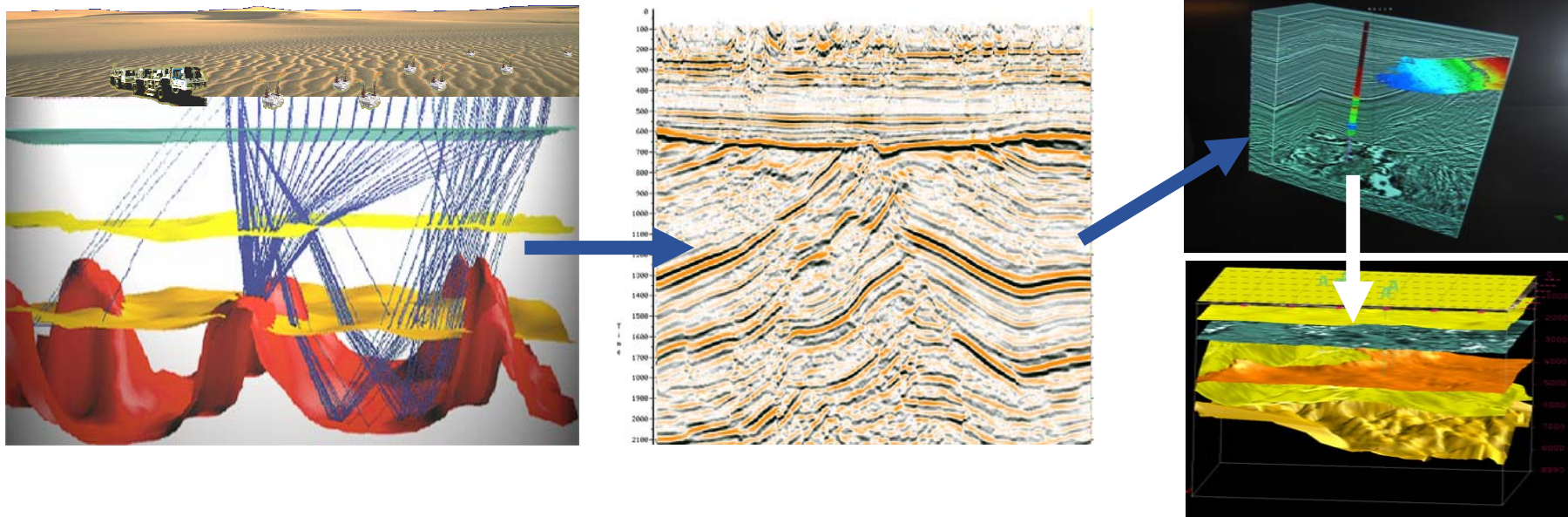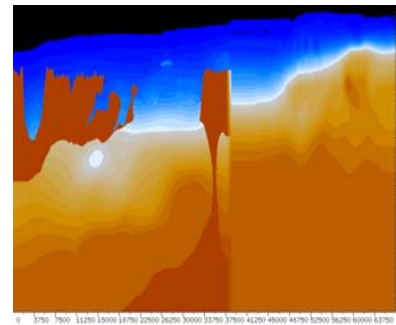
Seismic processing Generic Platform for research and education:

- Based on **Geocluster**, an industrial application, used in production

- Include several standard tools for signal processing, simulation and inversion (model optimization).

- Open: any user can write new algorithms in new modules (shared or not)

- Free access for academic research

- Controlled by license keys (opportunity to explore license issue at a grid level)
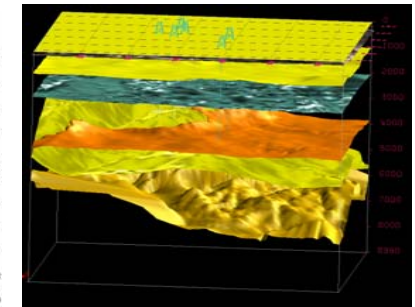
- Initial partners F, CH, NL, Russia

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Enabling Grids for E-sciencE

