



Making e-Infrastructures easy: the Science Gateway approach

Roberto Barbera (roberto.barbera@ct.infn.it)
University of Catania and INFN

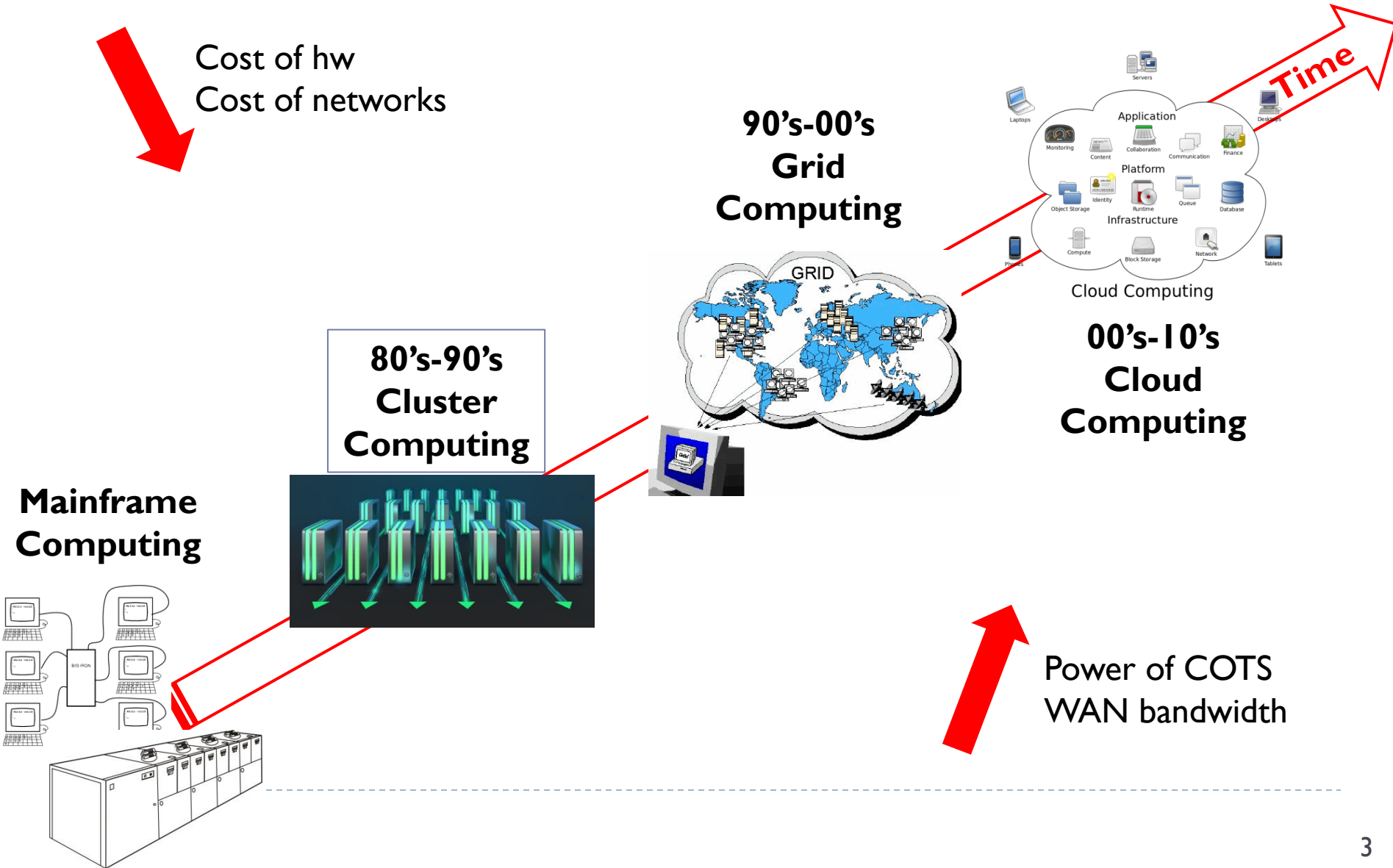
DECIDE Final Workshop – Rome, 22 February 2013

Outline

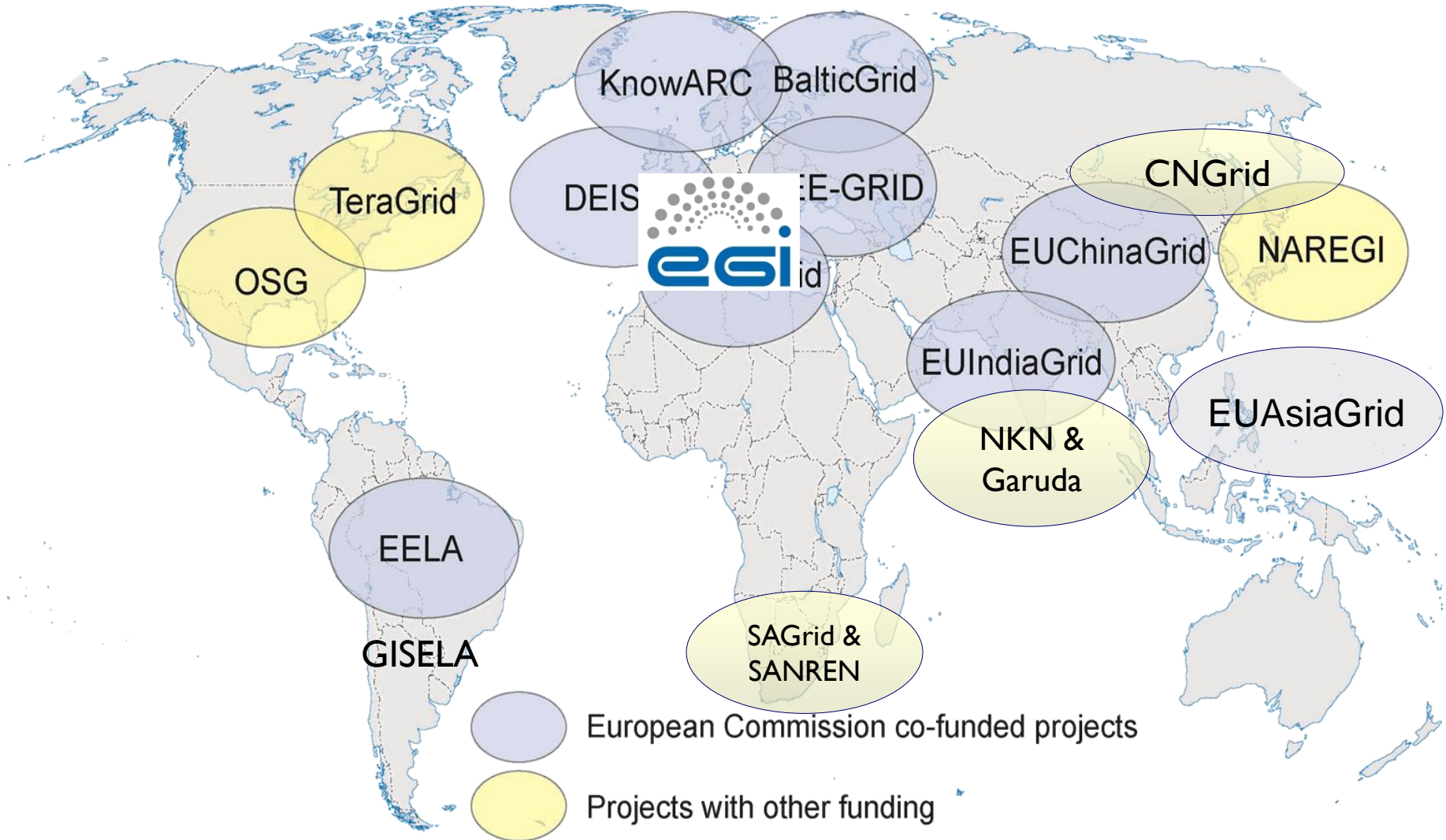
- ▶ Introductory considerations
- ▶ The Catania Science Gateway Framework
- ▶ Use cases from health:
 - ▶ DECIDE
 - ▶ IOERT
- ▶ Summary and conclusions



Evolution of distributed computing



The “Global” Grid





Using Grids is not straightforward ☹

```
Type = "Job";
JobType = "MPICH";
MPIType = "MVAPICH2_PGI706";
CpuNumber = 16;
MPIGranularity = 4;
Executable = "flash2";
StdOutput = "mpi.out";
StdError = "mpi.err";
InputSandbox =
{
  "watchdog"
  100
}
OutputS
Requirem
0
RetryCount
```

```
echo Staging Input Data \(\Courtesy of European Space
Agency\);
#edg-rm --vo=gilda copyFile lfn:$1.N1 file://$PWD/$1.N1;
lcp-cp --vo=gilda lfn:$1.N1 file://$PWD/$1.N1;
echo Staging Application;
gunzip beam20.tar.gz;
tar xvf beam20.tar;
cd beam-2.0/bin;
echo Starting Application;
./pds2jpg-ASAR-run.sh $1;
mv $1-b*.jpg ../
cd ../
rm -fr beam-2.0;
rm -fr $PWD
```

JDL

Script

CLI

Users have to cope with complex security procedures, execution scripts, job description languages, command line based interfaces and lack of standards. This makes the learning curve very steep and keeps non IT-experts away.

```
Reason(s):
Job terminated successfully
Exit code: 0
Status Reason: Job terminated successfully
Destination: grid010.ct.infn.it:2119/jobmanager-lcgpbs-gilda
Submitted: Tue Jun 29 15:34:40 2010 CEST
```

GSI

Request for the certificate

User's identity is confirmed by the RA

Certificate is emitted by the CA

Certificate is used as an access key to the grid

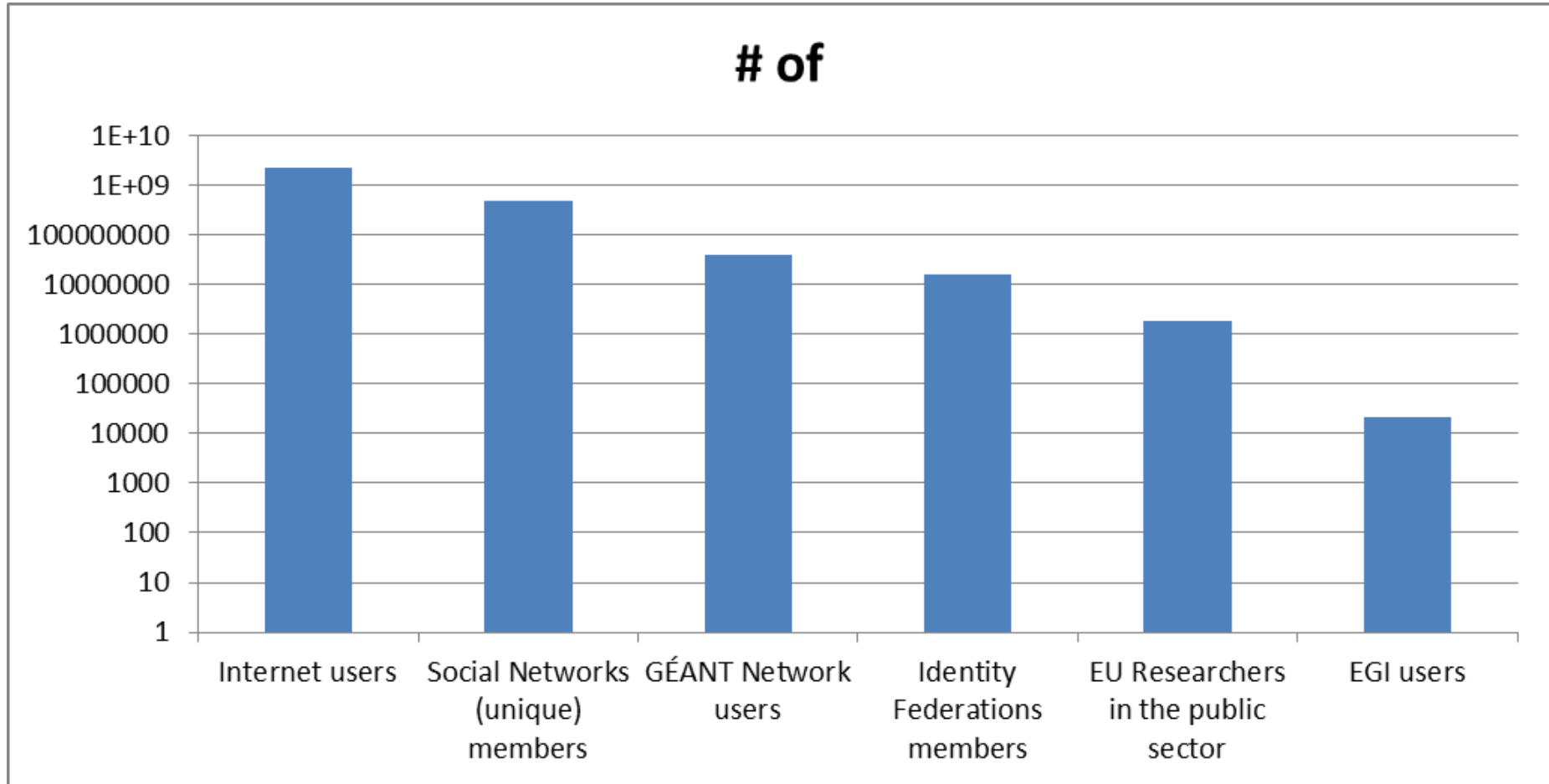
The eResearch2020 report

(<http://www.eresearch2020.eu/eResearch%20Brochure%20EN.pdf>)

- Some barriers in the adoption of Grids:
 - ▶ **Changes on Grids means changes on applications**
 - ▶ Time required to adapt usual workflows
 - ▶ Lack of structure to support anonymous access
 - ▶ Download and installation of applications
 - ▶ **Interface**
 - ▶ Slow to get to compared to other resources
 - ▶ **Difficult to use in the beginning**
 - ▶ **Time spent to get the application compiled and running**
-



Some figures...

