The Grid environment

and

the Grid Services for Computational Chemistry

CESGA

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CENTRO DE SUPERCOMPUTACIÓN DE GALICIA

CESGA

ESTABLISHED IN 1993

IN SANTIAGO DE COMPOSTELA [SPAIN]

CESGA

Legal entities

- **Public Company**
- **Public Foundation**

Partners

- **Regional Government of Galicia** 70 %

Xunta de Galicia

- **National Research Council of Spain** 30 %

CSIC

CESGA

mission statement

- **To provide** high performance computing, communications resources and services to the scientific community of Galicia and to the National Research Council, as well as, to institutions and enterprises with R&D activity.

- **To promote** the use of new information and communication technologies applied to research within the scientific community of Galicia.

- **To become** a consolidated RTD Centre of Excellence serving as international scientific and technological reference in the field of computing science and numerical simulation.

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CESGA Services

- HPC y HTC
- User Data Storage
- Communications Network (only in Galicia)
- E-Learning Rooms (Access Grid)
- GIS
- e-Business

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High Performance Computing Group

- Dr. Ignacio López Cabido (Physics)
- Dr. Andrés Gómez Tato (Physics)
- Dr. Carlos Fernández Sánchez (Physics)
- Dr. Javier López Cacheiro (Physics)
- Dr. José Carlos Mouriño Gallego (Computer Eng.)
- Dr. Aurelio Rodríguez López (Chemistry)

OUR POLICY

➲ **CESGA:**

- More than 40 technicians
- 22 avtive projects
- 35 ended projects in the last 5 years
- **ALWAYS in Collaboration**.

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13 years of history

1993

VP 2400

2,5 GFLOPS

1998

VPP 300

14,1 GFLOPS

AP 3000

12 GFLOPS

1999

HPC 4500

9,6 GFLOPS

STORAGETEK

51 TERABYTES

2001

SVG

9,9 GFLOPS

2002

HPC 320

64 GFLOPS

BEOWULF

16 GFLOPS

2003

SUPERDOME

768 GFLOPS

2004

SVG

512 GFLOPS

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VP-2400 AND Superdome 2003

1993: VP-2400 2,5 GFLOPS 0,5 GB RAM

Nº 1 in Spain and Nº 145 in the World

2003: SUPERDOME 768 GFLOPS 384 GB RAM

Nº 1 in Spain and Nº 227 in the World

XUNTA DE GALICIA
CONSELLERÍA DE INNOVACIÓN, INDUSTRIA E COMERCIO
Dirección Xeral de Investigación e Desenvolvemento

cofinanciado por
FEDER
Fondo Europeo de Desenvolvemento Rexional

CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS CSIC

MINISTERIO DE CIENCIA Y TECNOLOGÍA

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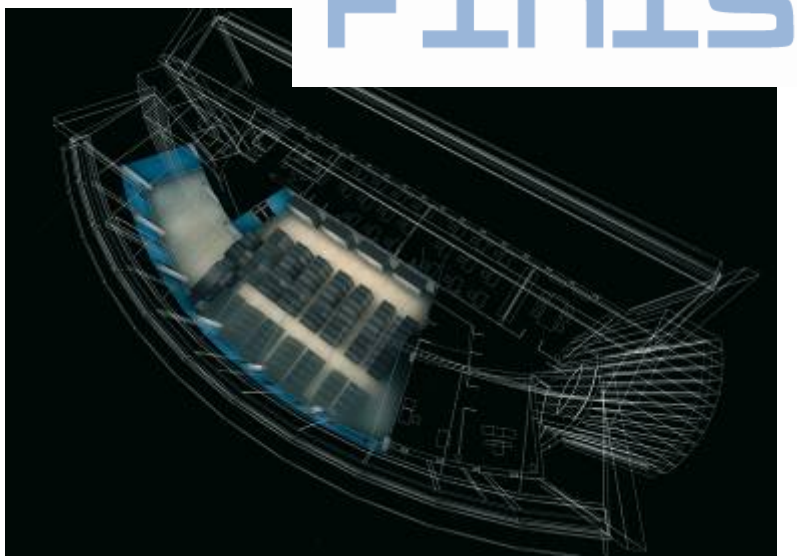
FinisTerrae 2007

