



**Making e-Infrastructures easy:
the Science Gateway approach**

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University of Catania and INFN

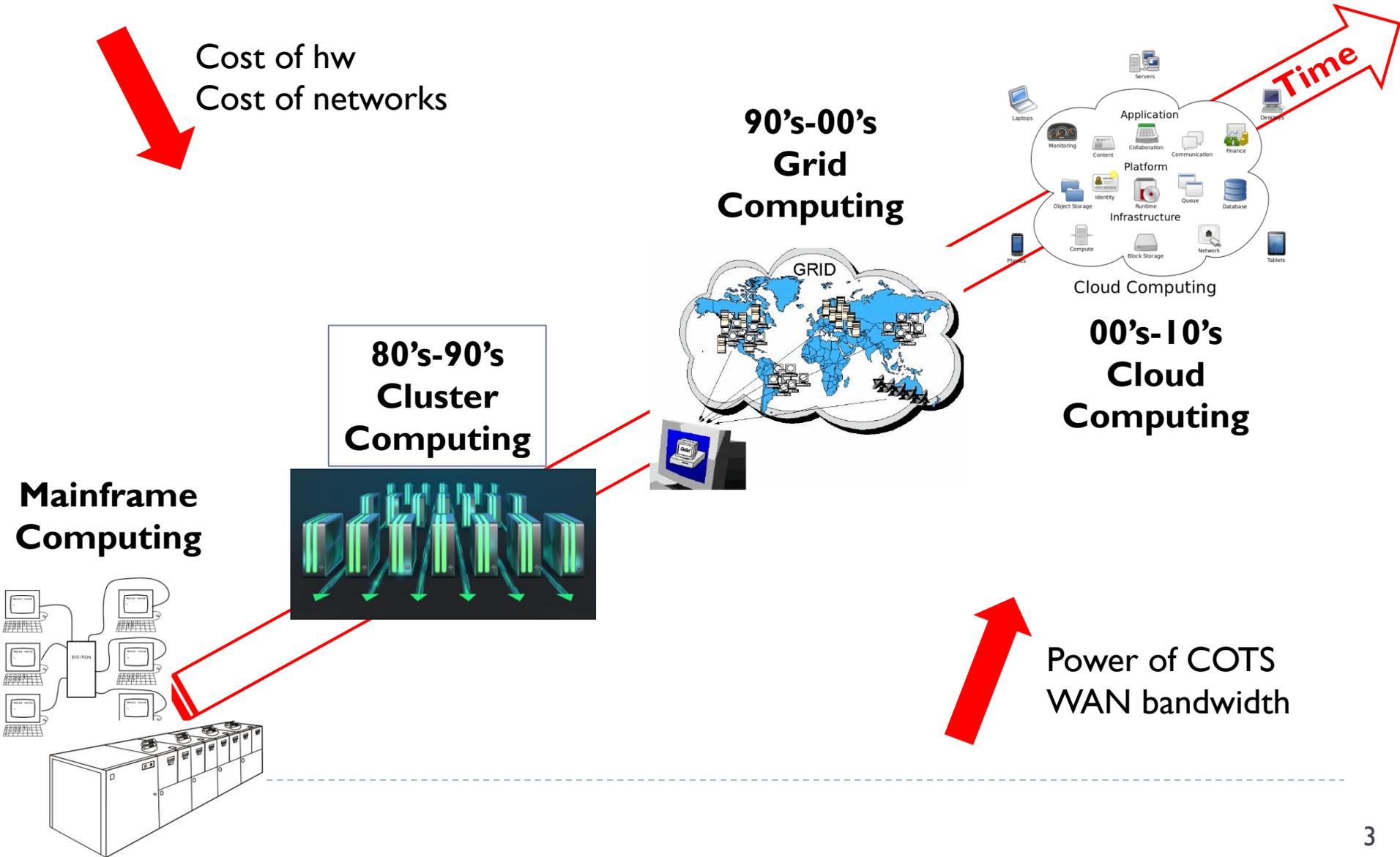
DECIDE Final Workshop – Rome, 22 February 2013

Outline

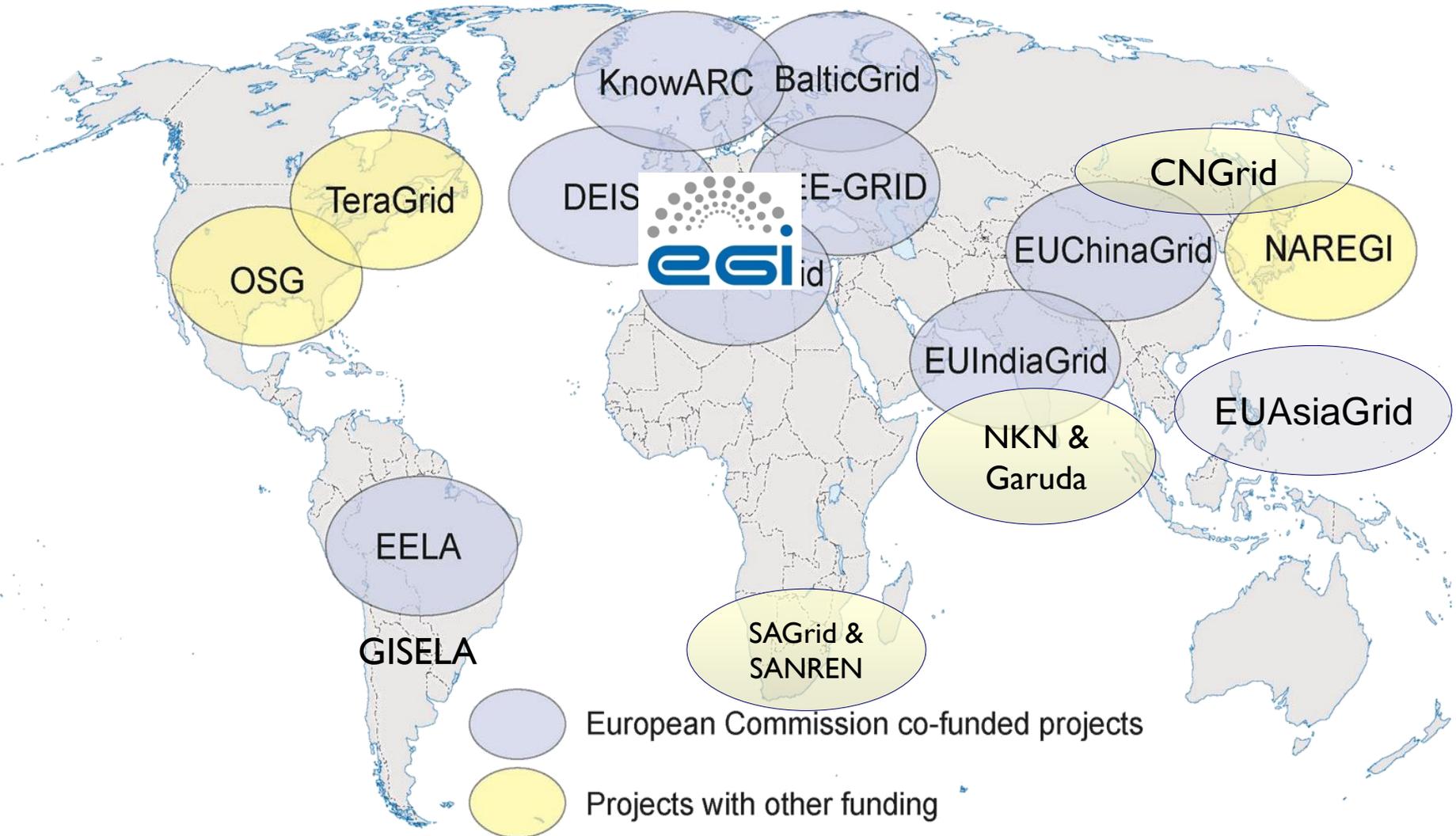
- ▶ **Introductory considerations**
- ▶ **The Catania Science Gateway Framework**
- ▶ **Use cases from health:**
 - ▶ **DECIDE**
 - ▶ **IOERT**
- ▶ **Summary and conclusions**



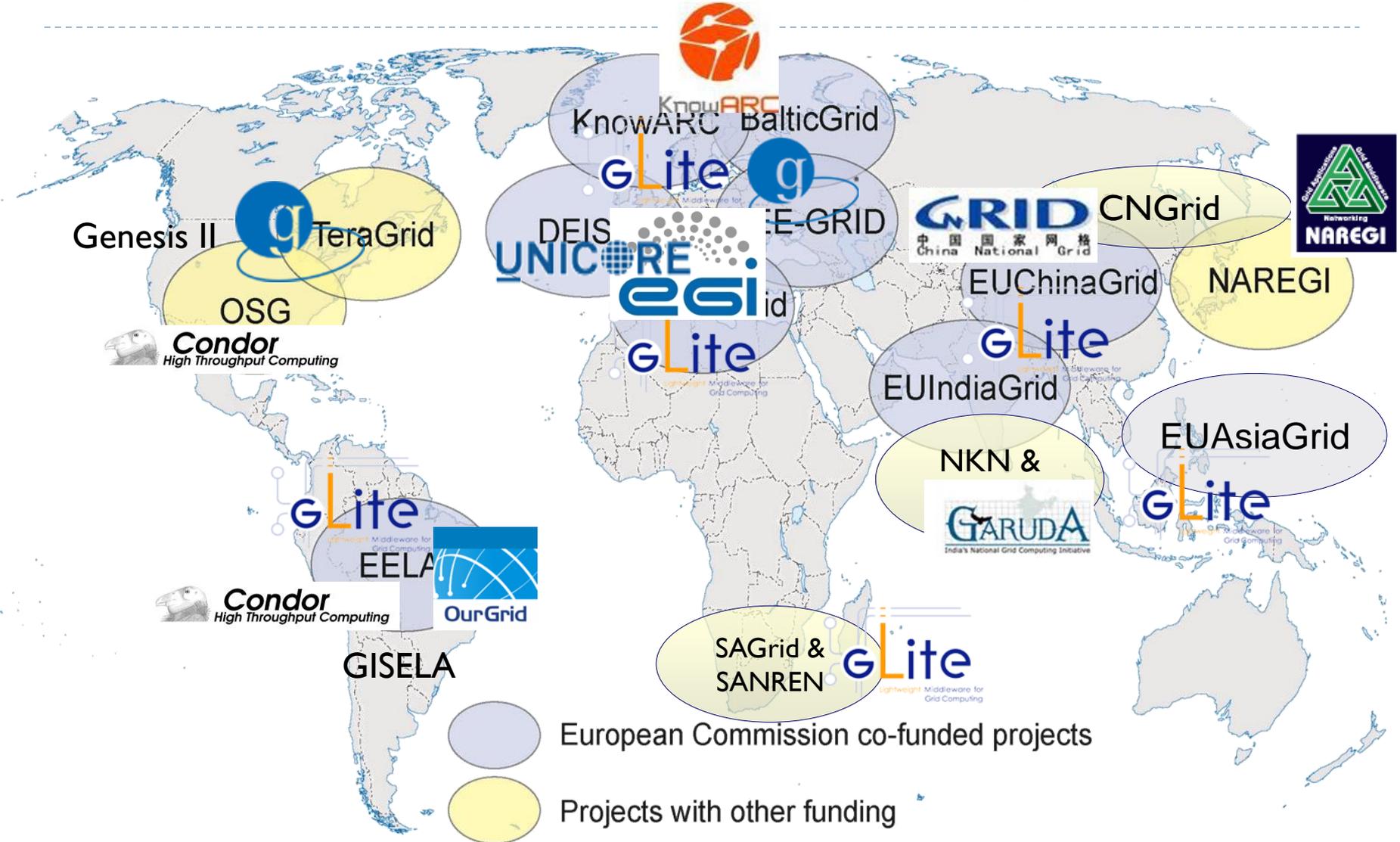
Evolution of distributed computing



The “Global” Grid



The “non-Global” middleware



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"  
160  
OutputS  
Requirem  
0;  
RetryCount
```

JDL

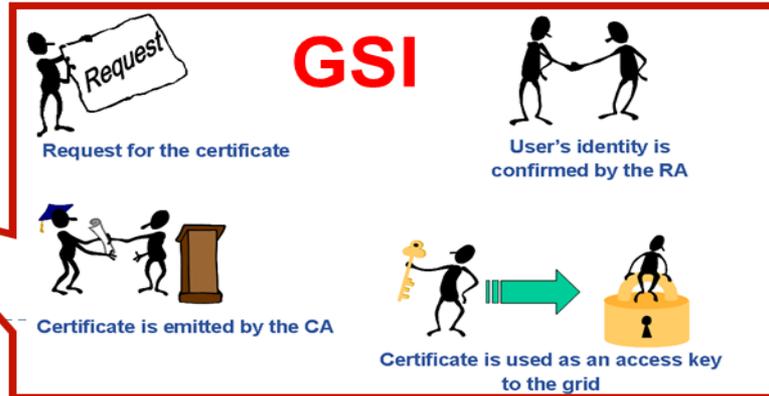
```
echo Staging Input Data \ (Courtesy of European Space  
Agency);  
#edg-rm --vo=gilda copyFile lfn:$1.N1 file://$PWD/$1.N1;  
lcg-cp --vo=gilda lfn:$1.N1 file://$PWD/$1.N1;  
echo Staging Application;  
gunzip beam20.tar.gz;  
tar xvf beam20.tar;  
cd beam-2.0/bin;  
echo Starting Application;  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

