P-GRADE Portal tutorial

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Agenda

- Basics of P-GRADE Portal (~45 minute)
- Workflow hands-on (~45 minute)

- Advanced applications with P-GRADE Portal (~15 minute)
- Hands-on cont'd – workflows, parameter studies (~20 minute)
- Next steps with P-GRADE (~10 minute)

P-GRADE overview and introduction: workflows & parameter sweeps (Basics)

Introduction of LPDS (Lab of Parallel and Distr. Systems)

- **Research division of MTA SZTAKI from 1998**
- **Head: Peter Kacsuk, Prof.**
  - 22 research fellows
- **Foundation member**
  - Central European Grid Consortium (2003)
  - Hungarian Grid Competence Center (2003)
- **Participant or coordinator in many European and national Grid research, infrastructure, and educational projects (from 2000)**
  - FP5: GridLab, DataGrid
  - FP6: EGEE I-II, SEE-GRID I-II, CoreGrid, ICEAGE, CancerGrid
  - FP7: EGEE III, SEE-GRID-SCI, EDGeS (coordinator), ETICS, S-CUBE
- **Central European Grid Training Center in EGEE (from 2004)**

www.lpds.sztaki.hu

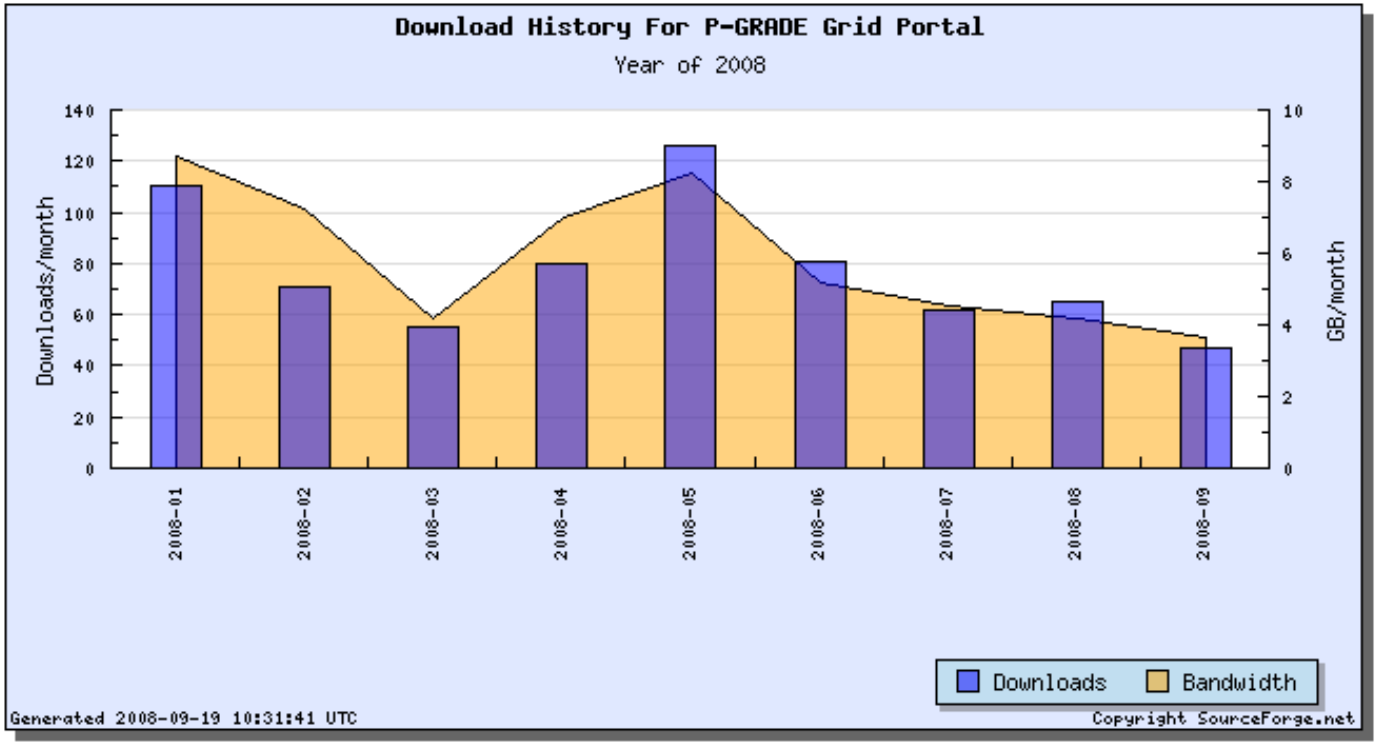
Short History of P-GRADE portal

- Parallel Grid Application and Development Environment
- Initial development started in the Hungarian SuperComputing Grid project in 2003
- It has been continuously developed since 2003
- Detailed information:

  http://www.portal.p-grade.hu/
- Open Source community development since January 2008:

  https://sourceforge.net/projects/pgportal/

Download of OSS P-GRADE portal



110 downloads within the first month

~697 total downloads until now

Main P-GRADE related projects

- **EU SEE-GRID-1** (2004-2006)
  - Integration with LCG-2 and gLite
- **EU SEE-GRID-2** (2006-2008)
  - Parameter sweep extension
- **EU CoreGrid** (2005-2008)
  - To solve grid interoperation for job submission
  - To solve grid interoperation for data handling: SRB, OGSA-DAI
- **GGF GIN** (2006)
  - Providing the GIN Resource Testing portal
- **EGEE 2,3** (2006-2010)
  - Respect program tool used for training and application development
- **ICEAGE** (2006-2008)
  - P-GRADE portal is used for training as official portal of the GILDA training infrastructure
- **EU EDGeS** (2008-2009)
  - Transparent access to any EGEE and Desktop Grid systems
  - **See Demo Booth 5: EDGes – Desktop Grid Extension of the EGEE Infrastructure**

Portal installations

-= P-GRADE Grid Portal =- - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Sear

Address http://portal.p-grade.hu/?m=3&s=0 Go Links

Portals under installation
- Documents
- Publications
- Download

For grid users
- Client requirements
- Try the Portal
- How to get access
- Trainings
- Workflow repository
- User Forum

