Open Grid

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Part of the slides came from:

- plenary lecture of Isabel Capos Plasencia at ICCSA08 Conference June – July 2008, Perugia, Italy
- Grid Security presentation of Rachana Ananthakrishnan, Argonne National Lab

1. Summary

1. **E-Science and E-Infrastructures**
   – Overview of Computational Grids
2. **Grid Communities**
   – COMPCHEM VO
3. **Computational Chemistry on Grid**
   – Common applications
4. **Advanced applications**
   – MPI on Grids
5. **Security on Grid**
   – Typical scenarios and adopted solutions
6. **Future an sustainability**
   – European context and perspectives

1. E-Science and e-Infrastructures

1. E-Science and e-Infrastructures

E-Infrastructure new generation of research infrastructures based on information and communication technologies

E-Science refers to scientific activities that are carried out by using resources distributed across the internet

- The utilization of those distributed resources is both a **necessity and an added value**

- More effective when associated to a global collaboration more than at the individual level

1. E-science and e-infrastructures

New concepts but

- The basics of scientific work is still the same
  - Observation, experiment,…
  - Analysis, Result Validation, Publication, discussion,…
    - In all the steps computing technologies are a key issue

Observation, Experiment

Complex detectors located in accelerators, cameras installed in satellites, deployment of sensors networks for Earth Observation,…

Analysis, Modelling Result Validation

Computing resources

Advanced Computing Projects require furthermore

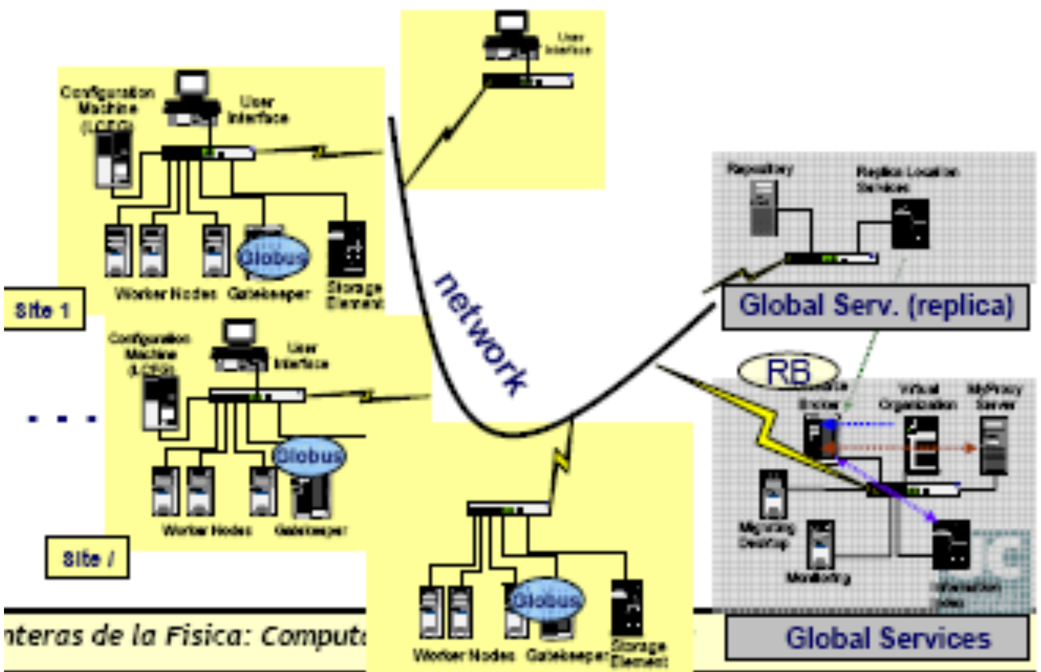
Specialized Hardware and Software

Methodology and Algorithmic developments

1. E-Science and e-infrastructures
What is a Grid ?

"A Grid is a set of resources, (digital instruments and elements attached to them or stored in them) which can be used in a combined way through a middleware to solve efficiently a particular problem"

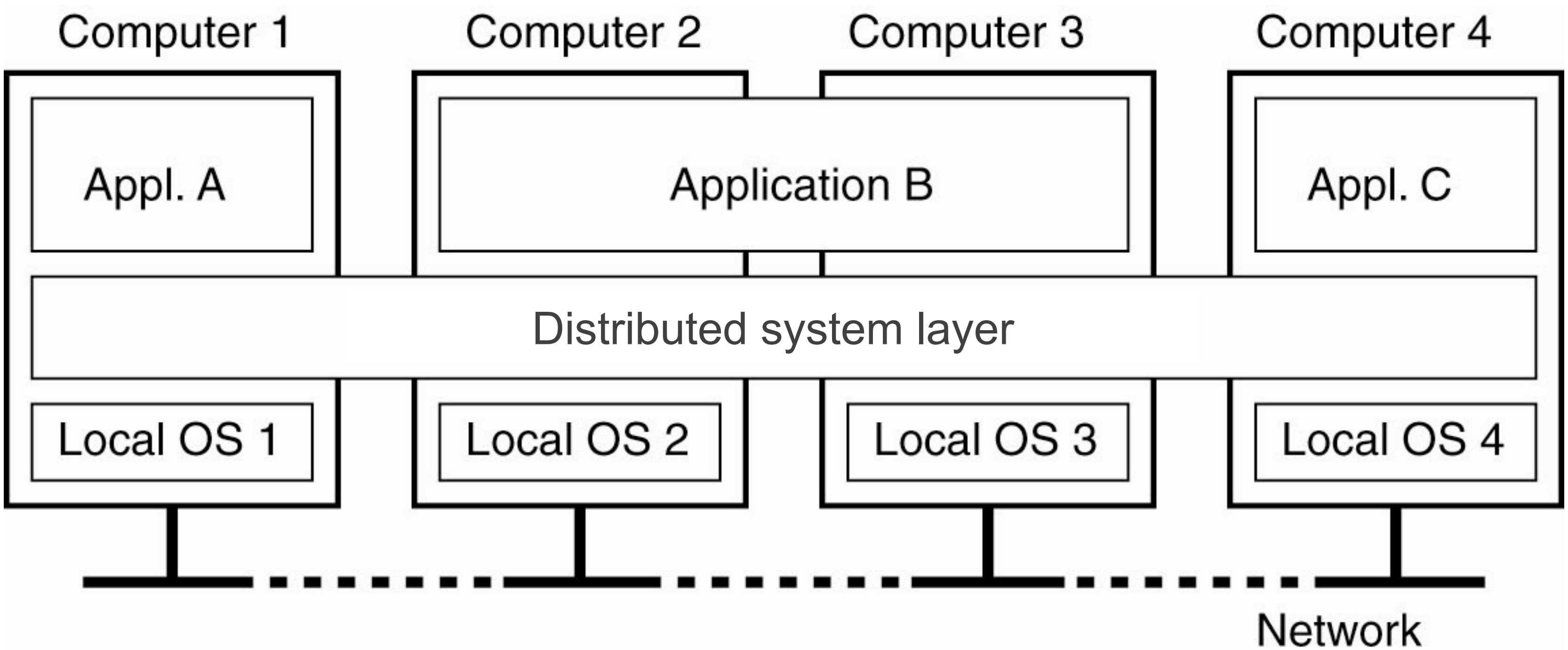
I. Foster



1. Distributed computing

Distributed computing is a field of computer science that studies distributed systems. A **distributed system** consists of multiple autonomous computers that communicate through a computer network.

1. Distributed computing



1. Distributed computing examples

Business Applications

- Airplane reservation system
- Banking system
- Storage management system
- Mail Servers

Other examples

- Grid computing
- Parallel computing

1. Parallel computing

Parallel computing is a form of computation in which many calculations are carried out simultaneously, operating on the principle that large problems can often be divided into smaller ones, which are then solved concurrently ("in parallel")

- High Performance Computing
- Clusters
- Single Multiprocessor machines

1. Grid Computing

Grid computing is afederation of computer resources from multiple administrative domains to reach a common goal. The **grid** can be thought of as a distributed system with non-interactive workloads that involve a large number of files.

1. Main Differences

What distinguishes grid computing from conventional high performance computing systems is that grids tend to be

- loosely coupled
- heterogeneous
- geographically dispersed

Although a single grid can be dedicated to a particular application, commonly a grid is used for a variety of purposes. Grids are often constructed with general-purpose grid middleware software libraries.

1. point checklist

1. Coordinates resources not subject to centralized control
2. Uses standard, open, general purpose protocols and interfaces
3. Deliver nontrivial qualities of service
   - e.g., response time, throughput, availability, security

1. Background: Related technologies

- Cluster computing
- Peer-to-peer computing
- Internet computing

1. Cluster computing

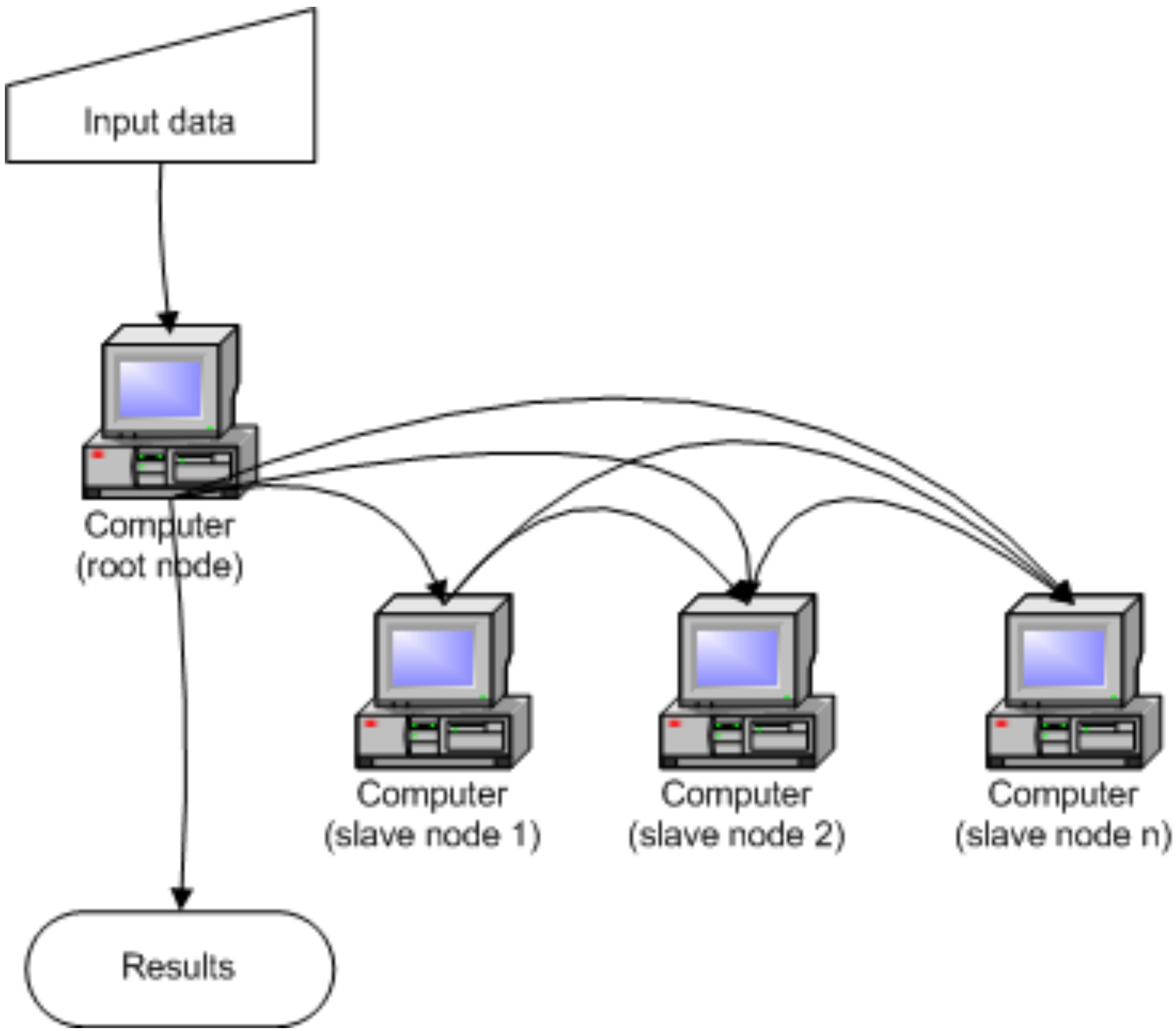
Idea: put some PCs together and get them to communicate