FINISTERRAE



New Server HPC 2007

More than 16 TFLOPS and 19TB RAM Memory

Joint Venture of

XUNTA DE GALICIA
CONSELLERÍA DE INNOVACIÓN, INDUSTRIA E COMERCIO
Dirección Xeral de Investigación e Desenvolvemento

intel

hp invent

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CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS CSIC

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FinisTerrae

FINISTERRAE

SUPERCOMPUTING:

146 ccNUMA Nodes with **Itanium II** CPUs connected through a high efficiency INFINIBAND network

- 1 node: 128 cores, 1.024 GB memory
- 1 node: 128 CPUs, 384 GB memory
- 142 nodes: 16 cores, 128 GB memory
- 2 nodes: 4 cores, 4 GB memory for testing

DATA STORAGE:

- 22 nodes with 44 cores for storage management
- 390 TB disk
- 1 PB Robot Tape Library

MORE TECHNICAL INFORMATION ON REQUEST

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PROJECTS:
-EGEE and CompChem
Int.eu.Grid
-CESGA-CESCA
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LARGEST GRID INITIATIVES in SPAIN (10/2006)

- EU DataGrid
- EU CrossGrid
- LCG (LHC Computing Grid)
- IRISGrid
- EGEE
- EGEE II
- DEISA
- Int.Eu.Grid
- IBERGrid Initiative
- Spanish Middleware Thematic Network
- EUMEDGrid
- EELA

CESGA is/was partner in all projects marked in red

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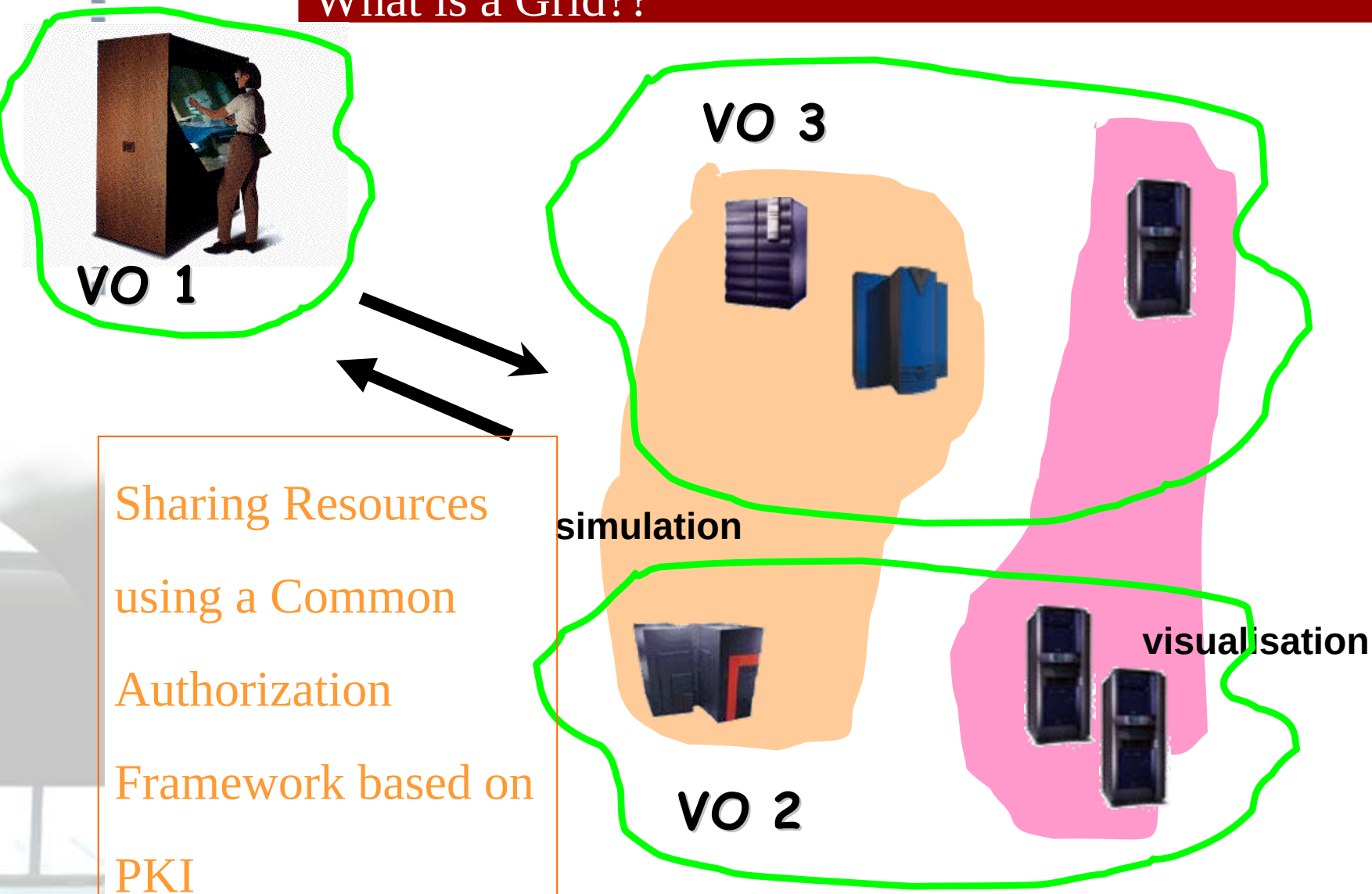
What is a Grid??