For grid administrators
- Install the portal
- Testing the portal

For grid system developers
- Developer Alliance
- Contributing to the software

Report Problems

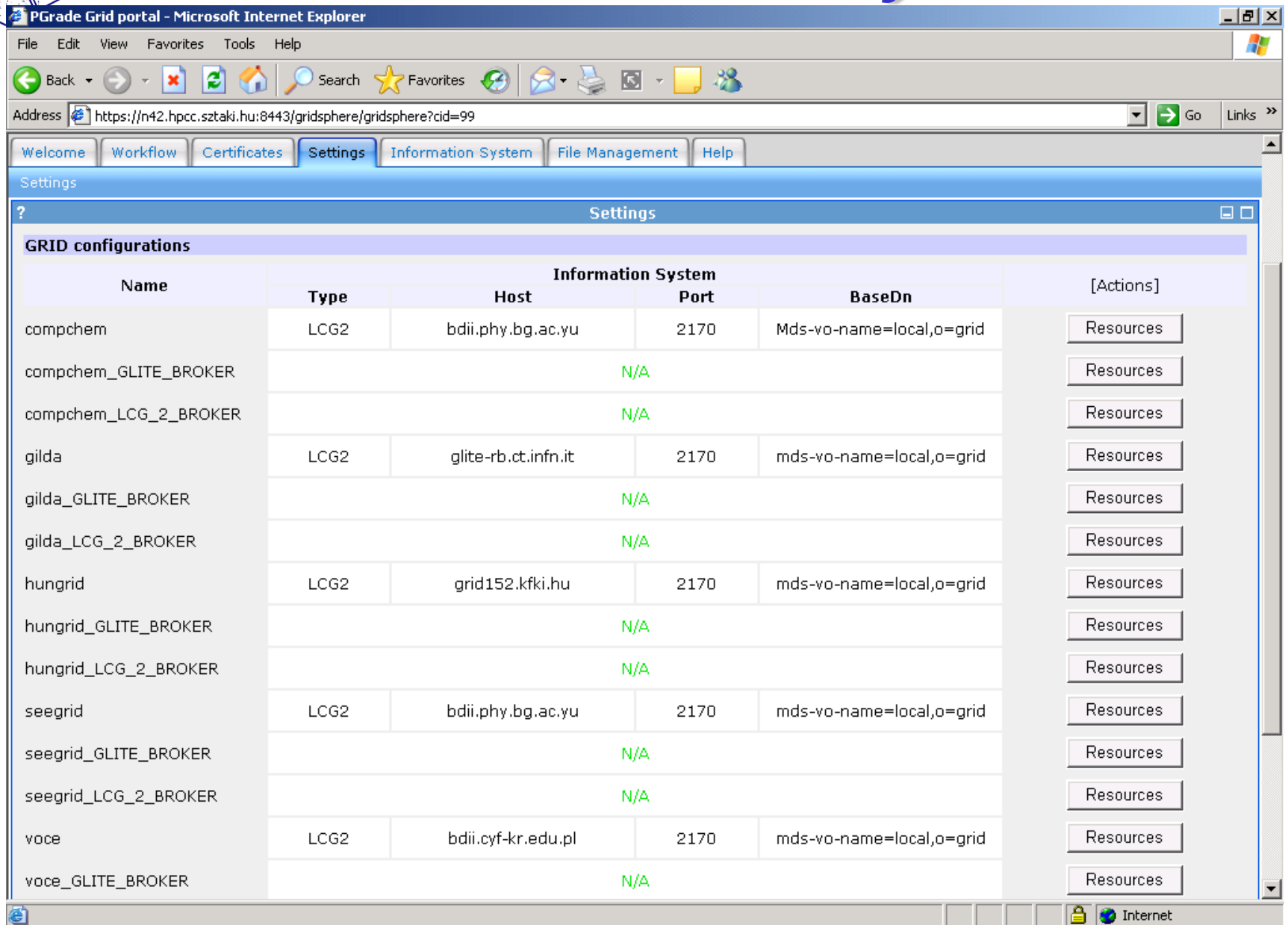
visitors » 69953

Name of the portal installation	Connected to the following grid(s)	Release
Multi-Grid portal operated by SZTAKI	**SEE-GRID** South-Eastern European Grid **VOCE** Virtual Organization Central Europe of EGEE **HunGrid** Hungarian Grid VO of EGEE **GILDA** Training VO of EGEE and other projects **Biomed** Biomedical VO of EGEE **Compchem** Computational Chemistry VO of EGEE	2.7
HunGrid Portal operated by Eötvös Loránd University	**HunGrid** Hungarian Grid VO of EGEE	2.5
Grid-Ireland Portal operated by Grid-Ireland	**Grid-Ireland**	2.6.1
EGRID Portal operated by Abdus Salam ICTP	**EGRID** Economics VO	2.4
WPI Portal operated by Worcester Polytechnic Institute	**OSG and SEE-GRID** Open Science Grid and South Eastern European Grid	2.5
Turkish Grid Portal operated by ULAKBIM & METU	**TR-Grid** Turkish Grid	2.6
NGS P-GRADE GEMLCA Portal operated by University of Westminster	**NGS and GILDA** UK National Grid Service and Training VO of EGEE and other projects	GEMLCA 2.4.1
GIN resource testing Portal operated by University of Westminster	**OGF GIN VO and NGS and OSG and TeraGrid and Westfocus Grid and Voce**	GEMLCA 2.4
Baltic Grid Portal operated by Estonian Educational and Research Network (EENet)	**Baltic Grid** Baltic Grid	2.6

Internet

Start User_Forum_... Quotation_fo... Adobe Reade... 2 Microsoft ... 3 Internet ... EN 3:33 PM

Multi-Grid service portal
To be used today!

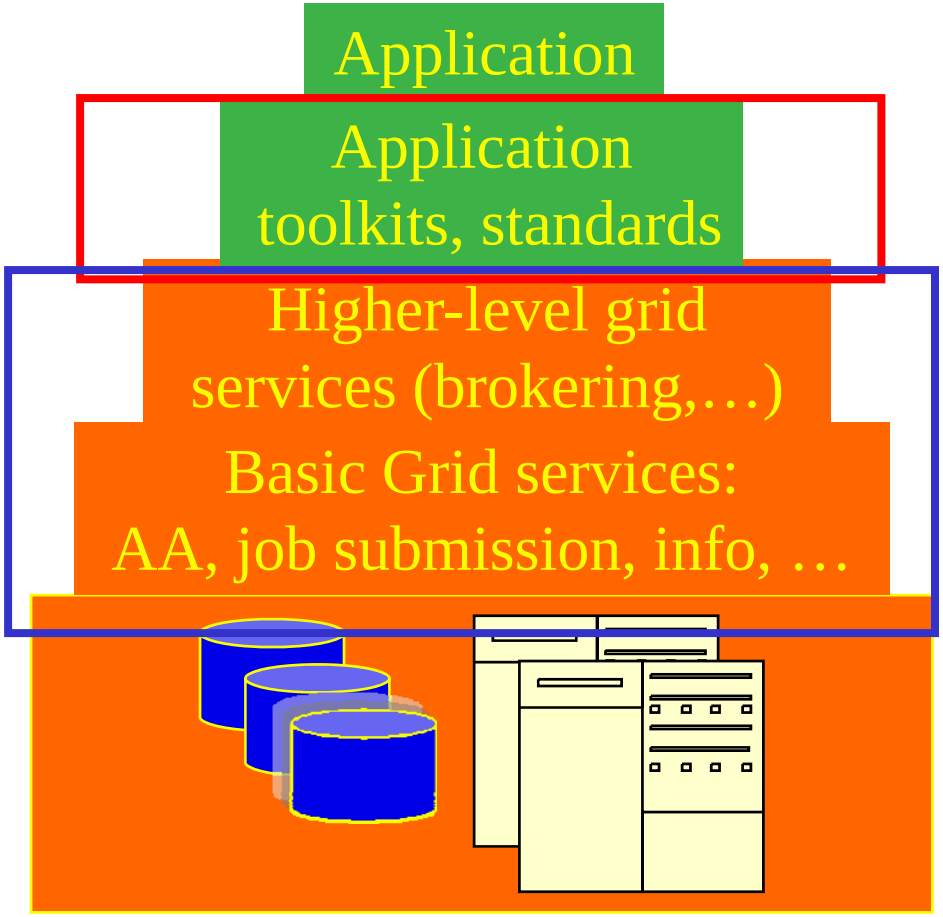


Name	Information System				[Actions]
	Type	Host	Port	BaseDn	
compchem	LCG2	bdii.phy.bg.ac.yu	2170	Mds-vo-name=local,o=grid	Resources
compchem_GLITE_BROKER	N/A				Resources
compchem_LCG_2_BROKER	N/A				Resources
gilda	LCG2	glite-rb.ct.infn.it	2170	mds-vo-name=local,o=grid	Resources
gilda_GLITE_BROKER	N/A				Resources
gilda_LCG_2_BROKER	N/A				Resources
hungrid	LCG2	grid152.kfki.hu	2170	mds-vo-name=local,o=grid	Resources
hungrid_GLITE_BROKER	N/A				Resources
hungrid_LCG_2_BROKER	N/A				Resources
seegrid	LCG2	bdii.phy.bg.ac.yu	2170	mds-vo-name=local,o=grid	Resources
seegrid_GLITE_BROKER	N/A				Resources
seegrid_LCG_2_BROKER	N/A				Resources
voce	LCG2	bdii.cyf-kr.edu.pl	2170	mds-vo-name=local,o=grid	Resources
voce_GLITE_BROKER	N/A				Resources

Motivations for developing P-GRADE portal

- P-GRADE portal should
  - Hide the complexity of the underlying grid middlewares
  - Provide a high-level graphical user interface that is easy-to-use for e-scientists
  - Support many different grid programming approaches:
    - **Simple Scripts & Control** (sequential and MPI job execution)
    - **Scientific Application Plug-ins**
    - **Complex Workflows**
    - **Parameter sweep applications:** both on job and workflow level
    - **Interoperability:** transparent access to grids based on different middleware technology (both computing and data resources)
  - Support several levels of parallelism