Cheaper to build than a mainframe supercomputer

Different sizes of clusters

Scalable – can grow a cluster by adding more PCs

1. Cluster Architecture



1. Peer-to-Peer computing

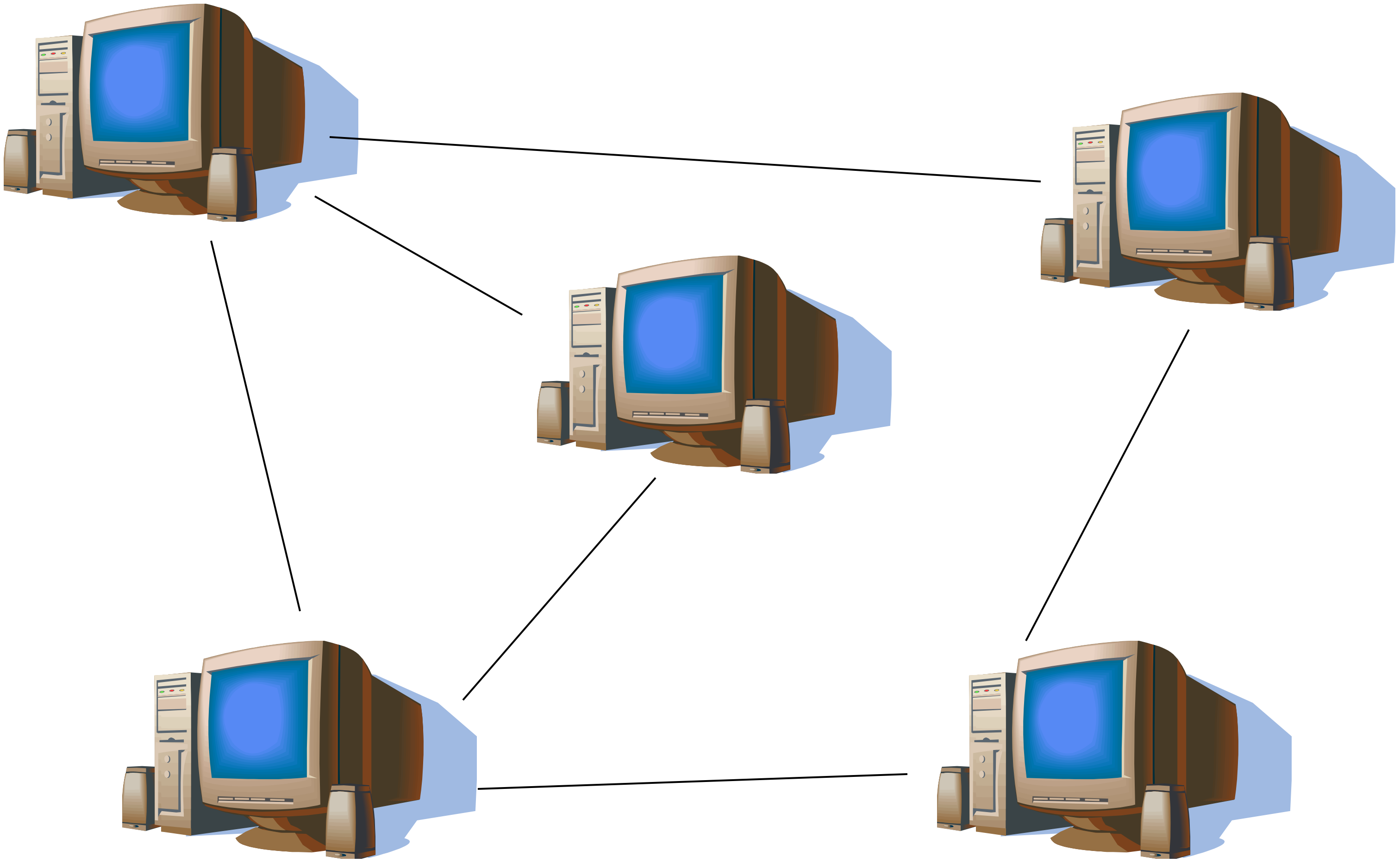
Connect to other computers

Can access files from any computer on the network

Allows data sharing without going through central server

Decentralized approach also useful for Grid

1. Peer to Peer architecture



1. Internet computing

Idea: many idle PCs on the Internet

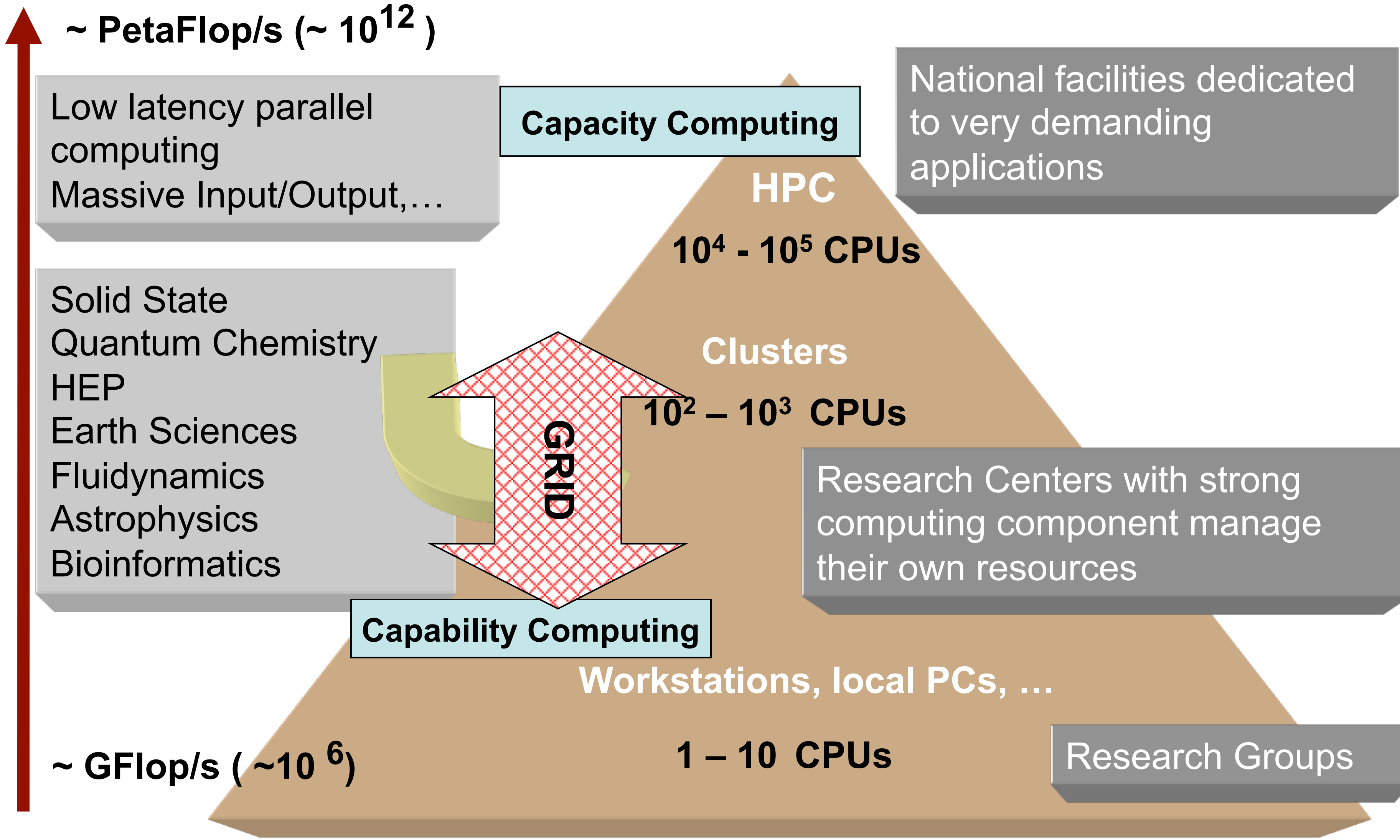
Can perform other computations while not being used

"Cycle scavenging" – rely on getting free time on other people's computers

Example: SETI@home

What are advantages/disadvantages of cycle scavenging?

1. E-Science and e-infrastructures Piramide Model



1. Some Grid Applications

- Distributed supercomputing
- High-throughput computing
- On-demand computing
- Data-intensive computing
- Collaborative computing

1. Distributed Supercomputing

- Idea: aggregate computational resources to tackle problems that cannot be solved by a single system
- Examples: climate modeling, computational chemistry
- Challenges include:
  - Scheduling scarce and expensive resources
  - Scalability of protocols and algorithms
  - Maintaining high levels of performance across heterogeneous systems

1. High-throughput computing

- Schedule large numbers of independent tasks
- Goal: exploit unused CPU cycles (e.g., from idle workstations)
- Unlike distributed computing, tasks loosely coupled
- Examples: parameter studies, cryptographic problems

1. On-demand computing

Use Grid capabilities to meet short-term requirements for resources that cannot conveniently be located locally

Unlike distributed computing, driven by cost-performance concerns rather than absolute performance

Dispatch expensive or specialized computations to remote servers

1. Data-intensive computing

- Synthesize data in geographically distributed repositories
- Synthesis may be computationally and communication intensive
- Examples:
  - High energy physics generate terabytes of distributed data, need complex queries to detect “interesting” events
  - Distributed analysis of Sloan Digital Sky Survey data

1. Collaborative computing

Enable shared use of data archives and simulations

Examples:

- Collaborative exploration of large geophysical data sets

Challenges:

- Real-time demands of interactive applications
- Rich variety of interactions

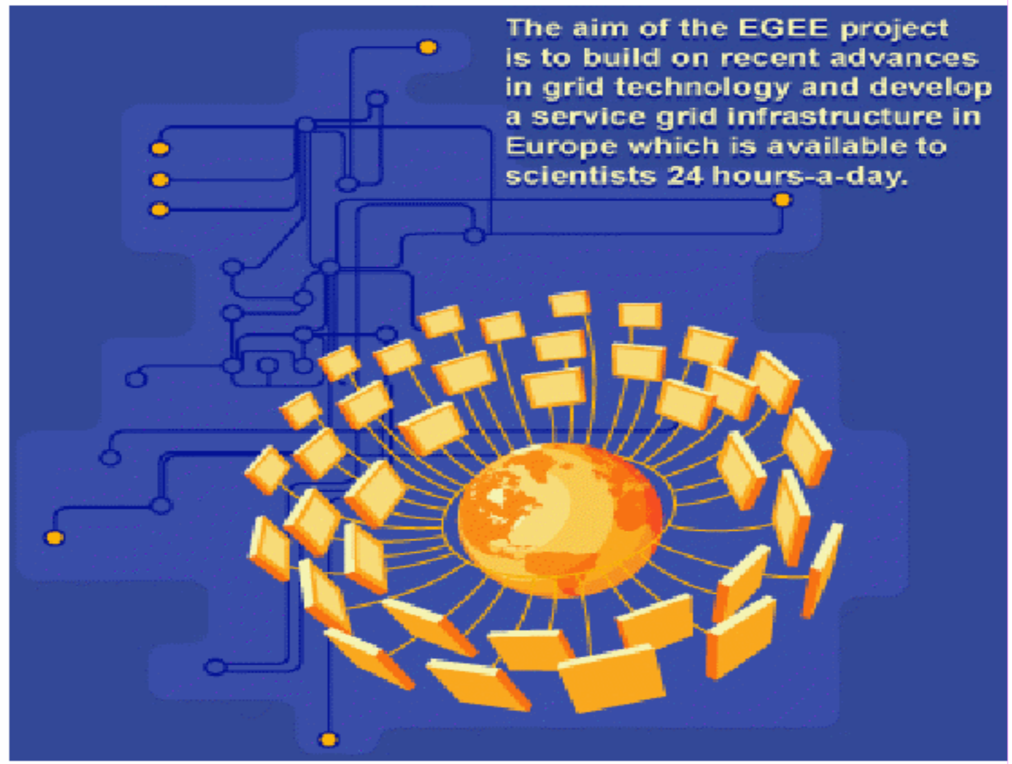
1. What do we expect from the Grid?

- Computing laboratory with almost infinite resources
- Access to distributed data
- Easy workload management
- Application interfaces easy to use

1. 2004-2010 The EGEE Project

Enabling Grids for E-sciencE

In order to create a seamless European Grid for the support of the European Research Area, the European Union founded the EGEE (Enabling Grids for E-Science in Europe) project that aims to integrate current national, regional and thematic Grid efforts.

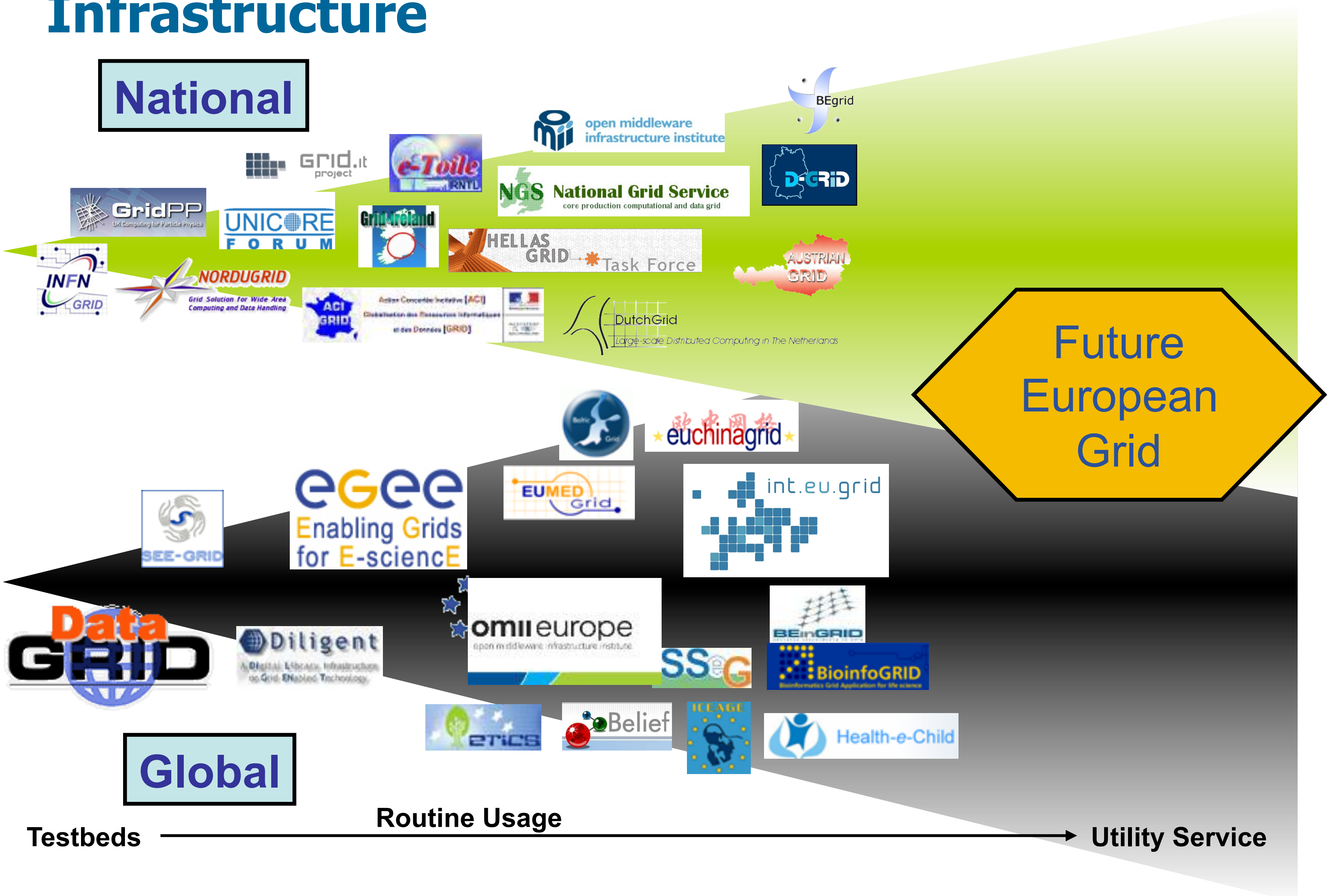


www.eu-egee.org

Information Society

University of Perugia

1. Evolution towards and European Grid Infrastructure



1. Future and Sustainability
European Grid Initiative

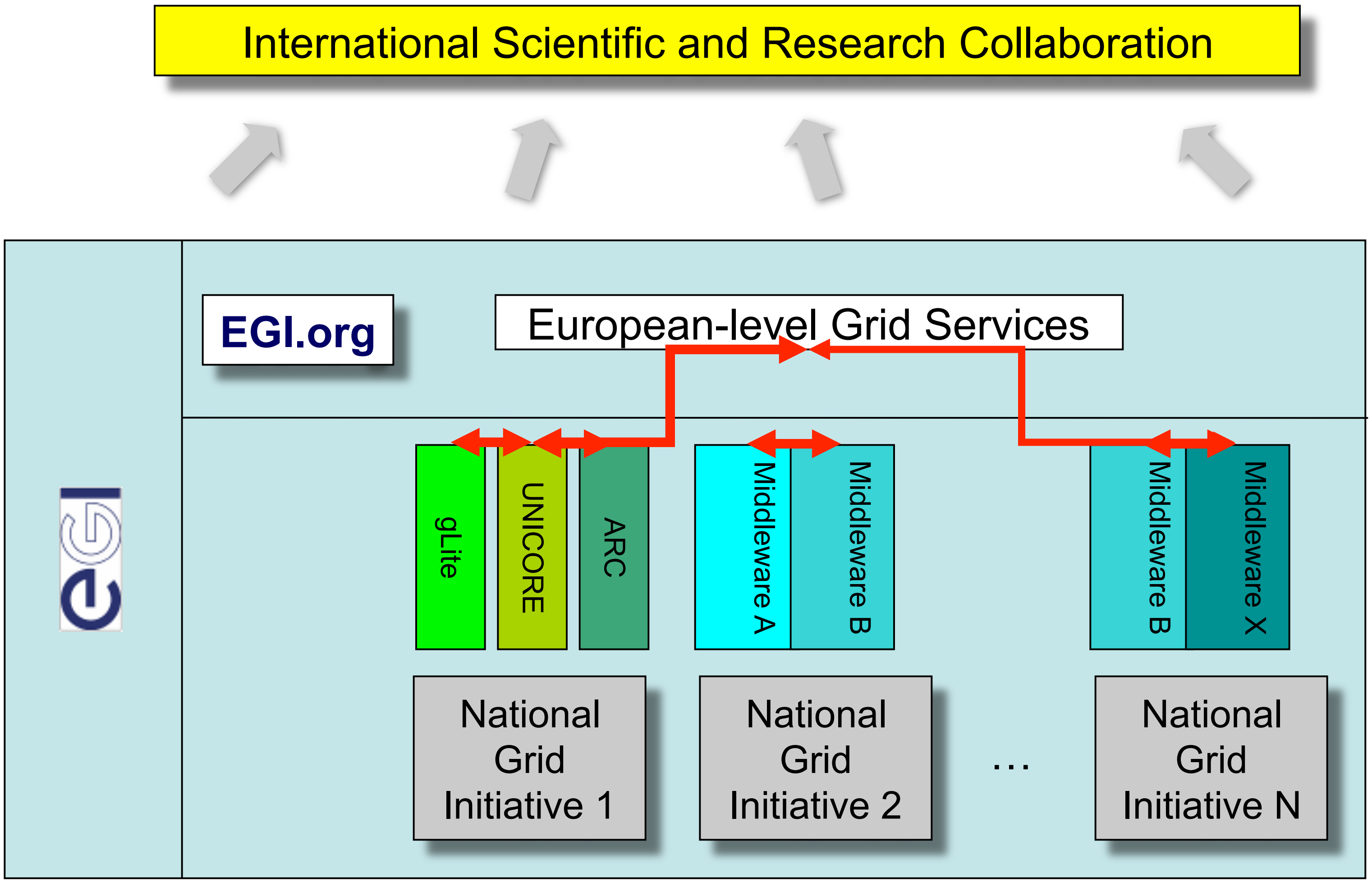
Goal:

- Ensure the long-term sustainability of grid infrastructures in Europe by establishing a new federated model bringing together NGIs to build the EGI Organization

Objectives:

- Ensure the long-term sustainability of the European e-infrastructure
- Coordinate the integration and interaction between National Grid Infrastructures
- Operate the European level of the production Grid infrastructure for a wide range of scientific disciplines to link National Grid Infrastructures

1. Future and Sustainability Model for EGI Infrastructure



1. Characteristics of NGIs

Each NGI

- … should be a recognized national body with a **single point-of-contact**
- … should mobilize national funding and resources
- … should ensure the operation of a national e-Infrastructure
- … should support user communities (application independent, and open to new user communities and resource providers)
- … should contribute and adhere to international standards and policies

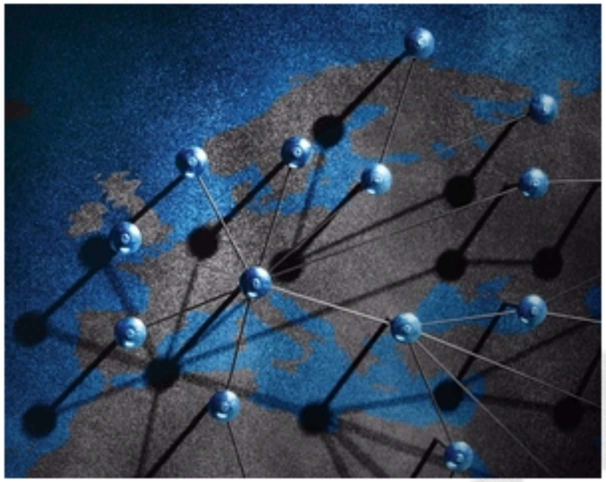
NGIs in Europe

www.eu-egi.eu

European Grid Initiative

»Towards a sustainable production grid infrastructure«

WELCOME TO EGI



Goal of EGI Design Study:

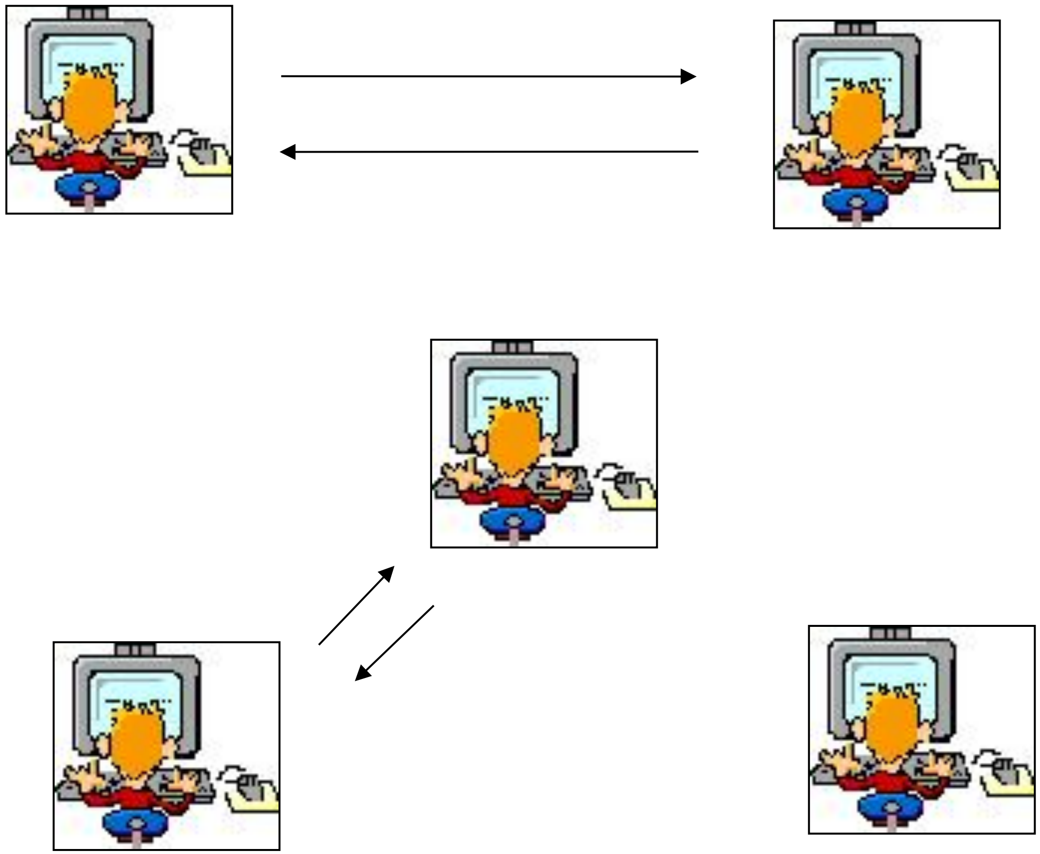
Conceptual setup and operation of a **new organizational model** of a sustainable pan-European **grid infrastructure**

- Objectives of EGI Design Study
- National Grid Initiatives
- Press releases
- Contact us

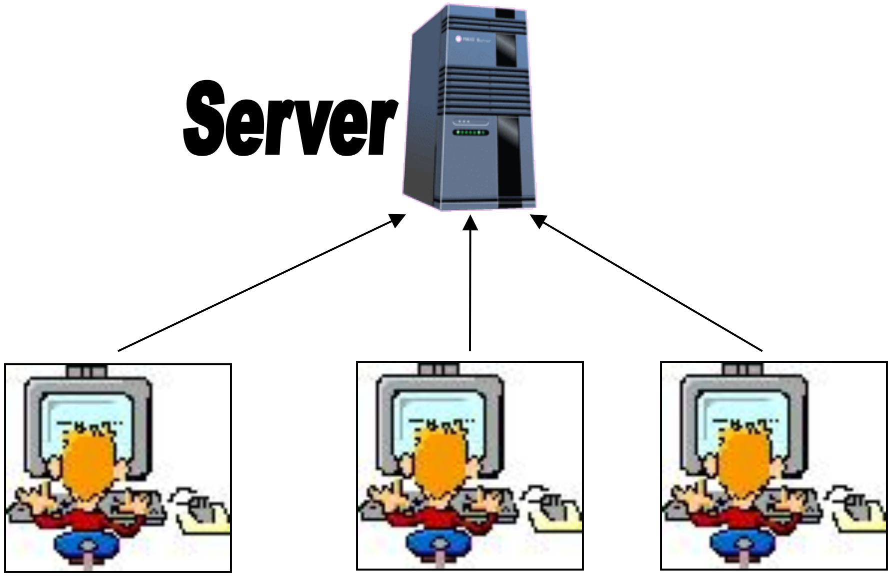
www.eu-egi.eu

e-infrastructure

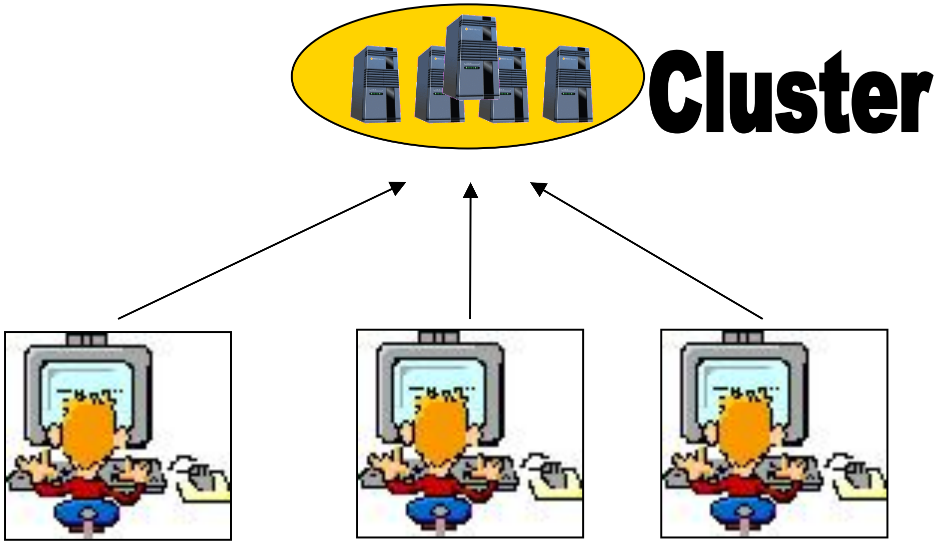
1. Deployment of Computational Grids
How was analysis before Grid ?

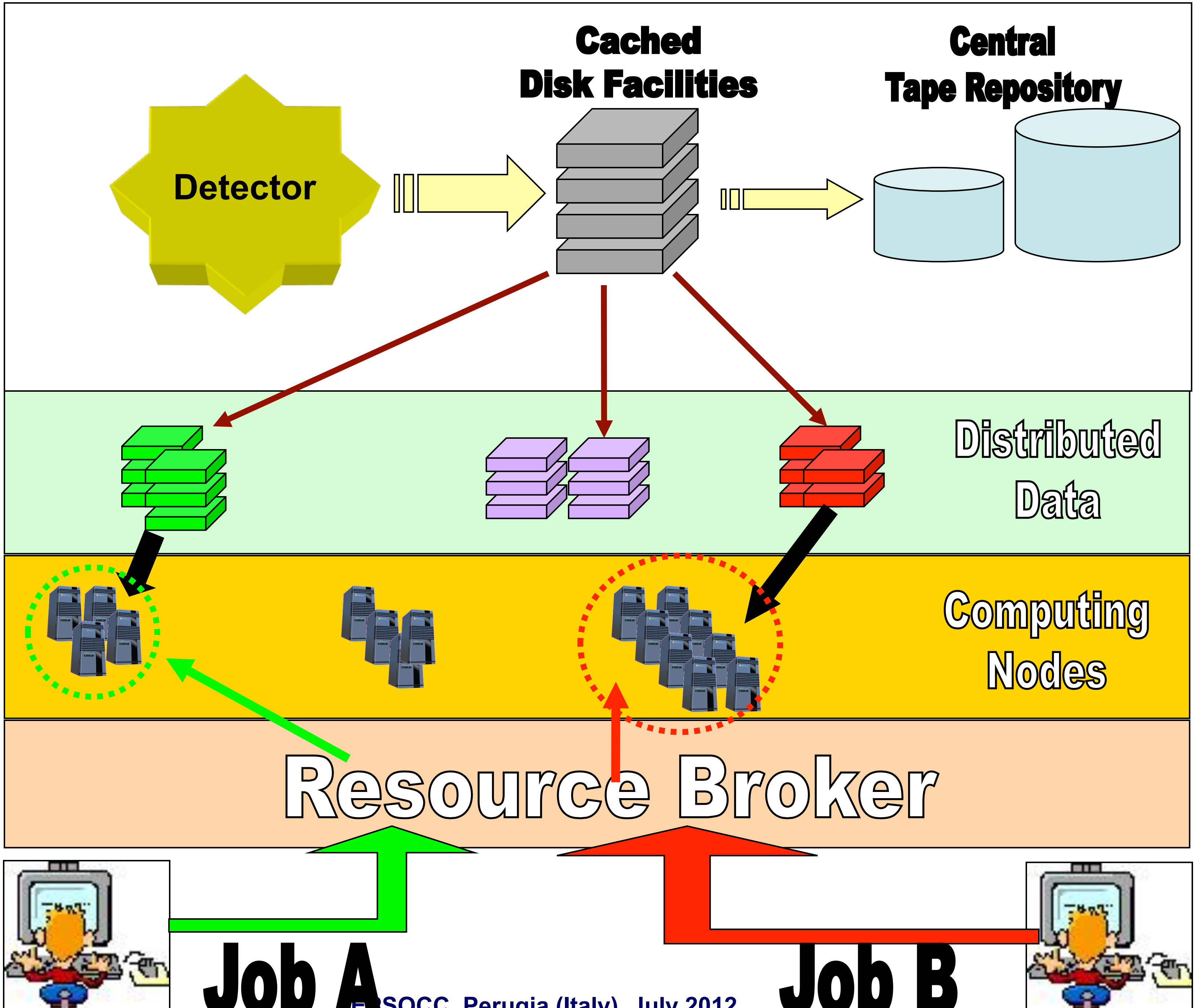


1. Deployment of Computational Grids
How was analysis without Grid ?



1. Deployment of Computational Grids
How was analysis without Grid ?

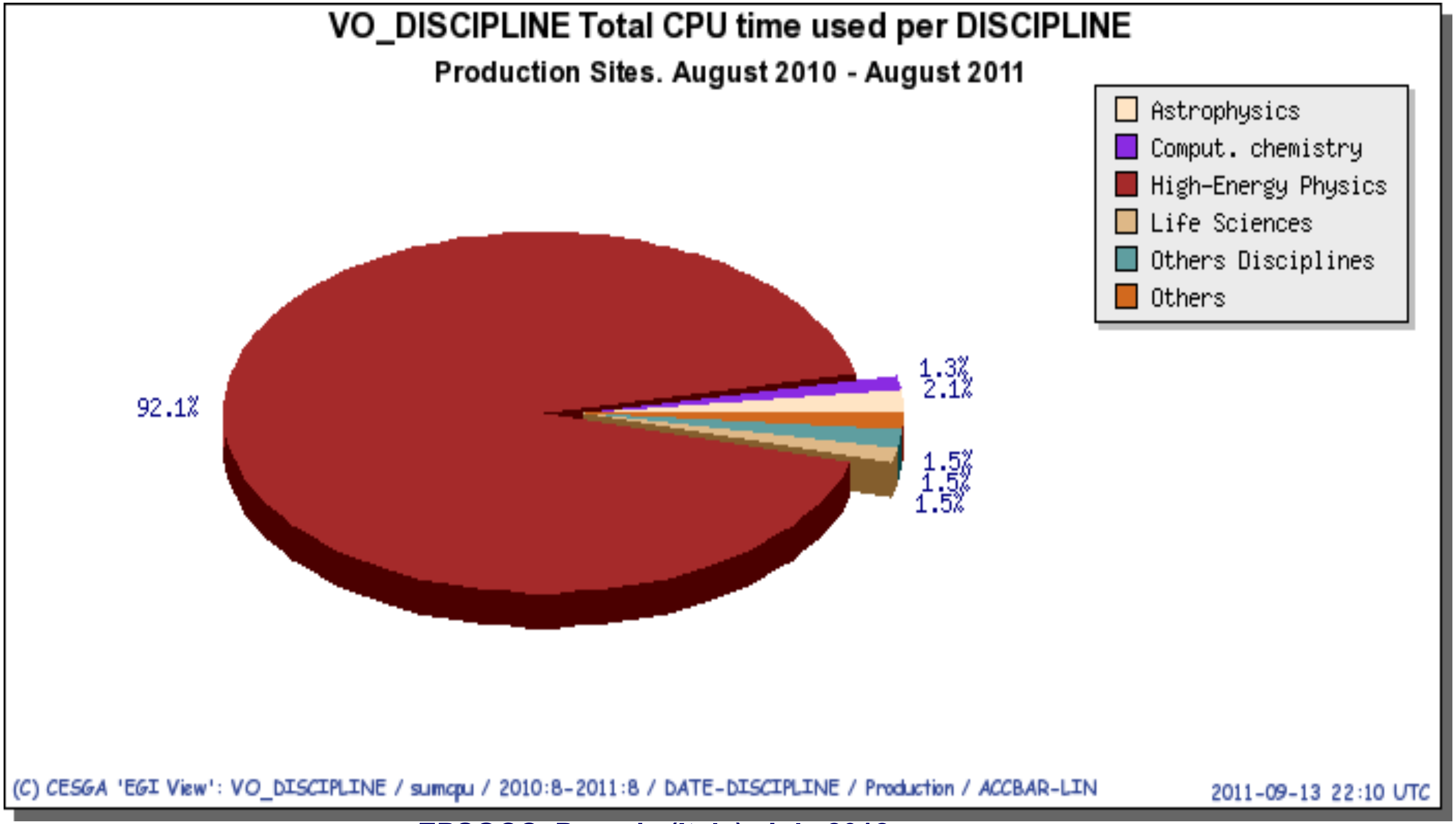



Cached
Disk Facilities
Central
Tape Repository
Detector
Distributed
Data
Computing
Nodes
Resource Broker
Job A
Job B

2. Grid Communities

2. Grid Communities

From the EGEE Accounting Portal at the *Centro de Supercomputación de Galicia*
http://www3.egee.cesga.es/gridsite/accounting/CESGA/egee_view.html