Sharing Resources using a Common Authorization Framework based on PKI

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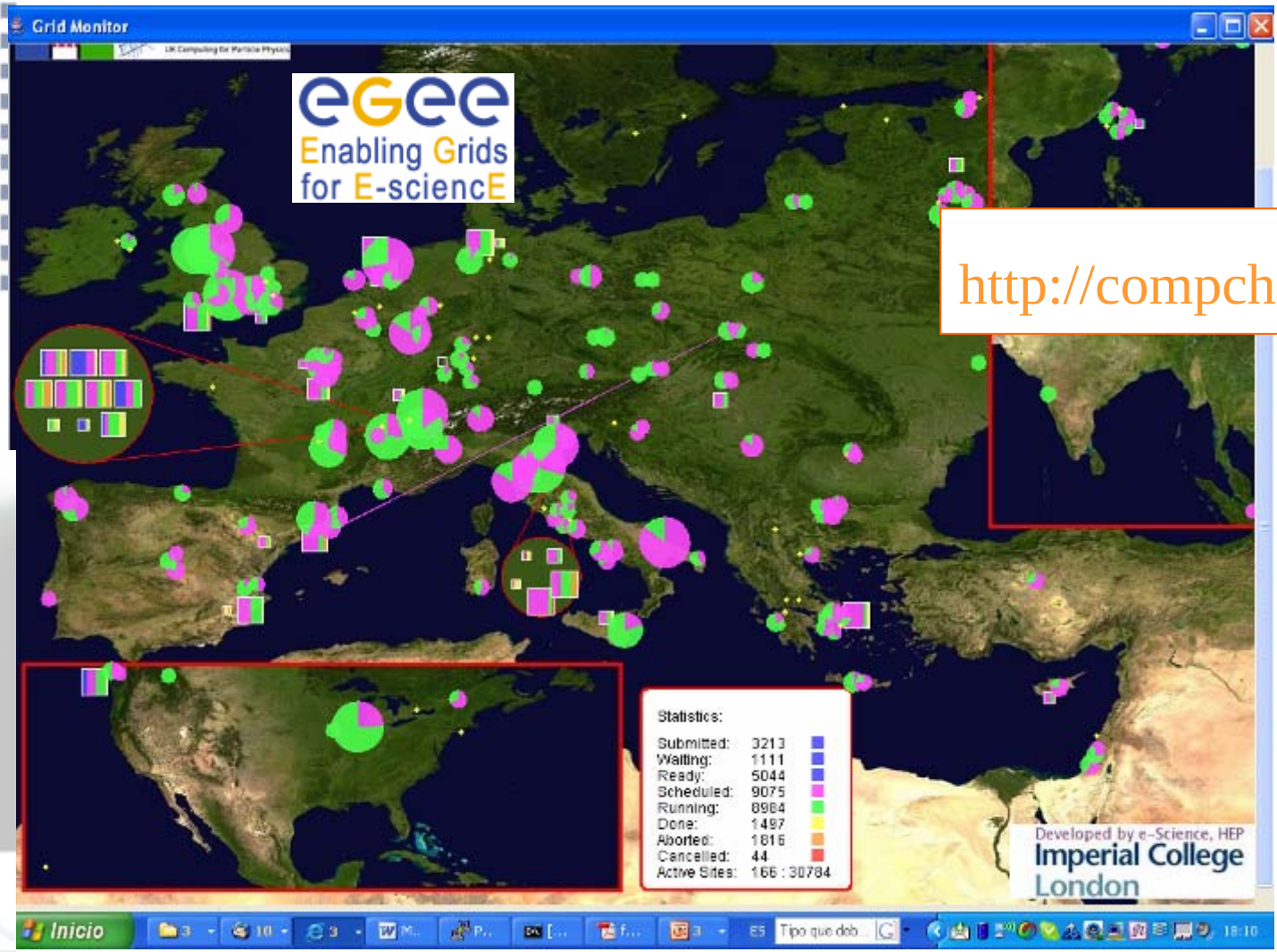
EGEE and CompChem