Layers in a Grid system

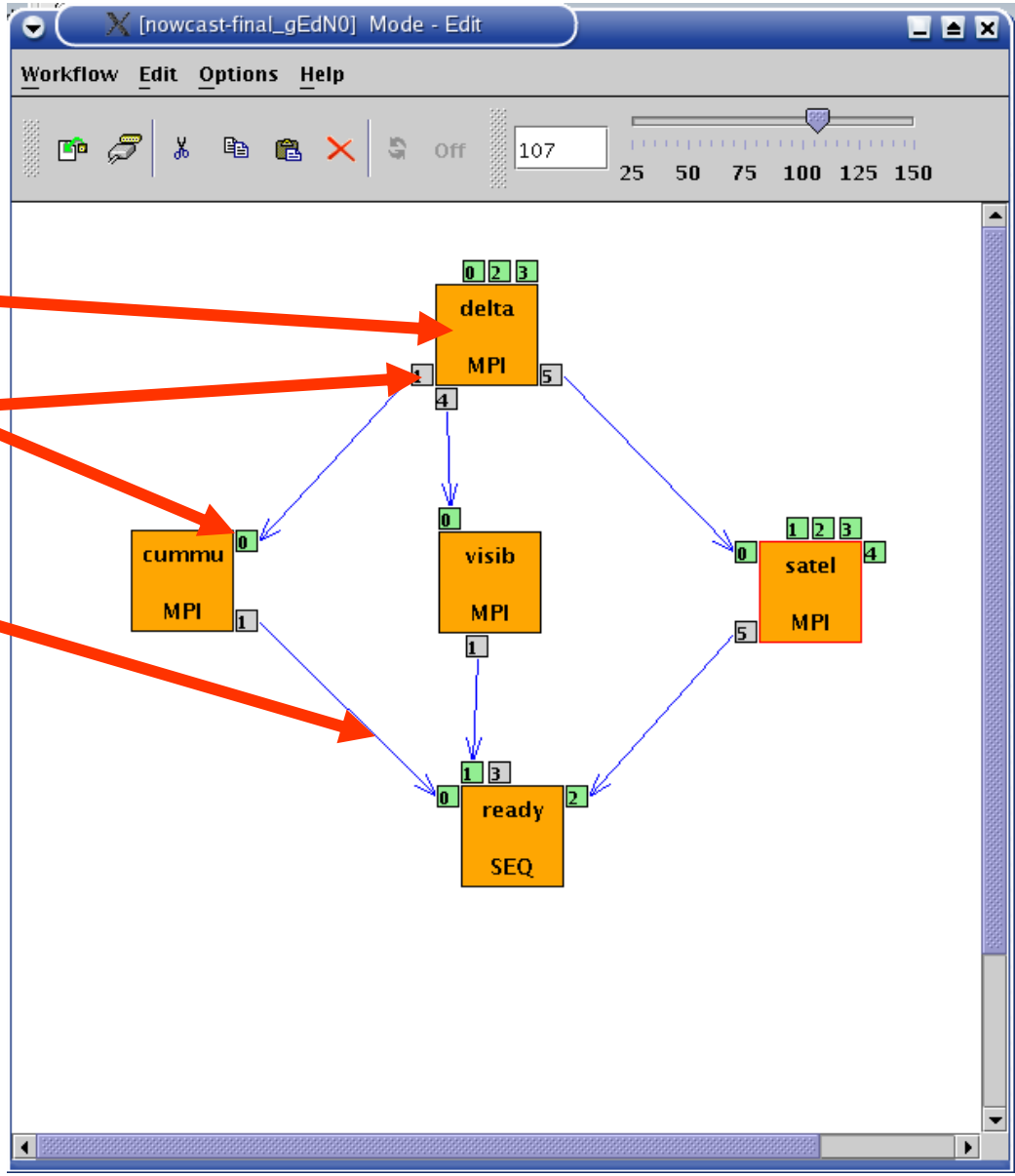


Graphical interface
P-GRADE Portal services

Command line tools
Grid middleware

What is a P-GRADE Portal workflow?

- **a directed acyclic graph where**
  - Nodes represent jobs (batch programs to be executed on a computing element)
  - Ports represent input/output files the jobs expect/produce
  - Arcs represent file transfer operations
- **semantics of the workflow:**
  - A job can be executed if all of its input files are available