2. Grid Communities

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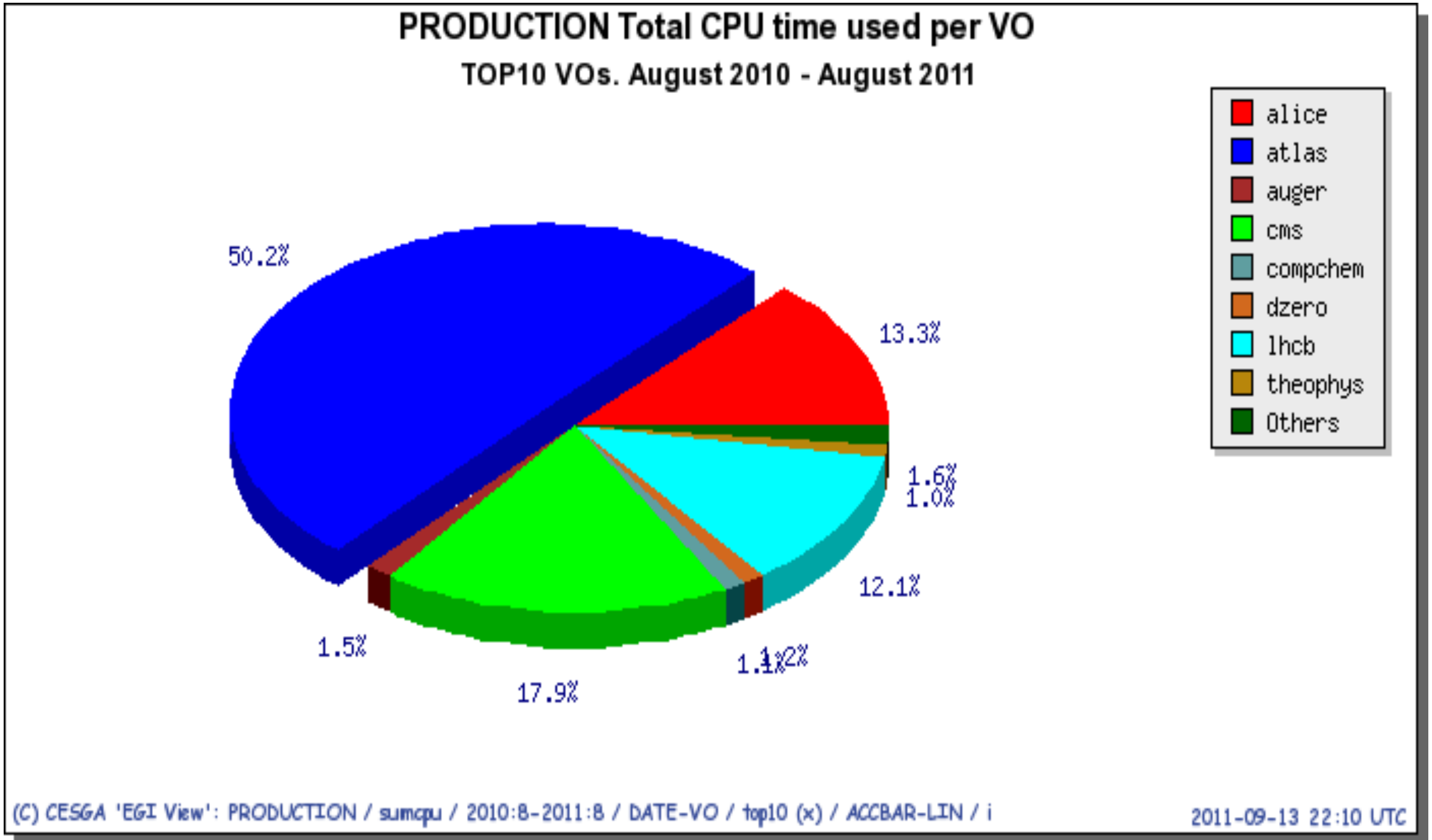
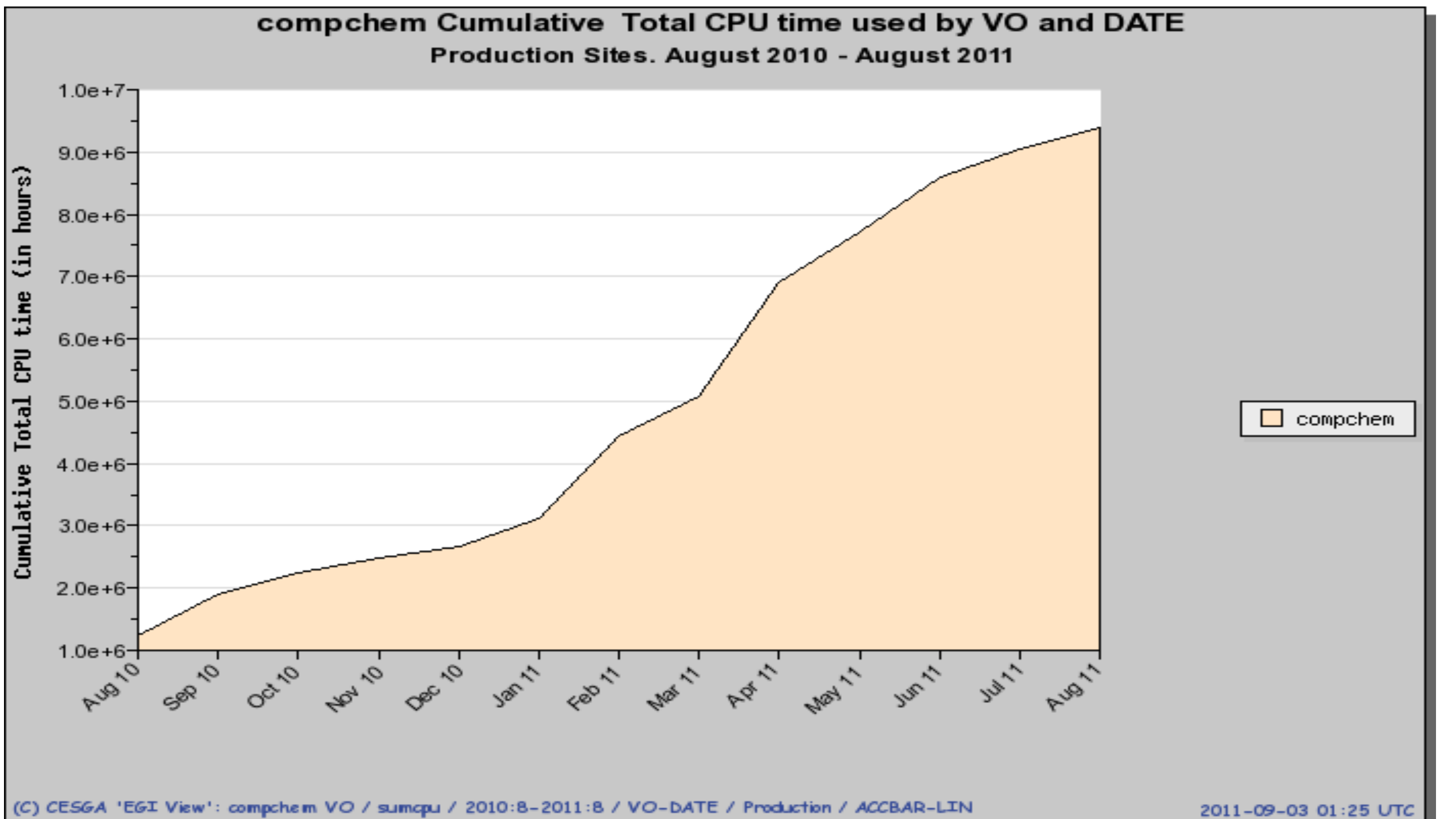


3. Statistics

From the EGEE Accounting Portal at the *Centro de Supercomputación de Galicia*
http://www3.egee.cesga.es/gridsite/accounting/CESGA/egee_view.html

9M hours/year ≈ 1000 Years



2. The Molecular Science Community and the European Grid project

- The Grid environment
  - Computational power
  - Middleware able to let people collaborate together
  - Secure access to common resources

- **COMPCHEM VO** has been created to pivoting the access to the Grid facilities.

2. COMPCHEM VO

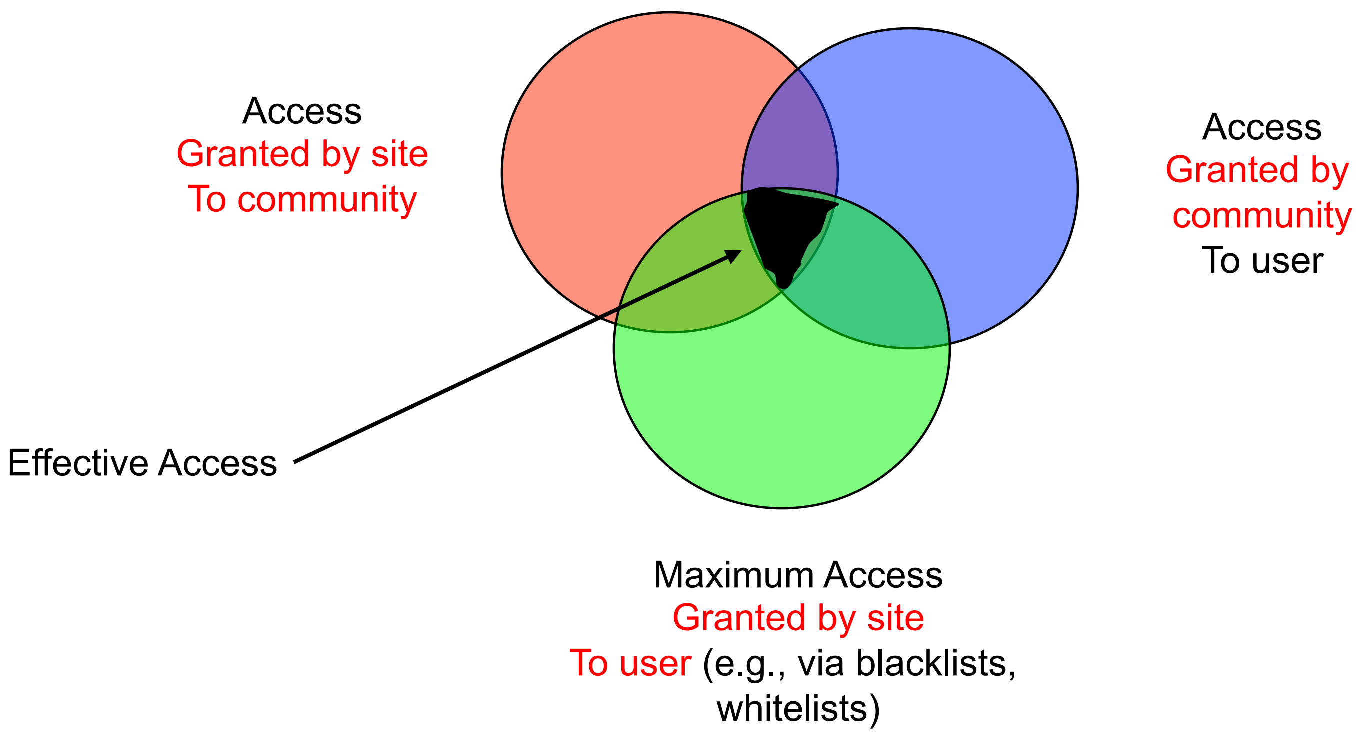
- **COMPCHEM VO** (http://compchem.unipg.it)
  - runs in the EGEE production Grid from the end of 2004
  - 40 active users
  - 32000 CPUs
  - Several Countries are supporting the VO
    - Italy (INFN), Spain (CESGA), France (IN2P3), Iteland (Trinity College of Dublin), Polland (CYFRONET and POZNAN Supercomputing Center), Greece (Hellas Grid and GRNET)...

2. Levels of COMPCHEM members

- Each partner may be involved at different levels:
  - Simple Usage: implementation on the Grid of a suite of codes of exclusive interest for the implementing laboratory
  - Code offer: the laboratory confers to the VO a stable suite of codes
  - Service offer: the laboratory participates to the management of the Grid infrastructure (manpower, hardware, service brokering and monitoring, etc), the development of joint projects etc.

2. Joint COMCHEM VO

- You need your personal Certificate released by a National CA



3. Computational Chemistry on Grid

3. Main features of COMPCHEM applications

- Both CPU-bound and data intensive jobs are present
  - Massive submission of sequential jobs running on different input datasets "parameter job study"
- Parallel jobs: some programs have been structured to run in parallel.
- Interactive jobs: graphical manipulation of chemical structures
- Implementation of Grid Services
  - to access the standard functionalities of the Grid
  - to create user-friendly visualization interfaces

3. COMPCHEM applications

COLUMBUS **Vienna (Austria)** **high-level *ab initio* molecular electronic structure calculations.**

GAMESS **Catania (Italy)** **high-level *ab initio* molecular quantum chemistry**

ABC **Perugia (Italy), Budapest (Hungary)** **quantum time-independent reactive dynamics**

RWAVEPR **Perugia (Italy), Vitoria (Spain)** **quantum time-dependent reactive dynamics**

MCTDH **Barcelona (Spain)** **multi-configurational time-dependent Hartree method**

FLUSS **Barcelona (Spain)** **Lanczos iterative diagonalisation of the thermal flux operator**

DIFF REAL WAVE **Melbourne (Australia)** **quantum differential cross-section**

VENUS **Vitoria (Spain)** **classical mechanics cross sections and rate coefficients**

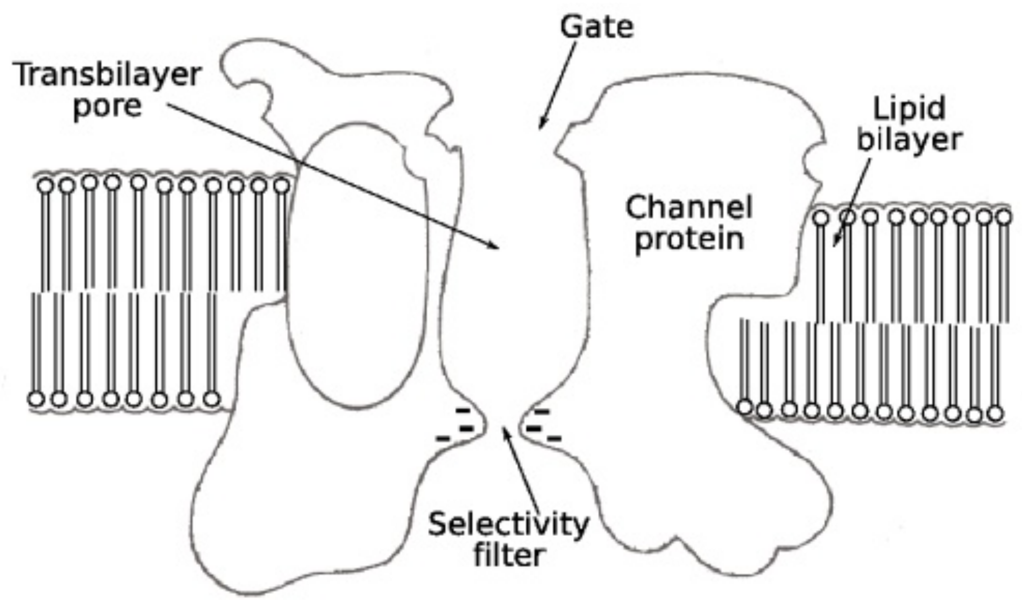
DL_POLY **Iraklion (Greece)** **molecular dynamics simulation of complex systems**

GROMACS **S. de Compostela (Spain)** **molecular dynamics simulation of complex systems**

CHIMERE **Perugia (Italy)** **chemistry and transport eulerian model for air quality simulations**

3.2. Ionic Biological Channels

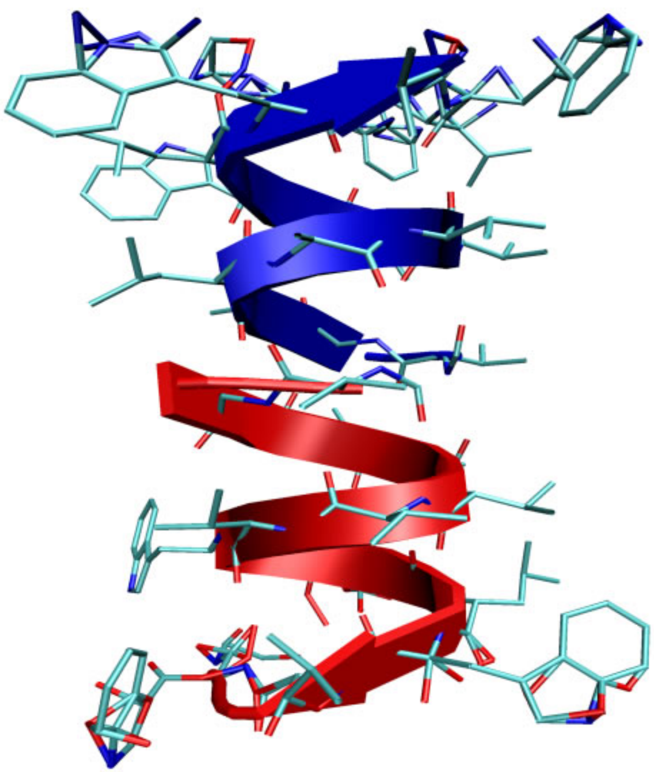
- Biological ionic channels play an important role in the control of ionic cellular concentrations and in synapses

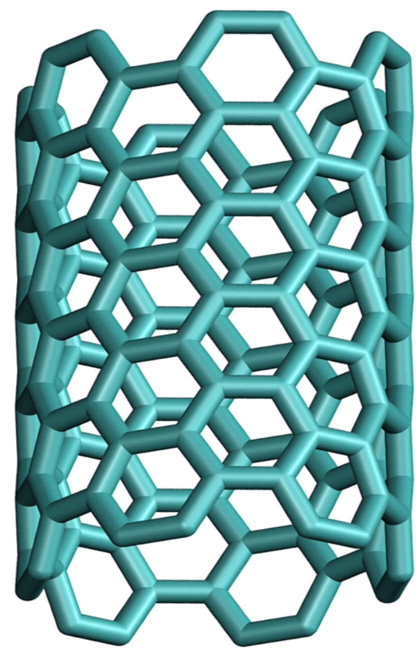


They are usually schematized as a sequence of:
Entrance gate
Bilayer pore
Selectivity filter

3.2. Ionic Biological Channels

We considered the CNT as a model for biological ionic channels (though it has also several interesting applications in itself)