- Pre-processing
- (1D, 2D)

- Velocity
- Analysis
- (1D,2D)

- Time
- Imaging
- (3D)

- Depth
- Imaging
- (3D)

- Reservoir
- Geophysics

- demo

- Rock properties
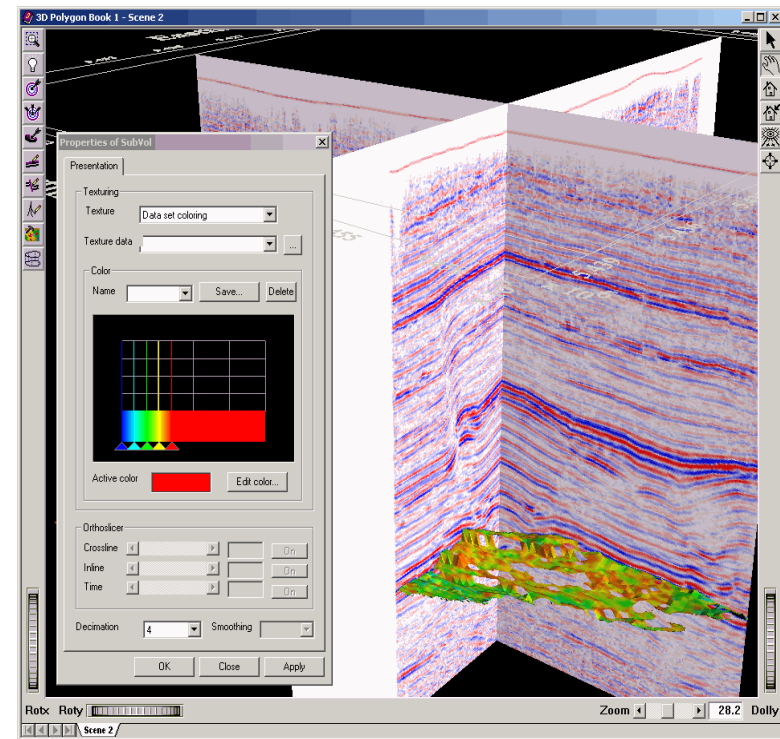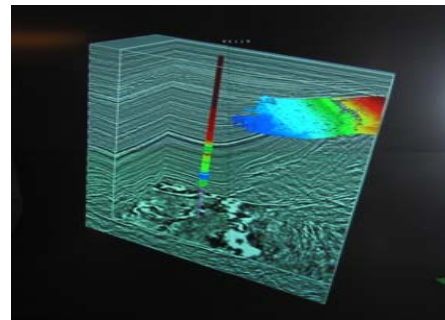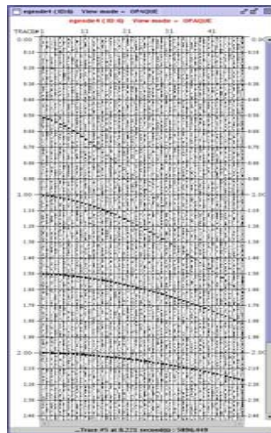
- 3D seismic