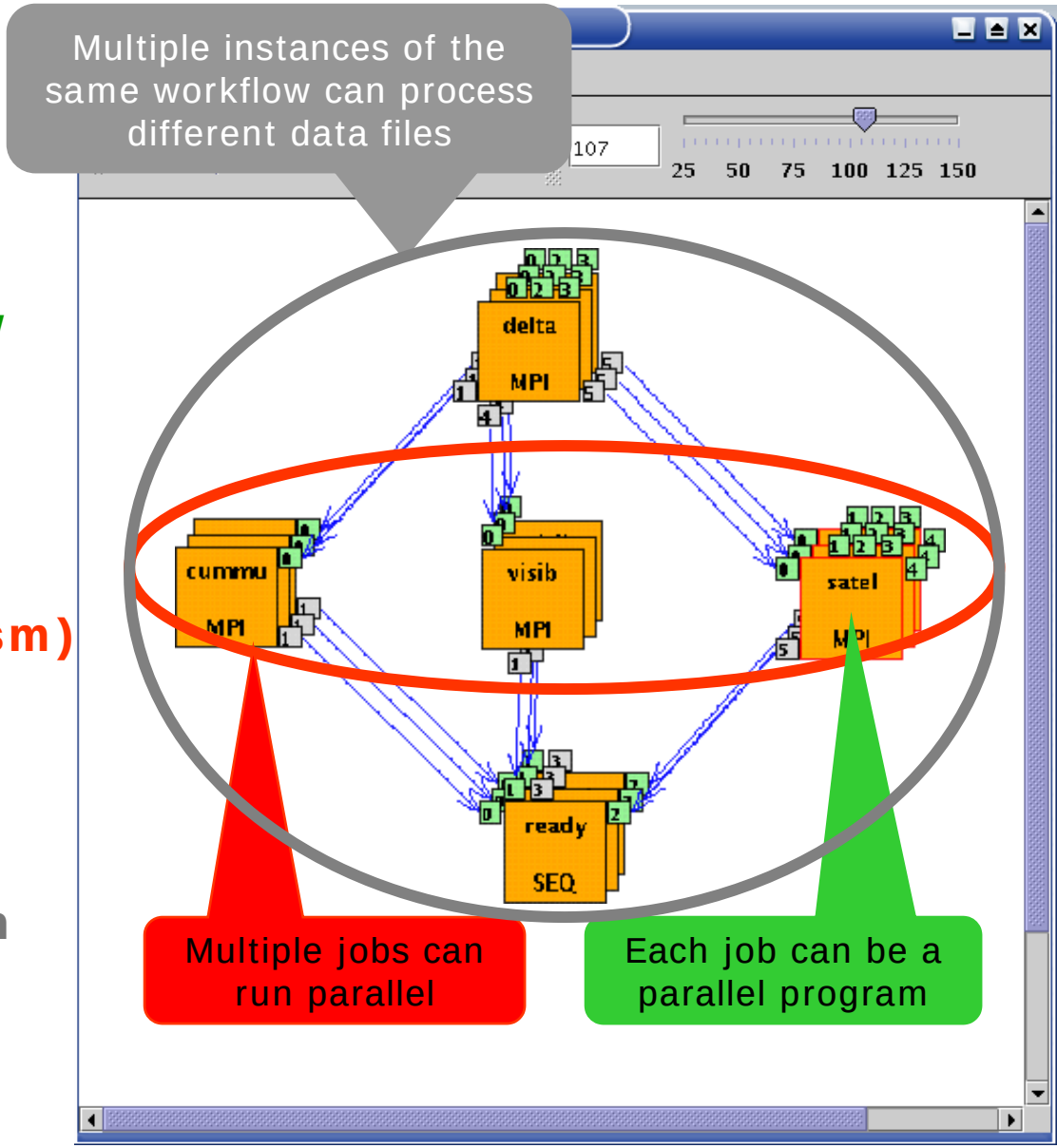


Three Levels of parallelism

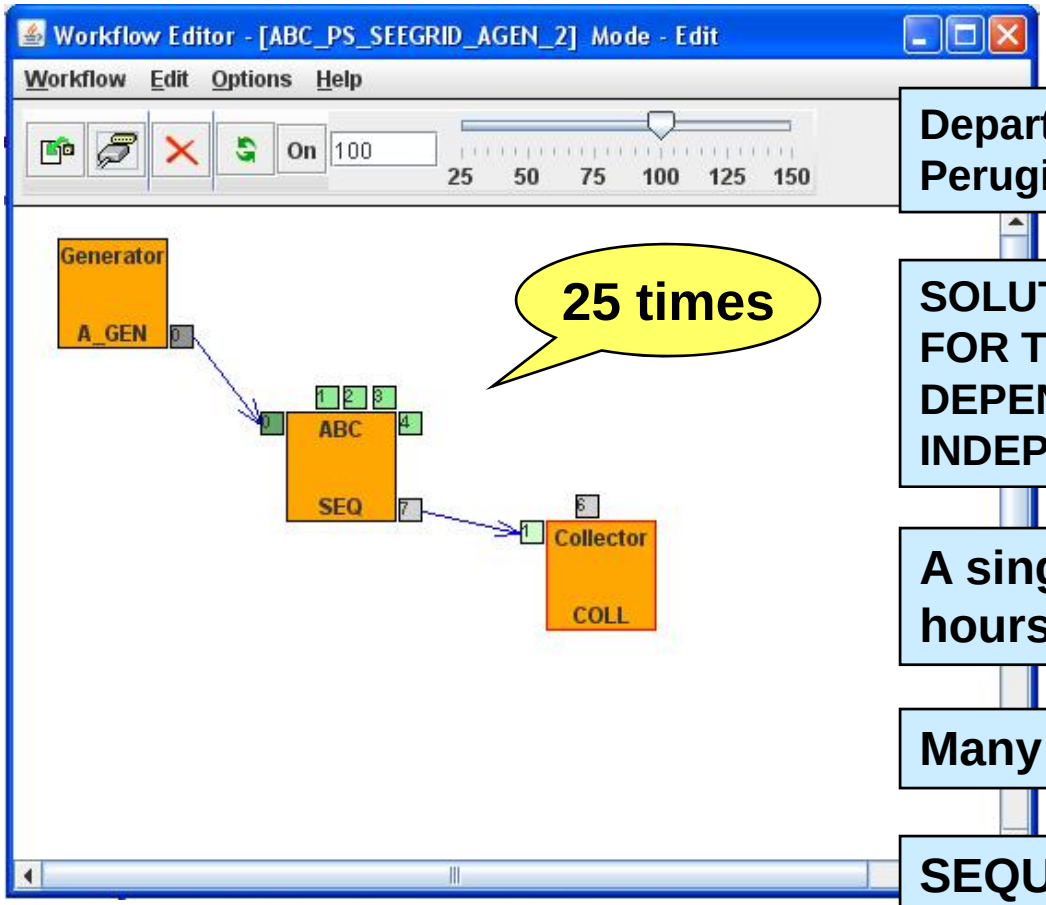
– **Job level: Parallel execution inside a workflow node (MPI job as workflow component)**

– **Workflow level: Parallel execution among workflow nodes (WF branch parallelism)**