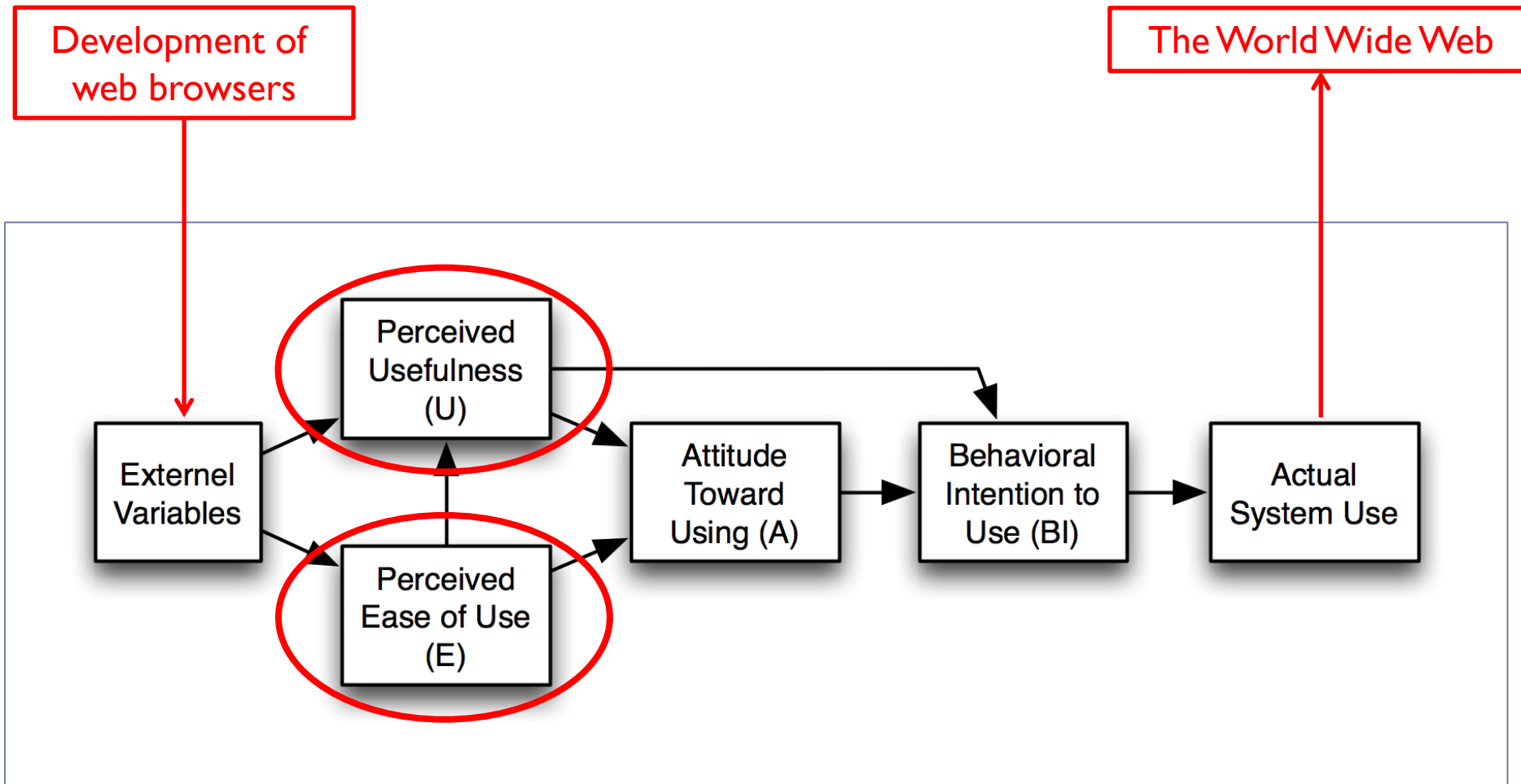


The path to technology uptake – Where are we with e-Infrastructures ?

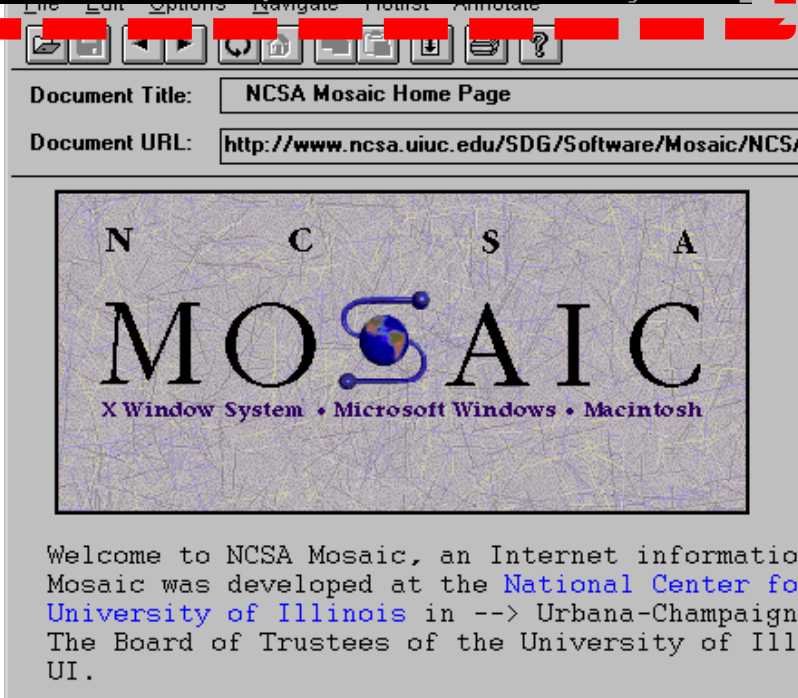
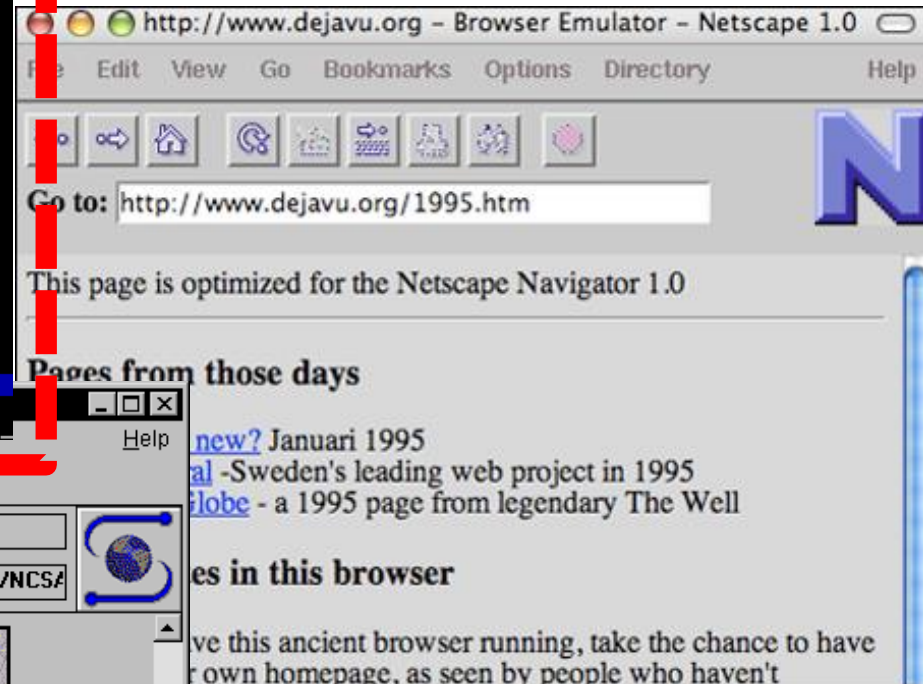
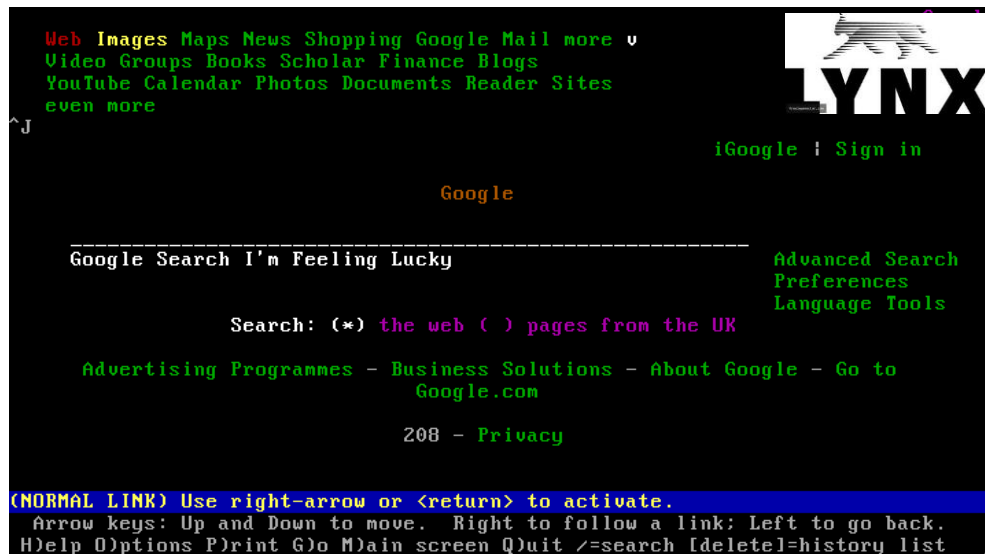


The Rogers "bell-shape" curve - Rogers, E. M. (1962), "Diffusion of Innovations", Glencoe: Free Press.