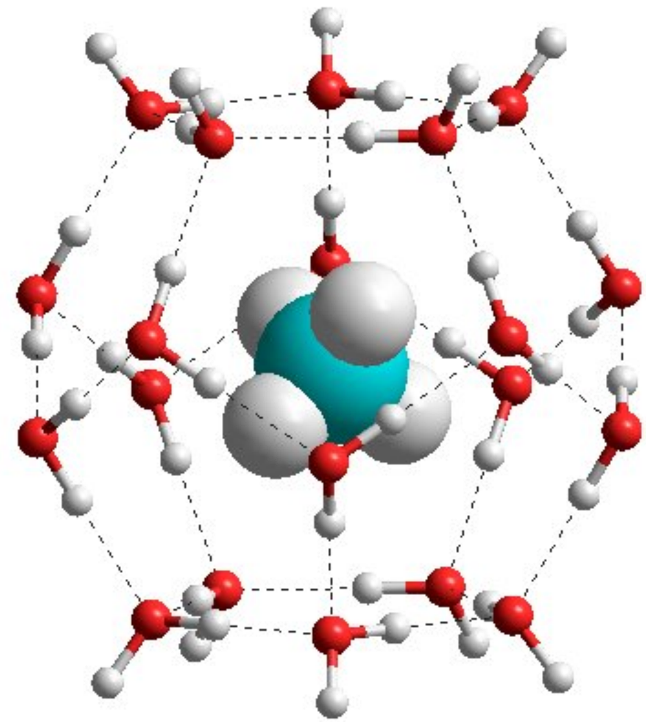




3.3. Methane Hydrates

***Gas hydrates (Clathrates)**: water hydrogen bonded structures caging gas molecules*

- Cl_2
- H_2S
- CO_2
- CH_4
- H_2
- *etc.*

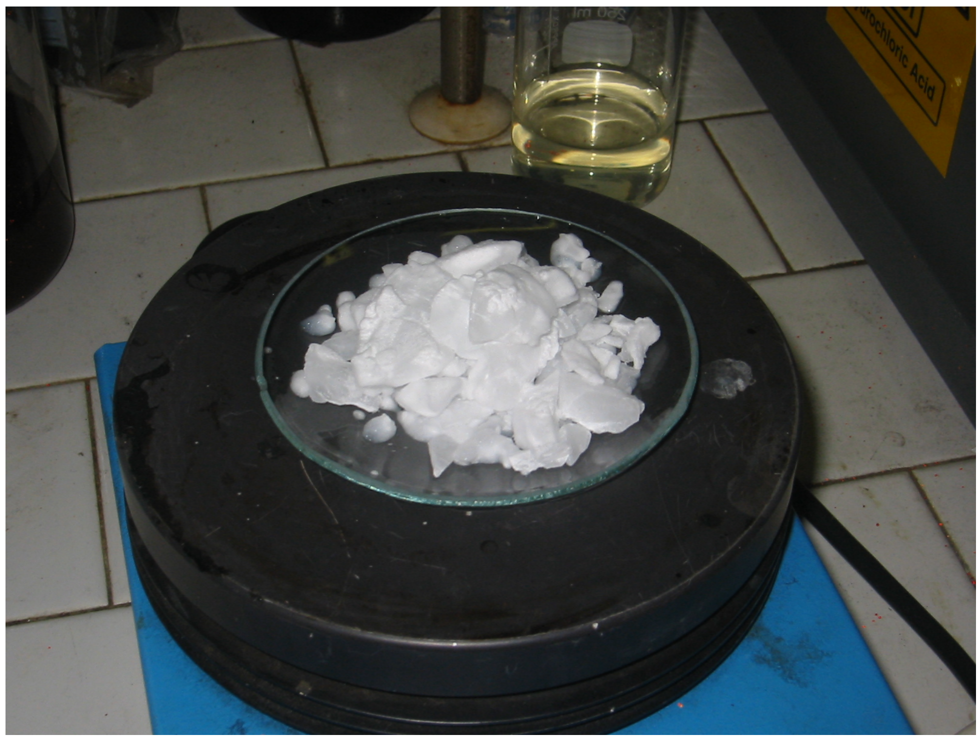


APPEARANCE: ice like

CAPTURING AND RELEASING: energetically cheap

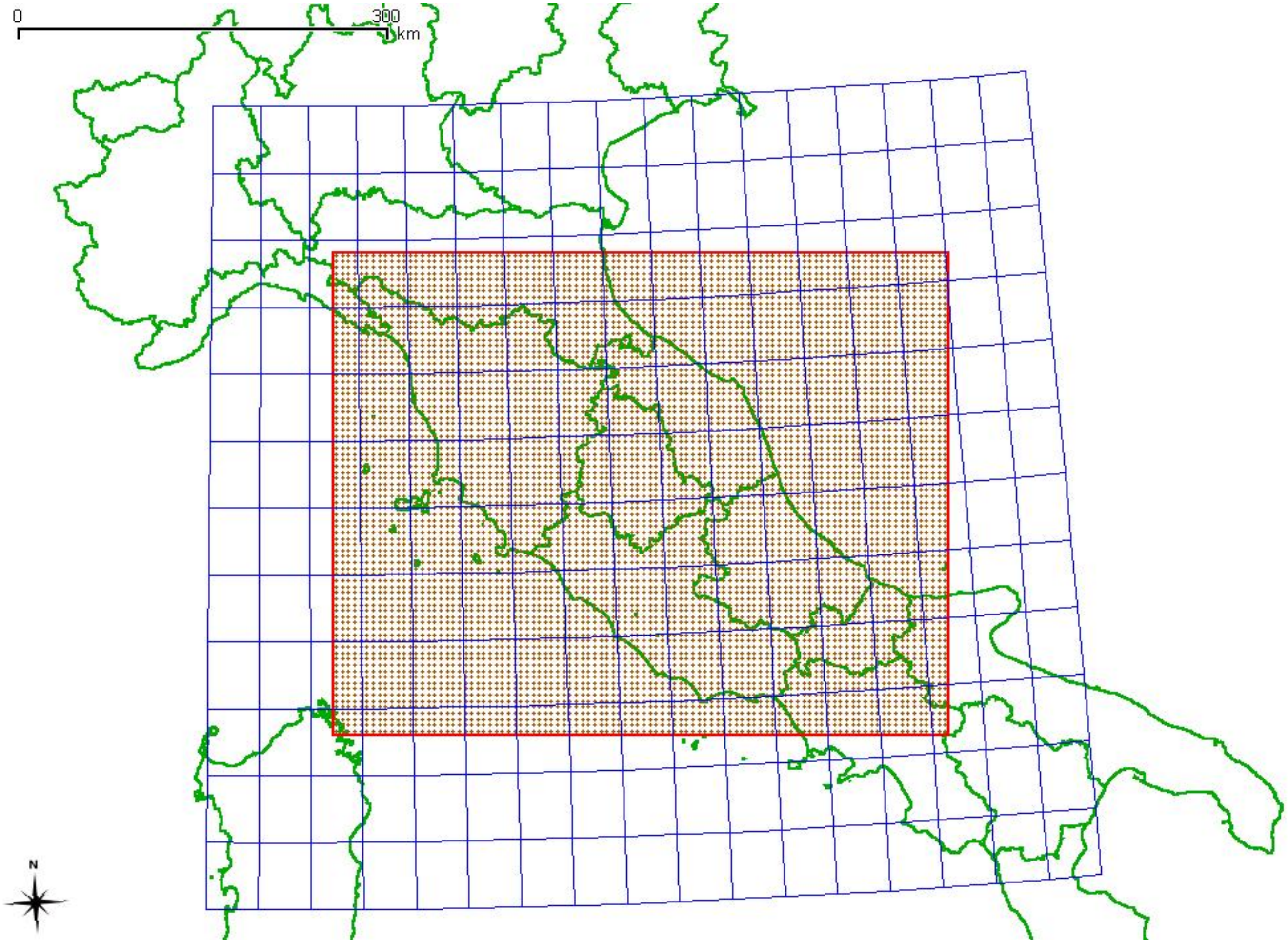
SAFET: no risks

UTILIZED TECHNOLOGIES: consolidated



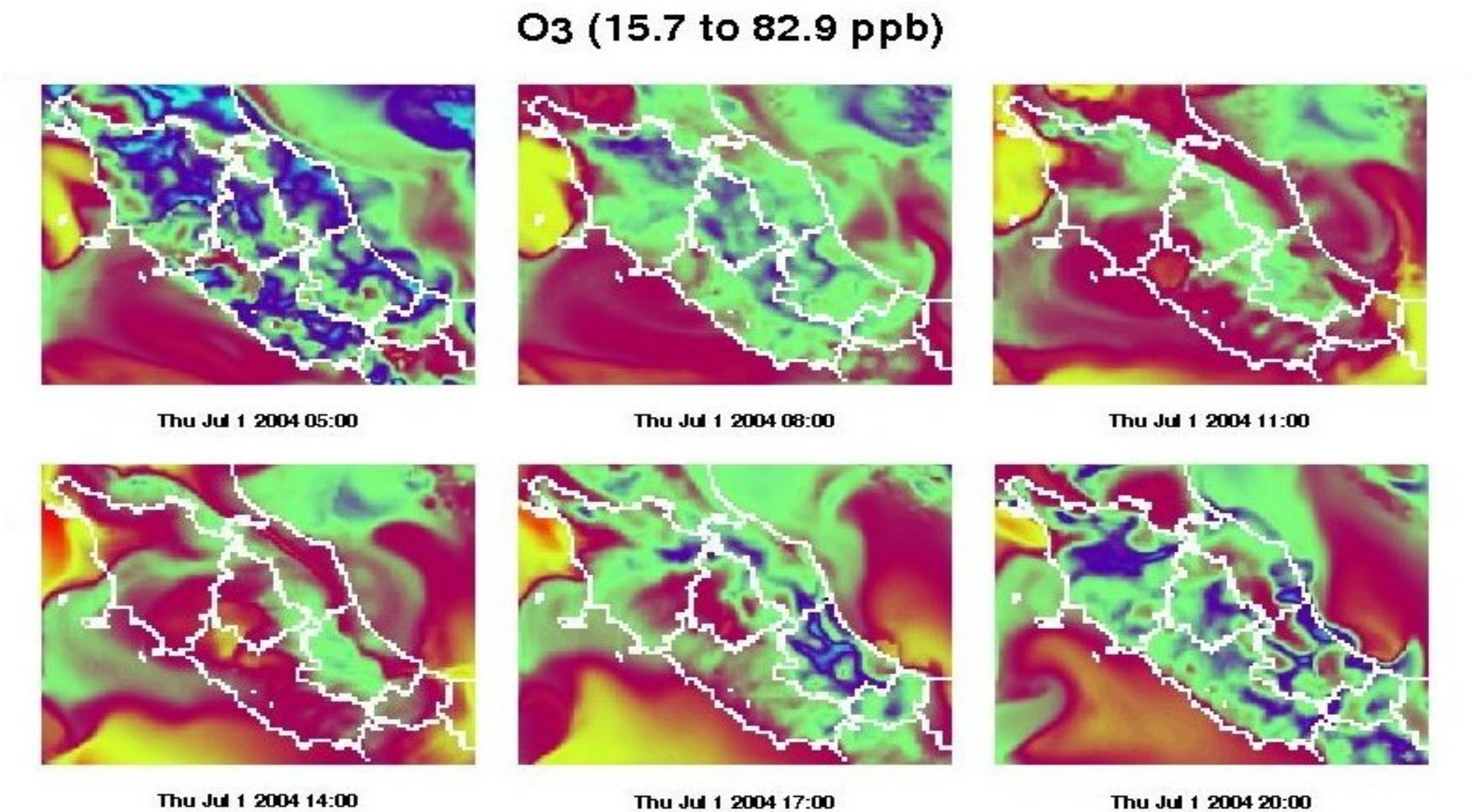
3.1. Atmospheric Modeling CHIMERE

- Simulated Center Itlay domain
- Four months (from May to August 2004)



3.1. Calculations and results

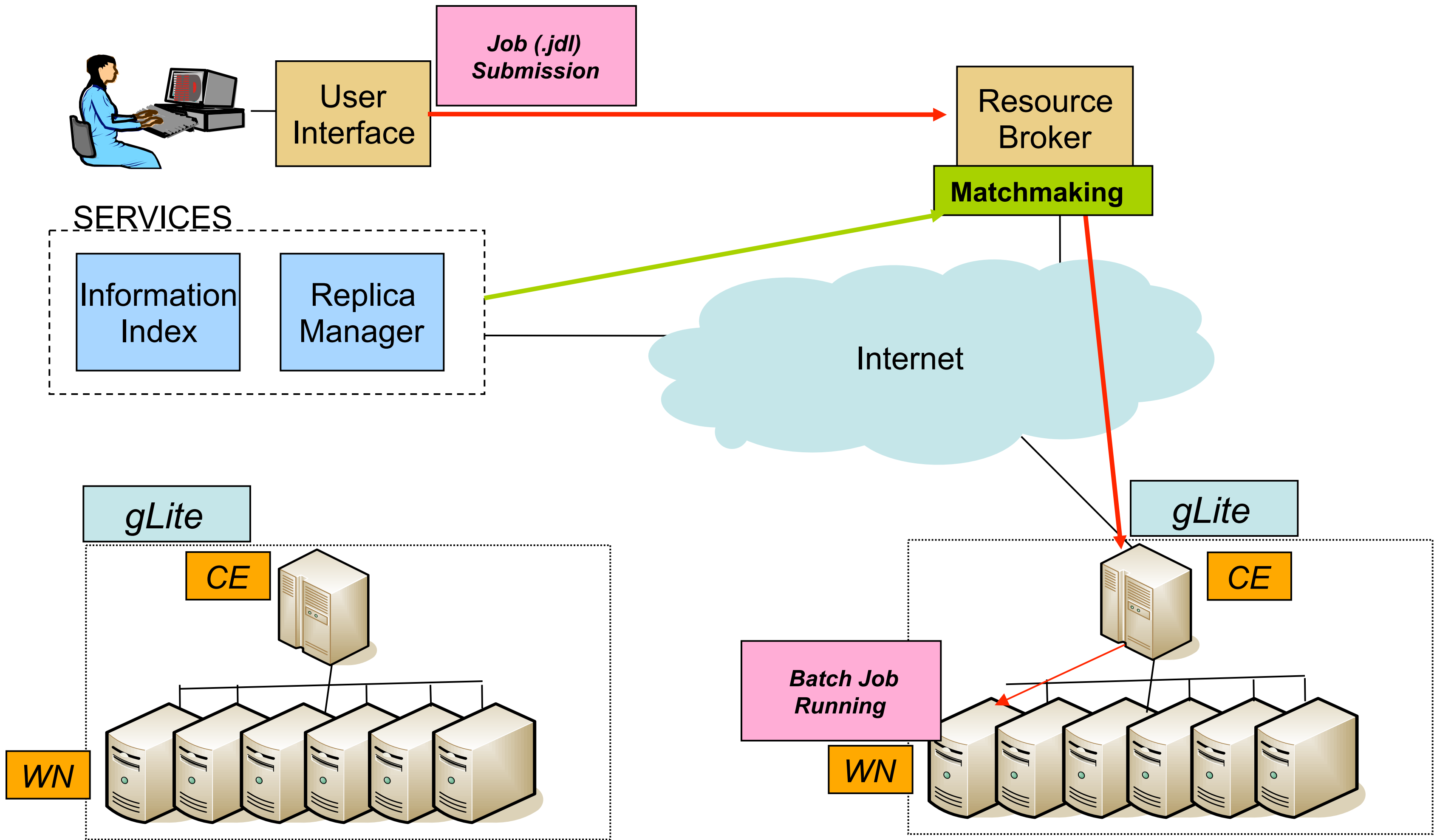
- Simulated July 2004 gas phase pollution (Ozone) on Center Italy domain



4. Advanced Applications

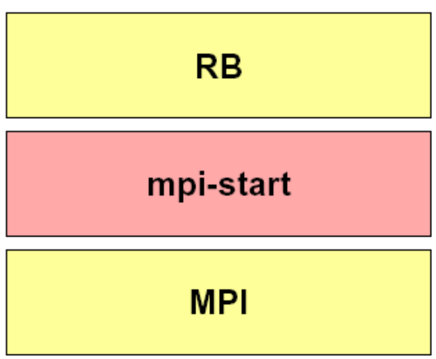
MPI Parallel Computing
Interactivity in Grids
Visualization and Steering

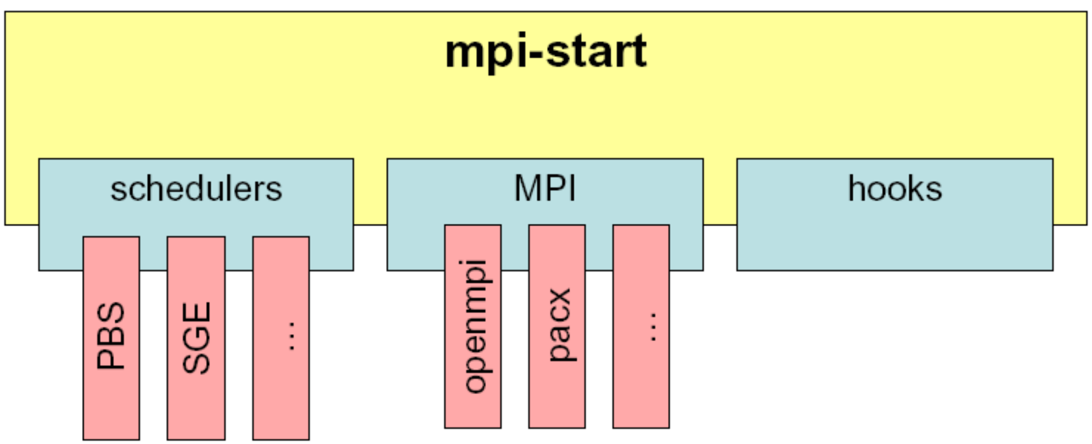
4. Advanced applications on Grids



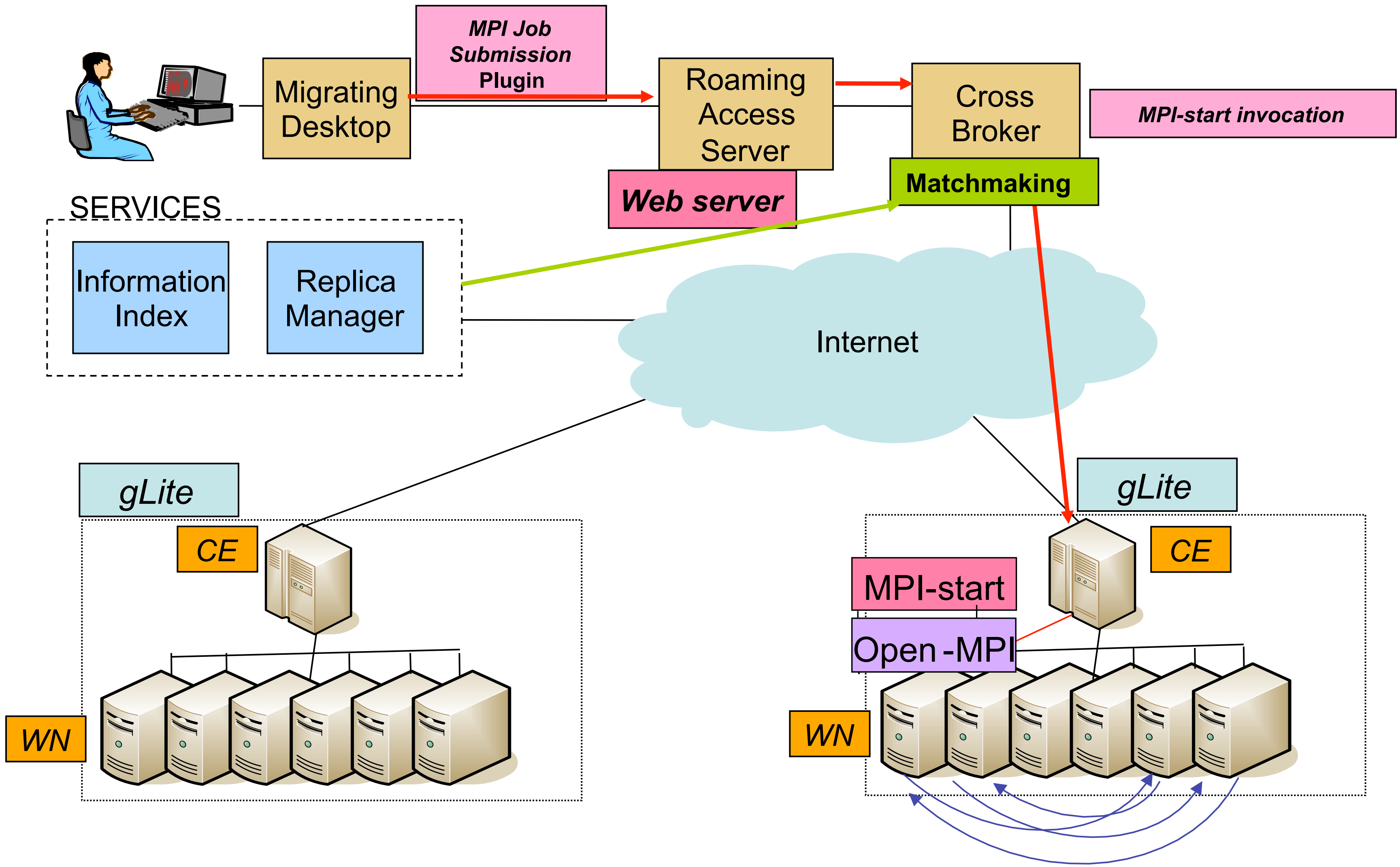
4. Advanced applications in Grid environment: Supporting MPI on Grids