– **PS workflow level: Parallel execution of the workflow**



Example: Computational Chemistry



Department of Chemistry, University of Perugia

SOLUTION OF SCHRODINGER EQUATION FOR TRIATOMIC SYSTEMS USING TIME-DEPENDENT (RWAVEPR) OR TIME INDEPENDENT (ABC) METHOD

A single execution can be between 5 hours and 10 hours

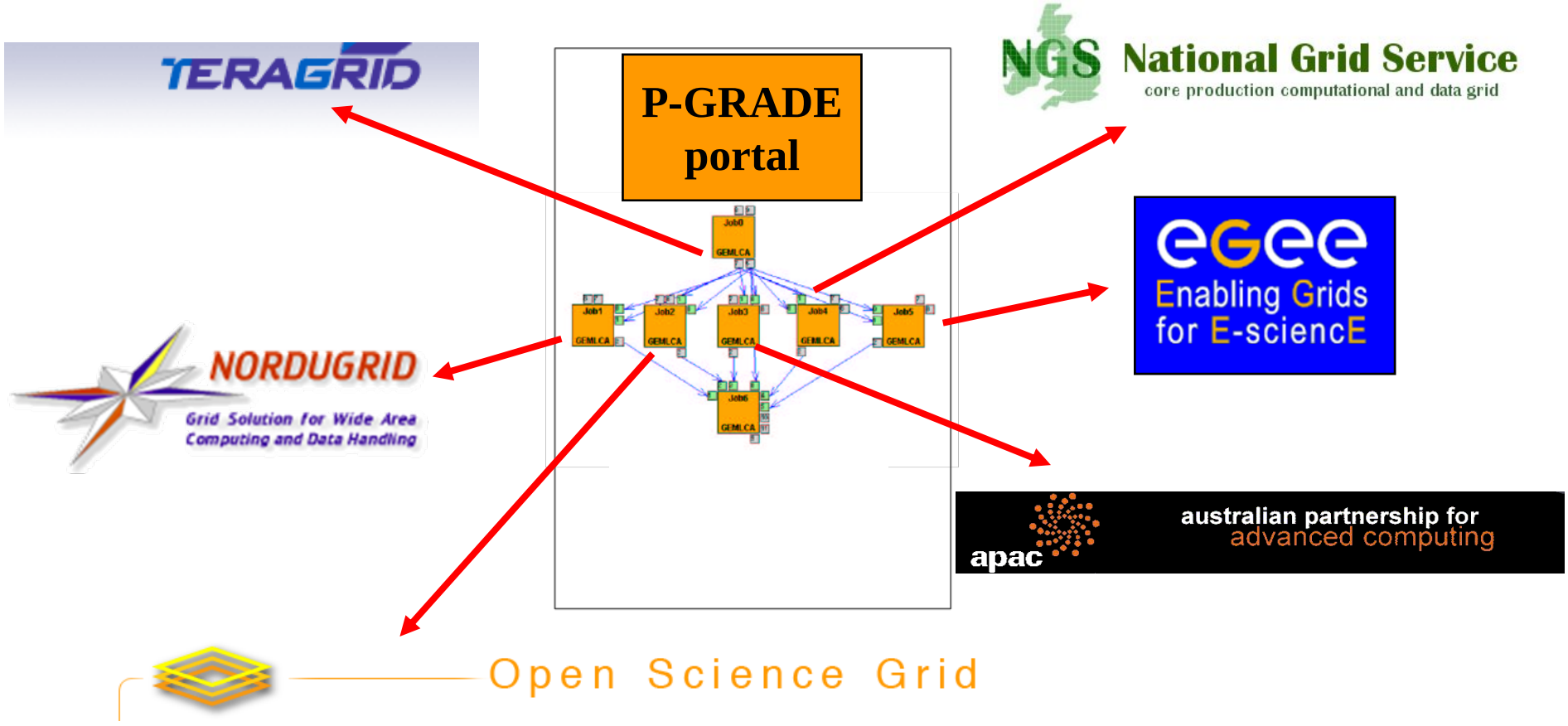
Many simulations at the same time

SEQUENTIAL FORTRAN 90

See at demo booth 11: EGEE Application Porting Support Group

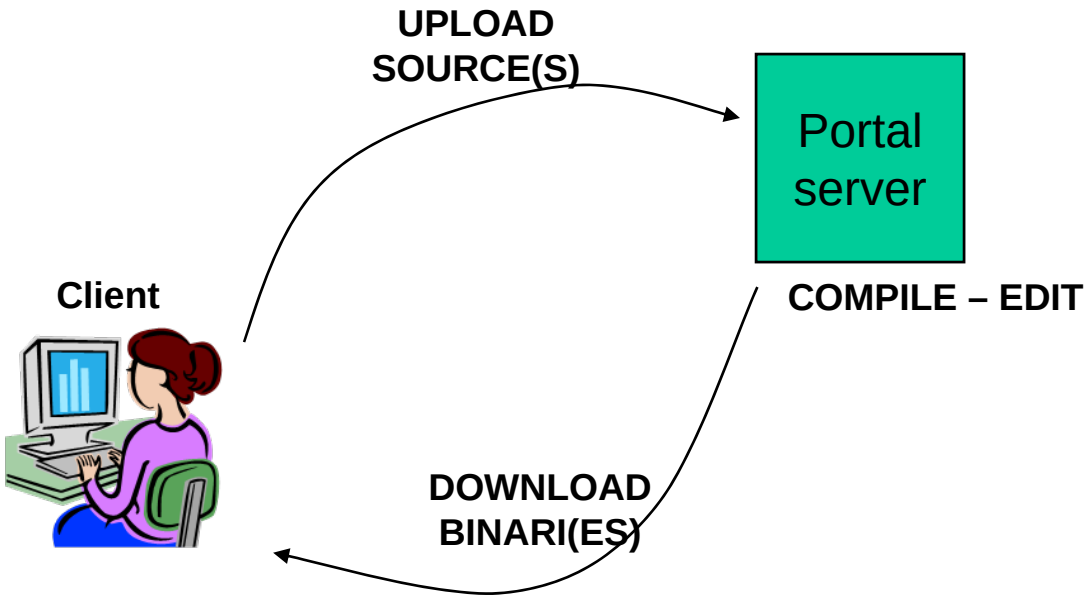
Grid interoperation by P-GRADE

Acccessing Globus, gLite and ARC based grids/VOs simultaneously



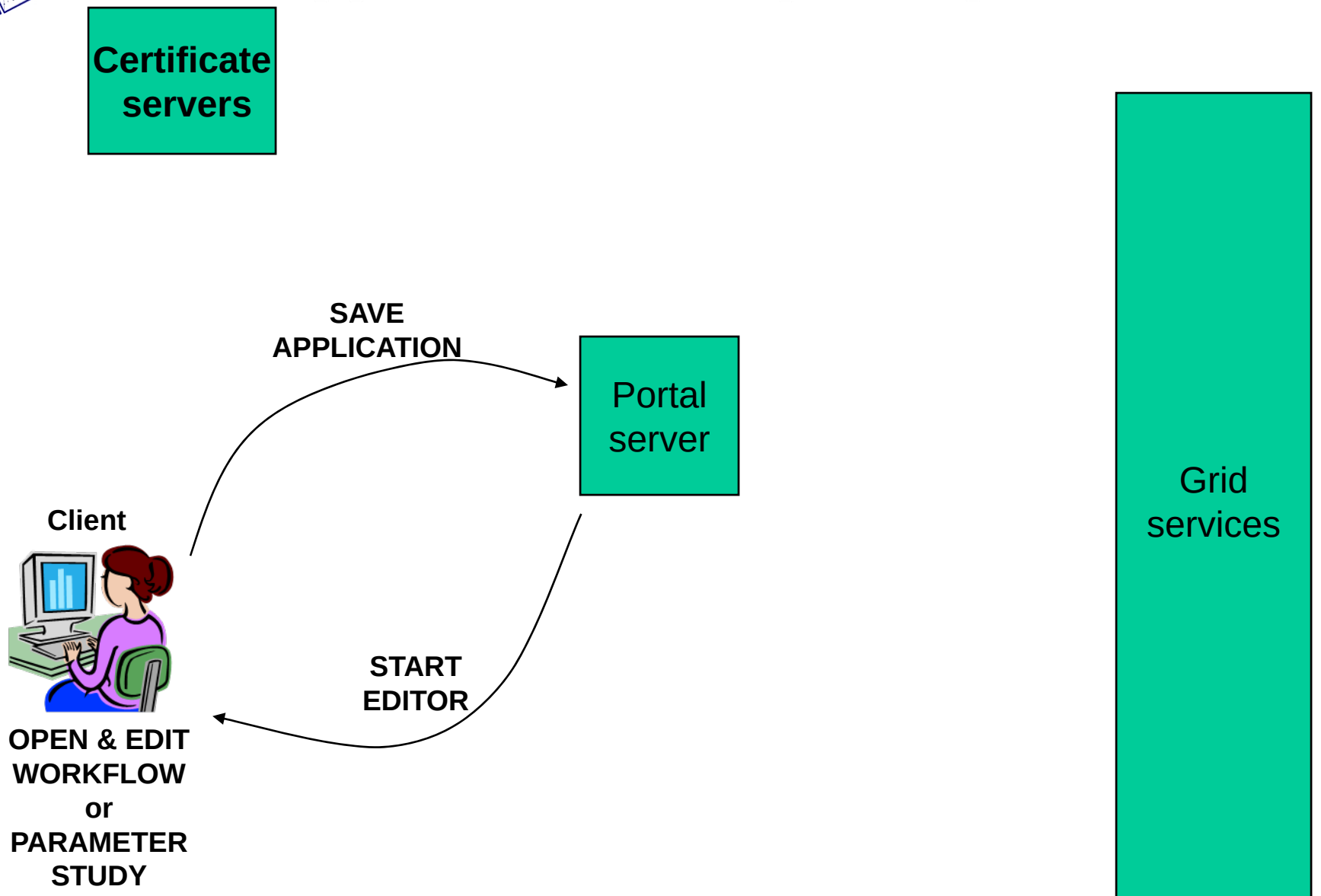
Typical user scenario
Job compilation phase