IT acceptance model – **the Web**



The evolution leap in web browsers

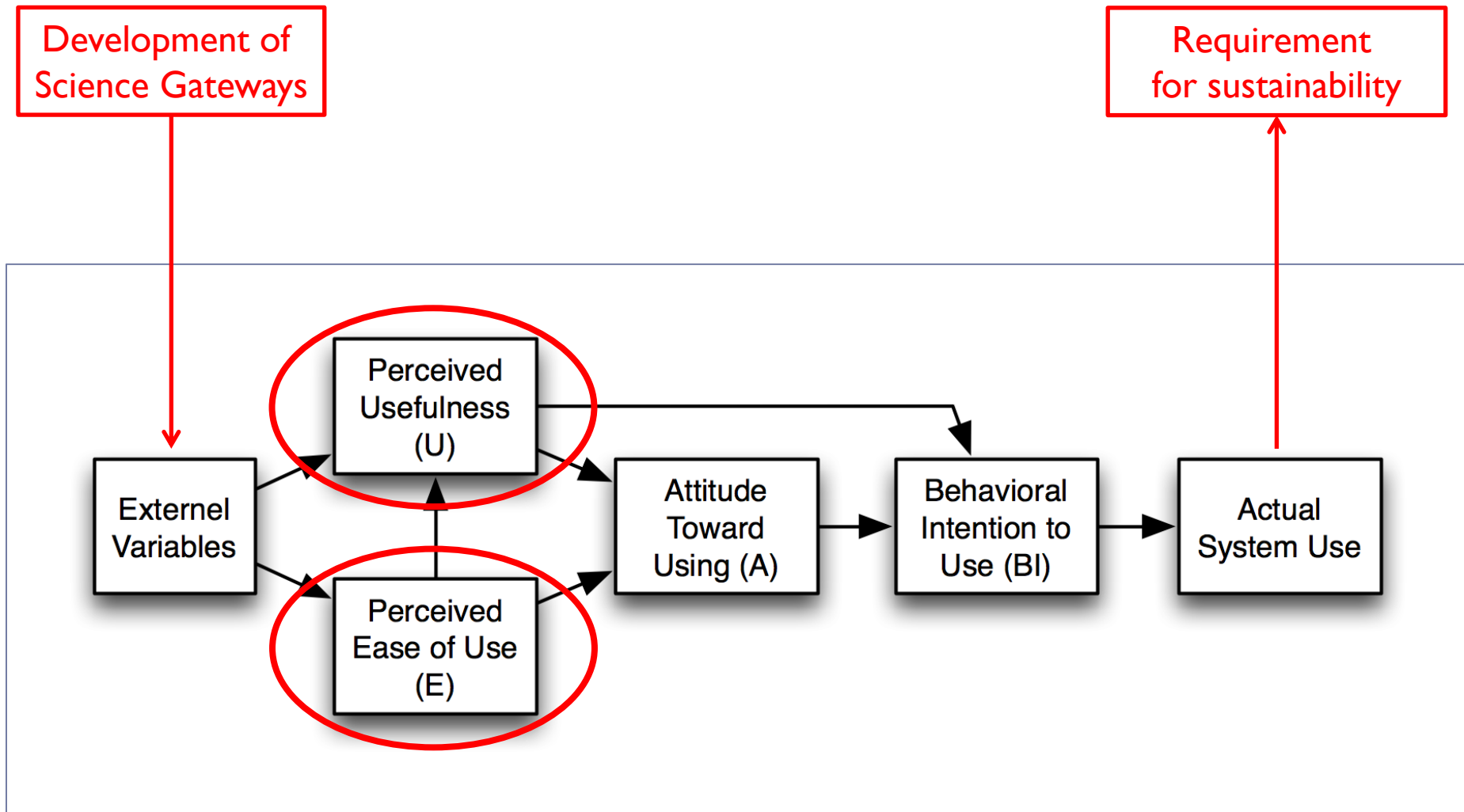


evolution leap

Community-driven web portals have started to integrate Grid Tools and Applications

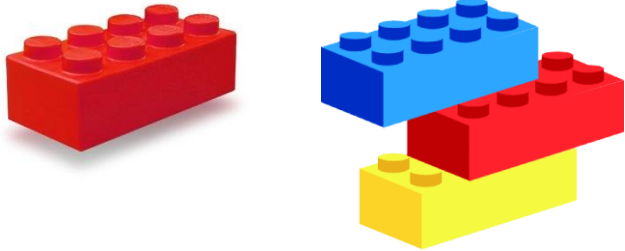


IT acceptance model – **the Grid**

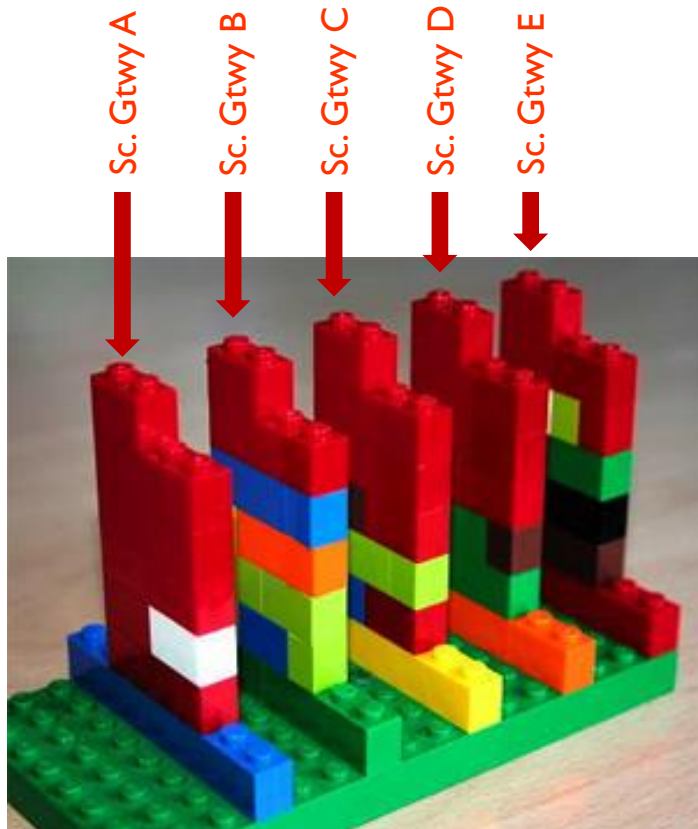


Davis, F. D. (1989), "Perceived usefulness, perceived ease of use, and user acceptance of information technology", *MIS Quarterly* 13(3): 319–340

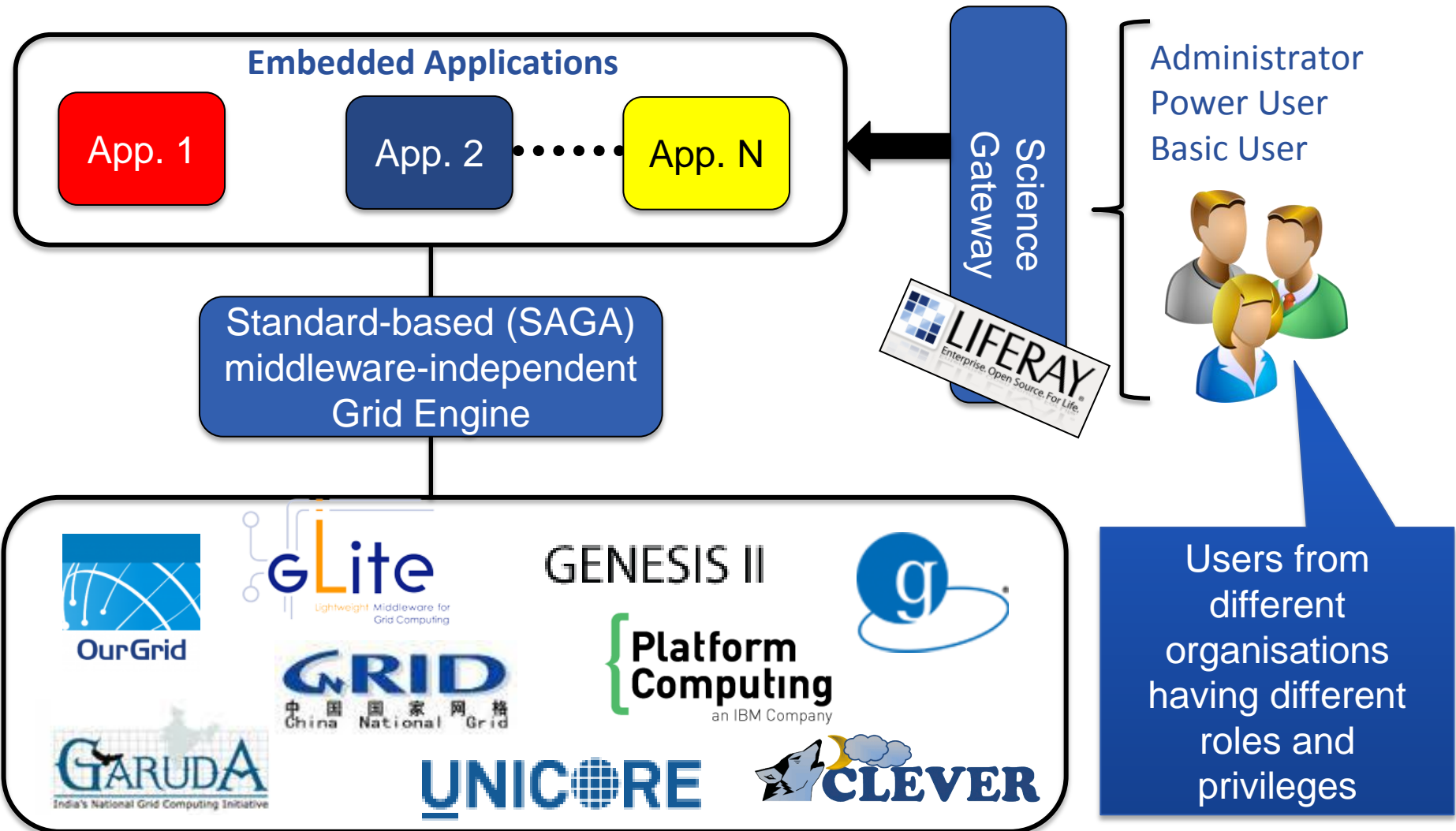
Primary requirement: building Science Gateways should be like playing with