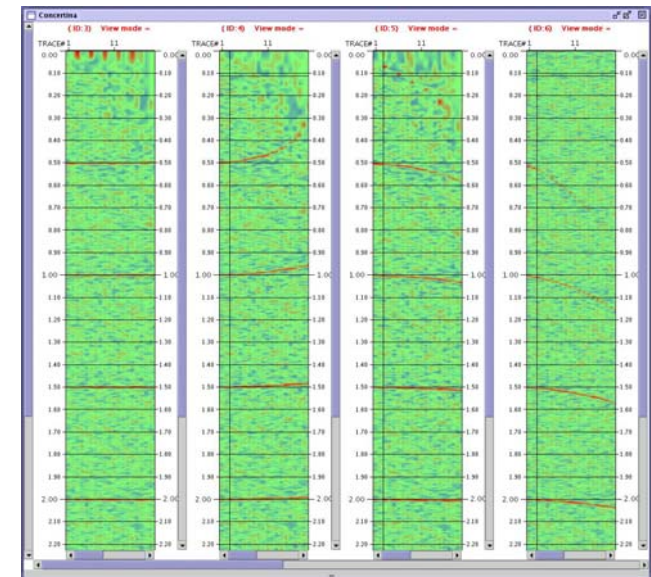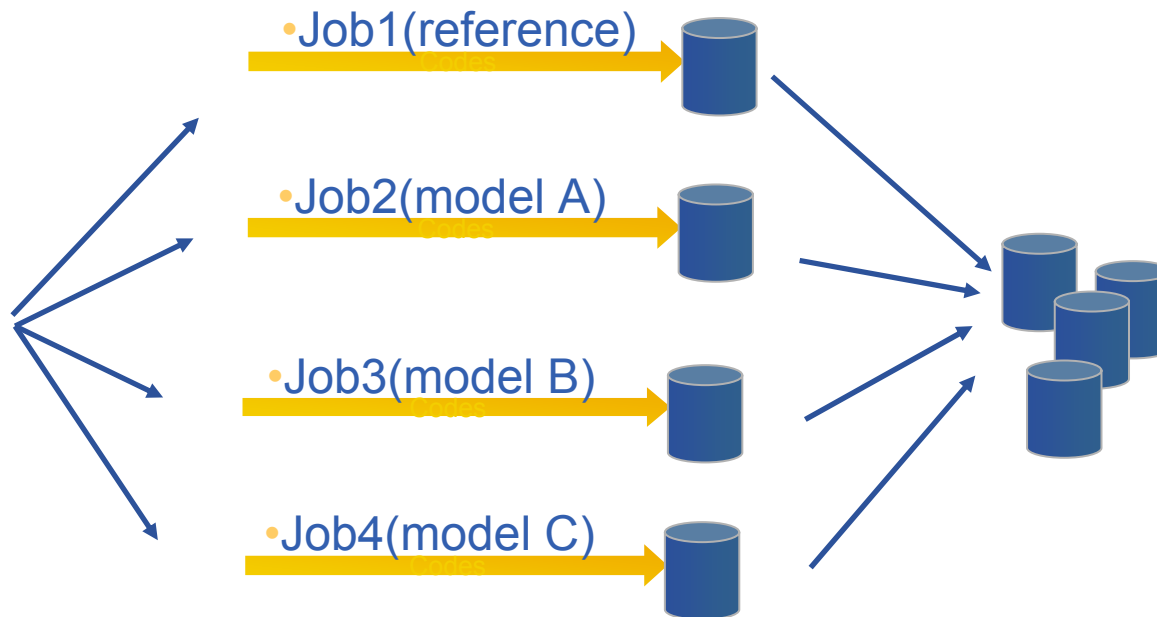- Velocity model