http://compchem.unipg.it/

Maybe Osvaldo can talk about it latter!

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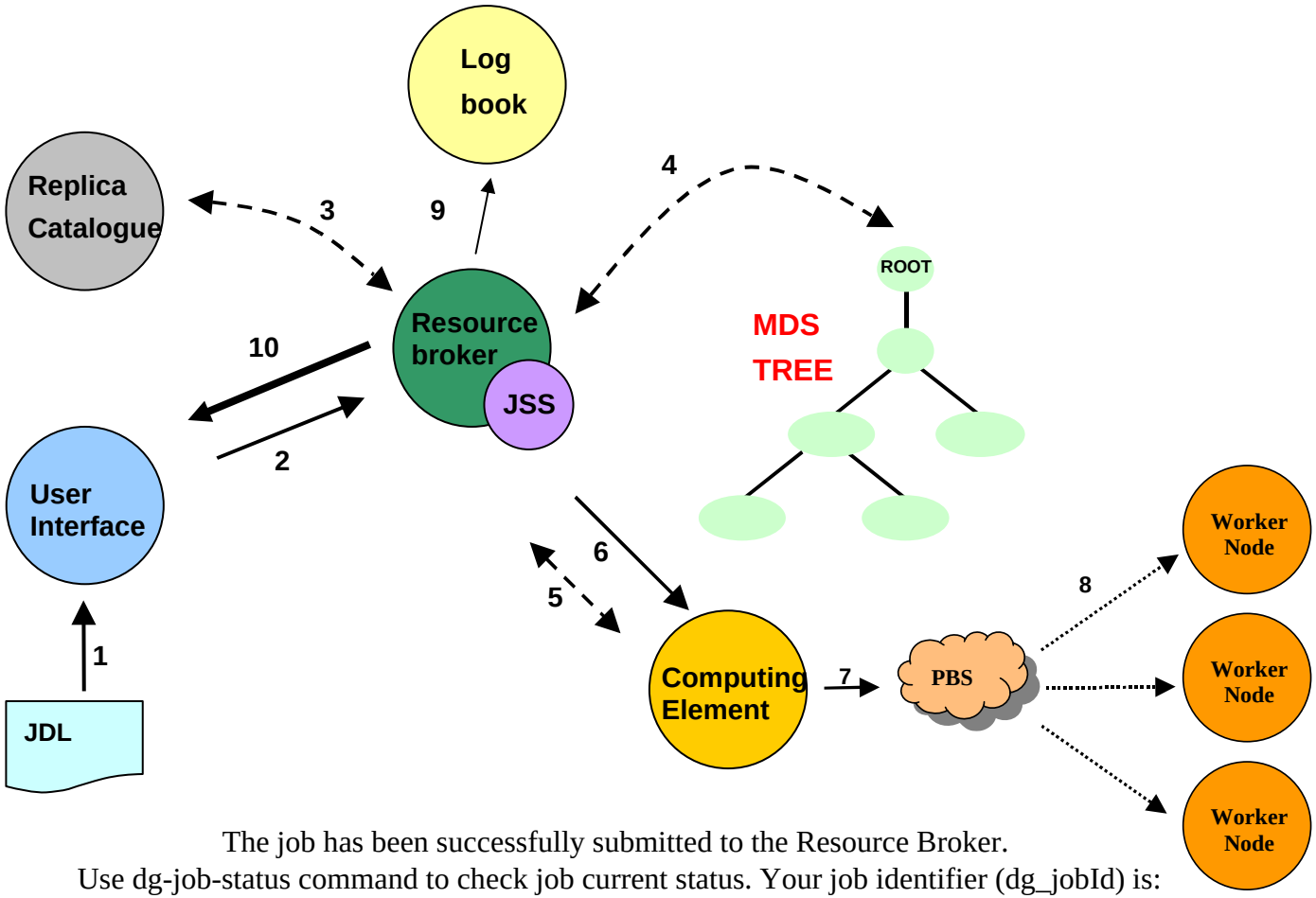
Grid Job Submission