- **Standards**
- **Simplicity**
- **Easiness of use**
- **Re-usability**

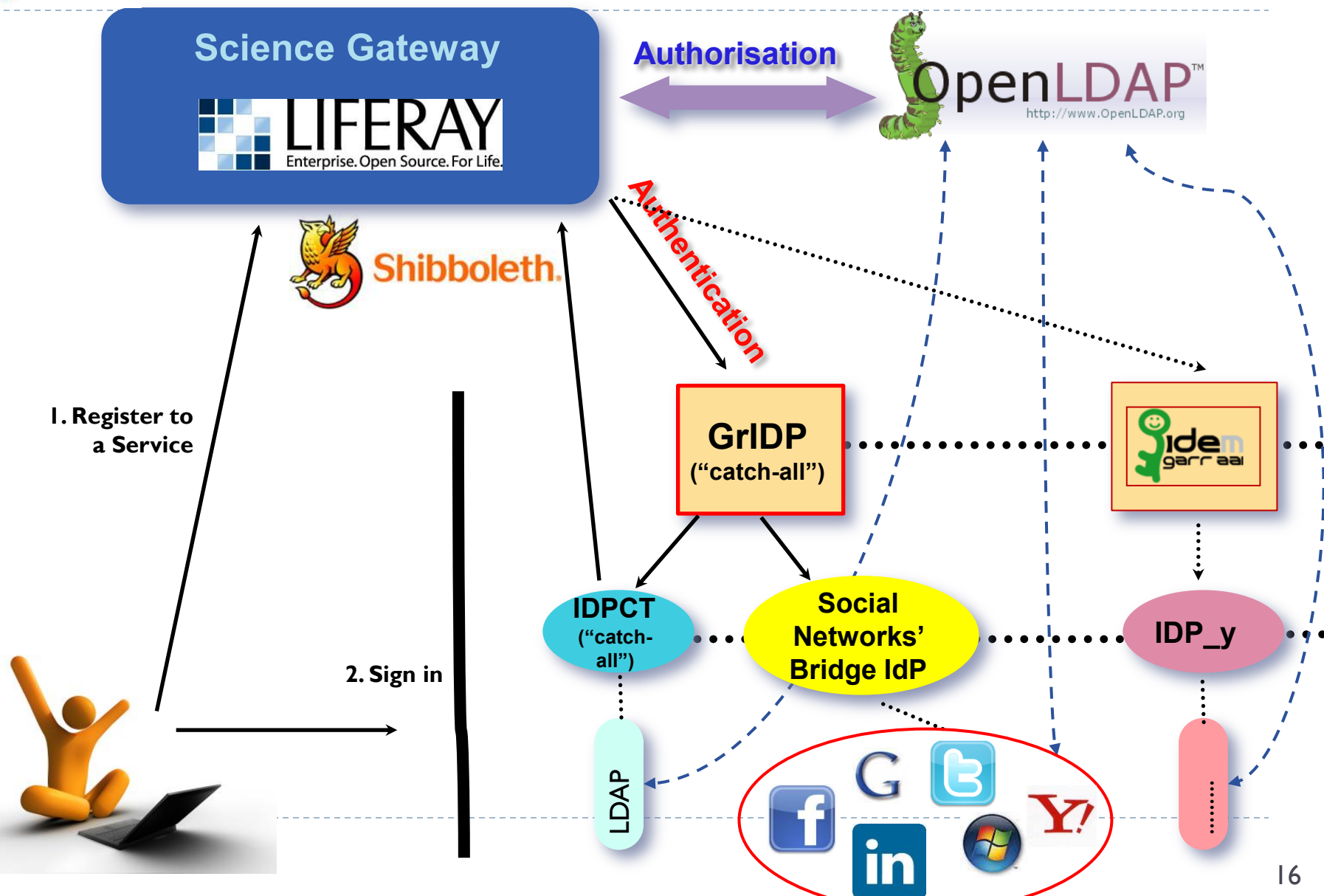


The Catania Science Gateway framework



► **Middleware supported so far**

AuthN & AuthZ Schema

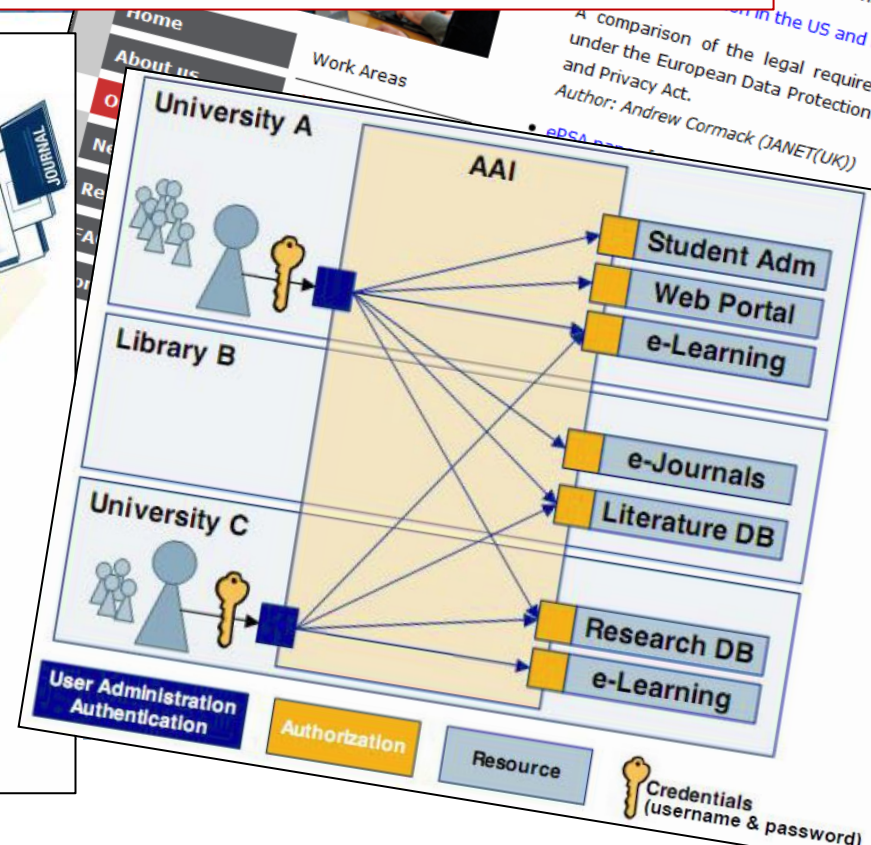
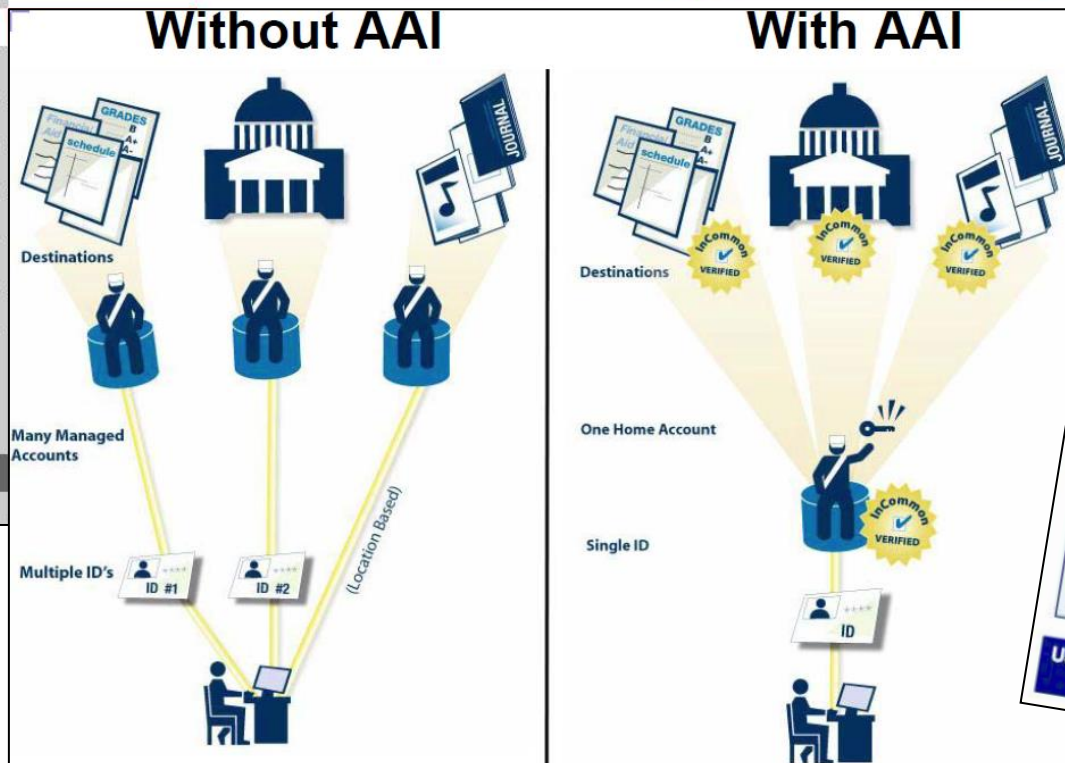


Identity Federations

(<https://refeds.org>)

An Identity Federation consists of “[...] the agreements, standards, and technologies that make identity and entitlements portable across autonomous domains.”

Burton Group



Official Identity Federations currently supported by Catania Science Gateways

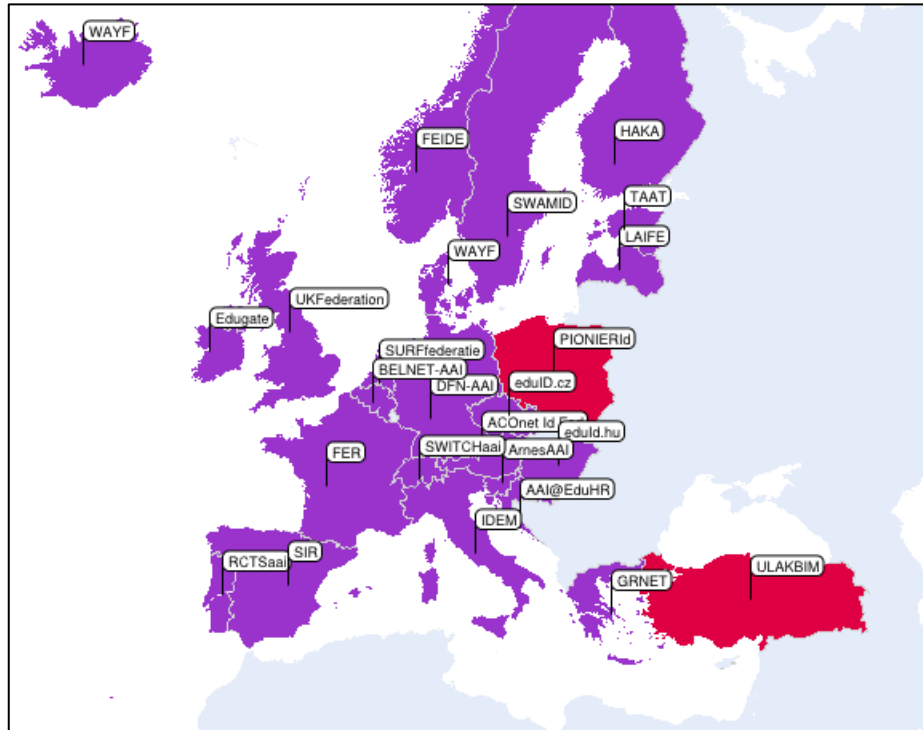


In progress



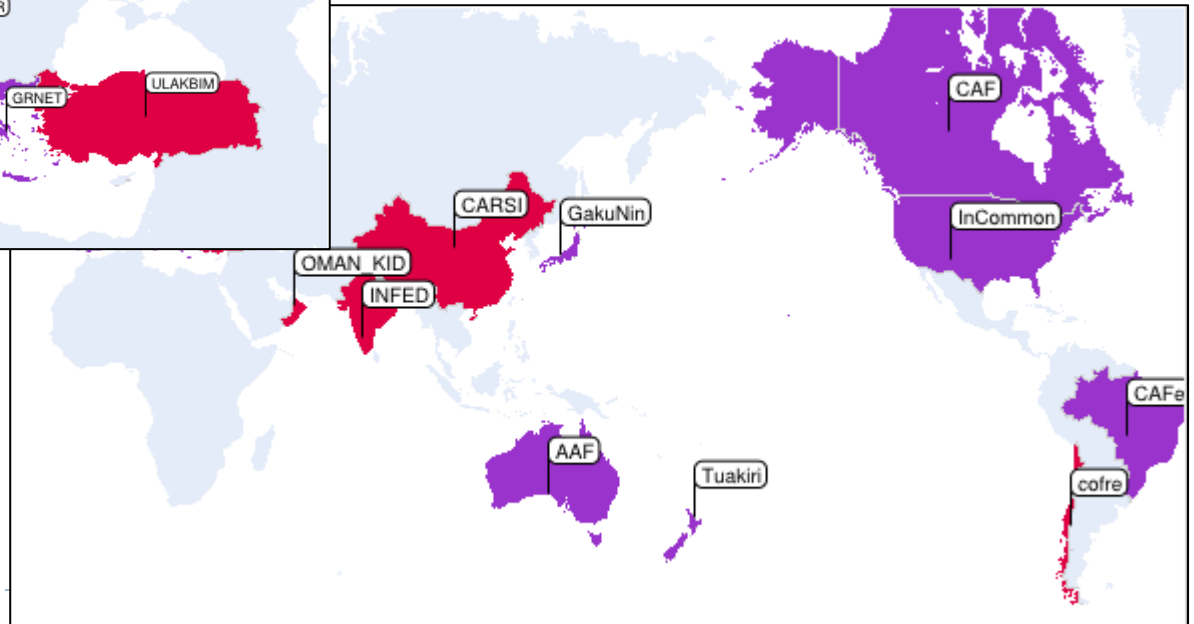
Identity Federations in the world

(<https://refeds.org>)