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.

```
...son(s):  
... 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
```



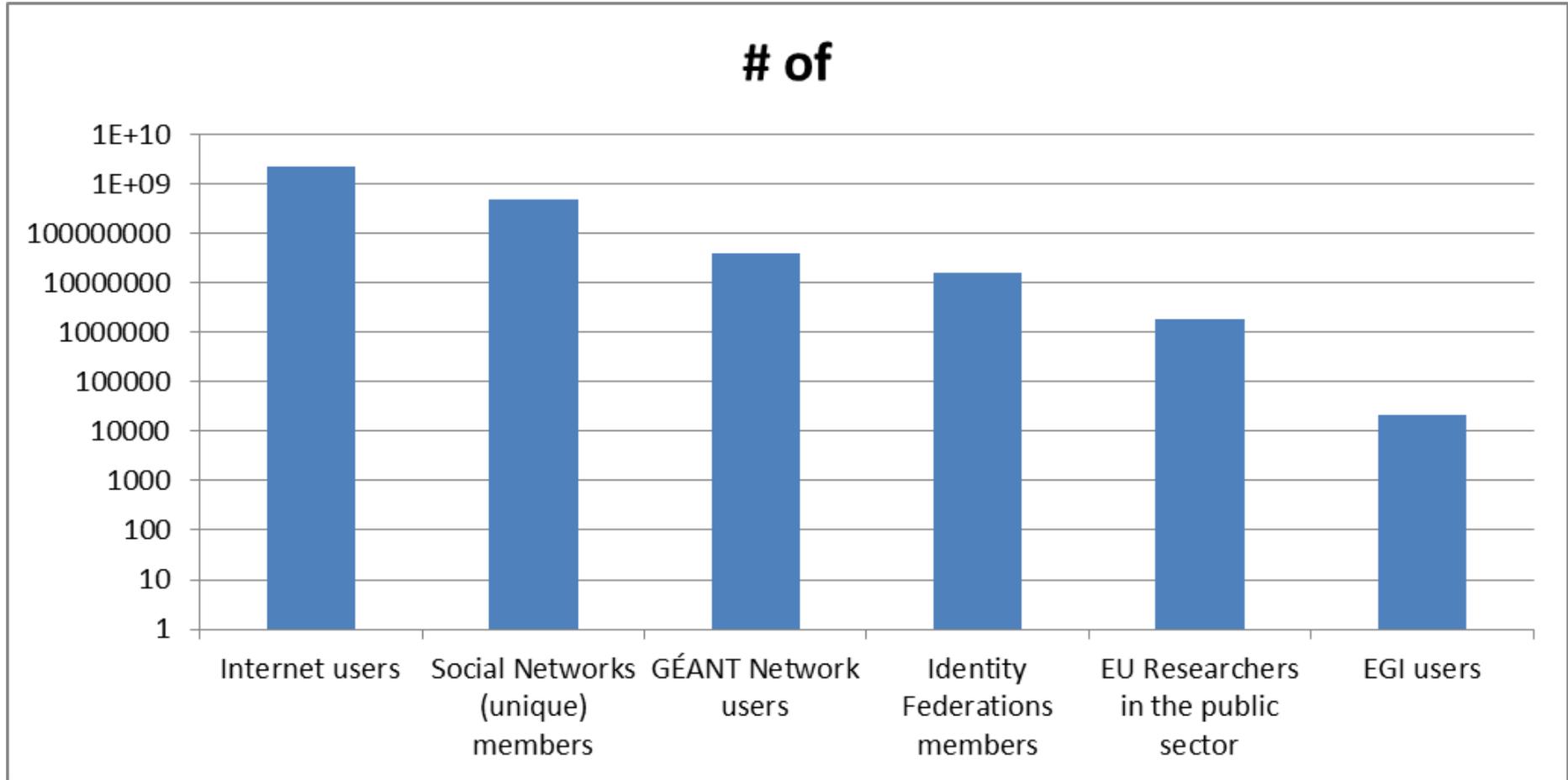
The eResearch2020 report

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

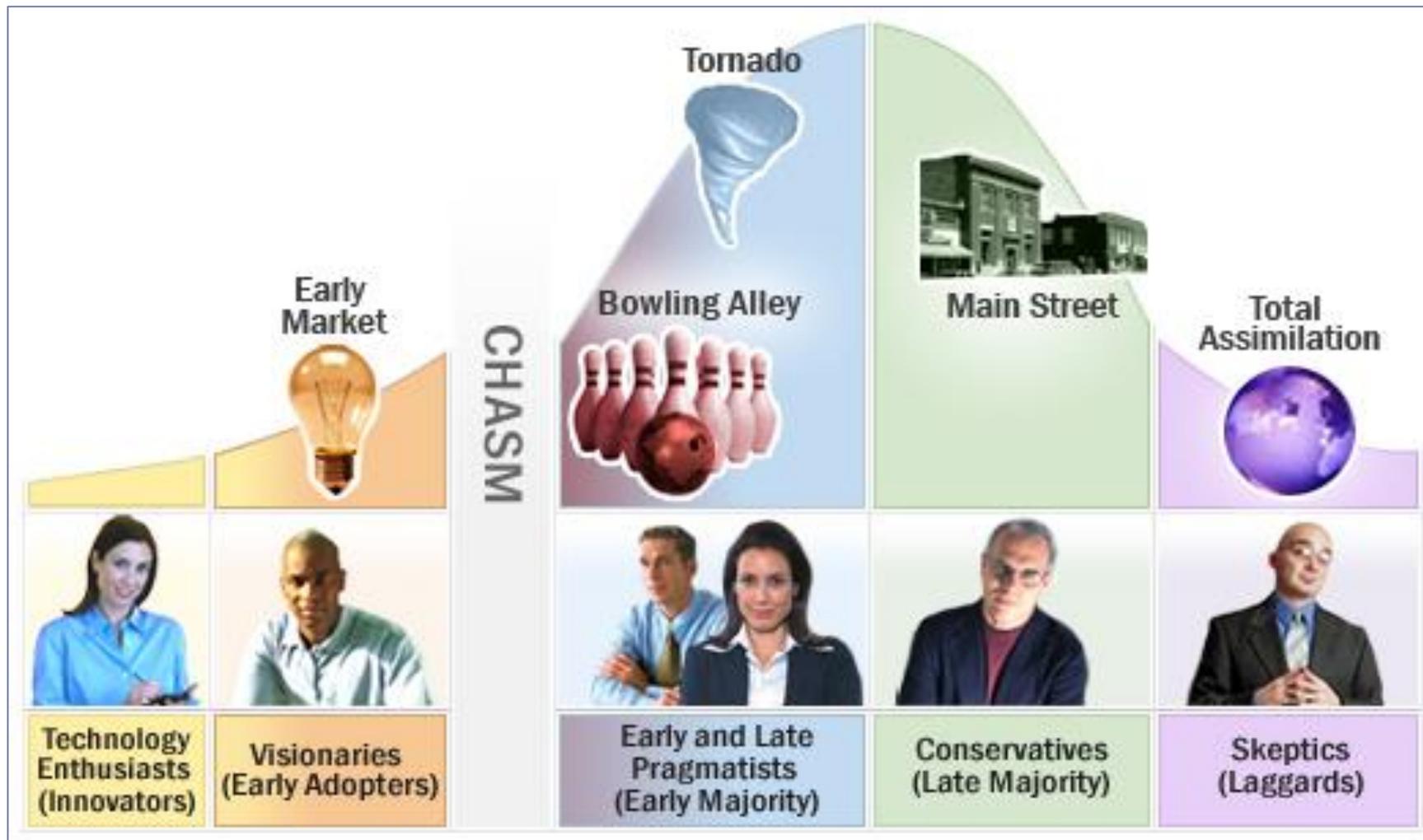
- Some barriers in the adoption of Grids:
 - ▶ **Changes on Grids means changes on applications**
 - ▶ Time required to adapt usual workflows
 - ▶ Lack of structure to support anonymous access
 - ▶ Download and installation of applications
 - ▶ **Interface**
 - ▶ Slow to get to compared to other resources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



Some figures...



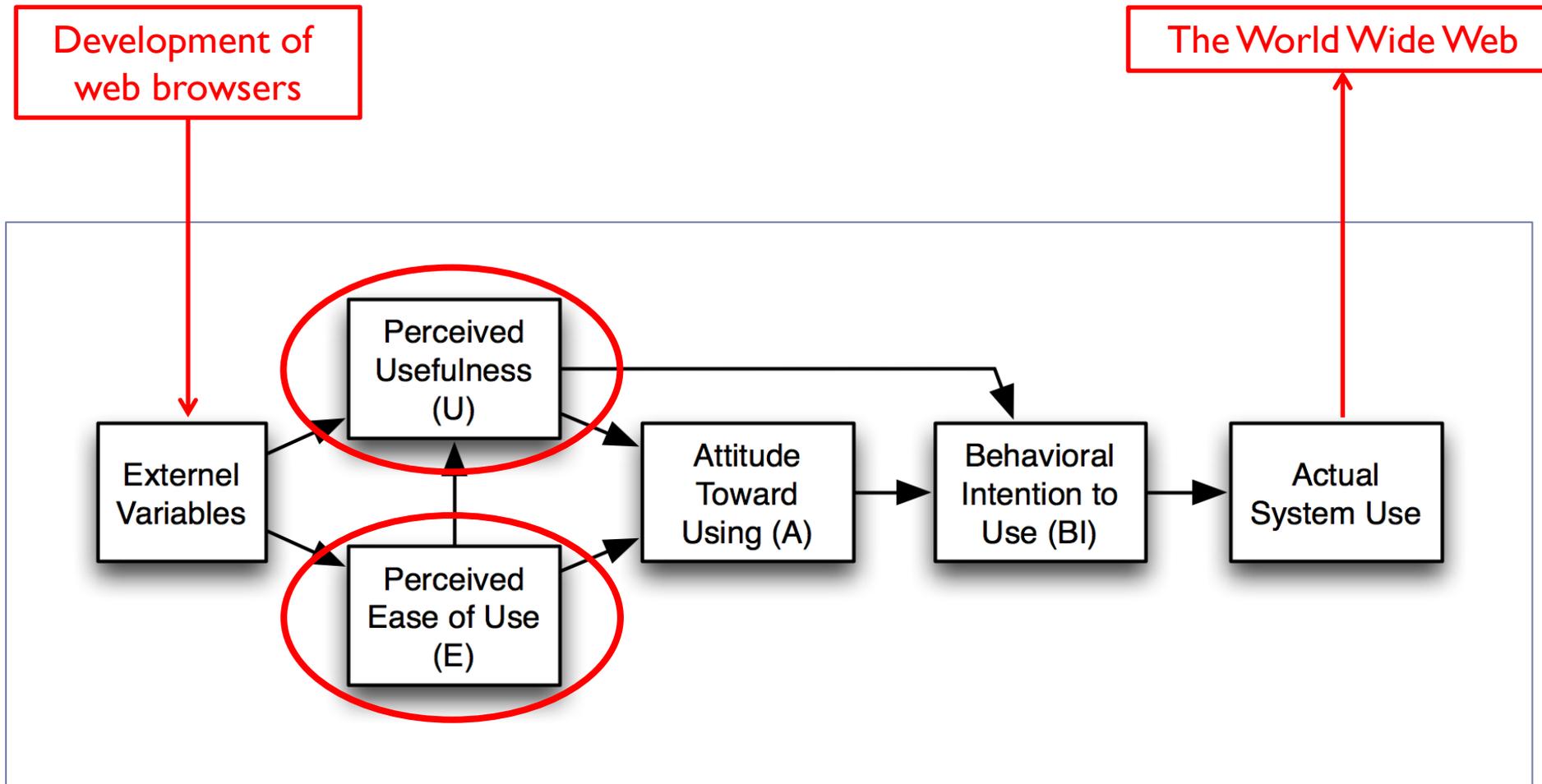
The path to technology uptake – Where are we with e-Infrastructures ?