The job has been successfully submitted to the Resource Broker.
Use dg-job-status command to check job current status. Your job identifier (dg_jobId) is:

- https://lngrid06.lip.pt:7846/192.168.4.252/15443164719173?lngrid06.lip.pt:7771

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The Interactive European Grid Project

"Interoperable production-level e-Infrastructure for demanding interactive applications to impact the daily work of researchers"

because researchers need answers in seconds, not in hours.

http://www.interactive-grid.eu

Instrument **I3**
Duration **2 years may ´06-april ´08**

- **Distributed Parallel (MPI) Interactive Computing & Storage at the Tera level**
- **User Friendly Access**
- **Grid Interactive Desktop**

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The Interactive European Grid Project

- the **int.eu.grid** project aims to ***change the way researchers can use the available e-Infrastructure***, exploiting the interactivity and collaboration possibilities
- **Researchers need to be convinced** that they can:
  - Transfer and process gigabytes of information in minutes
  - Foresee more complex algorithms on larger statistics, test and tune them, use more powerful visualization techniques
  - Collaborate across the network in a rewarding mode, from sharing information to discussing and presenting remotely through enhanced videoconference environments.

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The Interactive European Grid Project

*"To **deploy and operate a production-quality** Grid-empowered eInfrastructure oriented to **service** research communities supporting demanding interactive applications."*

- Deployment of e-Infrastructure
  - Oriented to interactive use
  - Site integration support
  - Grid operations service
- Middleware for interactivity and MPI
  - Adapt/integrate existing middleware
  - guarantee interoperability with EGEE
- Provide a complete interactivity suite
  - Desktop
  - roaming access
  - scheduler with prioritization services
  - complex visualization.
- Support for interactive applications:
  - setup of collaborative environment and VO
  - consideration of performance
  - interactivity and visualization requirements
  - identification and selection of research oriented interactive applications
- Support remote collaboration activities:
  - research, management, integration, training
- Approach target research communities
- Provide security measures for interactivity