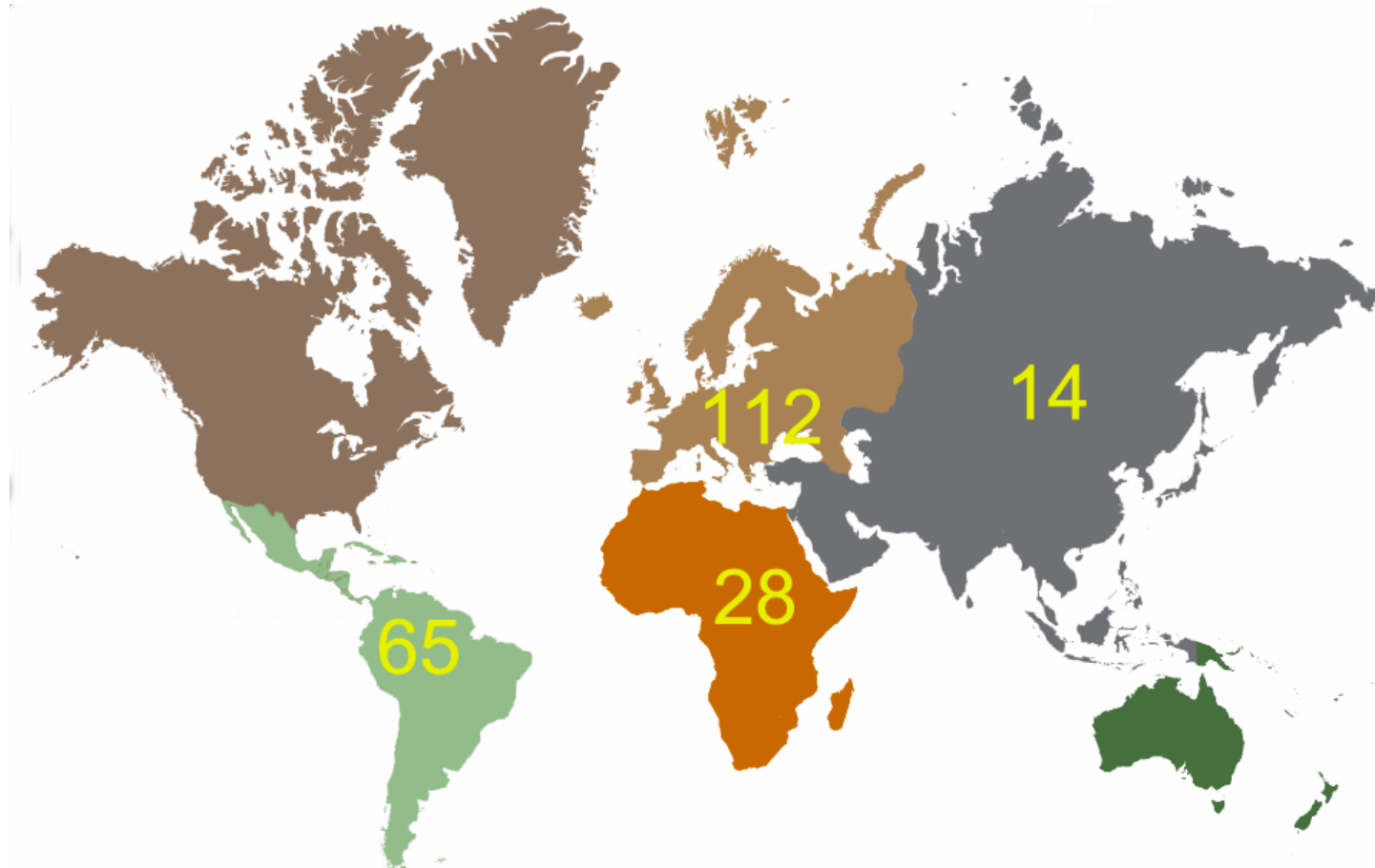
16 million people worldwide

■ Pilot ■ Production



Uptake of Catania Science Gateways (as of the end of 2012)

Users from 219 Organisations in 47 Countries

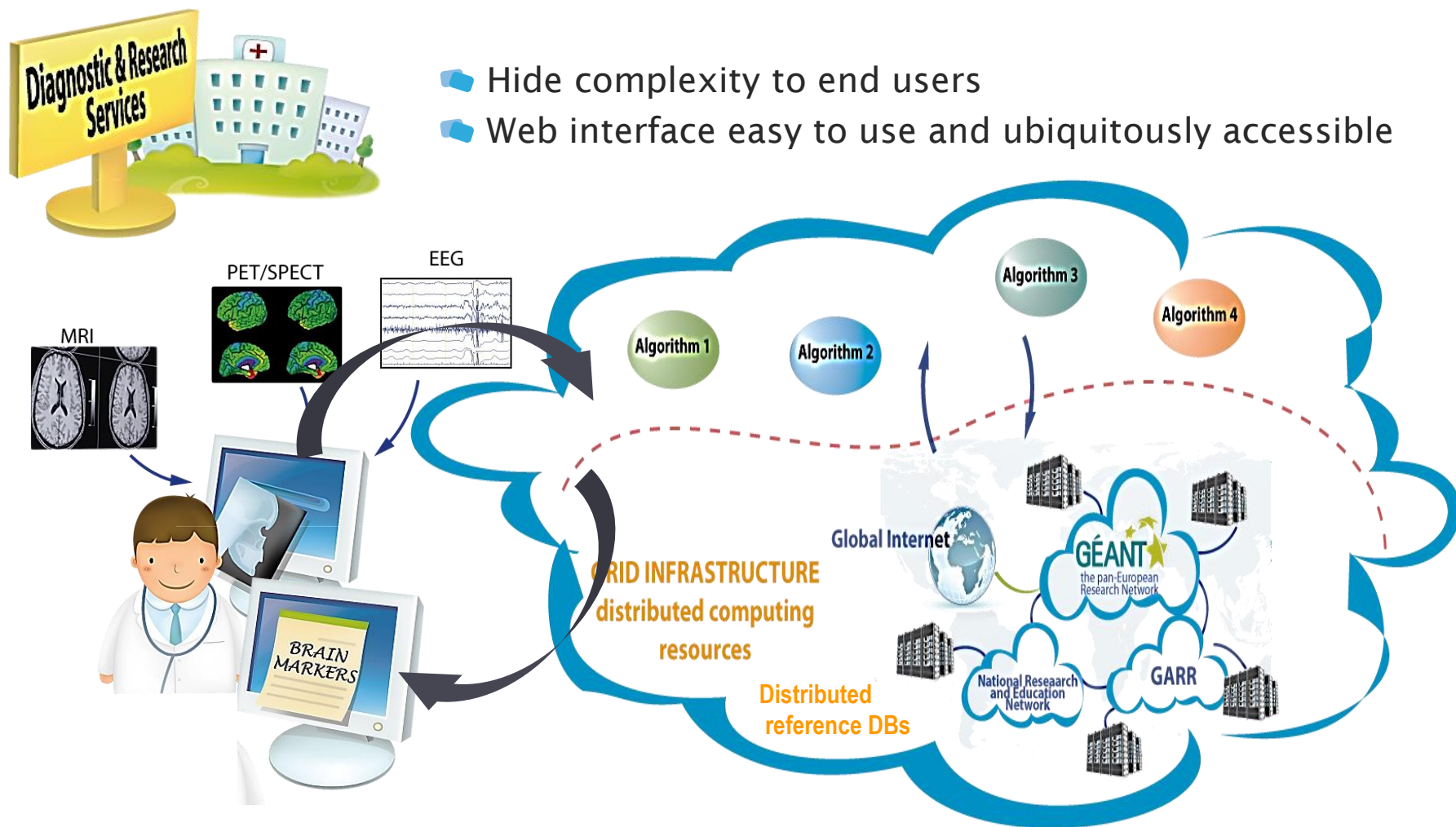


12 Science Gateways in production; 4 in preparation



The DECIDE Use Case

- Hide complexity to end users
- Web interface easy to use and ubiquitously accessible



The DECIDE Science Gateway

(<http://applications.eu-decide.eu>)

DECIDE Science Gateway | DECIDE Home | Project | Documents | Technical Wiki | Register | Sign In




DECIDE Science Gateway

- Home
- Applications**
- Grid Services
- User Support
- Collaborate with us

Social Networks

Follow us on the Social Networks

This Includes the possibility to access the Science Gateway from within the Social Network page.



 A una persona piace questo elemento. Di' che piace anche a te, prima di tutti i tuoi amici.

Welcome

Welcome to the DECIDE Science Gateway. If you do not yet have an account, find below the instructions to register and sign in.

1) Register

(If you have already registered)

In order to create an account appears on the top right of this page.

Once you are in the registration phase, you will be asked to choose a username and password, and to confirm the link which appears in the email you will receive. When the link is confirmed, you will be able to access the Science Gateway.

2) Sign In

(If you do not have yet an account)

Once you receive the email in which the link to the registration phase has been accepted by the administrator, you will be able to access the Science Gateway. There you have to sign in the registration phase, please choose the Organisation which are our partners. The button which will appear on the top right of the page will be the one to click.

DECIDE Science Gateway | DECIDE Home | Project | Documents | Technical Wiki | Register | Sign In



DECIDE Science Gateway


- Home
- Applications**
- Grid Services
- User Support
- Collaborate with us

Applications

Copy | Print | Save


Search:

Show 10 entries

NAME	RUN PAGE	DOMAIN	MIDDLEWARE	INSTITUTION
GridANN4ND		Life Sciences	EMI-gLite	Imperial College London Medical Research Council
GridEEG		Life Sciences	EMI-gLite	UWAR UNIFG UNIROMA1 AFAR
GridGDI		Life Sciences	EMI-gLite	Consortium GARR INFN
GridMRI Seg		Life Sciences	EMI-gLite	PLVODSGDD
GridSPM		Life Sciences	EMI-gLite	CNR

Showing 1 to 5 of 5 entries

First | Previous | 1 | Next | Last

This is a Service Provider of:    

22

The DECIDE Science Gateway in action

DECIDE Science Gateway
DECIDE Home
Project
Documents
Technical Wiki

Diagnostic Enhancement of Confidence by an International Distributed Environment

DECIDE Science Gateway

- Home
- Applications
 - GridANN4ND
 - GridEEG
 - Physician
 - Scientist
 - Manage Repository
 - GridMRISeg
 - GridSPM
 - GridGDI
 - test
- Grid Services
- User Support
- Collaborate with us

My Workspace

- Jobs
- JobsMap
- Data

GridEEG - Set Parameters

Welcome to Grid EEG

Welcome to the **GridEEG** DECIDE service. The service is running in **scientist** mode. In such mode you can vary the default values of the implemented algorithms. S

GridEEG is the application connected with porting of algorithms for the spectral analysis in the Grid environment.

In particular, these algorithms allow the estimation of the power spectral density as the computation of functional coupling of EEG rhythms by spectral coherence (DTF).

These algorithms provide EEG markers that are embedded into a multi-dimensional space for the subsequent classification of Alzheimer (AD) patients and normal elderly subjects using the Mahalanobis distance based classifier.

This procedure generates a statistical report whose clinical validity is under evaluation.

GridEEG application consists of the following tools:

- GridEEG-DATA (Gridified routine for EEG data conversion);
- GridEEG-QUALITY (Gridified routine for the selection of artifact free EEG segments);
- GridEEG-SOURCE (Gridified routine for estimation of Power Spectrum Density for each source cortical level);
- GridEEG-COHERENCE (Gridified routine for the estimation of Spectral Coherence);
- GridEEG-DTF (Gridified routine for the estimation of Directed Transfer Function);
- GridEEG-STAT (Gridified routine for the statistical comparison of the estimated EEG markers between the database of Alzheimer's diseased patients (n=100) and normal elderly subjects).

Alpha1: 8.5 Hz 10.5 Hz -
Alpha2: 11 Hz 13 Hz -
Beta1: 13.5 Hz 20 Hz -
Beta2: 20.5 Hz 30 Hz -
Gamma: 30.5 Hz 40 Hz -

Power Spectrum Density feature selection

Include? ☒

A feature is composed by a pair of values (cortical regions of interest, frequency band)

Area:	Band:
Occipital	Alpha1
Occipital	Delta
Parietal	Alpha1

Add - Remove

Partial Coherence feature selection

Include? ☒

A feature is composed by a triplet (electrode, electrode, frequency band)

Channel 1:	Channel 2:	Band:
P3	C3	Alpha1
T3	F3	Alpha2
Pz	Fz	Alpha2

Add - Remove

Directed Transfer Function feature selection

Include? ☒

A feature is composed by a triplet (electrode, electrode, frequency band)