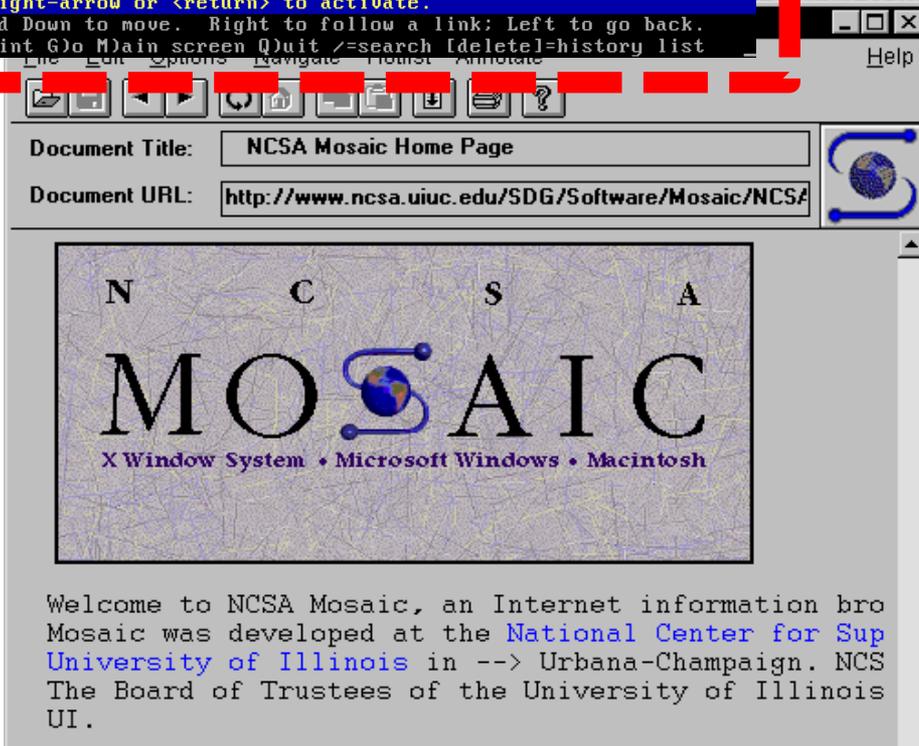
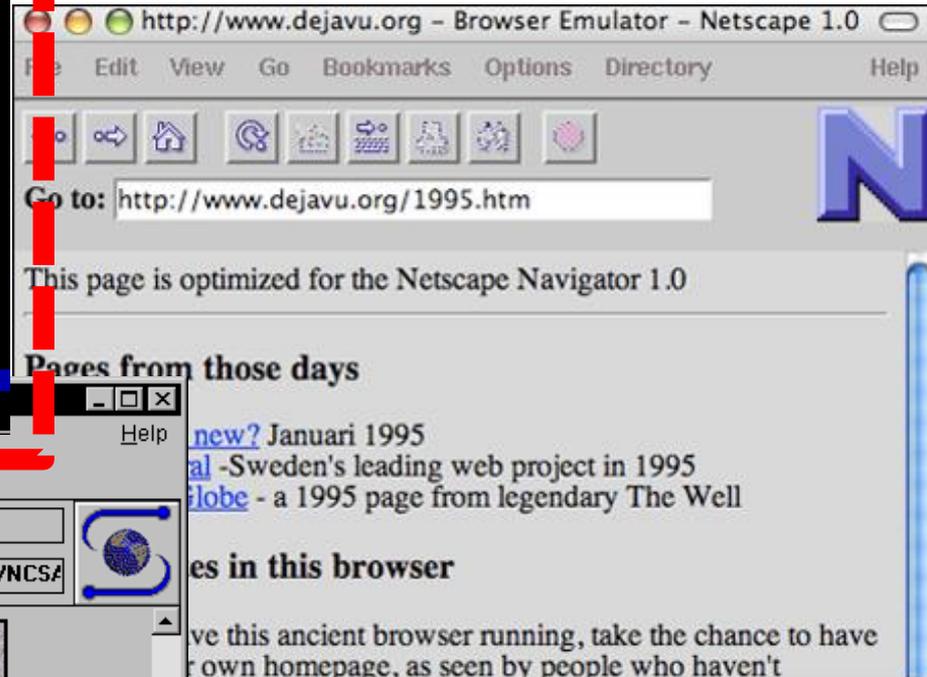
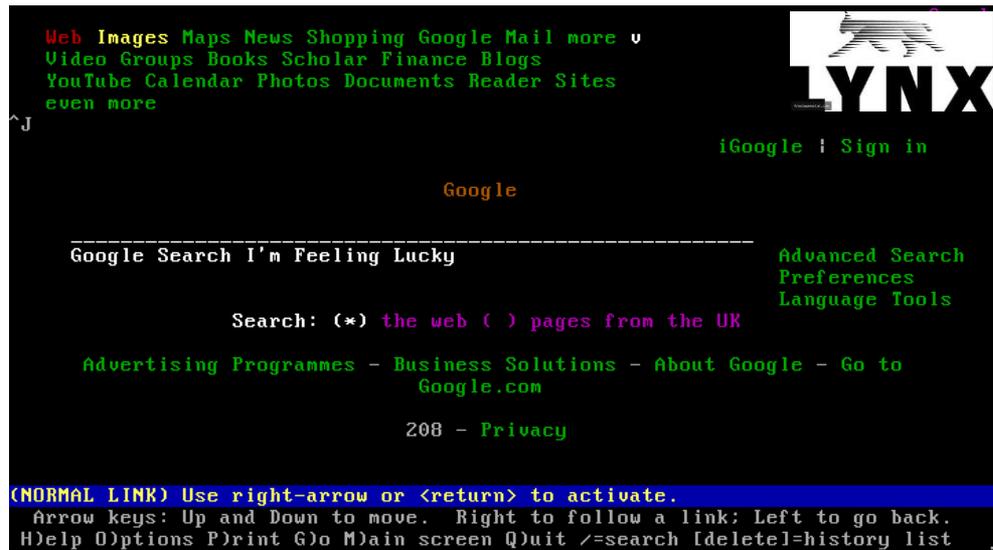
The Rogers "bell-shape" curve - Rogers, E. M. (1962), "Diffusion of Innovations", Glencoe: Free Press.



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



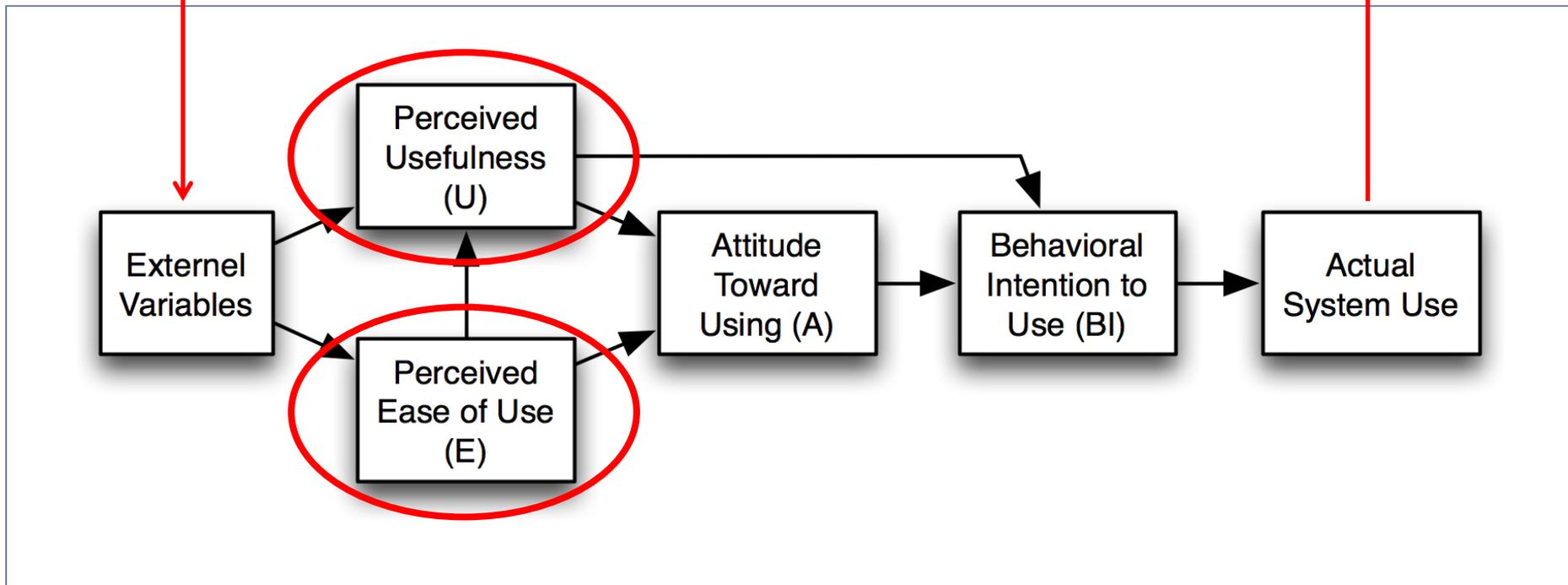
“A Science Gateway is a community-developed set of tools, applications, and data that is integrated via a portal or a suite of applications, usually in a graphical user interface, that is further customized to meet the needs of a specific community.”