Certificate servers

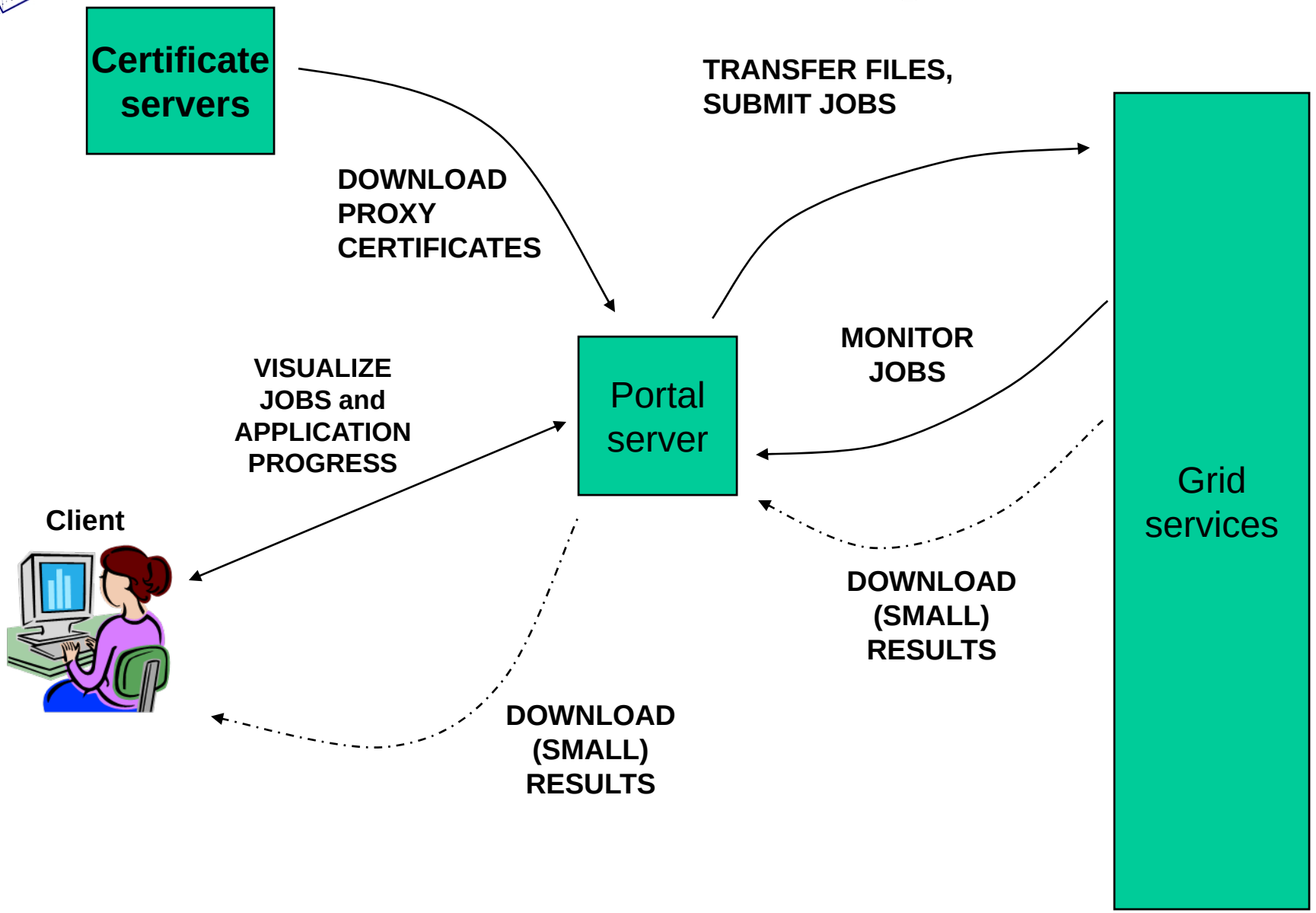


Grid services

Typical user scenario
Application development phase

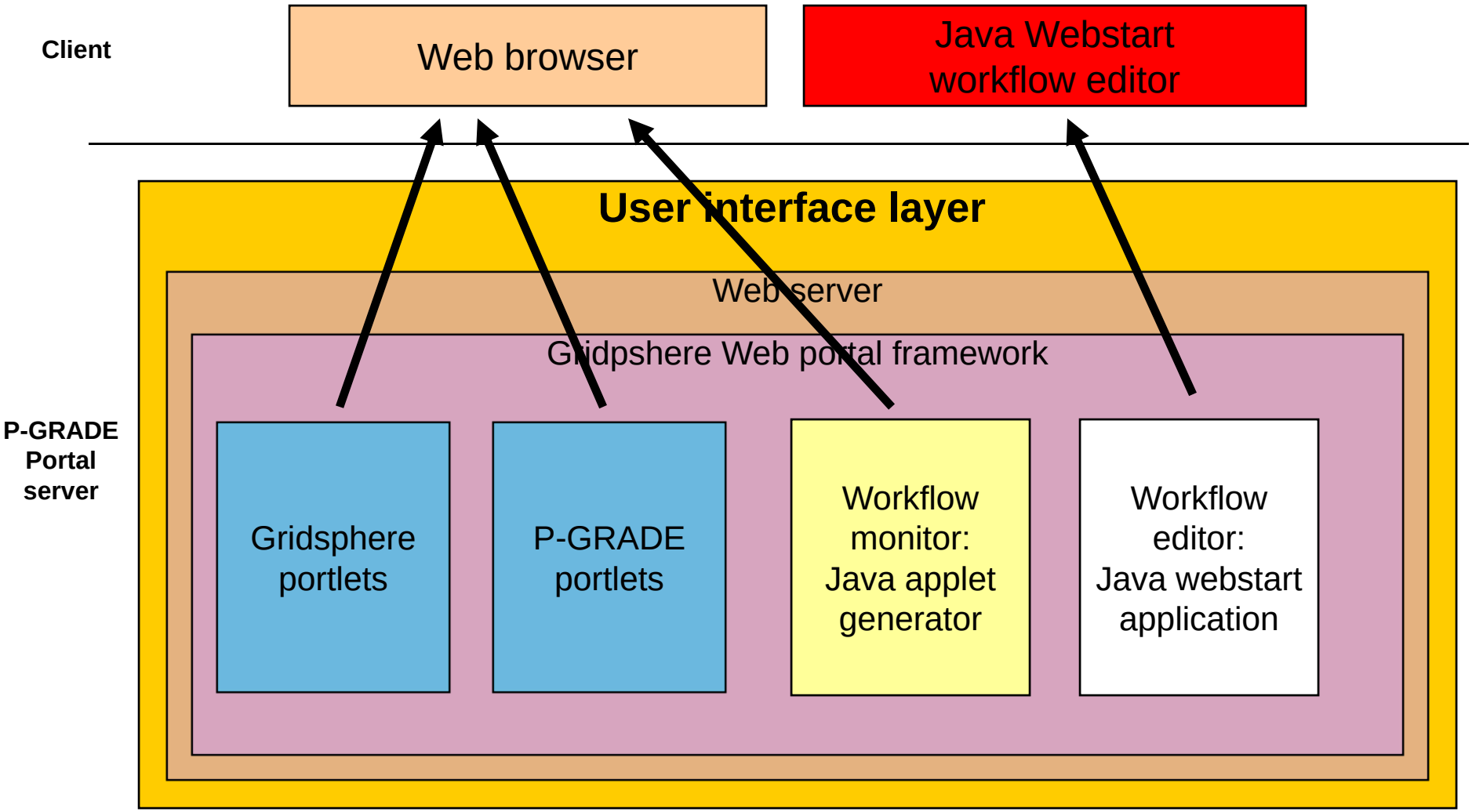


Typical user scenarios
Workflow execution phase

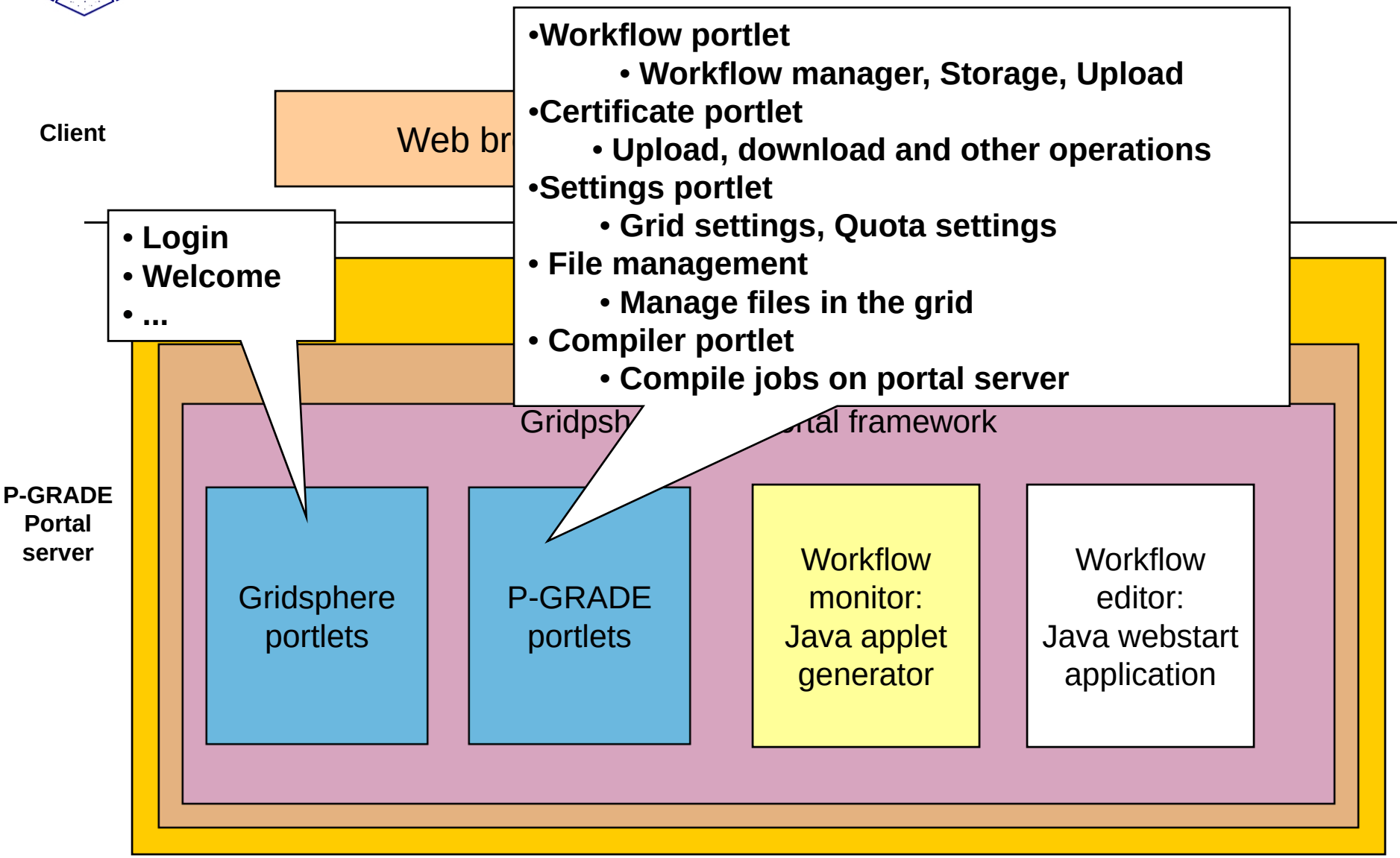


P-GRADE Portal structural overview

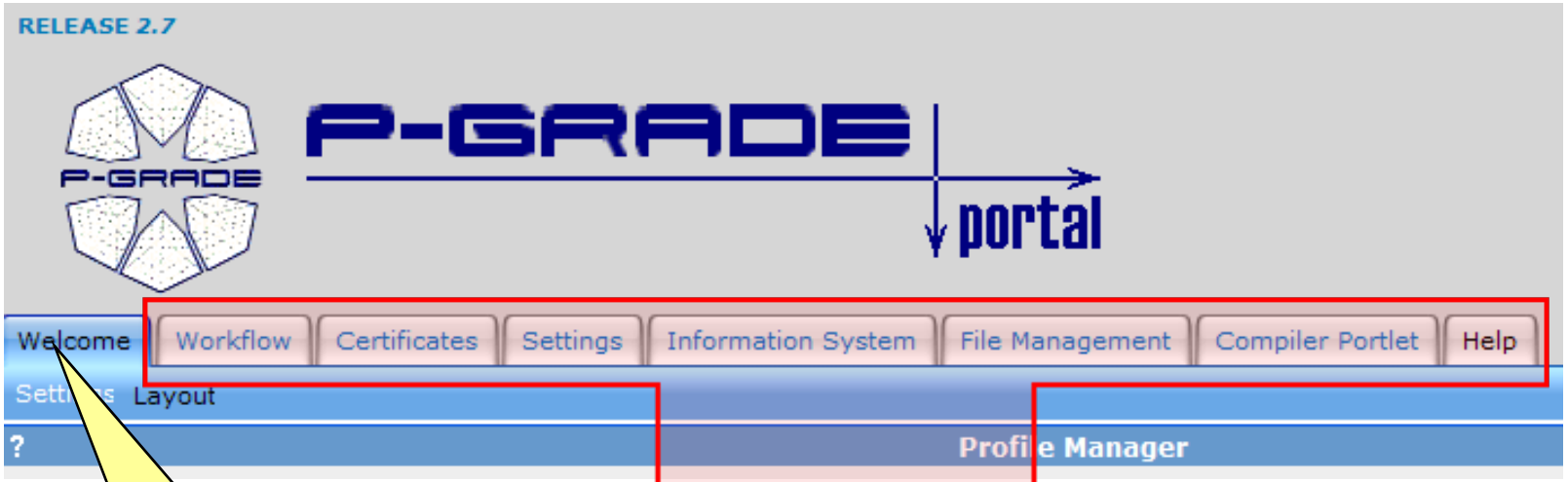
Interface layer



Interface layer functionalities



P-GRADE vs. Non-P-GRADE portlets



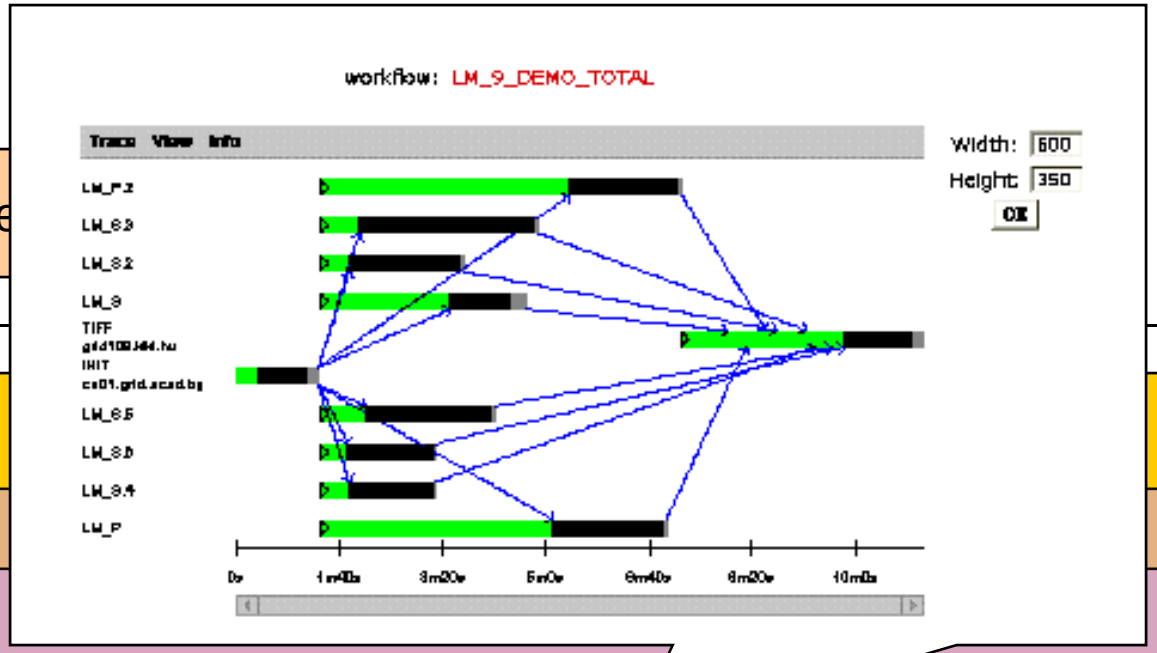