- Structural model

- **GeoCluster run on standard EGEE production grid and on GILDA for induction of new users**
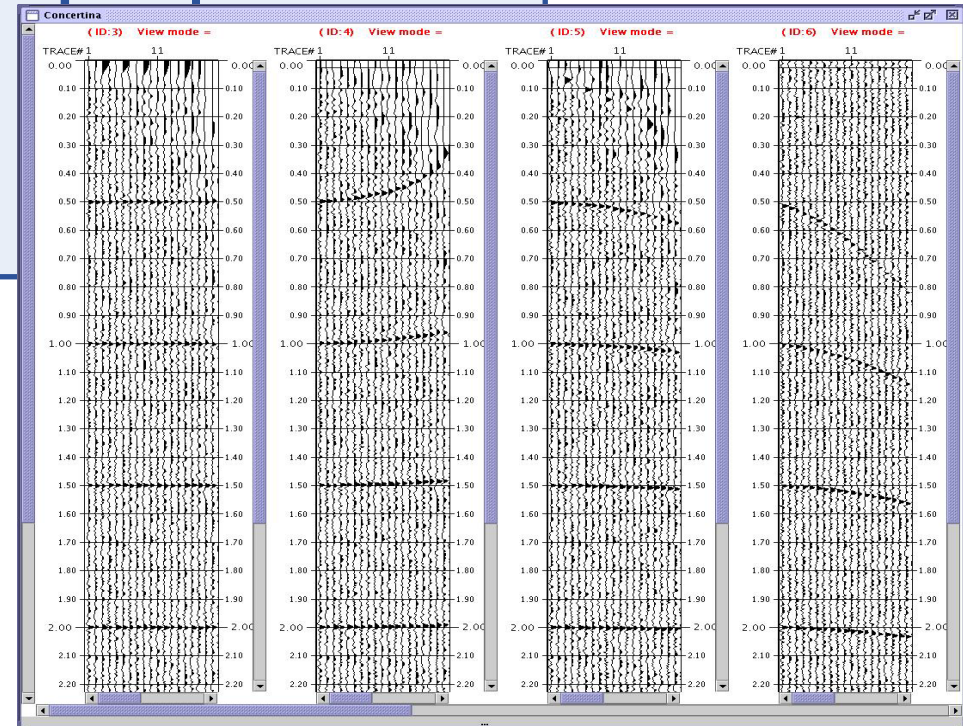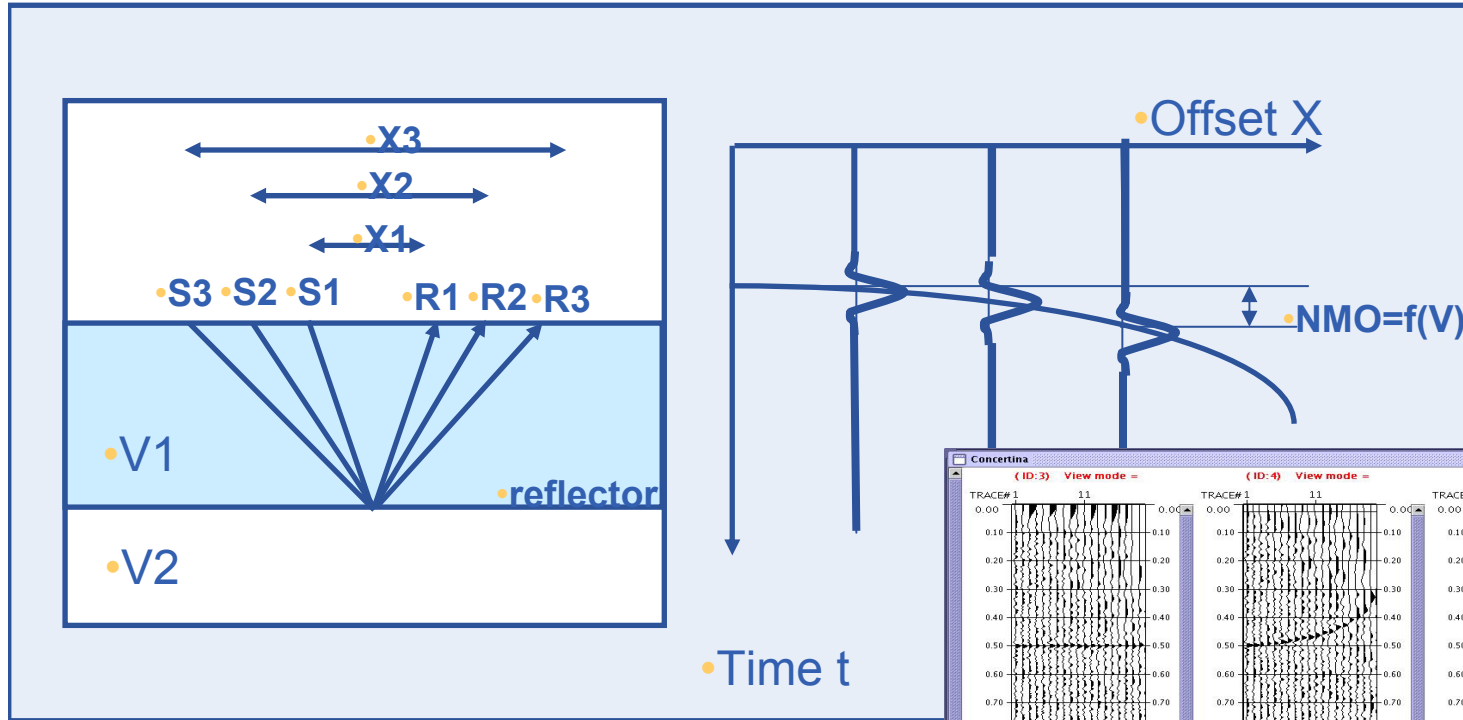 - Demonstration of a simple parametric study