Teragrid/XSEDE

IT acceptance model – the Grid

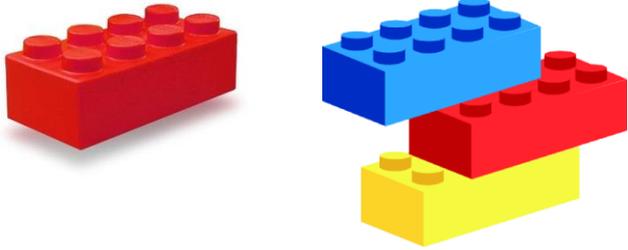
Development of
Science Gateways

Requirement
for sustainability

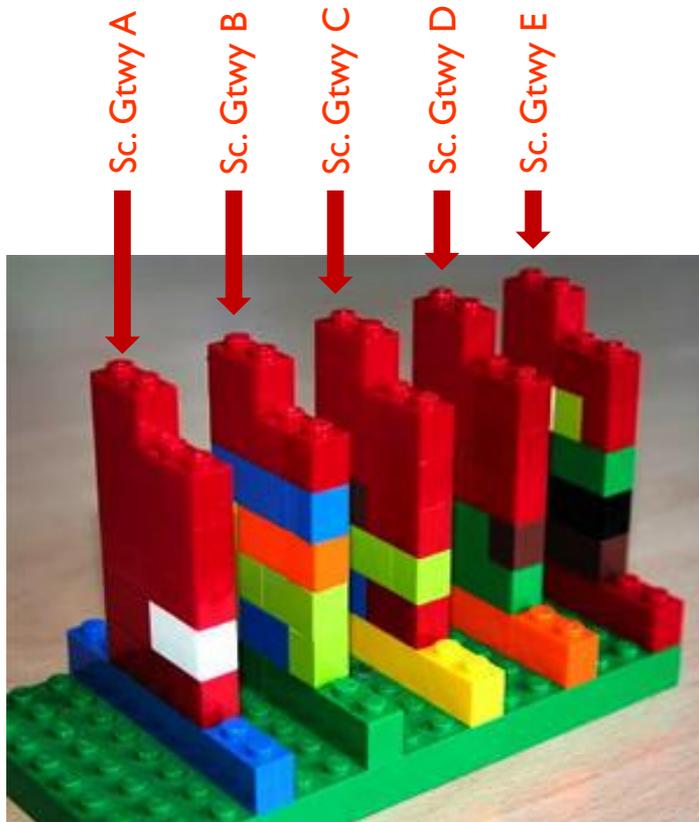


Davis, F. D. (1989), "Perceived usefulness, perceived ease of use, and user acceptance of information technology", *MIS Quarterly* 13(3): 319–340

Primary requirement: building Science Gateways should be like playing with



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



Embedded Applications

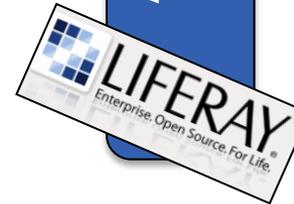
App. 1

App. 2

App. N

Standard-based (SAGA)
middleware-independent
Grid Engine

Science
Gateway



Administrator
Power User
Basic User



Users from
different
organisations
having different
roles and
privileges

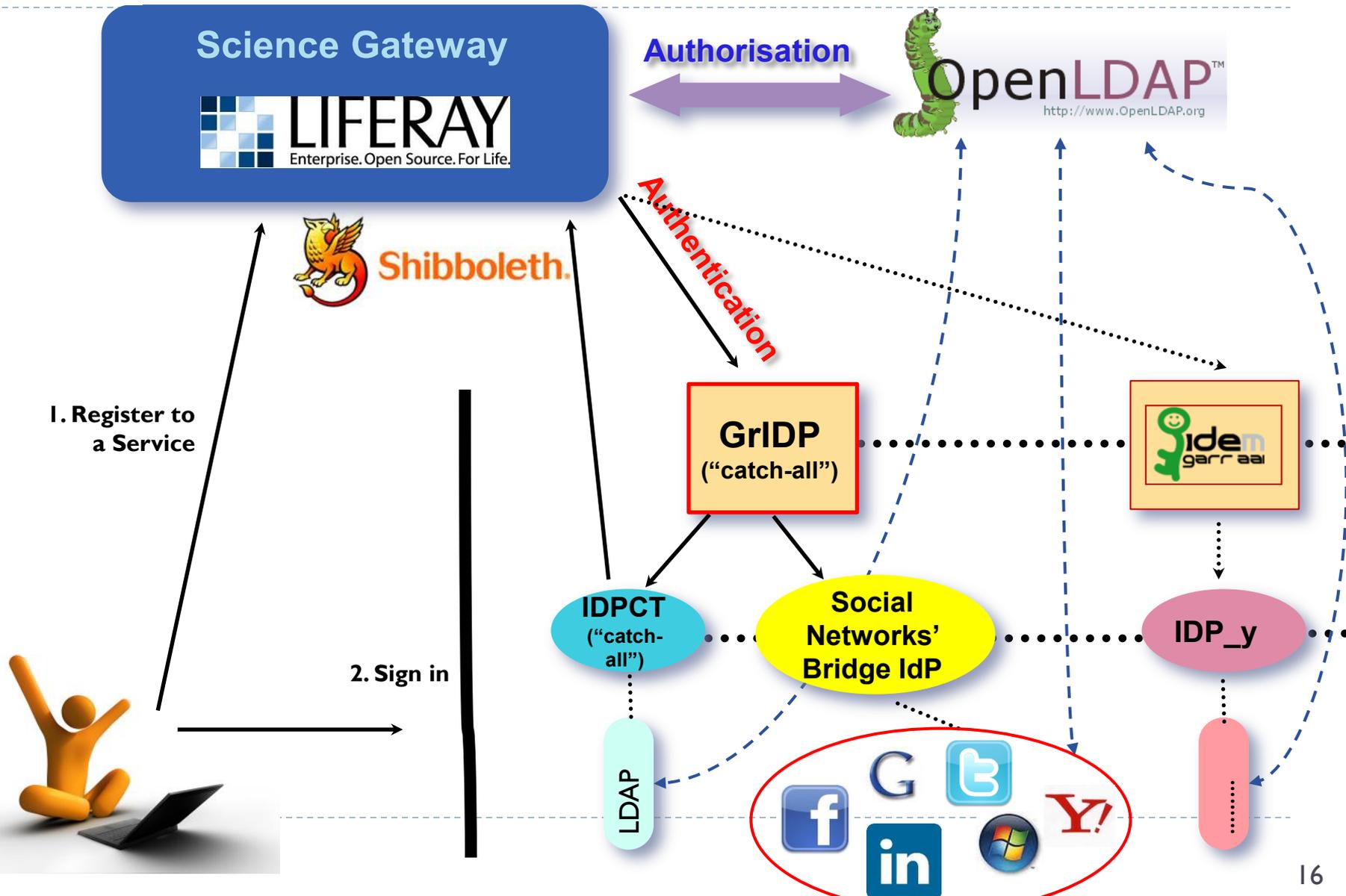


GENESIS II



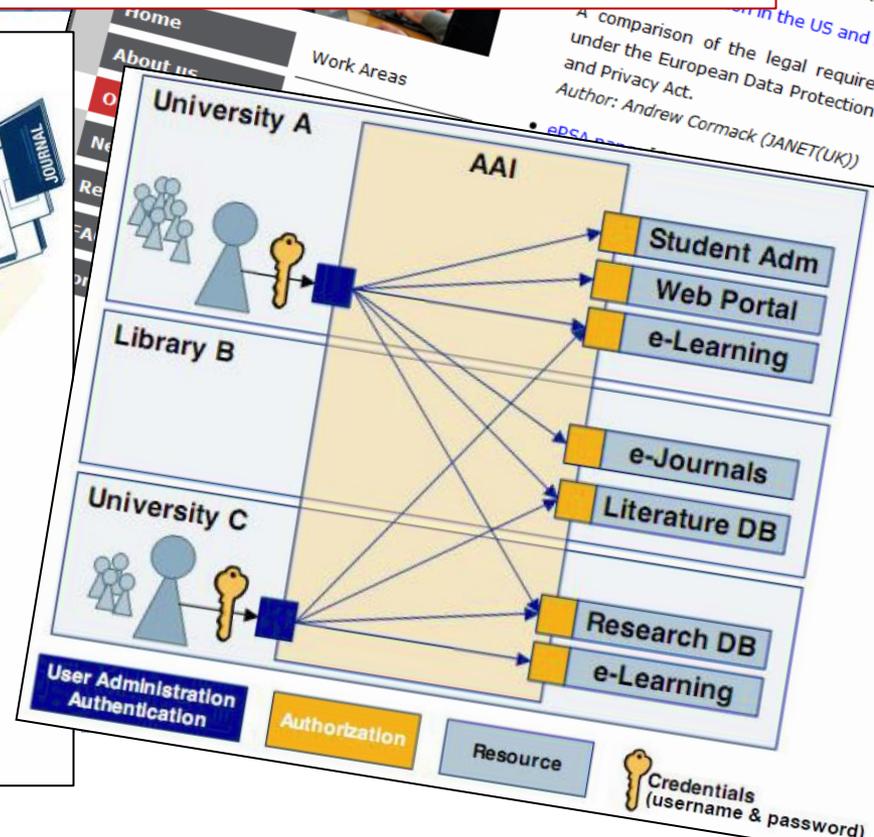
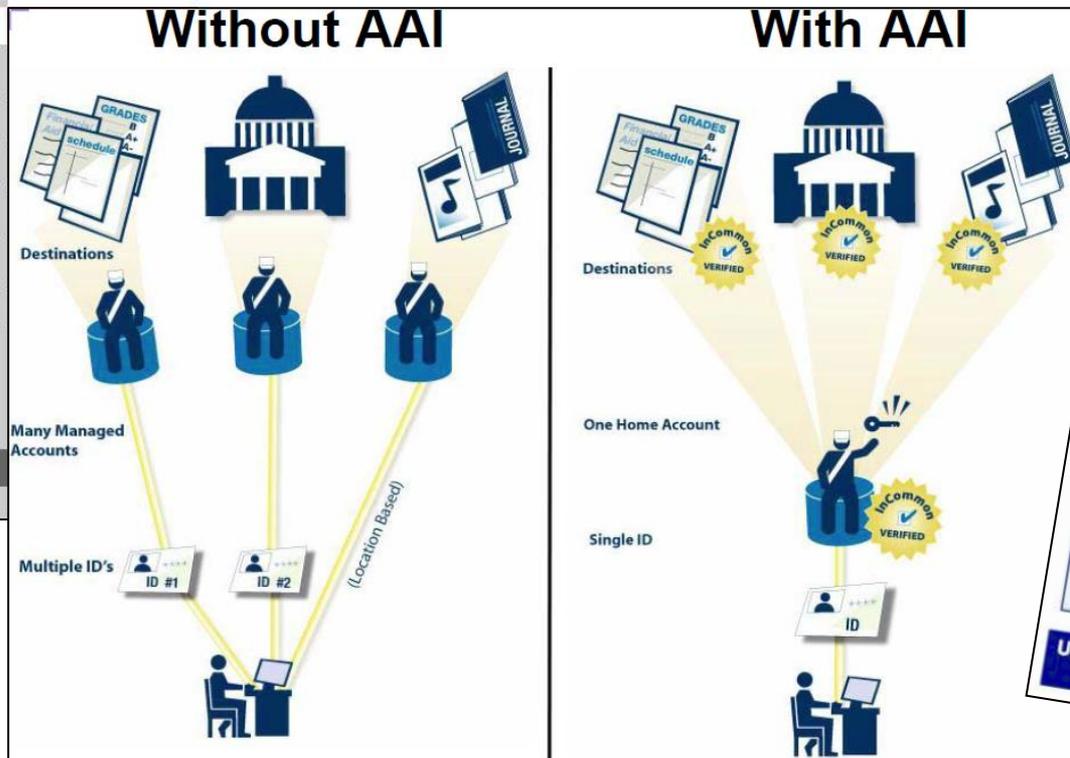
► **Middleware supported so far**