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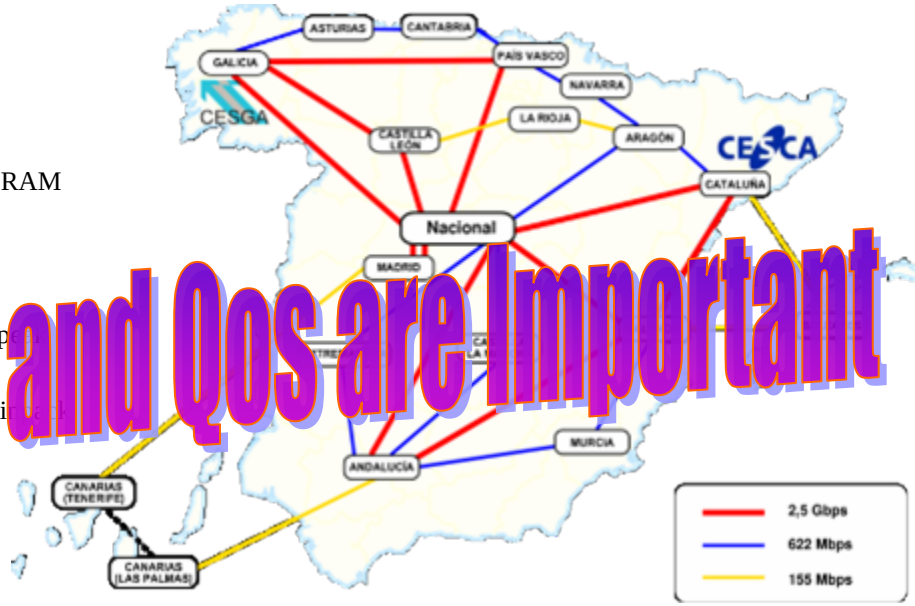
CESGA Experiences: a proof of the concept

Some time ago... Year 2003: Grid between 2 supercomputation centers CESGA/CESCA

Real application, a lot of memory required

- 2 HPC320
- 64 CPus
- 100 Gbytes RAM
- 4 TB disk



Latency and Qos are Important

- **Run OK**
- **Many initial tests needed (firewall, application start)**
- **QoS mechanism needed, high availability..**
- **The network behave very reasonably, no problem in that sense**