•*launch*   •*run*   •*move*   •*analyze*

•Job1(reference)

•Job2(model A)

•Job3(model B)

•Job4(model C)
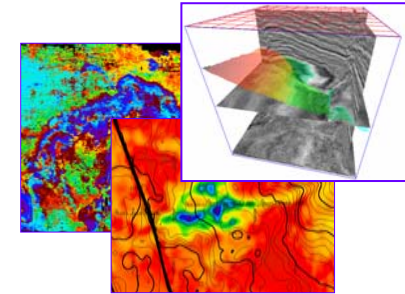
End 2004
20000+ cpus = 45 Tflops
1,5 Pb disc
5 Pb storage
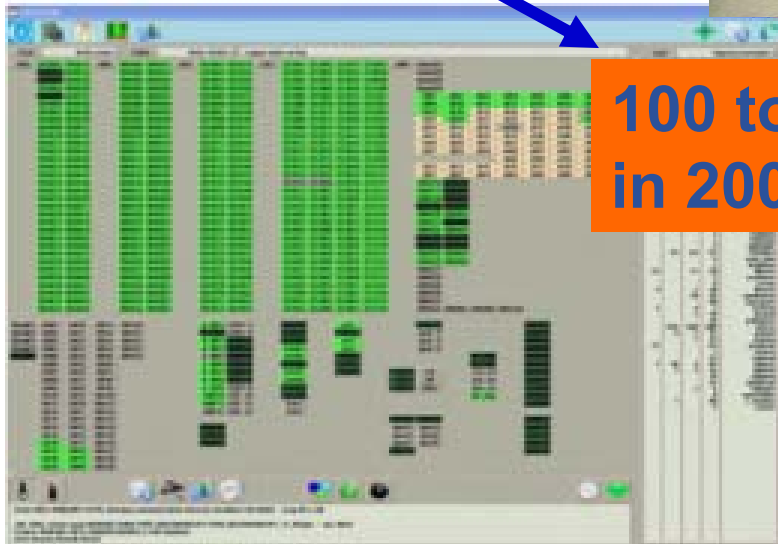
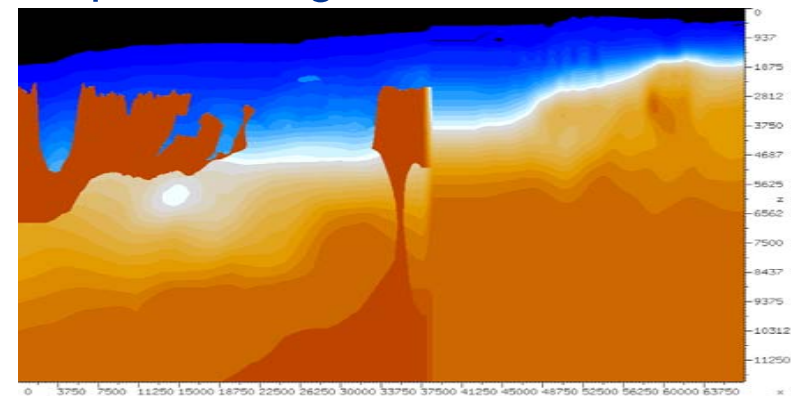**100 to 200 Tflops in 2006**

1Pflops in 2009?