Target:	Source:	Band:
O2	P4	Alpha1
Cz	Pz	Beta2
Pz	Fz	Alpha2

Add - Remove

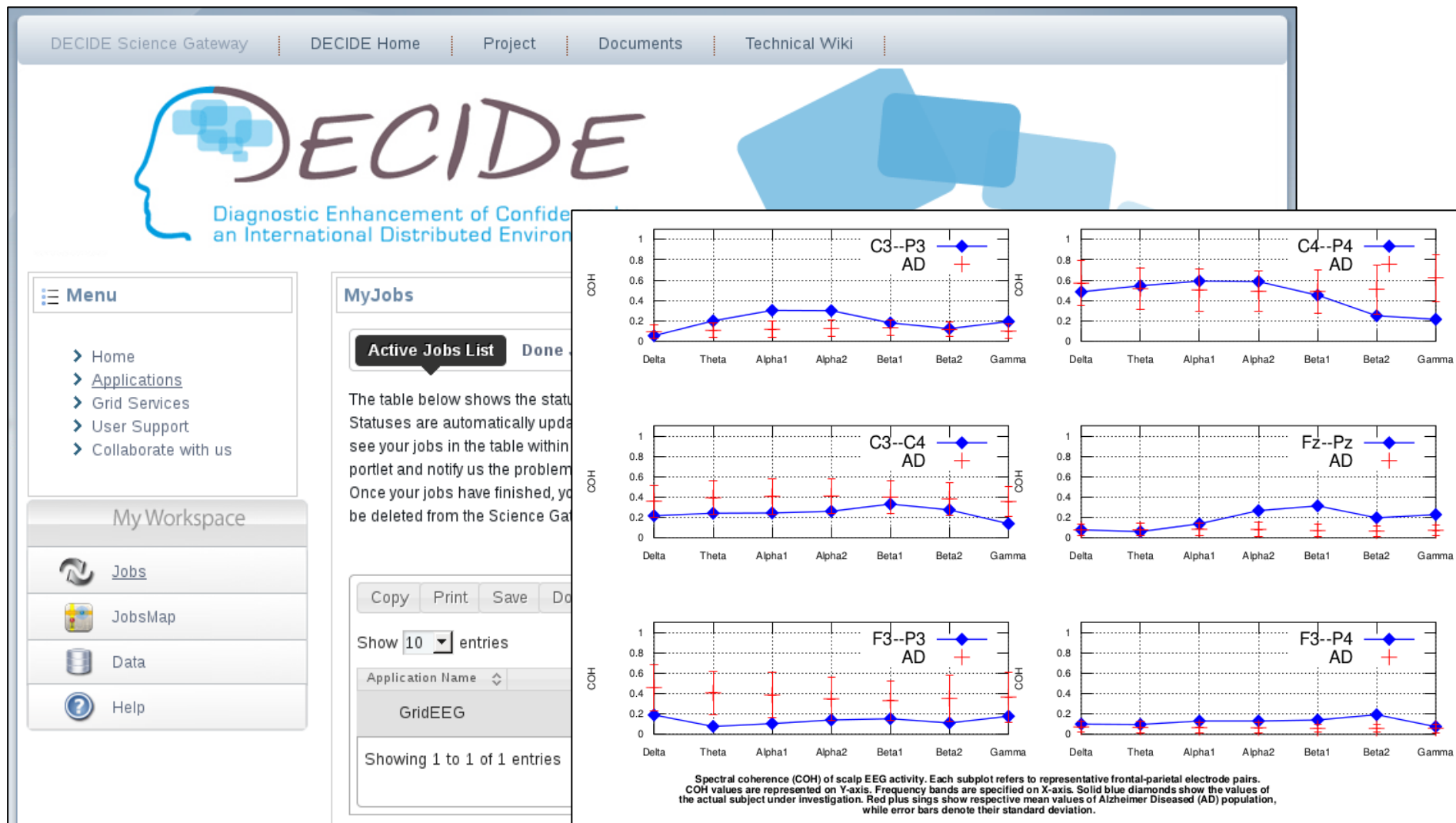
Upload here your EEG data archive

EEG data archive in .zip or .tgz Format:

Choose...

Start analysis

The DECIDE Science Gateway in action



The DECIDE Science Gateway in action

The screenshot displays the DECIDE Science Gateway interface. At the top, a navigation bar includes links for DECIDE Science Gateway, DECIDE Home, Project, Documents, and Technical Wiki. The main header features the DECIDE logo and the tagline "Diagnostic Enhancement of Confidence by an International Distributed Environment".

On the left, a sidebar menu lists various applications and services, including Home, Applications, GridANN4ND, GridEEG, GridMRISeg, GridSPM, Physician, Scientist (highlighted), Manage Repository, GridGDI, test, Grid Services, User Support, and Collaborate with us. Below this is a "MyWorkspace" section with buttons for Jobs, JobsMap, Data, and Help.

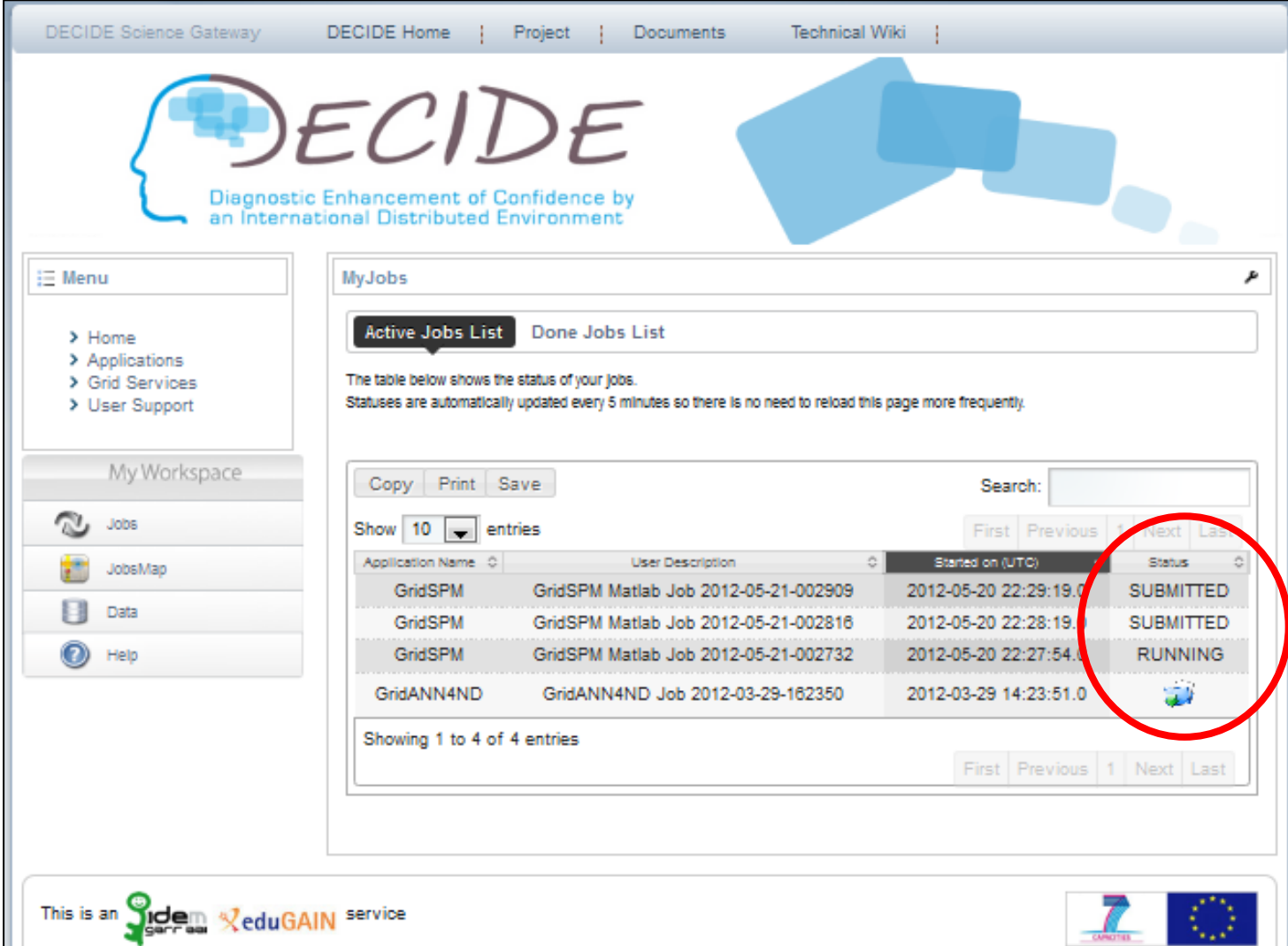
The main content area is titled "GridSPM - Scientist" and includes a welcome message, a purpose statement, and a list of steps for running the analysis. A red bracket highlights the "How to run the analysis" section, which is also titled "How to run the analysis" in a sub-header. This section provides instructions on uploading patient data and selecting analysis parameters.

The "How to run the analysis" section includes the following details:

- Normal subjects filter selection:** A dropdown menu set to "No, use all available subjects". A note states: "Please, note that currently filters are not applied due to the reduced number of normal subjects. Controls are shown for training purpose."
- Analysis parameters:** A section with a note: "Please note: currently some parameters cannot be selected. Default value is shown for your information." Parameters include:
 - Interpolation method: Bilinear Interpolation
 - Smothing (FWHM in mm): [8 8 8]
 - Define the contrast Name: Hypo-metabolism
 - Define the contrast Type: t-contrast
 - Corrected height threshold?: no
 - Set threshold (T or p value): 0.001
 - Threshold extent (voxels): 10
- Upload here your SPM data archive:** A section with a note: "Select your SPM data archive in .zip or .tgz format". A button labeled "Scegli file" is next to the text "Nessun file selezionato".

At the bottom of the "How to run the analysis" section, there is a "Start analysis" button.

The DECIDE Science Gateway in action



DECIDE Science Gateway | DECIDE Home | Project | Documents | Technical Wiki

DECIDE
Diagnostic Enhancement of Confidence by
an International Distributed Environment

Menu

- > Home
- > Applications
- > Grid Services
- > User Support

MyWorkspace

- Jobs
- JobsMap
- Data
- Help


MyJobs

Active Jobs List | Done Jobs List

The table below shows the status of your jobs.
Statuses are automatically updated every 5 minutes so there is no need to reload this page more frequently.



Copy | Print | Save | Search:



Show 10 entries

Application Name	User Description	Started on (UTC)	Status
GridSPM	GridSPM Matlab Job 2012-05-21-002909	2012-05-20 22:29:19.0	SUBMITTED
GridSPM	GridSPM Matlab Job 2012-05-21-002818	2012-05-20 22:28:19.0	SUBMITTED
GridSPM	GridSPM Matlab Job 2012-05-21-002732	2012-05-20 22:27:54.0	RUNNING
GridANN4ND	GridANN4ND Job 2012-03-29-162350	2012-03-29 14:23:51.0	