AuthN & AuthZ Schema



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

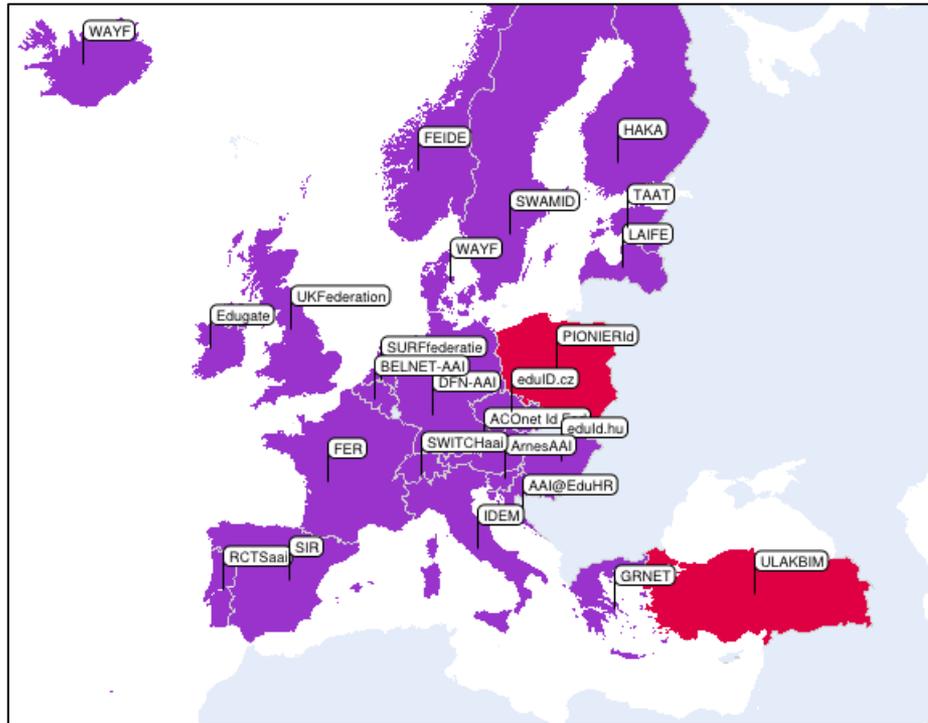


In progress

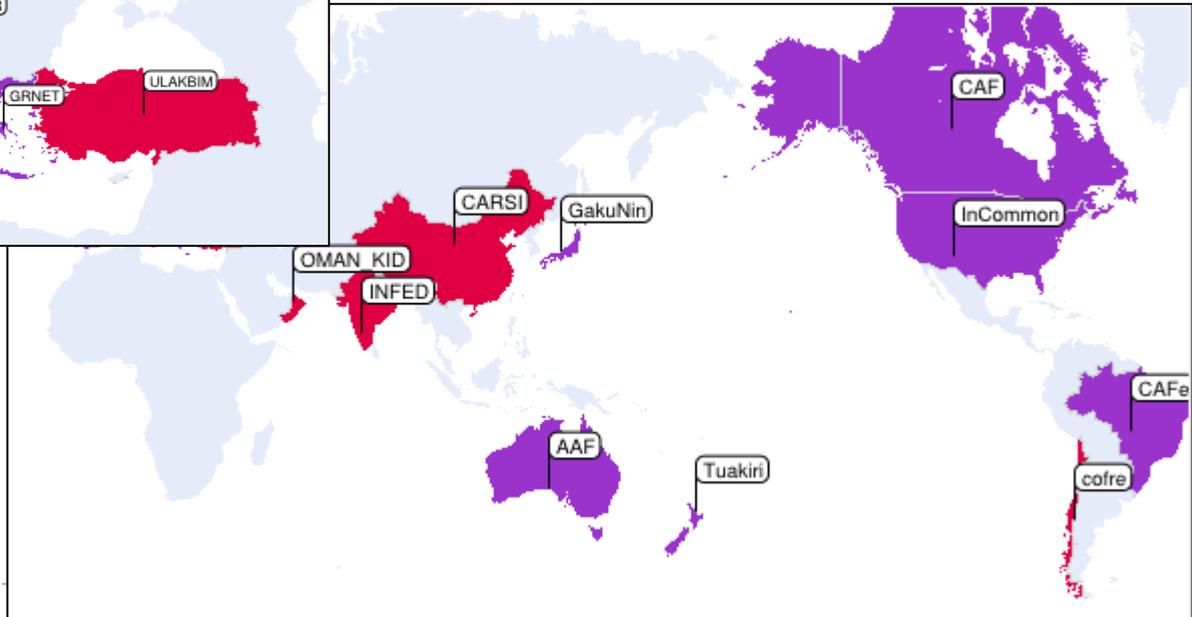


Identity Federations in the world

(<https://refeds.org>)



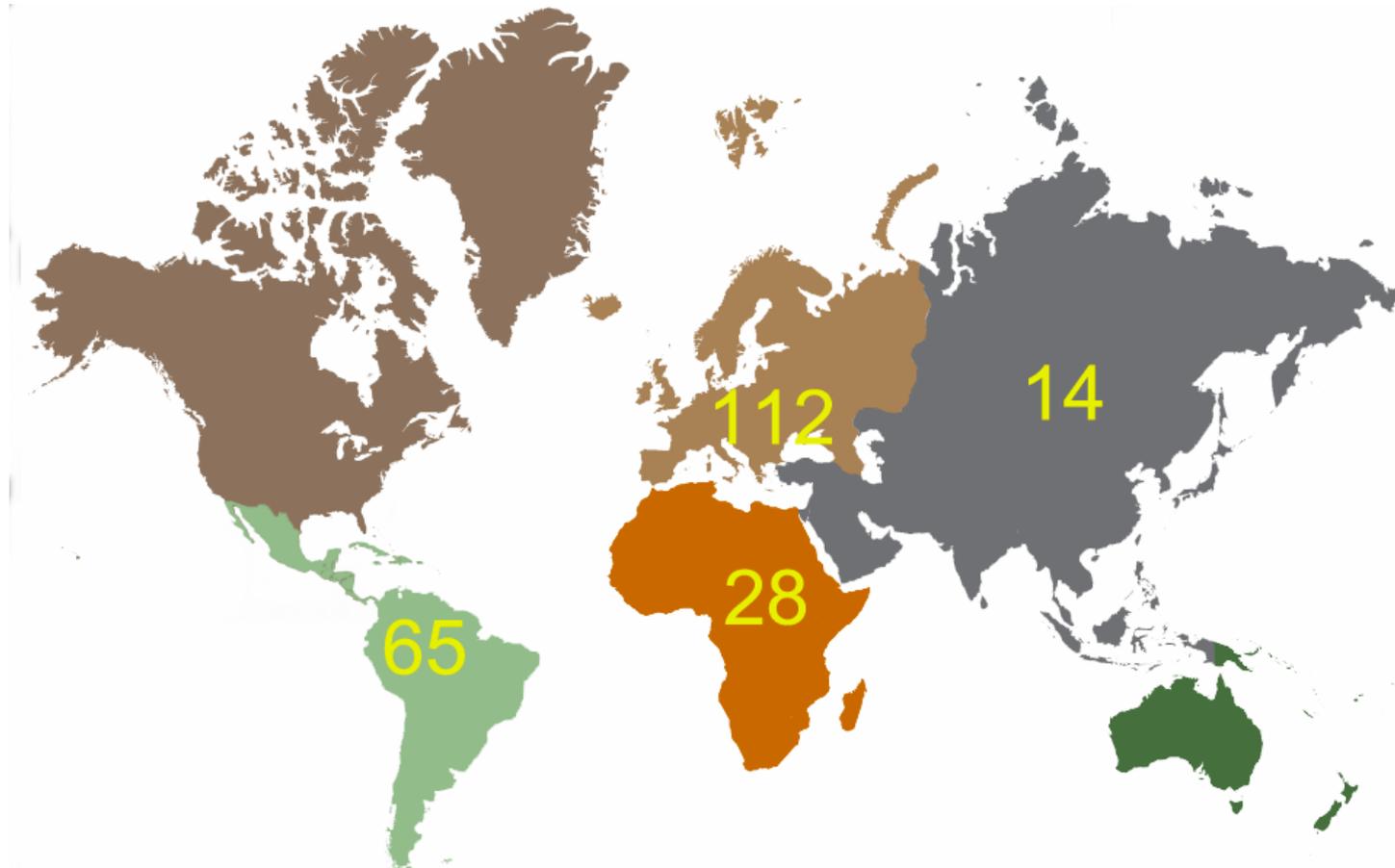
16 million people worldwide



■ Pilot ■ Production

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

Users from 219 Organisations in 47 Countries



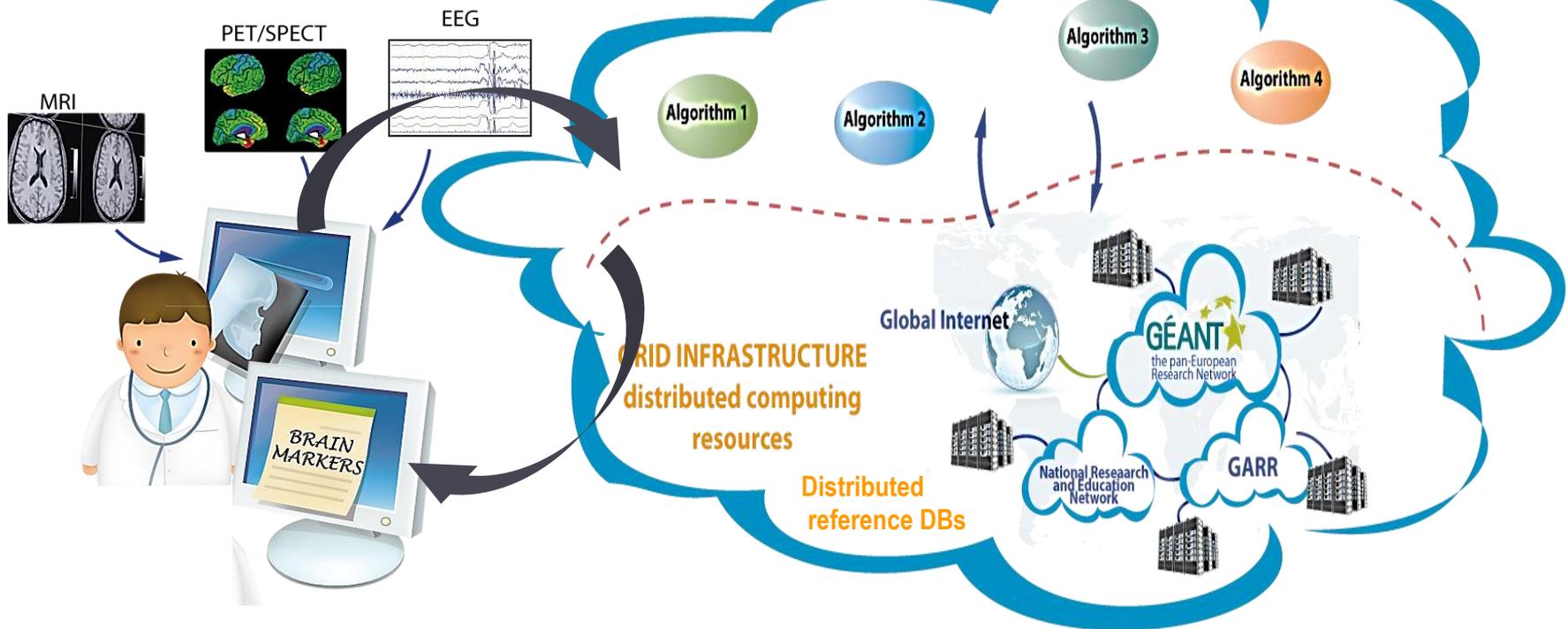
12 Science Gateways in production; 4 in preparation



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

Diagnostic Enhancement of Confidence by an International Distributed Environment

- 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.

Facebook Follow

Mi piace 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 select one of the Identity Federations supported by the DECIDE Science Gateway. You should select the one you would like to have. When you have selected the Identity Federation, you will be asked to confirm the link which appears in the registration form.

2) Sign In

(If you do not have yet an account)

Once you receive the email in your inbox, you should click on the link which has been accepted by the administrator. You will be asked to click on the "Sign In", at the top right of the page. There you have to specify your username and password. In the registration phase, please specify the Organisation which are our partners. The "Sign In" button which will appear on the page.

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

DECIDE

Diagnostic Enhancement of Confidence by an International Distributed Environment

- 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	PLWOODSGDD
GridSPM		Life Sciences	EMI-gLite	CNR

Showing 1 to 5 of 5 entries

First Previous 1 Next Last

This is a Service Provider of:

The DECIDE Science Gateway in action

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

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** 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 spectr in the Grid environment.