- **Another software layer between the site and the resource broker**
- **Takes care of making uniform the local specificities**
  - LRMS (PBS/Torque, SGE, …)
  - MPI implementation (OpenMPI, PACX-MPI, MPICH, …)
- **Hides the particularities of the infrastructure**
  - Shared/not shared $home
  - Location of MPI libraries and other local specificities





4. Advanced applications in Grid environment: MPI-START



4.1 Advanced Applications

Workflows

4.1 Workflows

- A workflow consists of a sequence of connected steps

- Workflows are designed to achieve processing intents of some sort, such as physical transformation, service provision, or information processing

- The term workflow is used in computer programming to capture and develop human-to-machine interaction

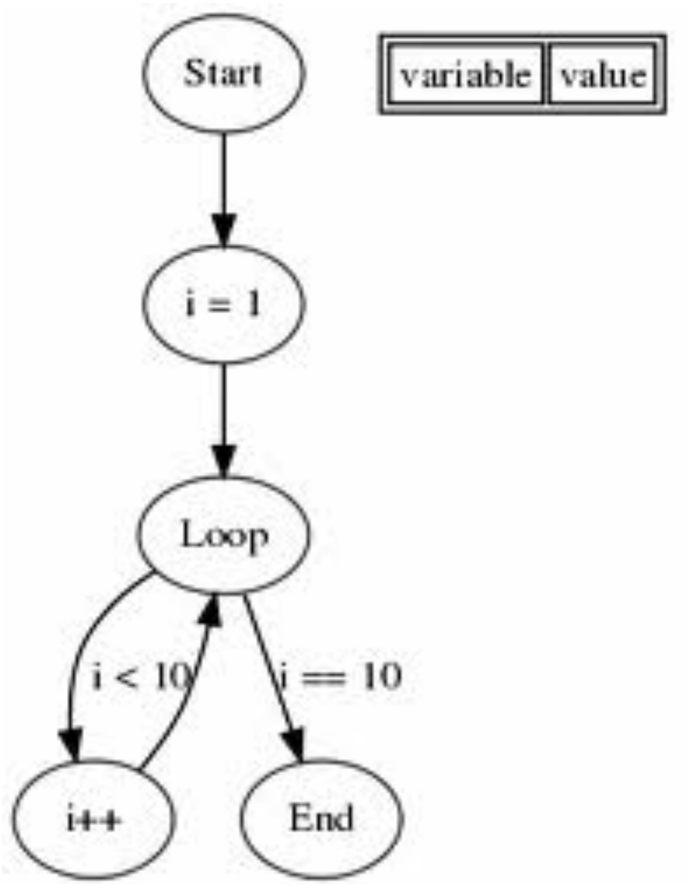
- Made use of a **workflow engine** that is a software application that manages and executes modeled computer processes

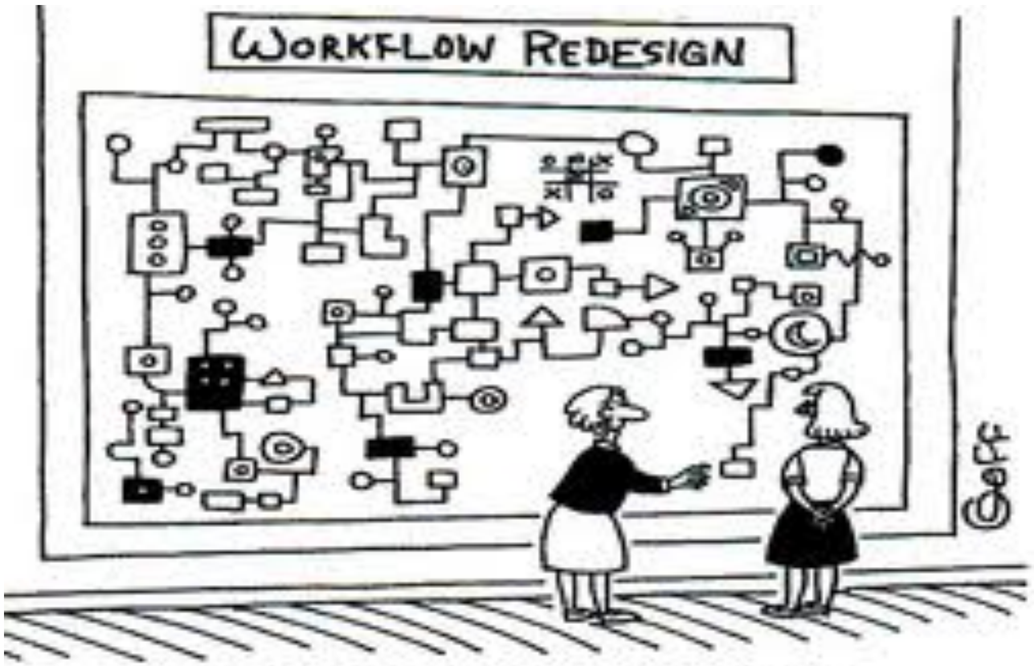
4.1 Workflows

The workflow engines mainly have three functions:

- Verification of the current status
    - Check whether the command is valid in executing a task
- Determine the authority of users
    - Check if the current user is permitted to execute the task
- Executing condition script
    - workflow engine begins to evaluate condition script in which two processes are carried out

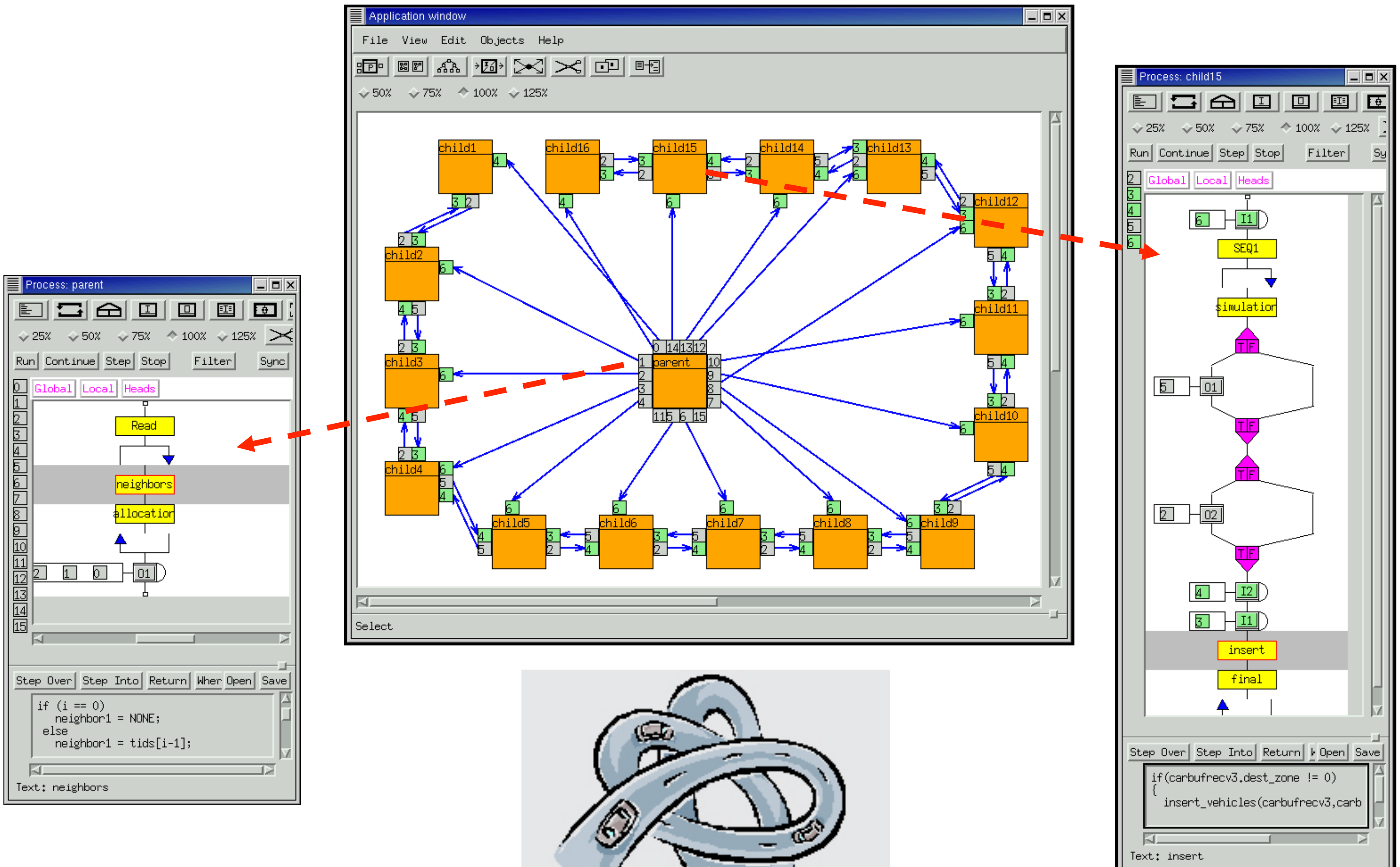
4.1 Workflows





"And this is where our ED workflow redesign team went insane."

Application: Urban traffic simulation



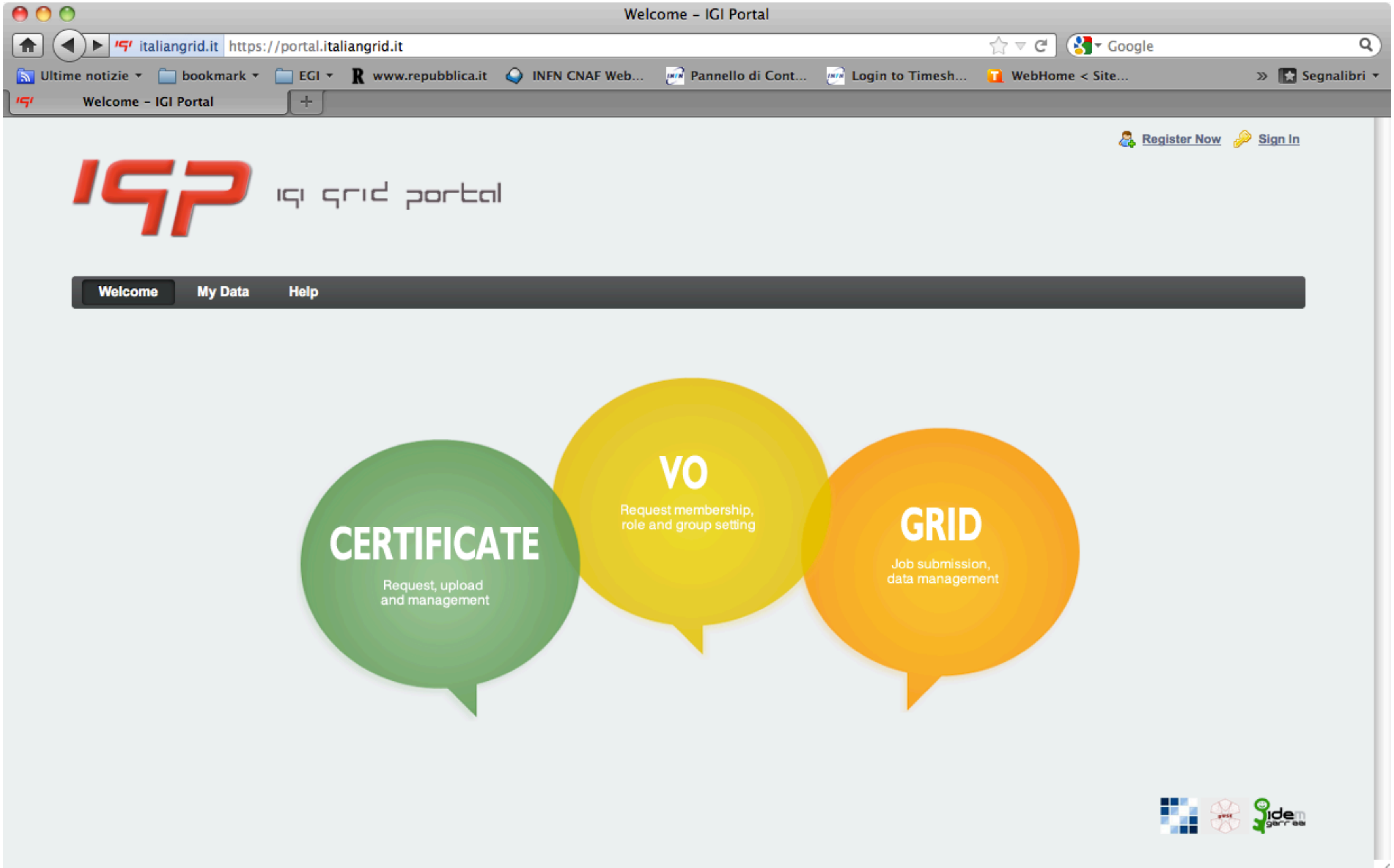
4.1 Science Gateways and Protals

Workflows and Workflow engines can be integrated in Science Gateway and Web-Portals

- Web Portal
  - A web site that brings together information from diverse sources in a unified way

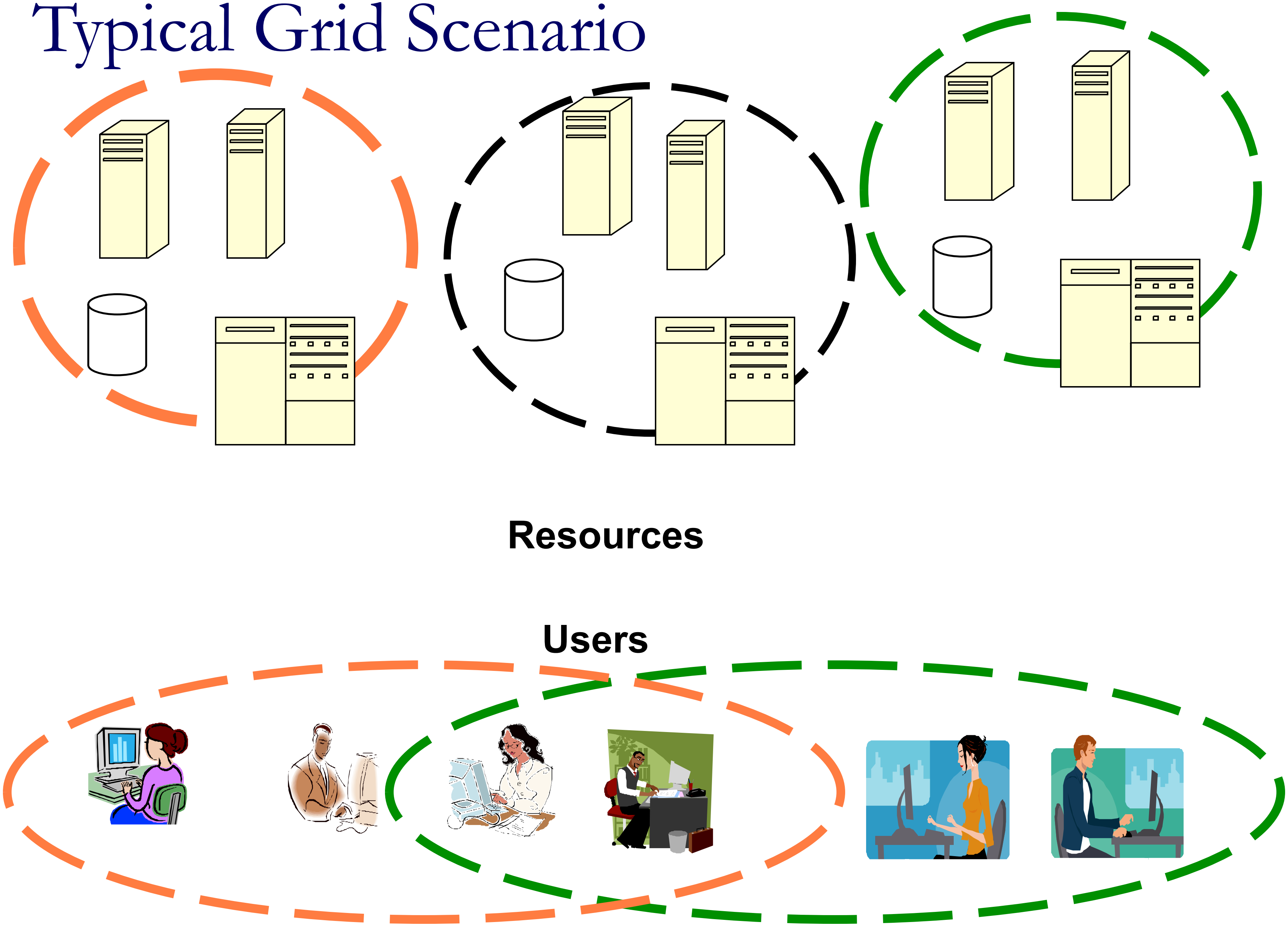
- Scientific Gateway
  - Web site with specific scientific-area related information