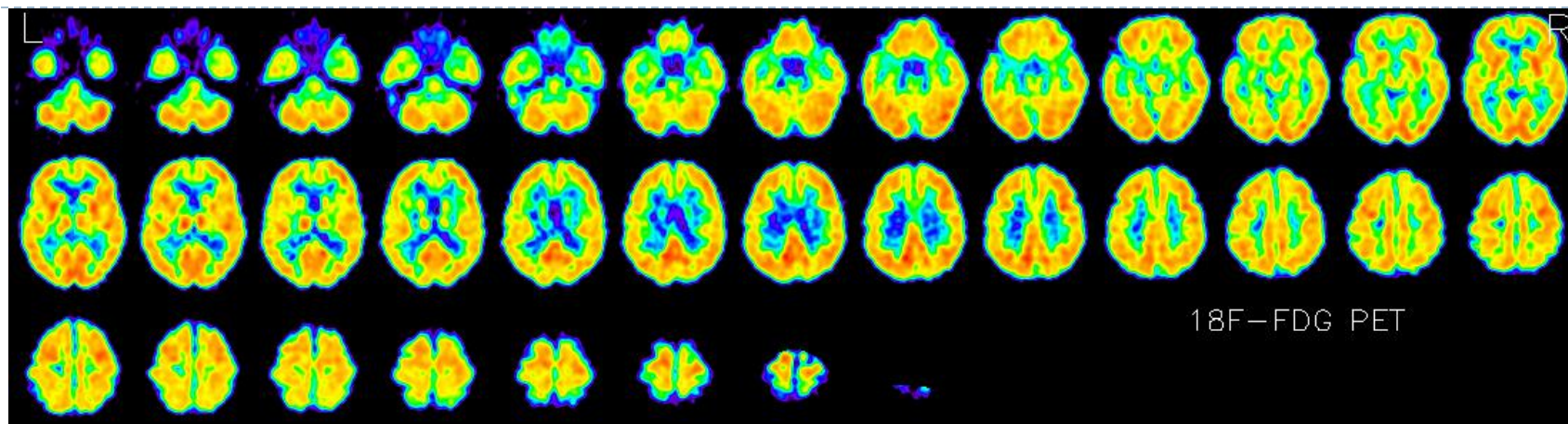
Showing 1 to 4 of 4 entries

First | Previous | 1 | Next | Last

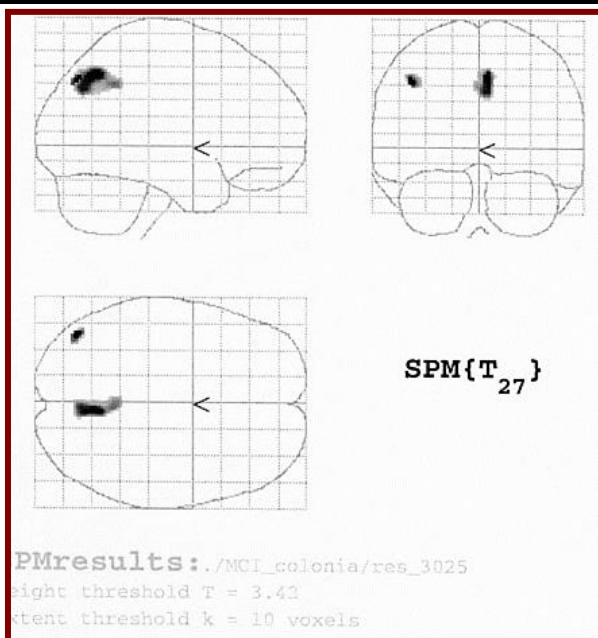
This is an   service

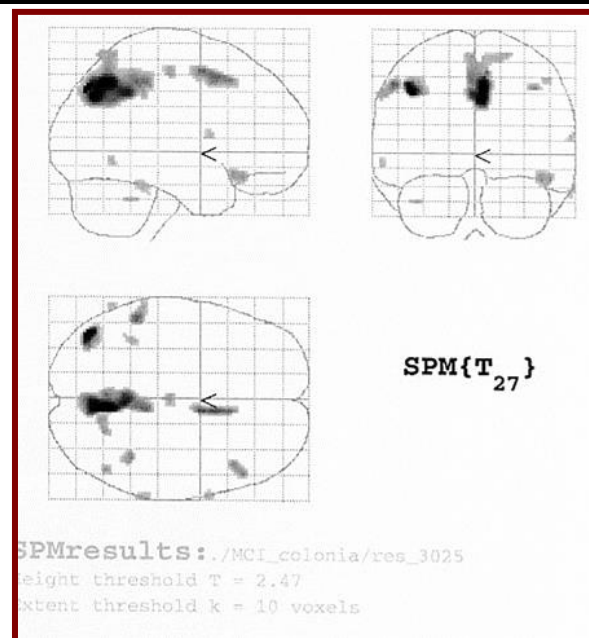
The DECIDE Science Gateway in action



GridSPM report



p = 0.001



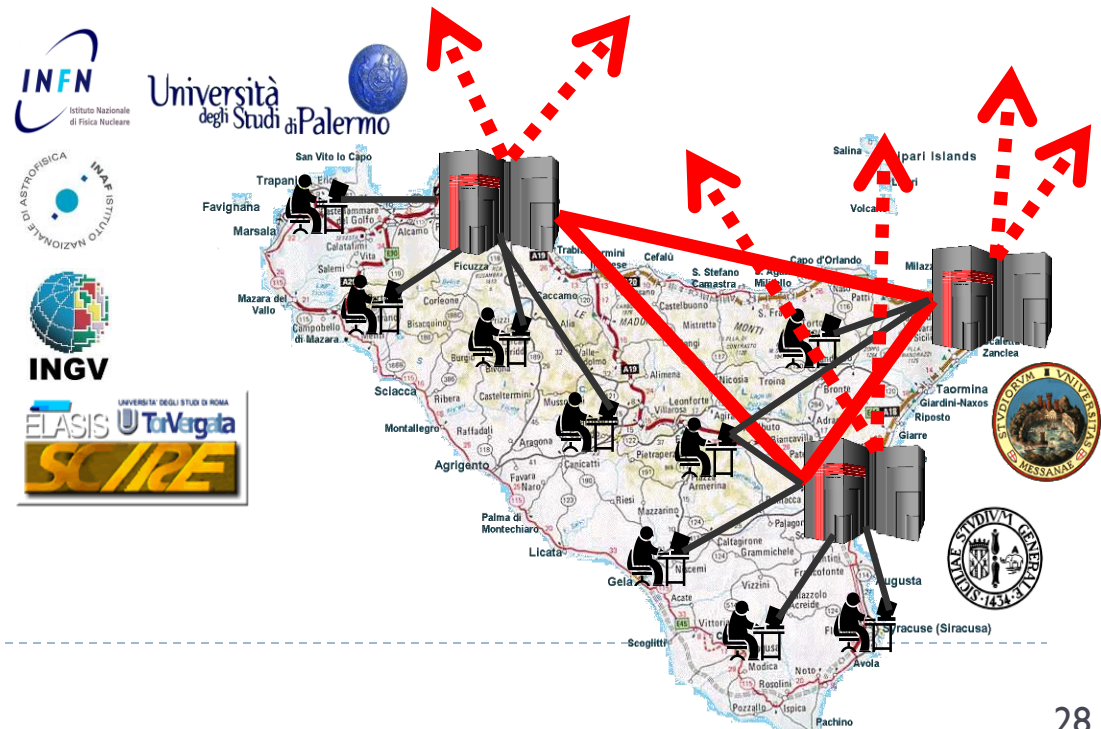
p = 0.01

The IOERT Use Case



**Laboratorio di Tecnologie
Oncologiche (LATO)**
@ HSR Giglio - Cefalù (PA)

Consorzio COMETA- Catania

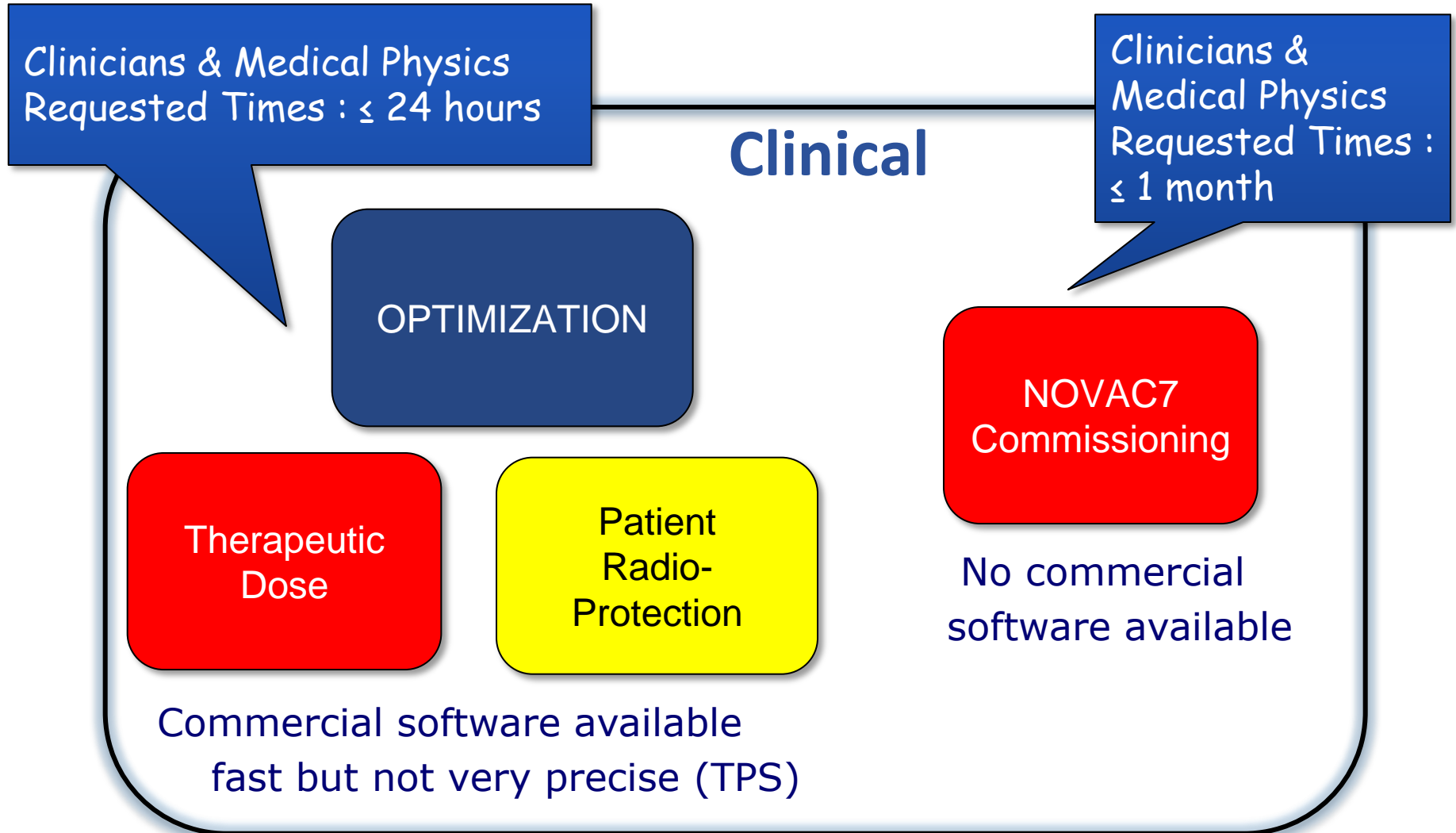


The Intra-Operative Electron Radio-Therapy (IOERT) technique in a nutshell

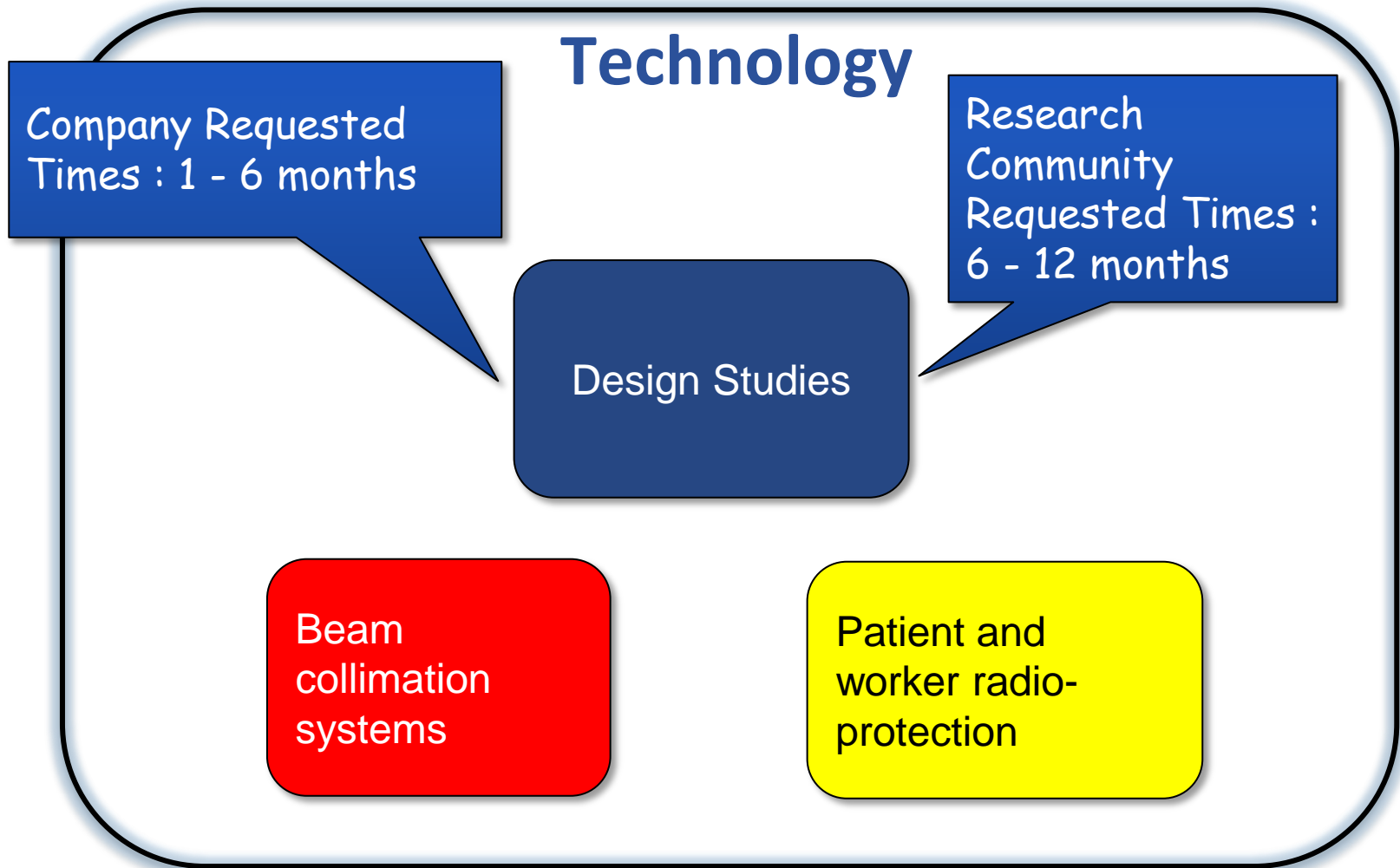
- ❖ **Intra-Operative Electron Radiotherapy (IOERT)** is an advanced radiation therapy technique that allows treatment of tumors after surgery, directly in the surgery room, delivering a high dose to the target (*Veronesi et al., 2001*);
- ❖ Treatment of breast, stomach, prostate cancers;
- ❖ The electron beam is produced through dedicated and mobile accelerators, such as **NOVAC7** (NRT, Aprilia - Italy);
 - ✓ Electron beams of 4, 6, 8 e 10 MeV with different diameters (from 3 to 10 cm) and slant angles collimators (0°, 15°, 22.5°, 30° and 45°)