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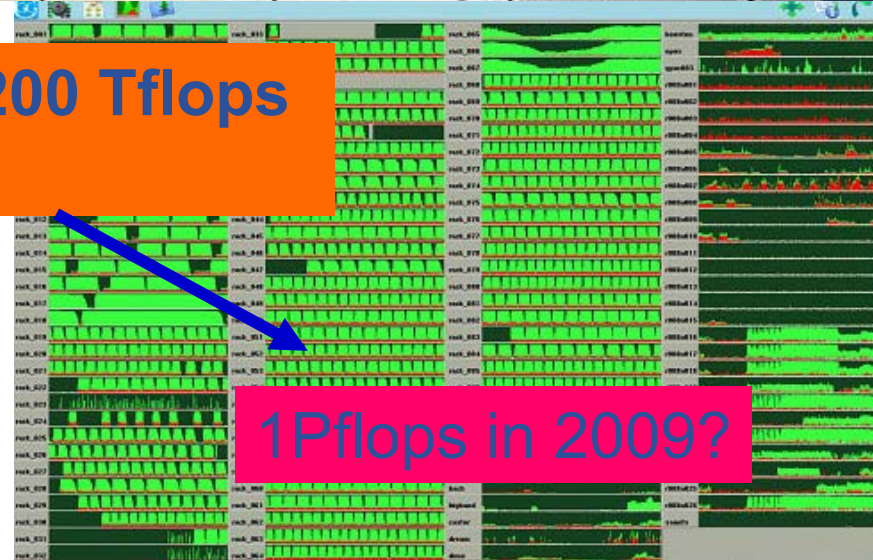
- **Who are the targeted users:**
  - Researchers in seismic processing algorithms
  - Researchers in geosciences *using* seismic processing
- **Few hundred, very scattered**

- **Imaging benchmark example:**

- **CGG**
  - R&D team has access to large production facilities
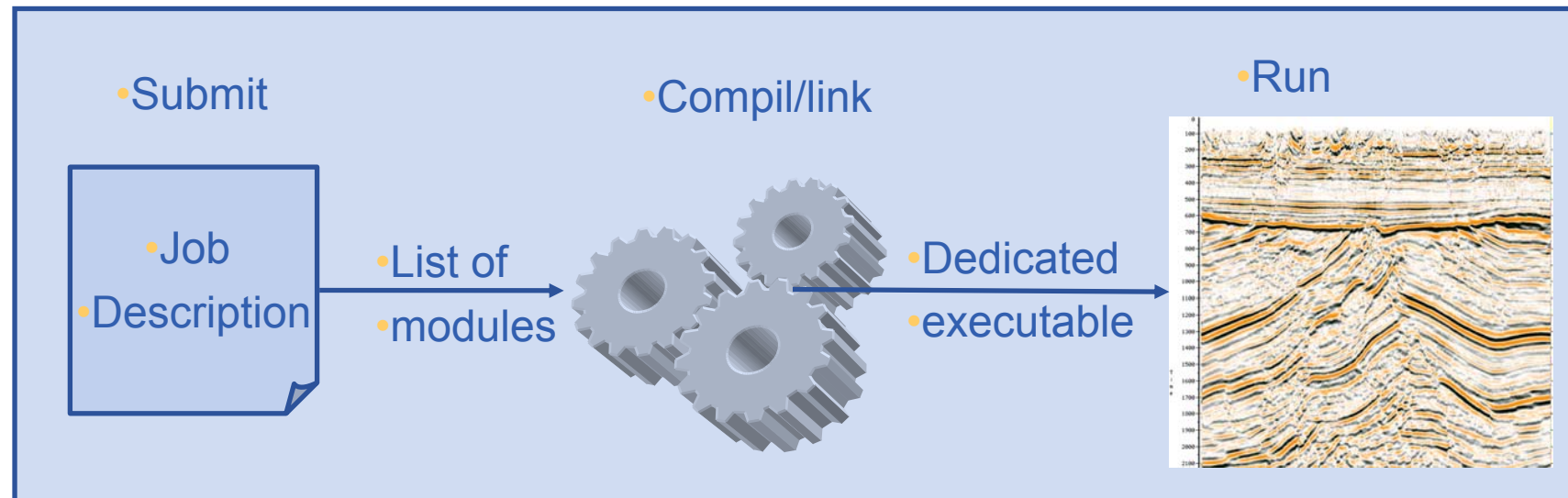 - Use state of the art technology in the full sequence
- **University**
  - Process a small part of data, hiding potential quality of results
  - Use basic processing except for imaging
  - Has a very innovative algorithm for imaging