GridSphere 2.x Grid Portal framework

P-GRADE Portal portlets

Interface layer

Client

We



P-GRADE Portal server

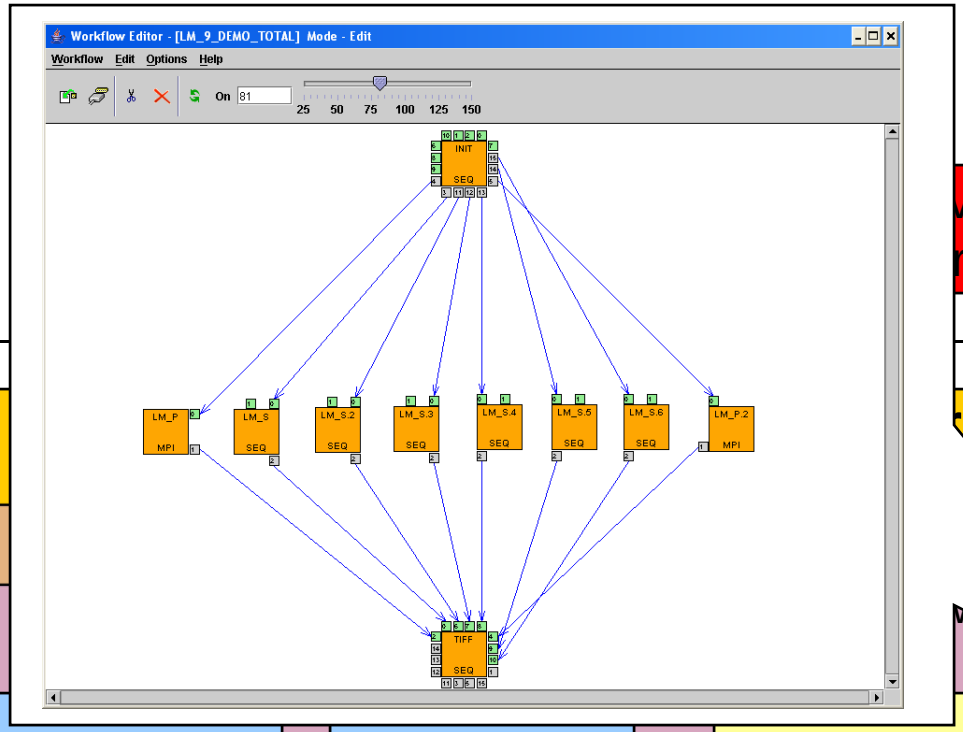
Gridsphere portlets

P-GRADE portlets

Workflow monitor: Java applet generator

Workflow editor: Java webstart application

Interface layer



Client

va Webstart
rkflow editor

P-GRADE Portal server

Gridsphere portlets

P-GRADE portlets

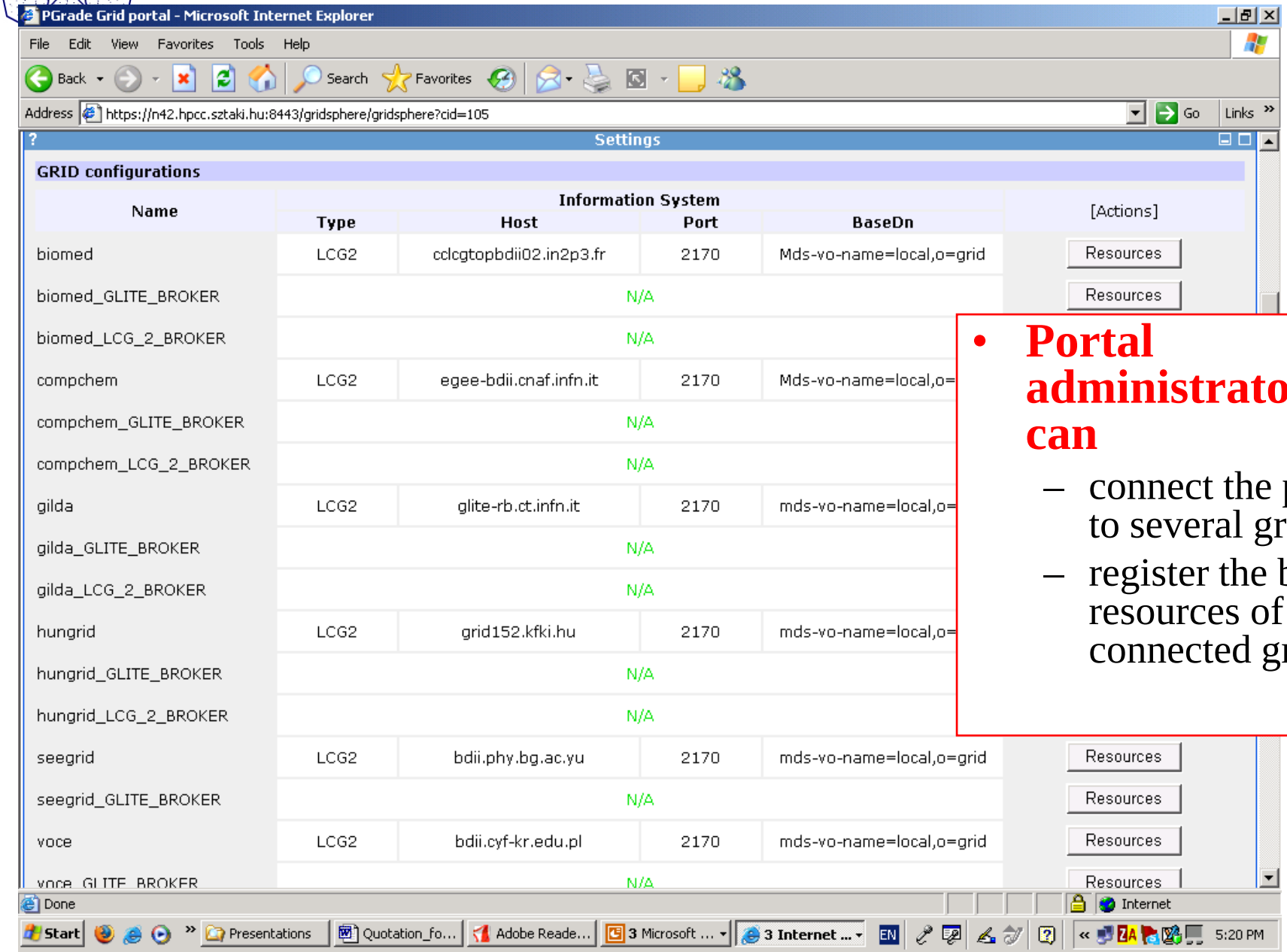