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

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

This procedure generates a statistical report whose clinical validity is under ev

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 s
- GridEEG-SOURCE (Gridified routine for estimation of Power Spectrum De source cortical level);
- GridEEG-COHERENCE (Gridified routine for the estimation of Spectral Co signals);
- GridEEG-DTF (Gridified routine for the estimation of Directed Transfer Fun signals);
- GridEEG-STAT (Gridified routine for the statistical comparison of the estim database of Alzheimer's diseased patients (n=100) and normal elderly su

Alpha1 -

Alpha2 -

Beta1 -

Beta2 -

Gamma -

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
Area:	Band:
Occipital	Delta
Area:	Band:
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
Channel 1:	Channel 2:	Band:
T3	F3	Alpha2
Channel 1:	Channel 2:	Band:
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
Target:	Source:	Band:
Cz	Pz	Beta2
Target:	Source:	Band:
Pz	Fz	Alpha2

Add - Remove

Upload here your EEG data archive

EEG data archive in .zip or .tgz Format:

The DECIDE Science Gateway in action

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



Diagnostic Enhancement of Confidence
an International Distributed Environment



Menu

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

MyJobs

Active Jobs List

Done

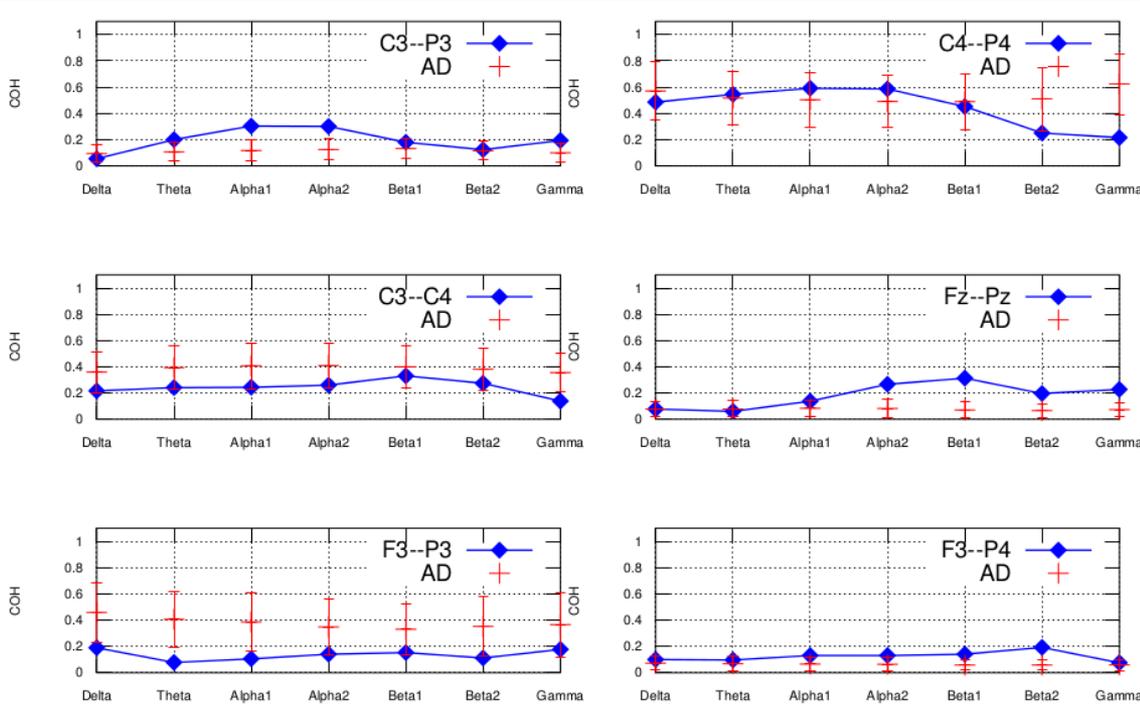
The table below shows the status of your jobs. Statuses are automatically updated. You can see your jobs in the table within the portal and notify us the problem. Once your jobs have finished, your jobs will be deleted from the Science Gateway.

Copy Print Save Download

Show entries

Application Name GridEEG

Showing 1 to 1 of 1 entries



Spectral coherence (COH) of scalp EEG activity. Each subplot refers to representative frontal-parietal electrode pairs. COH values are represented on Y-axis. Frequency bands are specified on X-axis. Solid blue diamonds show the values of the actual subject under investigation. Red plus signs show respective mean values of Alzheimer Diseased (AD) population, while error bars denote their standard deviation.



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

DECIDE Science Gateway x

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

MyWorkspace MYWORK

- Jobs
- JobsMap
- Data
- Help

JobsMap

Data

Help

GridSPM Scientist - Set P

Grid SPM - Scientis

Welcome to the Grid SPM DECIDE

Purpose

This service allows the statistical Mapping (SPM) system. The use of the service is allowed

The workflow of the service consists of:

1. Data upload step: your PET/SPECT data is uploaded in DICOM and Interfile format.
2. The system automatically performs a process of spatial normalization, as the normal subject Gaussian kernel in order to perform normalization.
3. Statistical procedures (statistical parametric mapping) report in PDF format is generated and registered on a standard and secure environment.

How to run the analysis

Please upload your patient's data in DICOM and Interfile format. DICOM and Interfile format have to be archived together in .tgz format.

Follow the information on screen in order to follow-up your analysis and retrieve results.

Normal subjects filter selection

Please select:

Please, note that currently filters are not applied due to the reduced number of normal subjects. Controls are shown for training purpose.

Analysis parameters

Please note: currently some parameters cannot be selected. Default value is shown for your information.

Interpolation method:

Smoothing (FWHM in mm):

Define the contrast Name:

Define the contrast Type:

Corrected height threshold?

Set threshold (T or p value):

Threshold extent (voxels):

Upload here your SPM data archive

Select your SPM data archive in .zip or .tgz format:

Nessun file selezionato

Start analysis

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

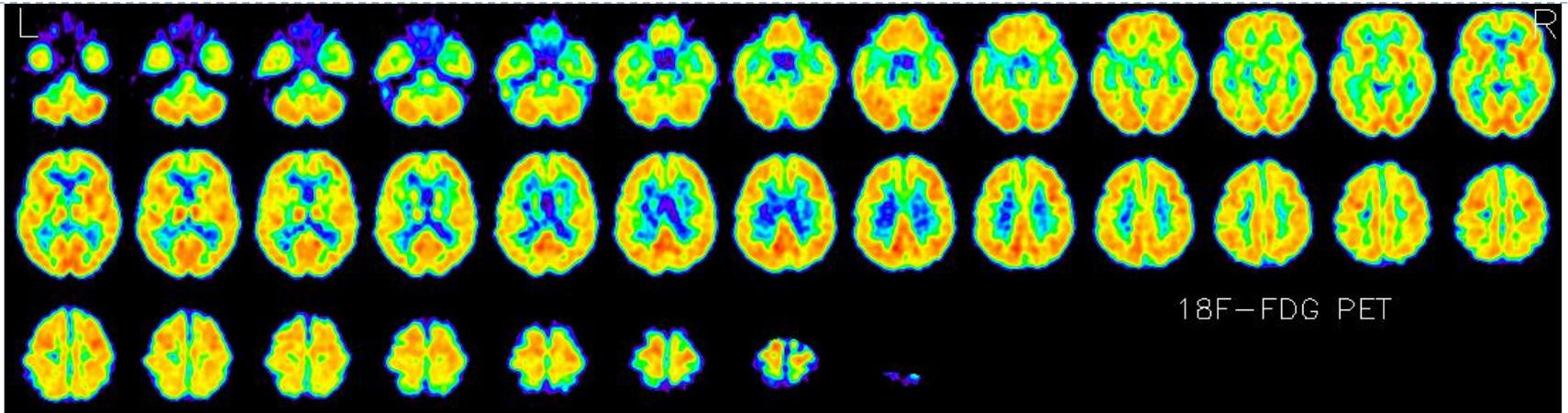
Application Name	User Description	Started on (UTC)	Status
GridSPM	GridSPM Matlab Job 2012-05-21-002909	2012-05-20 22:29:19.0	SUBMITTED
GridSPM	GridSPM Matlab Job 2012-05-21-002818	2012-05-20 22:28:19.0	SUBMITTED
GridSPM	GridSPM Matlab Job 2012-05-21-002732	2012-05-20 22:27:54.0	RUNNING
GridANN4ND	GridANN4ND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