- **The general benefits of grid computing:**
  - *Access to computing resources without investing in large IT infrastructure*
  - Lower the total cost of IT by sharing available resources

- **And the specific benefits for Research community:**
  - *Access to a comprehensive, industrial software*
  - Free the researcher from the additional burden of managing IT hardware and software complexity and limitations.
  - Have a framework to share data and project resources with other teams across Europe and the rest of the world,
  - Share best practices, support and training more easily.
  - Enable cross-organizational teamwork and partnership.

Deployment layout

- **Just started: the application is not yet fully available on the Grid**

- **3 Sites on production grid +GILDA**
  - CGG (CE/WNs; SE; UI), IPGP(CE/WN;UI), SCAI (CE/WN;SE)
  - GILDA(« get started »: easy access via portal for new grid user)
- **Key services**
  - Based on standard LCG-2
  - 2 RB (LAPP, LAL, CGG in Q1)
  - VOMS expected (managing sub-projects?)
  - MPI expected (for Imaging)
  - Licence server not yet implemented
  - Compilation/Link server implemented (not part of LCG-2)

- **A running application**
  - Gridifying: depedencies on run-time environment (WN!)
    - (new version of Geocluster: full availability: mid-2005)
  - Commercial software
    - (licence management must be implemented)
  - Size of the binary executable (>2Gb by default)
    - (two phases: compil/link + run => compilation server)

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Enabling Grids for E-sciencE