4.1 IGP: the Grid-Protal



5. Security on Grid

Typical Grid Scenario



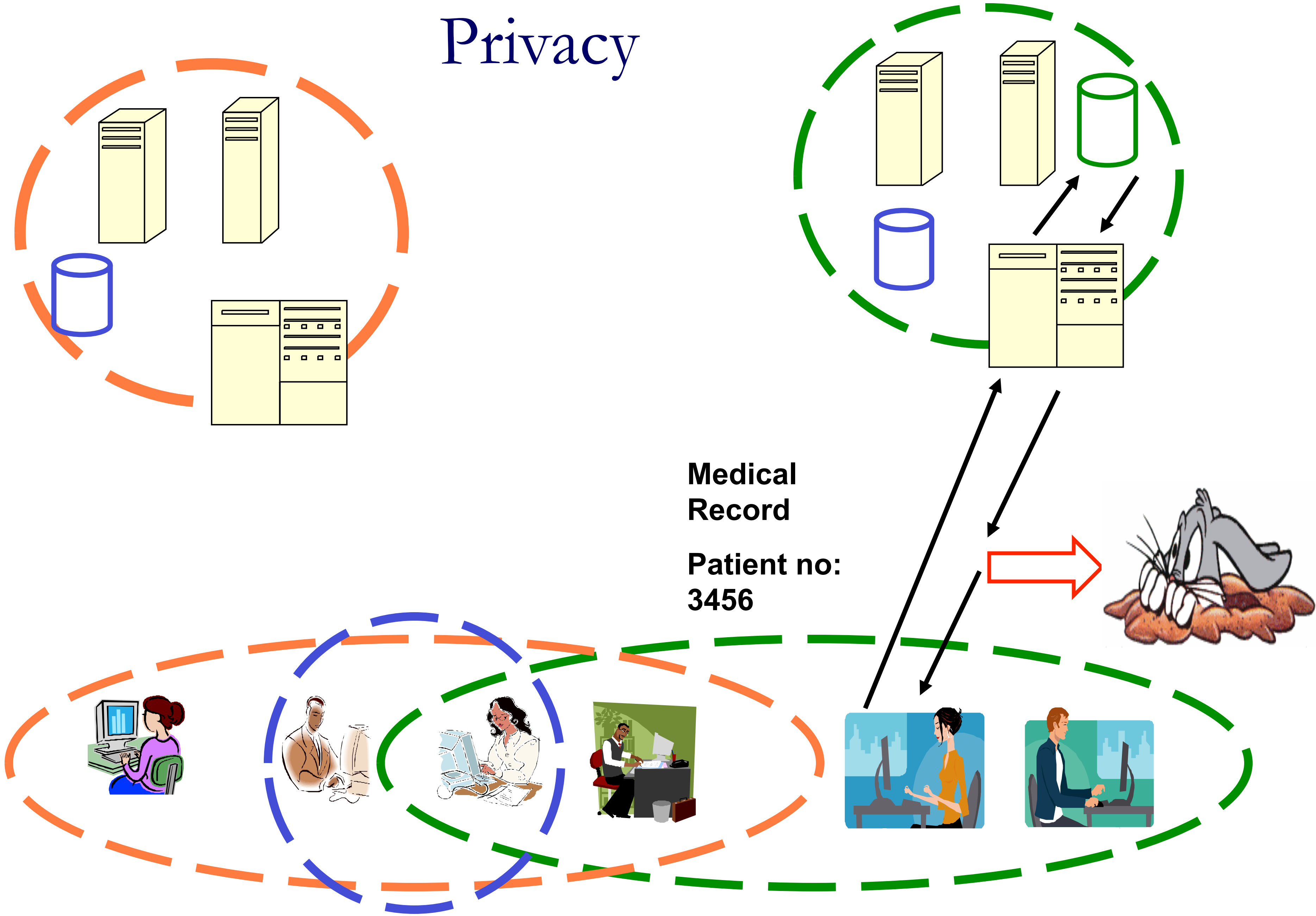
What do we want from security?

- Identity
- Authentication
- Privacy
- Integrity
- Authorization
- Single Sign-On
- Delegation

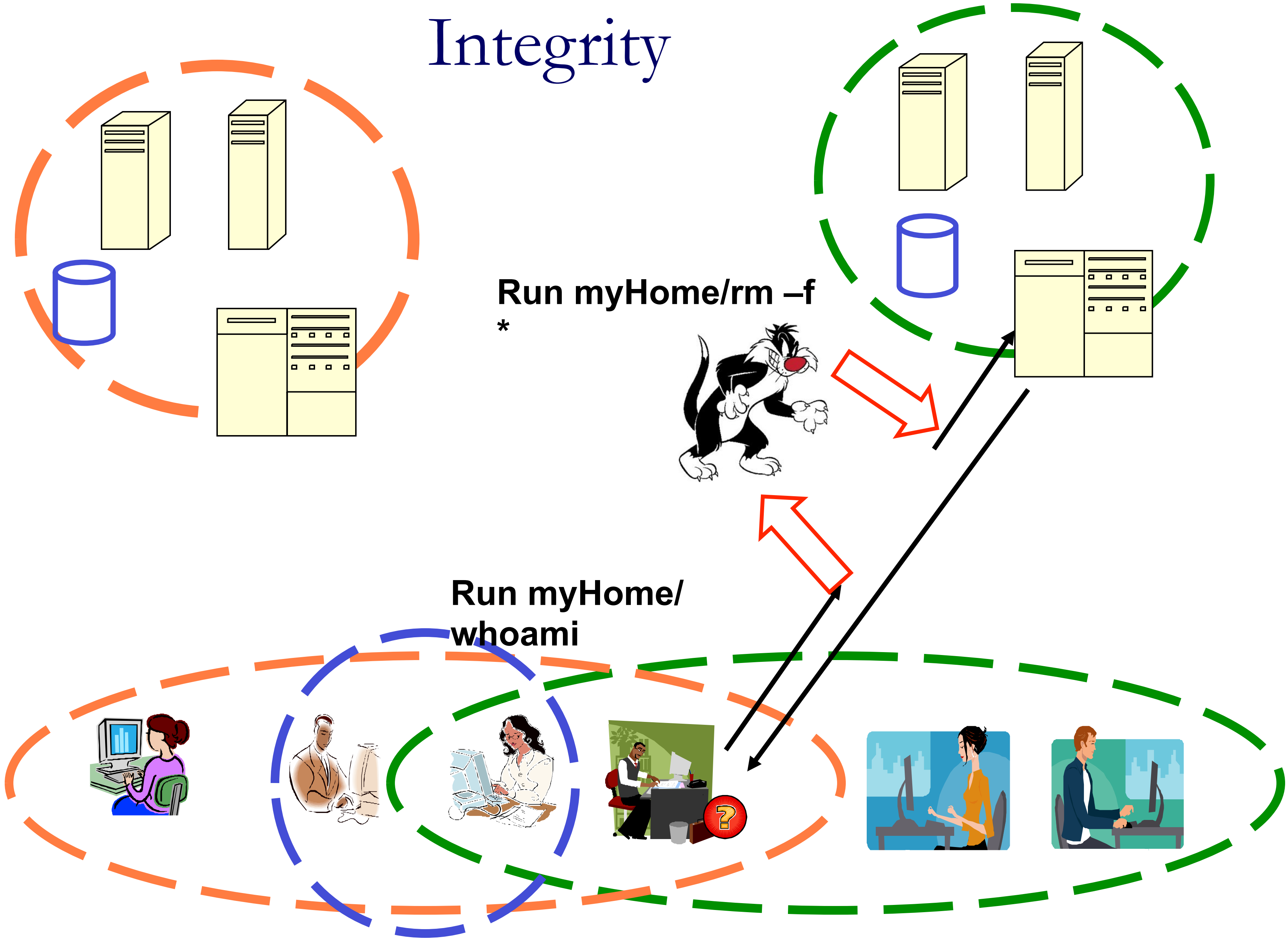
Identity & Authentication

- Each entity should have an identity
  - Who are you?
  - Example: Unix login name
- Authentication:
  - Prove your identity
  - Stops masquerading imposters
- Examples:
  - Passport
  - Username and password

Privacy



Integrity



Message Protection

- Sending message securely
- Integrity
  - Detect whether message has been tampered
- Privacy
  - No one other than sender and receiver should be able to read message

Authorization establishes rights to do actions

- What can a particular identity do?

Examples:

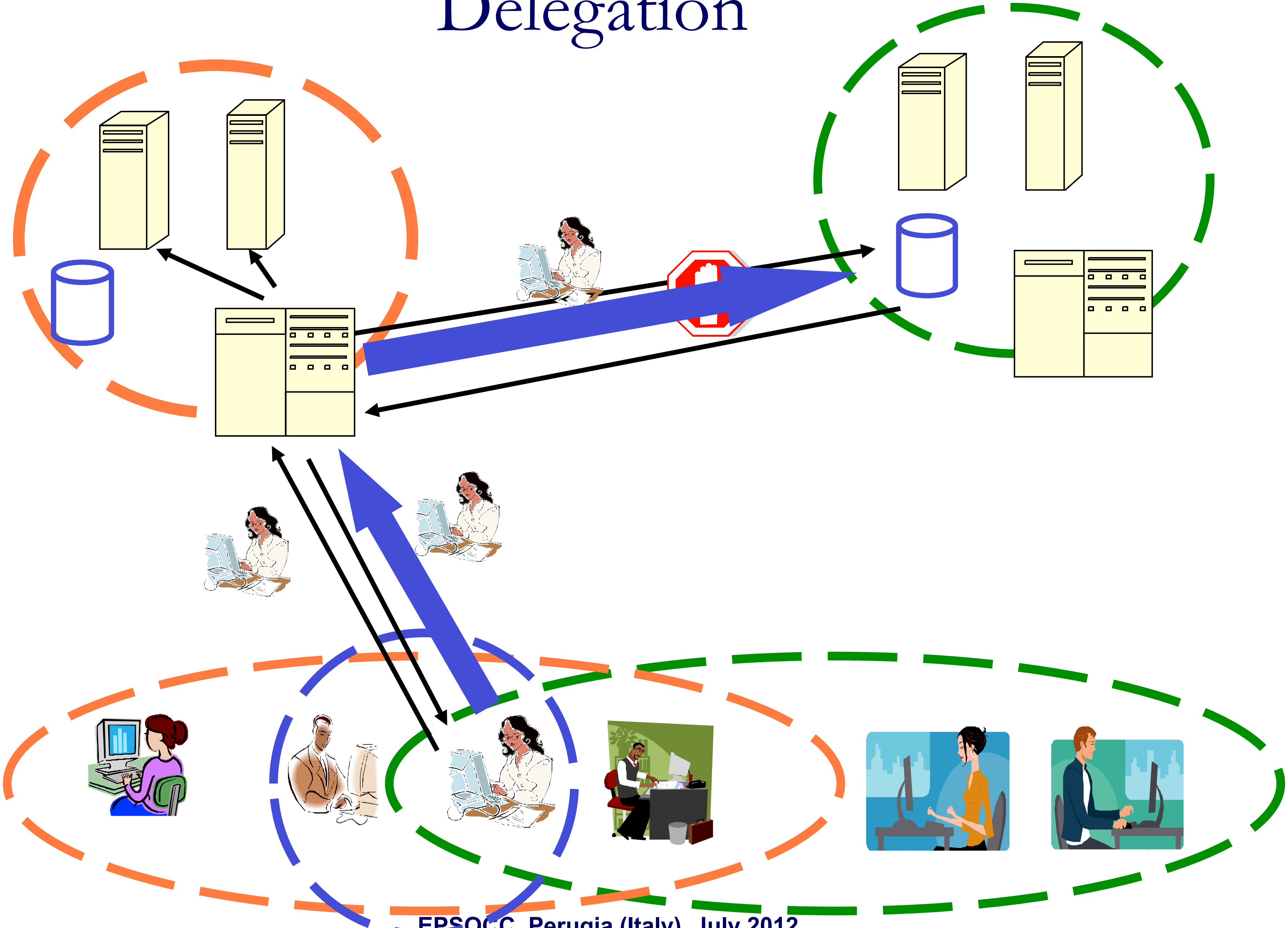
  - Are you allowed to read this file?
  - Are you allowed to run a job on this machine?
  - Unix read/write/execute permissions

- Must authenticate first
  - Authentication != authorization

Single sign on

- Log on once
  - Type password once
- Use any grid resource without typing password again

Delegation



Delegation

- Resources on the grid can act as you
- Example: Execution jobs can transfer files
- Delegation can be restricted
  - For example: Delegation only valid for a short period of time

5.1 Solutions using cryptography

Cryptographic Keys, the building block of cryptography, are collections of bits

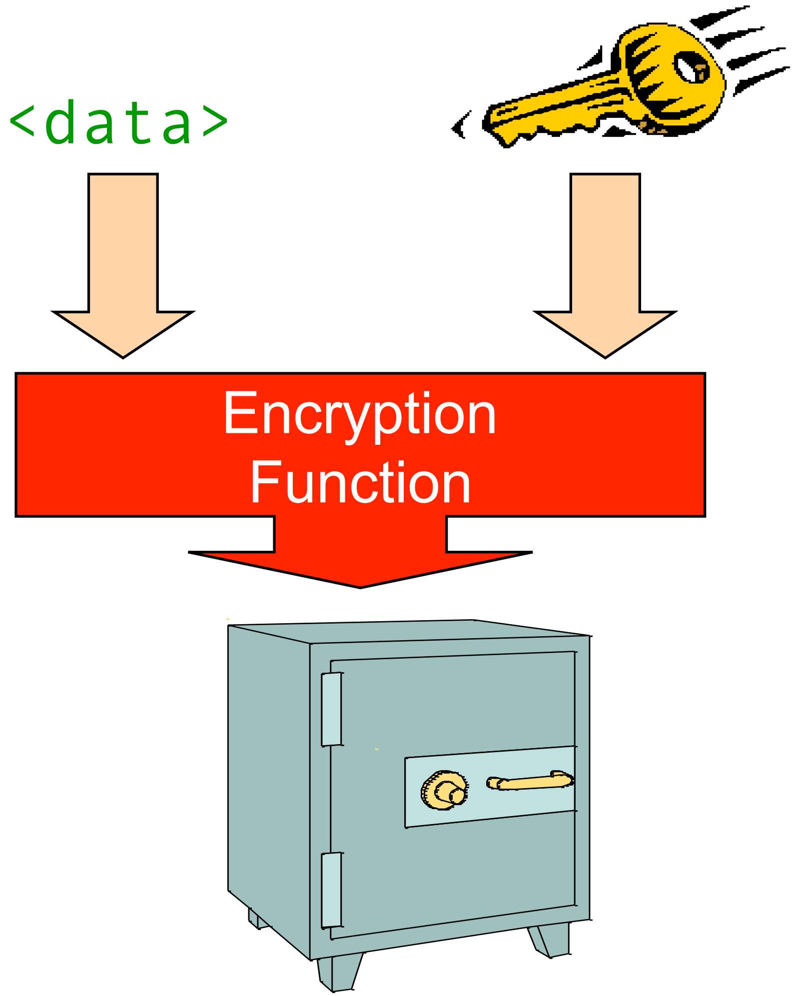
- The more bits that you have, the stronger is the key
- Public key cryptography has two keys:
  - Public key
  - Private key