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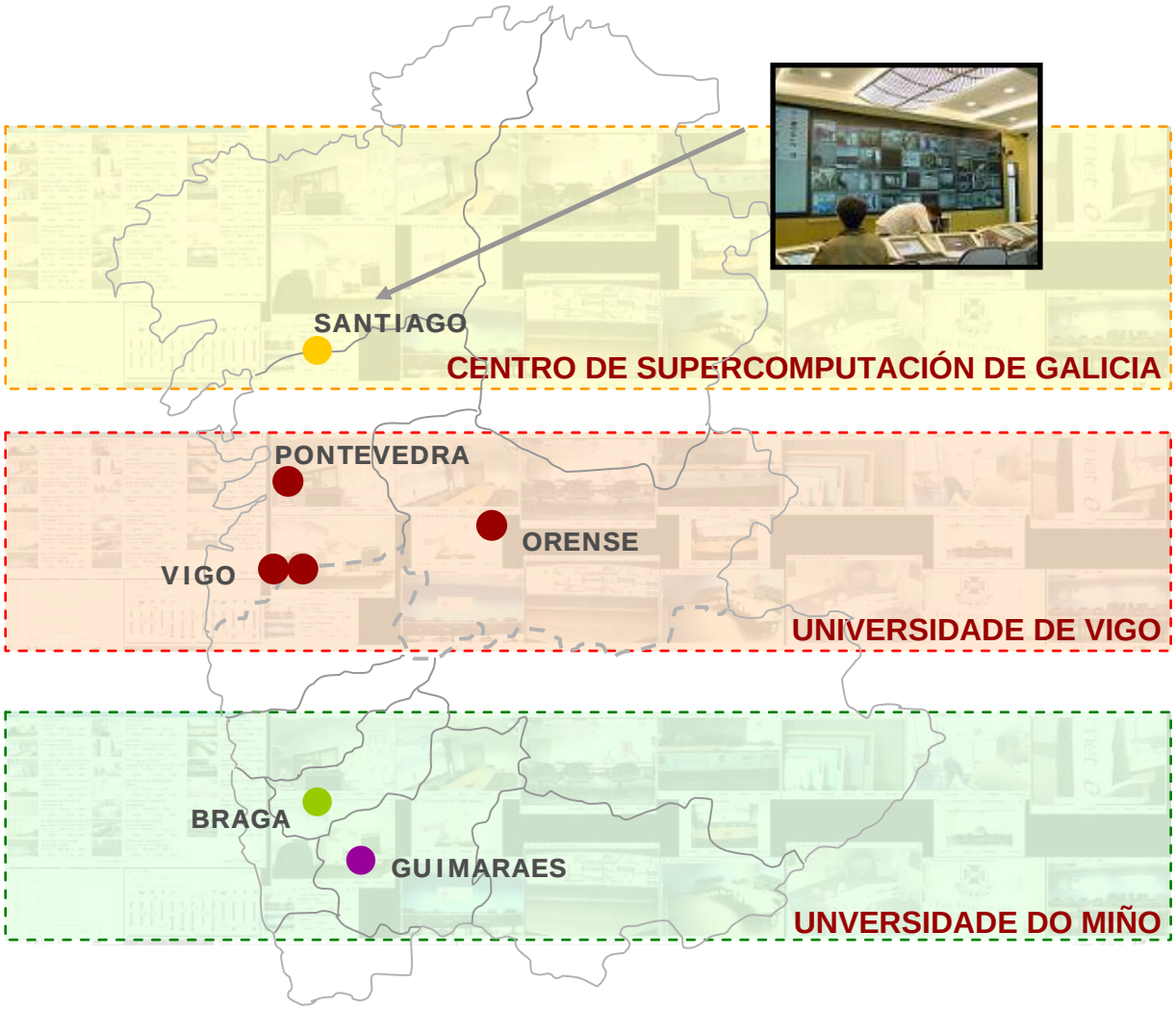
ACCESS GRIDS



- CCG
- Universidad de Miño
- Universidad de Vigo
- CESGA

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ACCESS GRID ROOM NETWORK



GRID SERVICES

CESGA Experiences with Web Services and Grid

- **RENDERGRID.** Based on GT3. Services to render scenes for SMEs. Filesize too large for commercial networks.

- **FUNCMOV.** Web services for off-board car route calculation. Filesize using SOAP too large for GPRS.

- **eIMRT.** In process. Remote computational platform for treatment VERIFICATION and OPTIMIZATION in RadioTherapy. 1000s of simultaneous jobs block EGEE scheduler.

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USUAL Grid Services

- **Job Submission and Job Monitoring.**
- **File Transfer**
- **Data access**

But

THEY ARE KERNELS TO MAKE NEW SERVICES On TOP

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What a Chemistry Grid Service Needs

- A Clear WSDD Definition.
  - Messages
  - Methods
- An infrastructure
- A Middleware:
  - WSRF/GT4
  - OMII
  - LCG
  - gLite
  - ....
- Thin/Fat Client

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What is a fashion NOW

- **Scientific WorkFlow/Problem Solving Environments**
  - **Informnet (SDSC)**
  - **SOMA (Workflow for Small Molecule Property Calculations on a Multiplatform Computing Grid)**
  - **ECEE ("A Problem Solving Environment's Evolution Toward Grid Services and a Web Architecture")**
  - **SIMBEX (ask Olvaldo)**
- **Semantic Grid**

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What next for ELAMS?

- **Choose a Grid Environment for working (GT4, EGEE, Int.eu.grid, other?)**
- **Make a simple test of Grid visualization without services: Input file in one institution, Render in a 2nd institution, visualize in a 3rd institution.**
- **If EGEE, create a new VO?**

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What can we provide?

- **Storage and CPU cycles**
- **Access Grid room**
- **Grid Knowledge**
- **Limited man-power (if not external funding)**

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Thanks for your attention!! Questions??