Blue=LCG-2; green = EGEODE

RB

UI

CE

- List of modules

Compilation Server

- Executable

WN

Licence Server

- Runtime key

Enabling Grids for E-sciencE
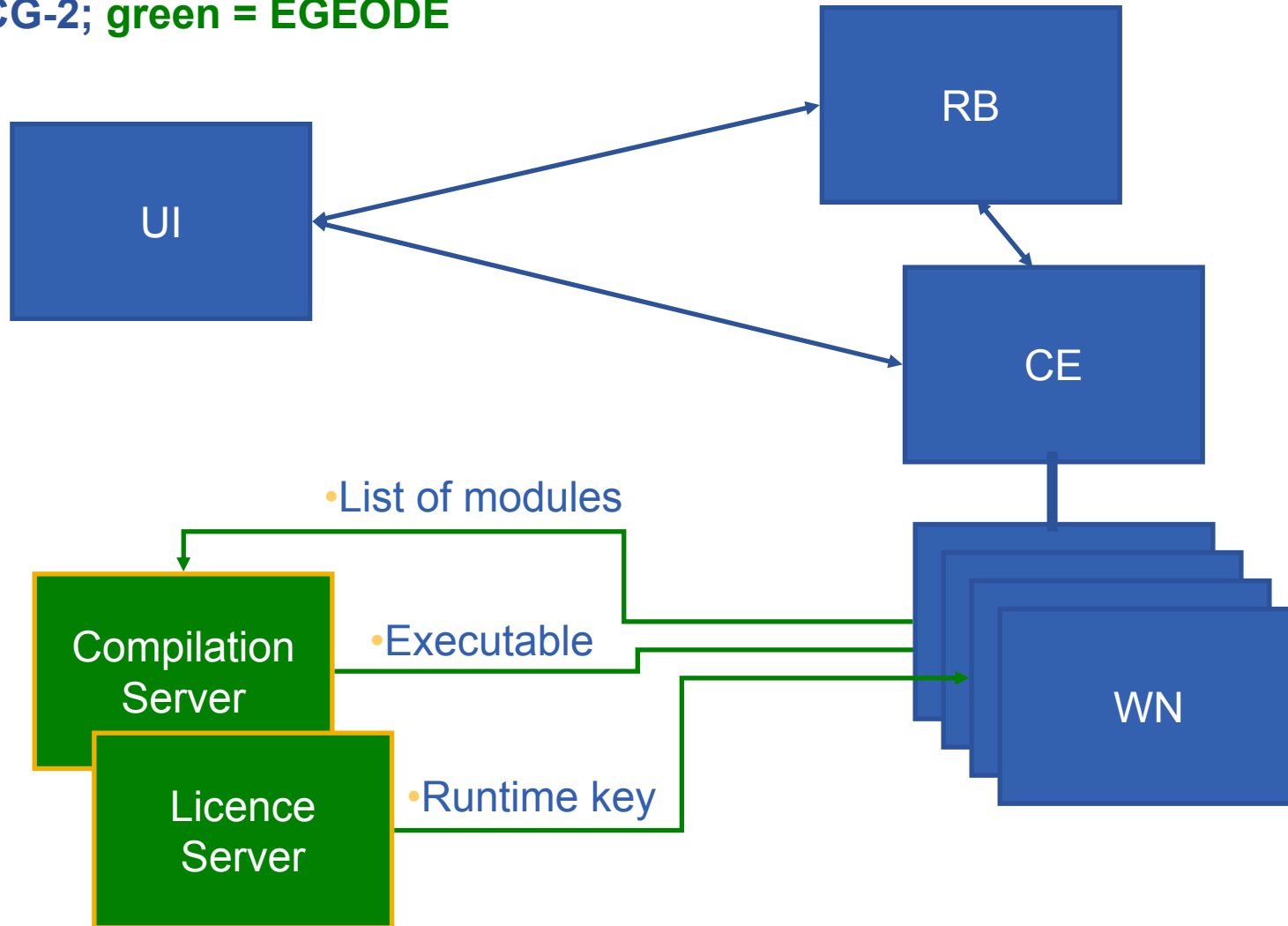
- **No figure available**
  - Accounting system not yet used,
  - What are the relevant indicators (->TCO) ?

- **Significant cost saving expected from centralized software management**

Enabling Grids for E-sciencE

- **Lessons learned**
  - It works
  - The learning curve is significant

- **Next activities (in collaboration with ESR and EGEE)**
- **1 – Application**
  - Finalize the porting of the application to the grid
  - Implement a licence management system
  - Implement an accounting system
  - Work on the data management issues (data servers, SE,..)

- **2 – Users/deployment**
  - Train a support team aware of both application and grid topics
  - Create a web based, support and information system (as any other VOs)
  - Consolidate and Formalize membership

eGee

Enabling Grids for E-sciencE

- **what's missing to go to full production:**
  - The validated application

  - An economical/usage model (and accounting tool)
    - To support a good balance between users and providers of resources
    - To include cost of network transfer

  - A mean to manage projects inside a VO: authorization for a user to access a project, accounting and licence management at a project or user level.

  - Middleware to implement local policies about dynamic priorities and resources allocation to VOs or Projects

- **Expected deployment of EGEODE (with SA1 and NA4 support)**
  - 5 sites, 100 nodes, 10 users Q2-2005
  - Up to 25 sites, 500 nodes, 100 users Q1-2006

- **Early examples of EGEE infrastructure usage from various scientific disciplines**

- **Development and deployment of Grid applications still require a significant amount of effort: not yet Plug-and-Play!!**

- **Common issues**
  - Interactive jobs
  - Outbound connectivity
  - Security (data privacy)
  - Commercial license issues