0 1 0 1 0 0 1 1 1 0

1 0 1 1 1 1 0 1 1 1

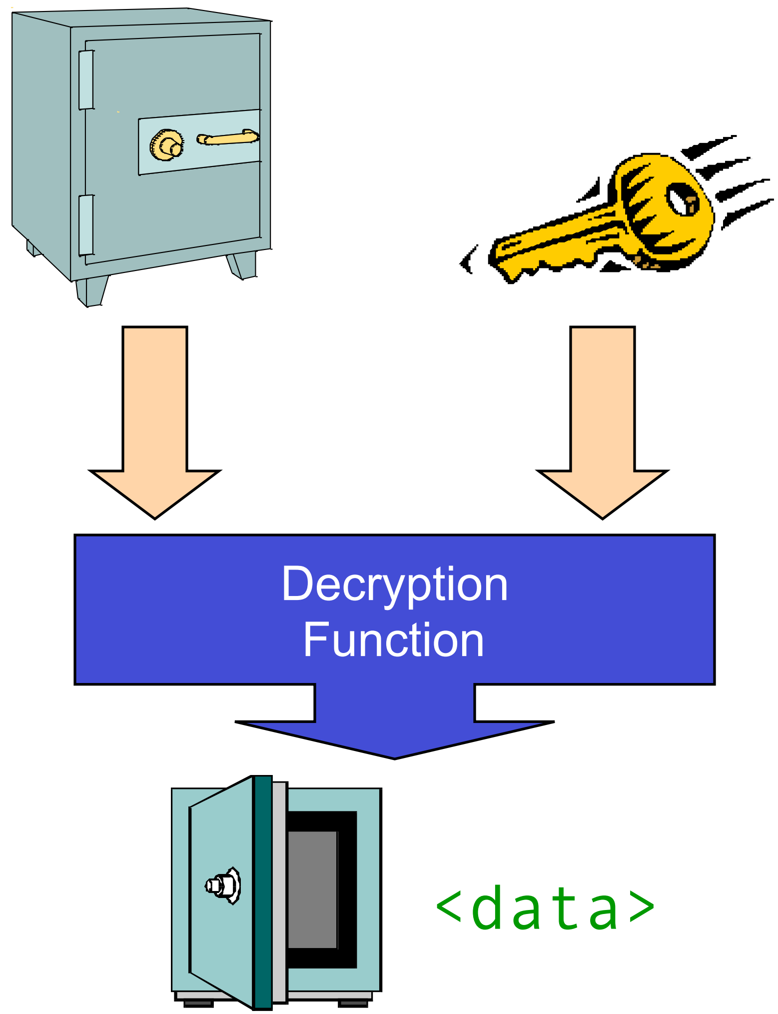
Encryption takes data and a key, feeds it into a function and gets encrypted data out

- Encrypted data is, in principal, unreadable unless decrypted



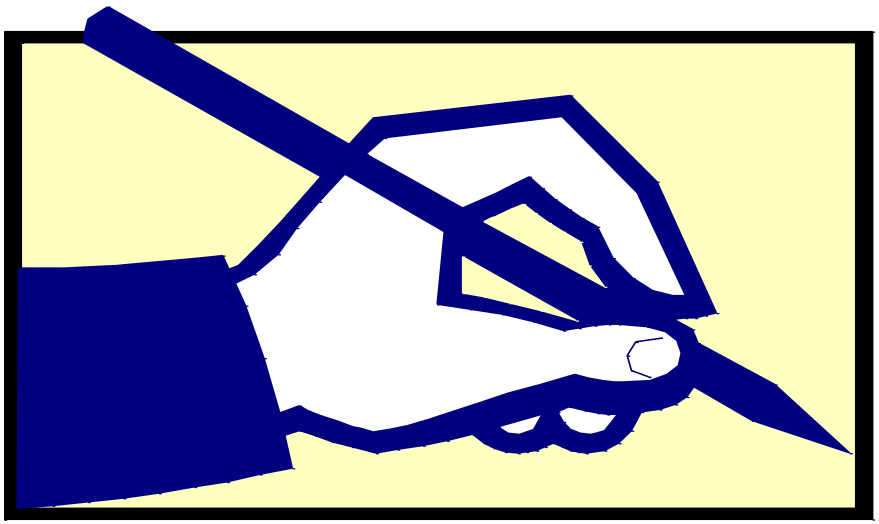
Decryption feeds encrypted data & a key into a function and gets the original data

- Encryption and decryption functions are linked



Digital Signatures let you verify aspects of the data

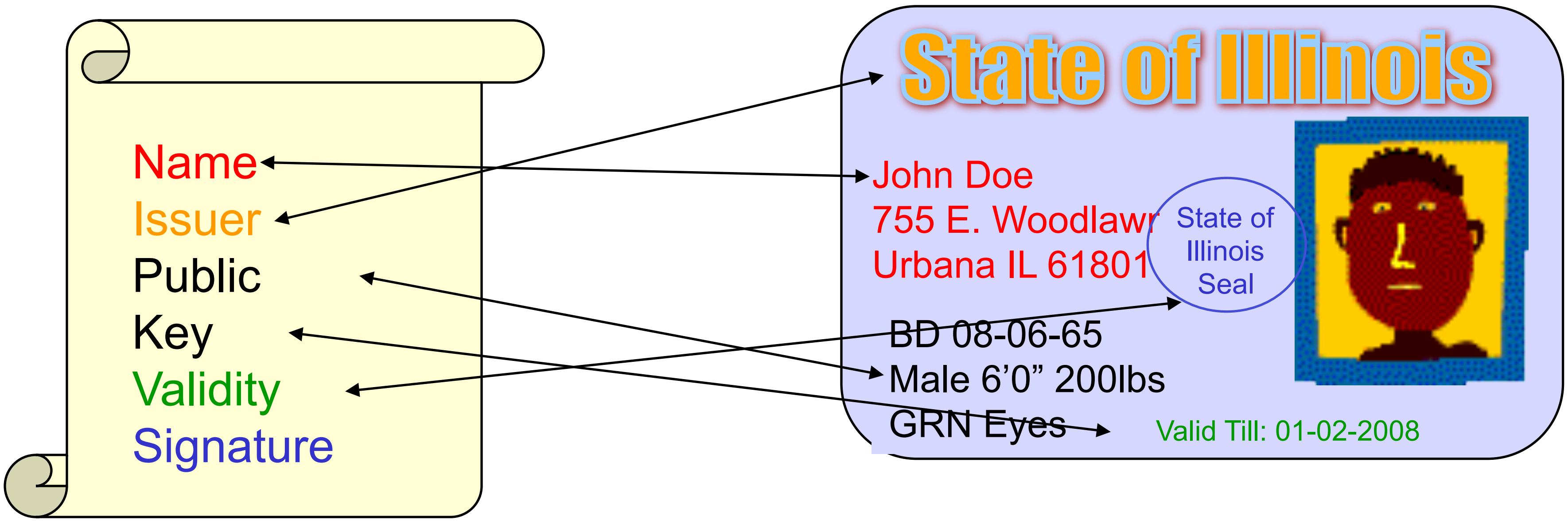
- Who created the data
- That the data has not been tampered with
- Does not stop other people reading the data
  - Combine encryption +signature



Public Key Infrastructure (PKI) provides Identity

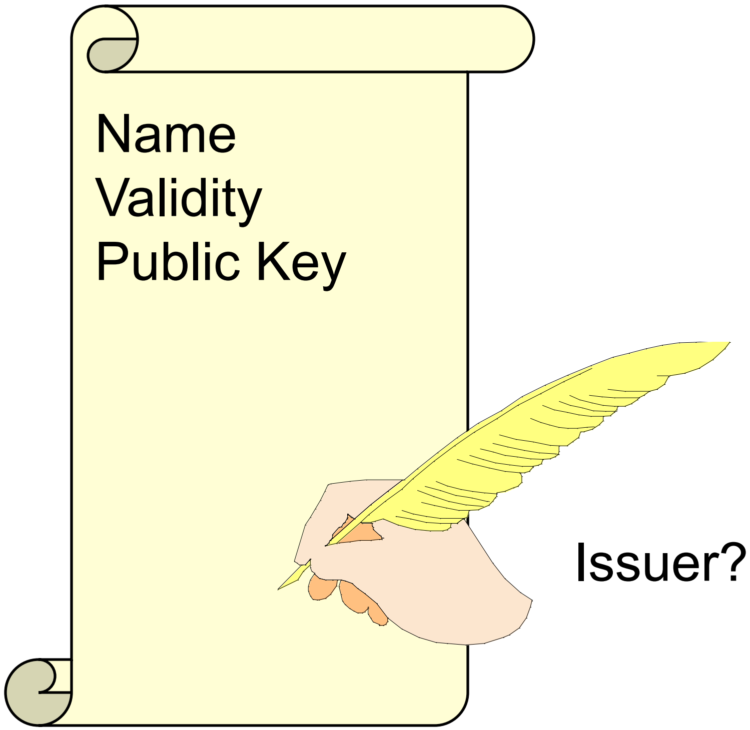
- X.509 certificate
  - Associates an identity with a public key
  - Signed by a Certificate Authority

Certificates are similar to passports or identity cards



Certification Authorities (CAs) sign certificates

- CAs are small set of trusted entities
- CA certificates must be distributed securely



Each CA has a *Certificate Policy (CP)*

- The Certificate Policy states:
  - To whom the CA will issue certificates
  - How the CA identifies people to whom it will issue certificates
- Lenient CAs don’t pose security threat because resources determine the CAs they trust.

Grid Security Infrastructure (GSI) allows users & apps to securely access resources

- Based on PKI
- A set of tools, libraries and protocols used in Globus
- Uses SSL for authentication and message protection
- Adds features needed for Single-Sign on
  - Proxy Credentials
  - Delegation

In GSI, each user has a set of credentials they use to prove their identity on the grid

- Consists of a X509 certificate and private key
- Long-term private key is kept encrypted with a pass phrase
  - Good for security, inconvenient for repeated usage

GSI Proxy credentials are short-lived credentials created by user

- Short term binding of user’s identity to alternate private key
- Same identity as certificate
- Stored unencrypted for easy repeated access
- Short lifetime in case of theft

GSI *delegation* allows another entity to run using your credentials

- Other entity gets a proxy with your identity
- Other entity can run as you
  - only for limited time
  - for specific purpose
- For example, a compute job might want to transfer files on your behalf.

Gridmap is a list of mappings from allowed DNs to user name

```
"/C=US/O=Globus/O=ANL/OU=MCS/CN=Ben Clifford"  benc
"/C=US/O=Globus/O=ANL/OU=MCS/CN=MikeWilde"  wilde
```

- Commonly used in Globus for server side
- ACL + some attribute
- Controlled by administrator
- Open read access

MyProxy: Use Cases

- Credential need not to be stored in every machine
- Used by services that can only handle username and pass phrases to authenticate to Grid. E.g. web portals
- Handles credential renewal for long-running tasks
- Can delegate to other services

6. Future sustainability of Scientific Grids

6. Future Sustainability Interoperability

- More than 20 Grid projects in Europe
  - Different fields of science, different objectives
  - different middlewares, different services
  - Users using more than one Grid, going towards interdisciplinarity
- Modern scientific/industrial/economic applications need higher number of resources. Users will want to:
  - Use/share/join multiple Grid resources
  - Transparently migrate between Grids according to their needs

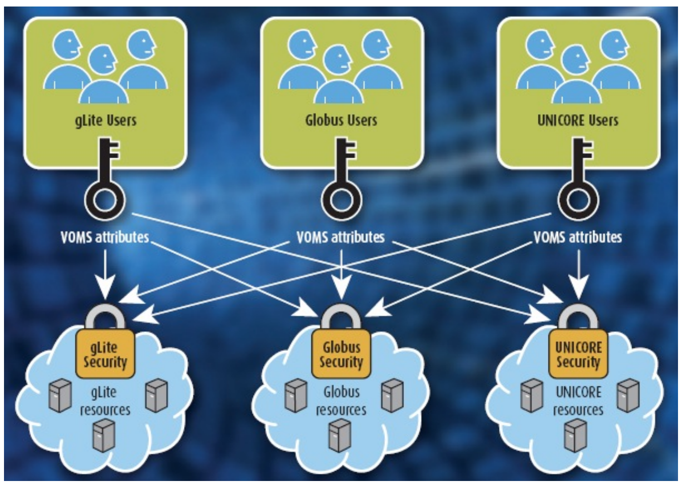
6. Future Sustainability
Who Benefits from Interoperability?

- Grid Developers
  - A single standard set of services on all Grid middleware systems
  - Applications portable across different Grid middleware systems
- E-Science application users
  - Common ways for accessing any e-infrastructure resources
  - Potential access to a significantly larger set of resources
- E-infrastructure owners
  - Reduced management overheads as only a single Grid middleware system needs deployment
  - Potential for greater resource utilisation

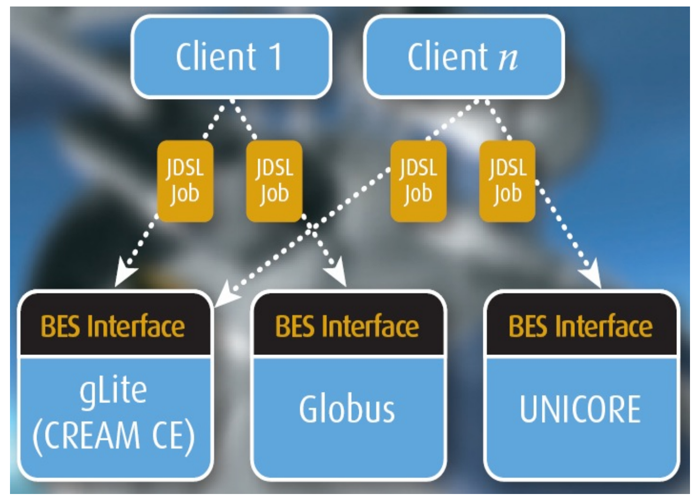
6. Future and sustainability
How are standards defined?

Standards are discussed and defined at the Open Grid Forum, OGF: **http://www.ogf.org**

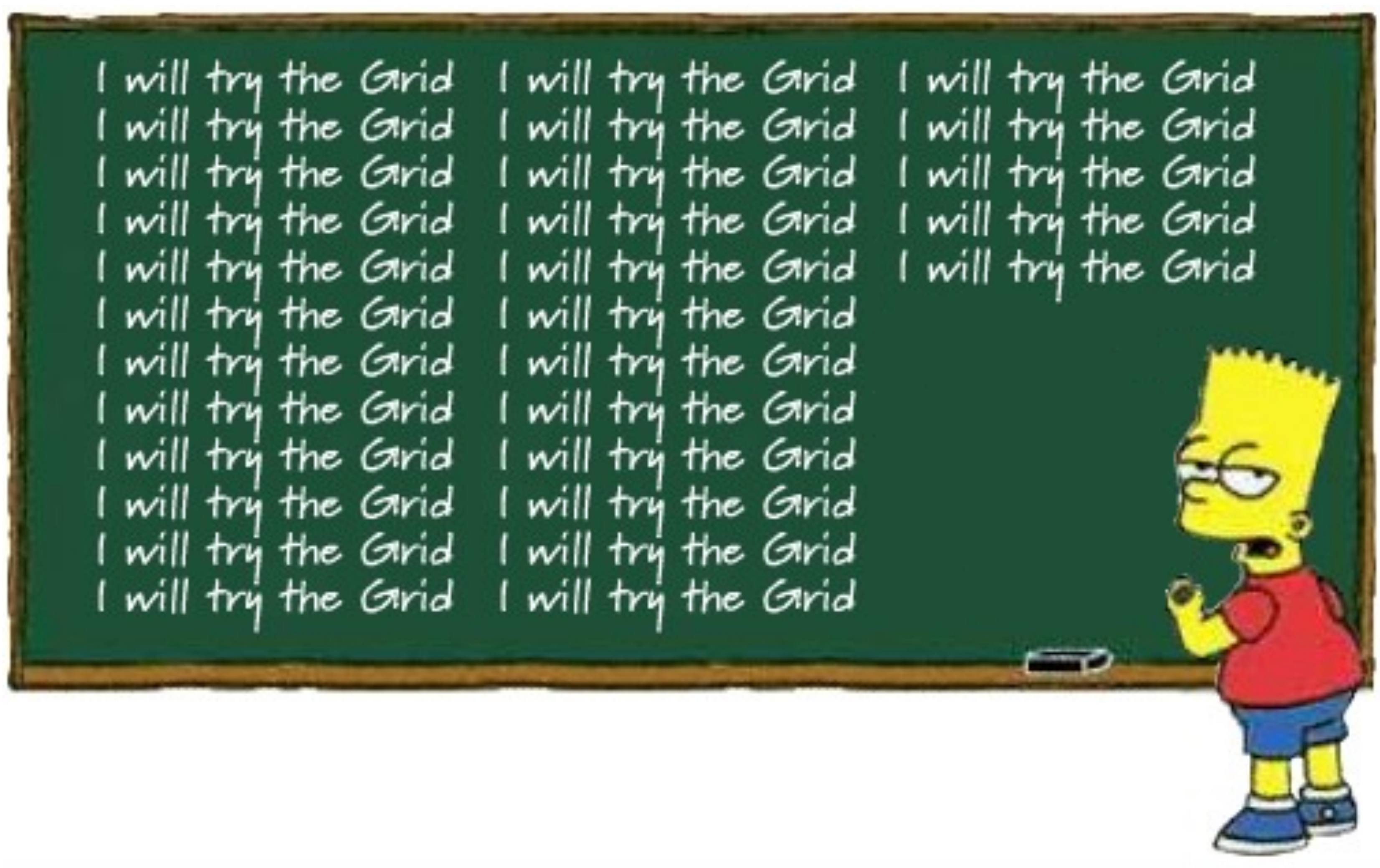
- Open Forum to discuss about Open Standards
- Standards are now defined by the Open Grid Services Architecture OGSA:
  - Based on Web Services concepts



A common Virtual Organisation management across different middlewares



Unifying Job Submission and Monitoring Interface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