Clinical Activities



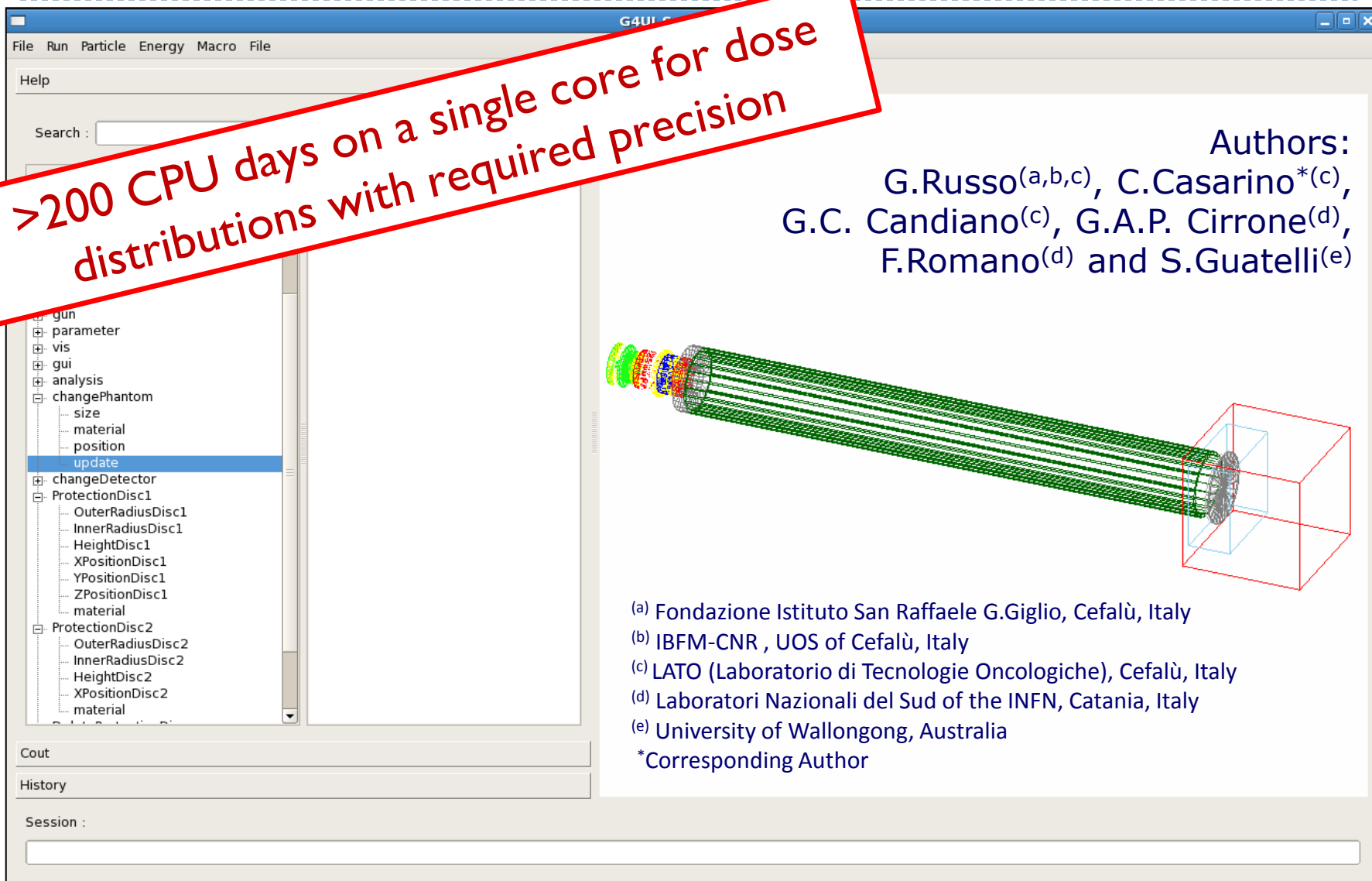
Technological Activities



❖ No commercial software available

The IOERT simulator with Geant4

>200 CPU days on a single core for dose distributions with required precision



The IOERT Science Gateway in action

The screenshot shows a web browser window at the URL `gw.ct.infn.it/run-ior_t_therapy`. The page has a breadcrumb trail: `Science Gateway to IGI > Applications > Life Sciences > iort_therapy > run_iort_therapy`. On the left is a sidebar with a 'My Workspace' section containing links for 'Jobs', 'JobsMap', 'Data', and 'Help'. The main content area is titled 'The iort Project' and features a 'Iort_Therapy Input Form'. This form is divided into three numbered sections: 1. 'Display Settings', 2. 'Worldwide Software Distribution', and 3. 'Specify your Input Settings'. The 'Display Settings' section is expanded and contains the following text:

The current IORT_THERAPY portlet has been configured for:

- ☒ The COMETA Grid Infrastructure ✓

Instructions for users:

- ~ This portlet aims to address typical needs related to the IntraOperative Radio-Therapy (IORT) technique. This technique delivers a single dose of radiation directly to the tumor bed, or to the exposed tumor, during surgery.

The portlet takes as input:

- ~ a GEANT4 macro file (.mac);
- ~ the number of run to be submitted in grid ([0, 200]).

Each run will produce:

- ~ .std.txt: the standard output file;
- ~ .std.err: the standard error file;
- ~ results.tar.gz: containing the results of the generic Monte Carlo simulation.

For further information, please refer to the output.README file produced during the run.

If you need to change some preferences, please contact the administrator

Your Rating: ★★★★★ Average (1 Vote): ★★★★★

IORT_THERAPY portlet ver. 1.1.8



running on <http://gw.ct.infn.it>

1

It provides some explanation about the application

The IOERT Science Gateway in action

 **Science Gateway**
running on <http://gw.ct.infn.it>

Science Gateway to IGI > Applications > Life Sciences > iort_therapy > run_iort_therapy

My Workspace **MYWORK**

- Jobs
- JobsMap
- Data
- Help

The iort Project

Iort_Therapy Input Form


- 1 Display Settings
- 2 Worldwide Software Distribution
- 3 Specify your Input Settings

Please, paste the macro you want to run in the textarea below, OR upload it in an ASCII file

☒ Upload macro * defaultMacro.mac


☐ Insert macro *

Description

☒ Notification 

N *

Number of GEANT4 jobs to be submitted: 20



All rights reserved

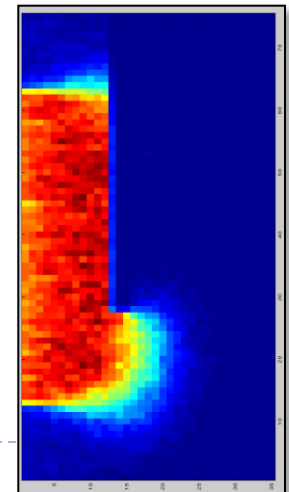
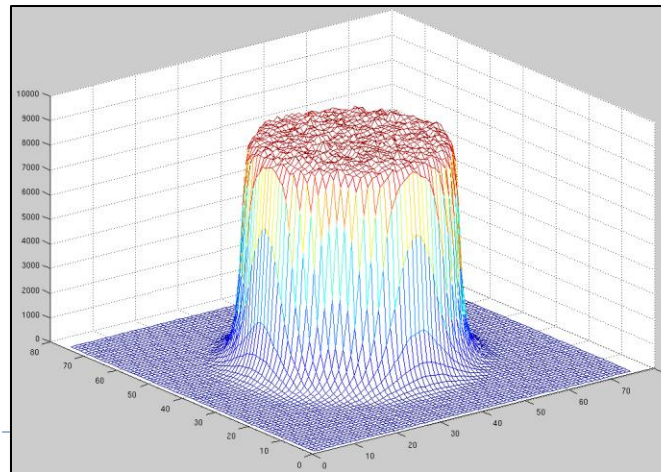
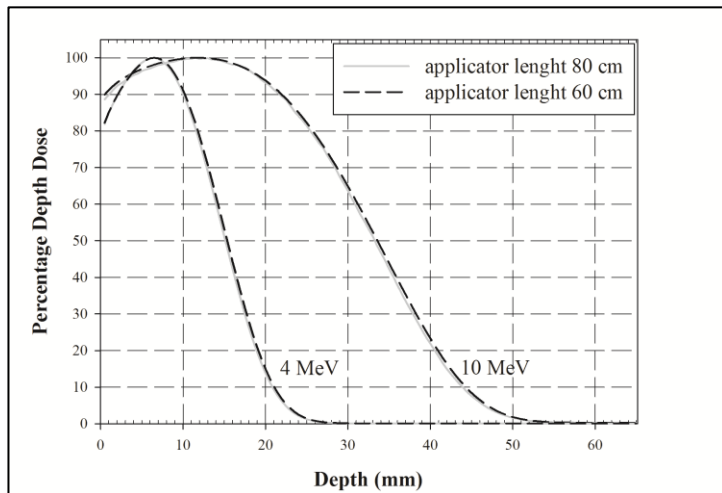
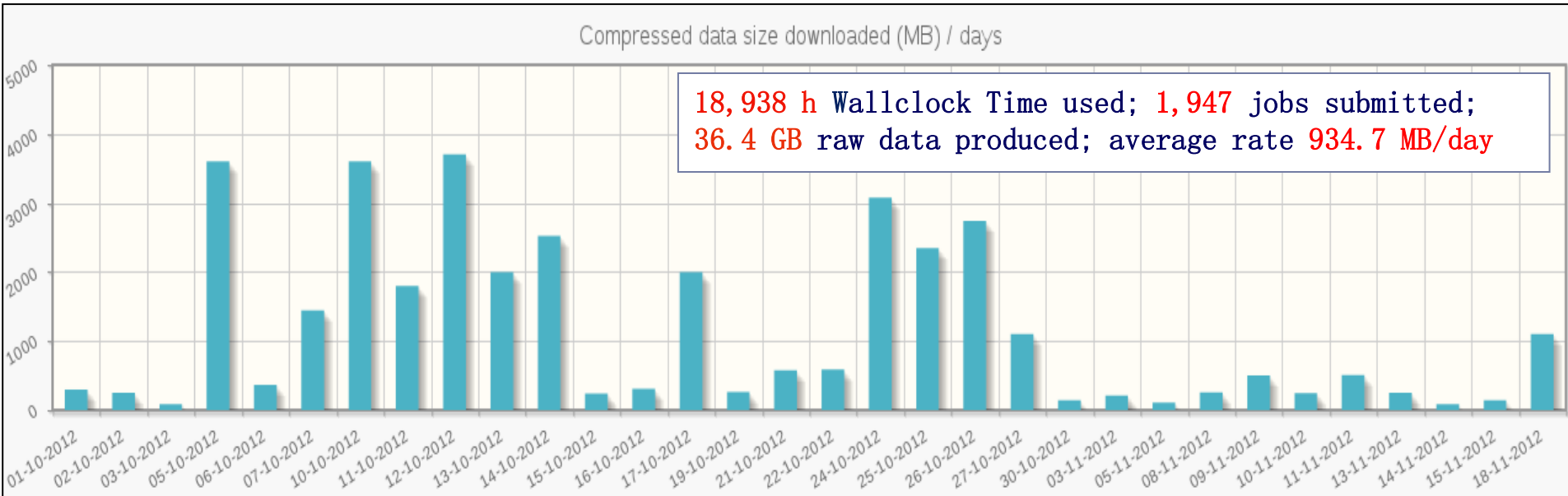
3 Uploading a GEANT4 macro as ASCII file or via the text-area

Job description

Enable e-mail notification

of Monte Carlo jobs to submit

The IOERT Science Gateway in action



Summary and conclusions

- ▶ e-Infrastructures can be very beneficial platforms for many users, provided they are really «easy to use» and users are at their centre
- ▶ The Catania Science Gateway framework, with support for Identity Federations, changes the way e-Infrastructures can be used, hugely widening their potential user base across continents and organisations, especially non-IT experts
- ▶ The adoption of standards (JSR 286, SAGA, SAML, etc.) represents a concrete investment towards sustainability
- ▶ Concrete use cases demonstrate the usefulness of the Science Gateway paradigm for next generation e-health



Thank you !