Showing 1 to 4 of 4 entries

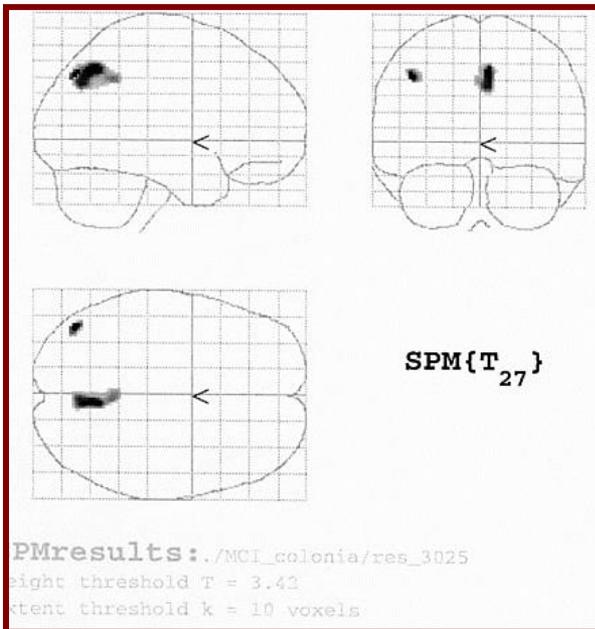
First | Previous | 1 | Next | Last

This is an service

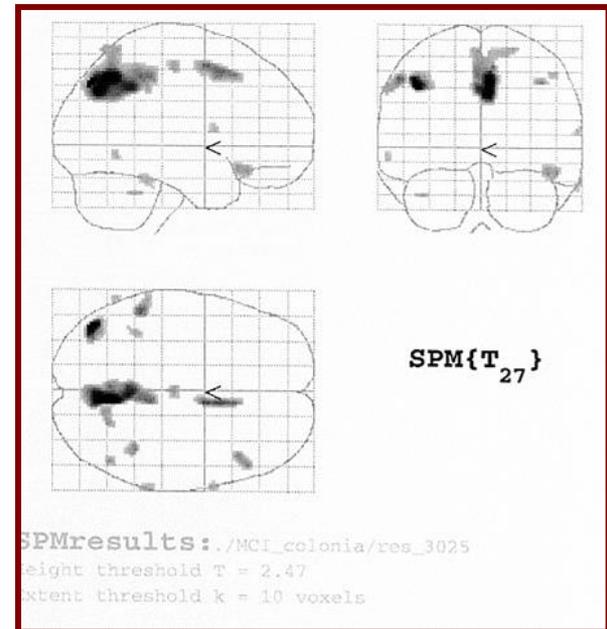
The DECIDE Science Gateway in action



GridSPM report



p = 0.001



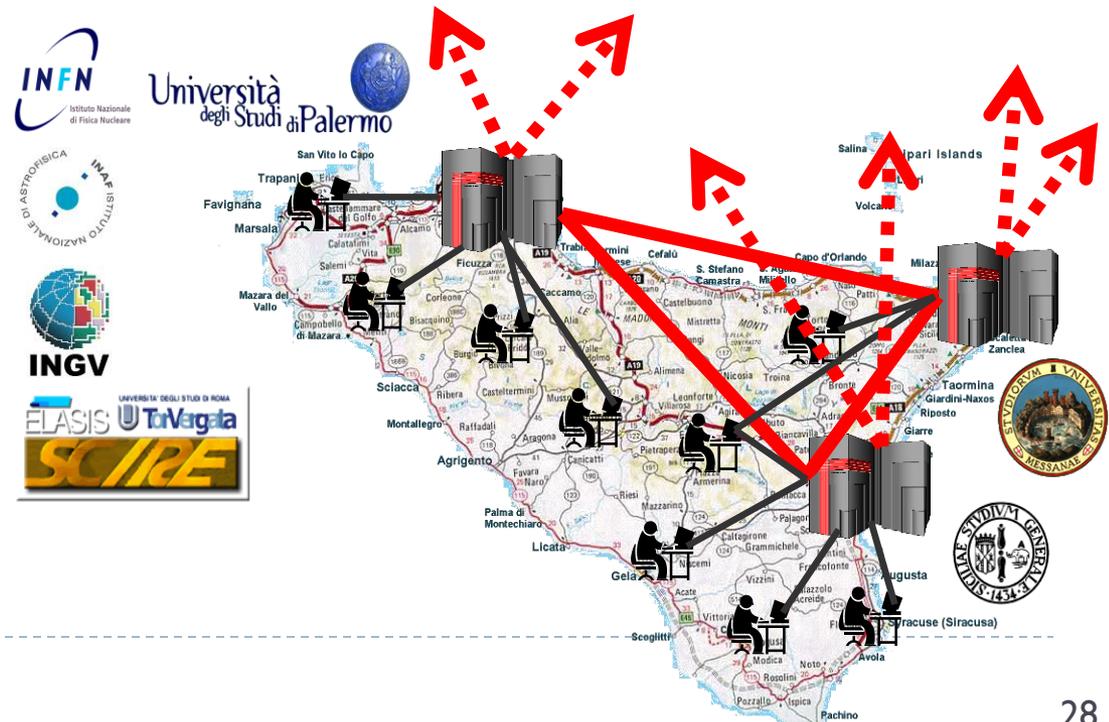
p = 0.01

The IOERT Use Case



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

Consorzio COMETA- Catania

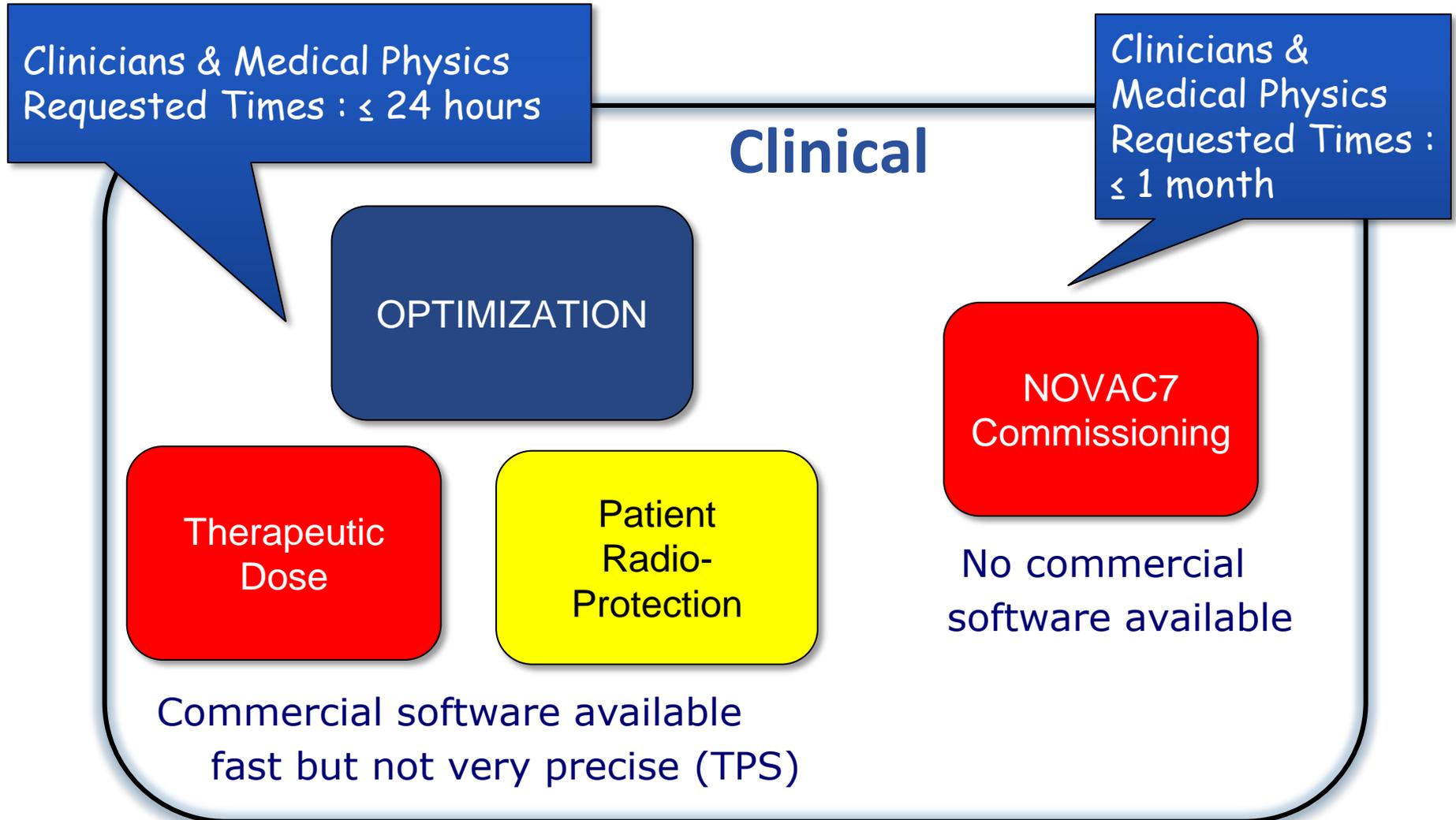


The Intra-Operative Electron Radio-Therapy (IOERT) technique in a nutshell

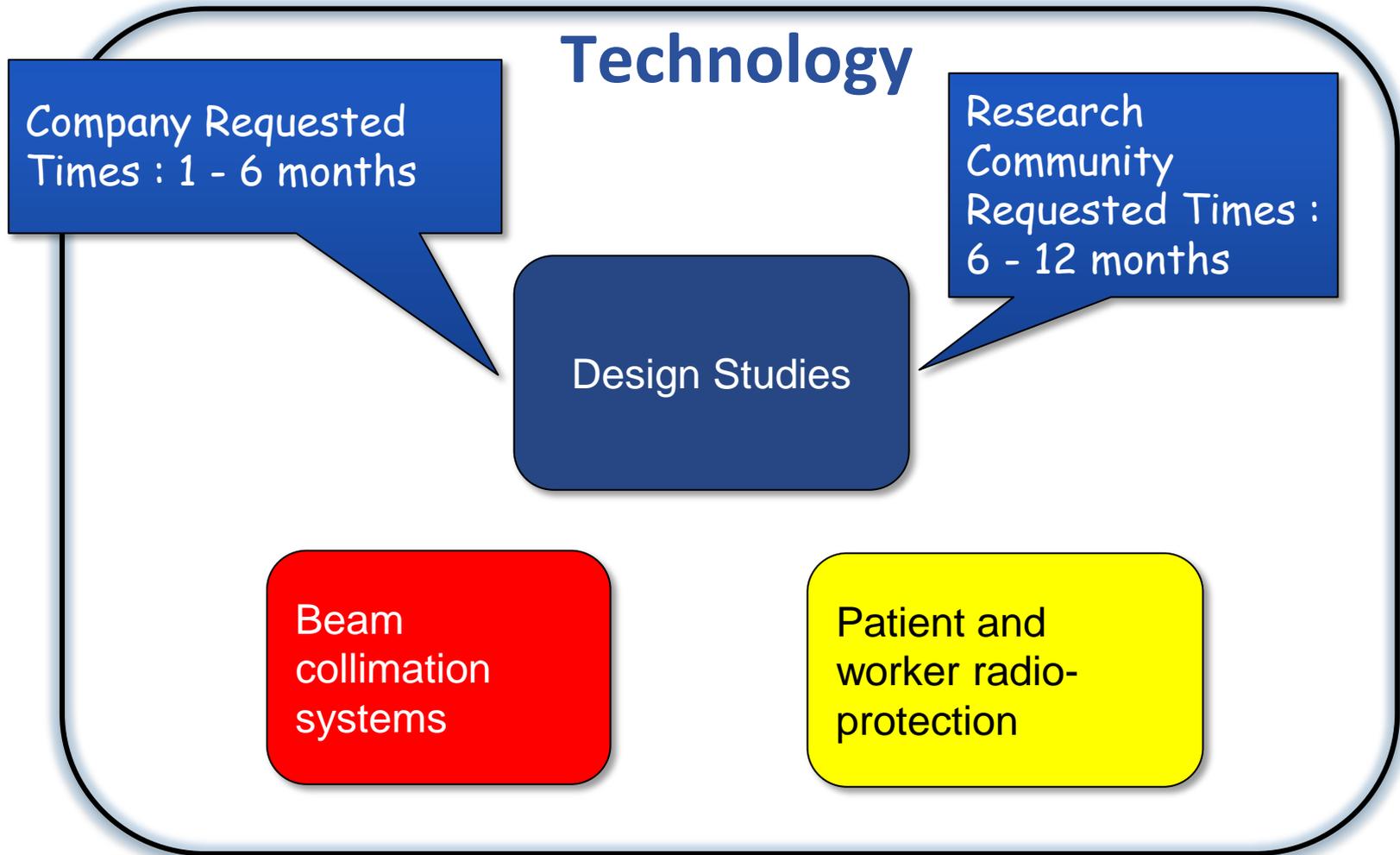
- ❖ **Intra-Operative Electron Radiotherapy (IOERT)** is an advanced radiation therapy technique that allows treatment of tumors after surgery, directly in the surgery room, delivering a high dose to the target (*Veronesi et al., 2001*);
- ❖ Treatment of breast, stomach, prostate cancers;
- ❖ The electron 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



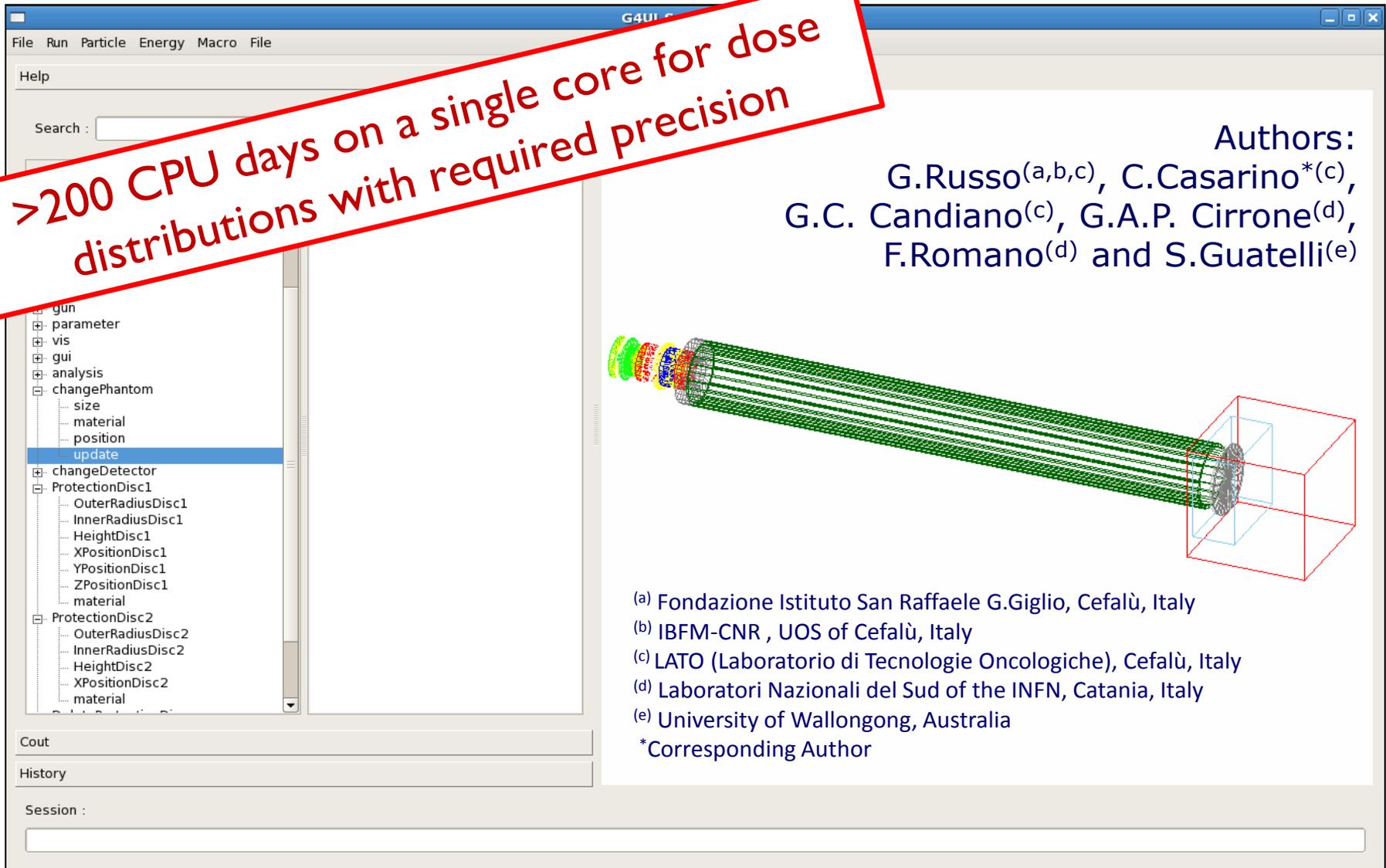
Technological Activities



❖ No commercial software available

The IOERT simulator with Geant4

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



Authors:

G.Russo^(a,b,c), C.Casarino^{*(c)},
G.C. Candiano^(c), G.A.P. Cirrone^(d),
F.Romano^(d) and S.Guatelli^(e)

- (a) Fondazione Istituto San Raffaele G.Giglio, Cefalù, Italy
 - (b) IBFM-CNR , UOS of Cefalù, Italy
 - (c) LATO (Laboratorio di Tecnologie Oncologiche), Cefalù, Italy
 - (d) Laboratori Nazionali del Sud of the INFN, Catania, Italy
 - (e) University of Wallongong, Australia
- *Corresponding Author

The IOERT Science Gateway in action

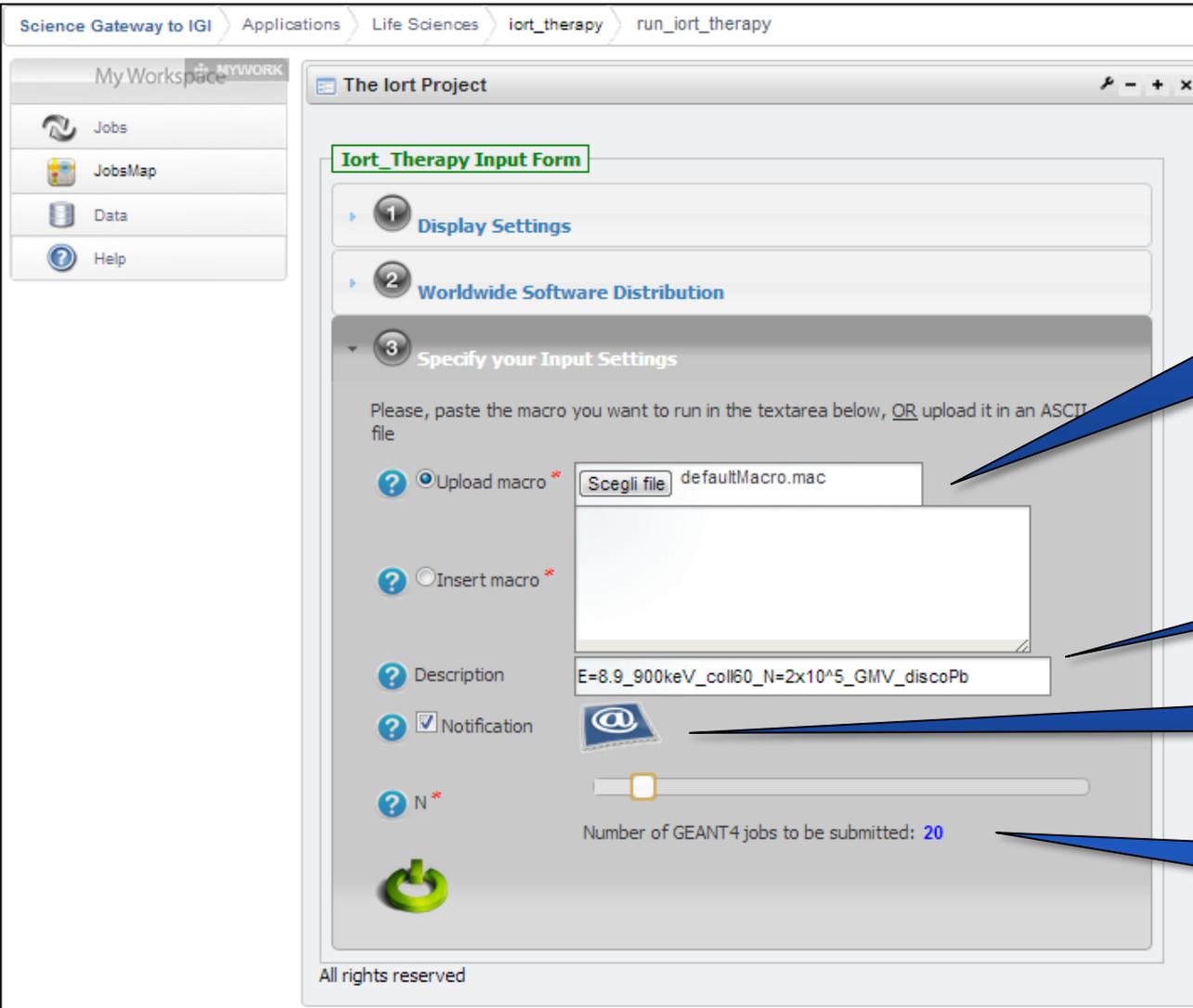
The screenshot shows a web browser window at gw.ct.infn.it/run-iort_therapy. The breadcrumb navigation is: Science Gateway to IGI > Applications > Life Sciences > iort_therapy > run_iort_therapy. On the left, there is a 'My Workspace' sidebar with links for Jobs, JobsMap, Data, and Help. The main content area is titled 'The Iort Project' and contains an 'Iort_Therapy Input Form'. The form is divided into sections: '1 Display Settings', '2 Worldwide Software Distribution', and '3 Specify your Input Settings'. The 'Display Settings' section is expanded and shows that the current IORT_THERAPY portlet is configured for 'The COMETA Grid Infrastructure' (indicated by a green checkmark). Below this, there are instructions for users, input requirements (a GEANT4 macro file and a number of runs), and output files. A rating section shows 'Your Rating' and 'Average (1 Vote)' with five stars each. The version number 'IORT_THERAPY portlet ver. 1.1.8' is visible at the bottom of the page.

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

1

It provides some explanation about the application

The IOERT Science Gateway in action



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

My Workspace MYWORK

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 *

Insert macro *

Description

Notification 

N *
Number of GEANT4 jobs to be submitted: 20

All rights reserved

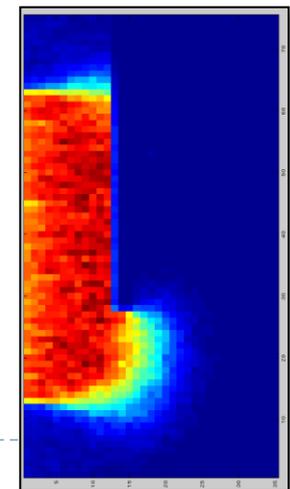
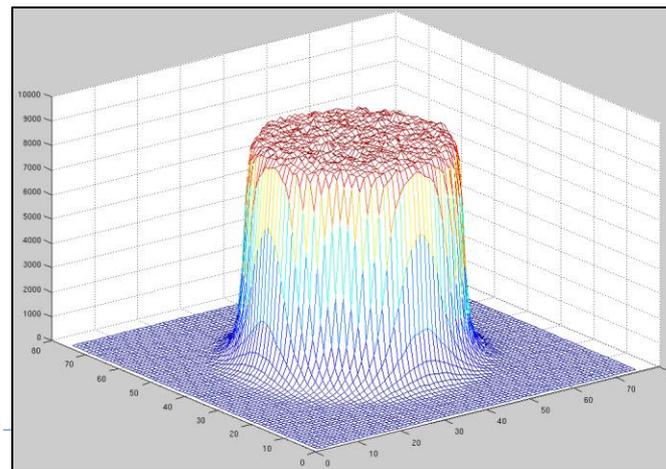
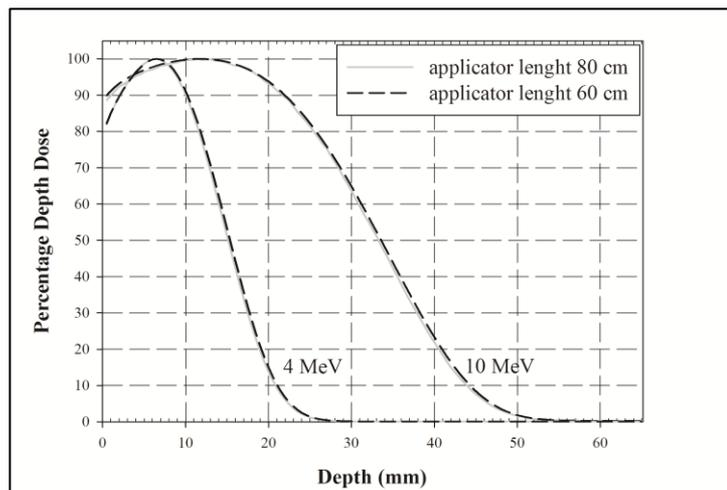
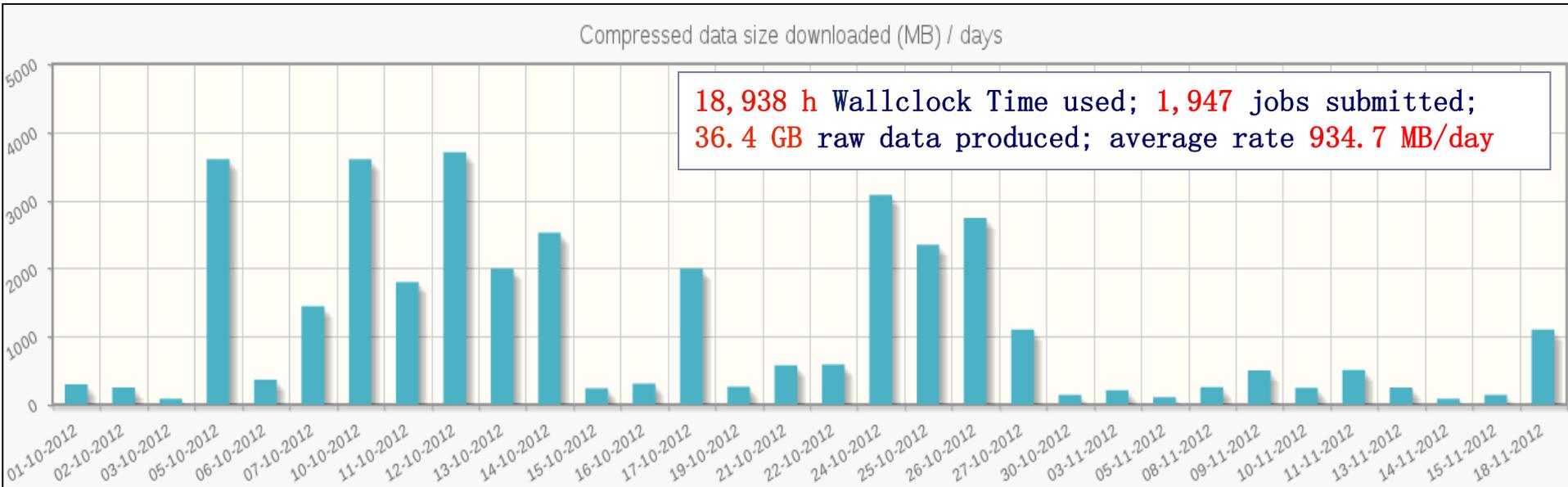
3 Uploading a GEANT4 macro as ASCII file or via the text-area

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 !