Workflow monitor: Java applet generator

Workflow editor: Java webstart application

Portlets/functionalities of P-GRADE portal

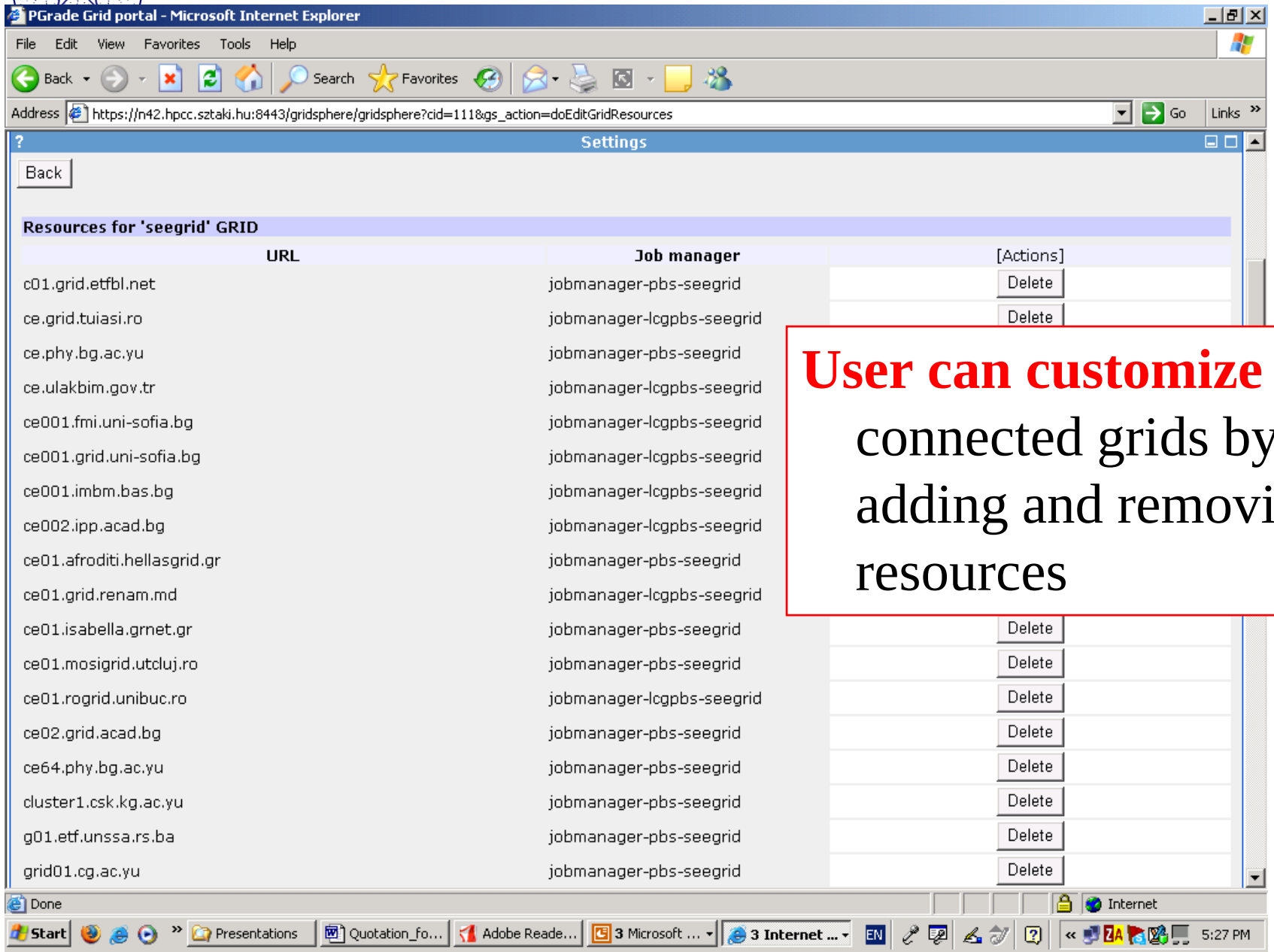
- Settings (portlet)
- Certificate and proxy management (portlet)
- Information system visualization (portlet)
- Graphical workflow editing
- Workflow manager (portlet)
- LFC (EGEE) file management (portlet)
- Compilation support (portlet)
- Fault-tolerance support

Settings Portlet



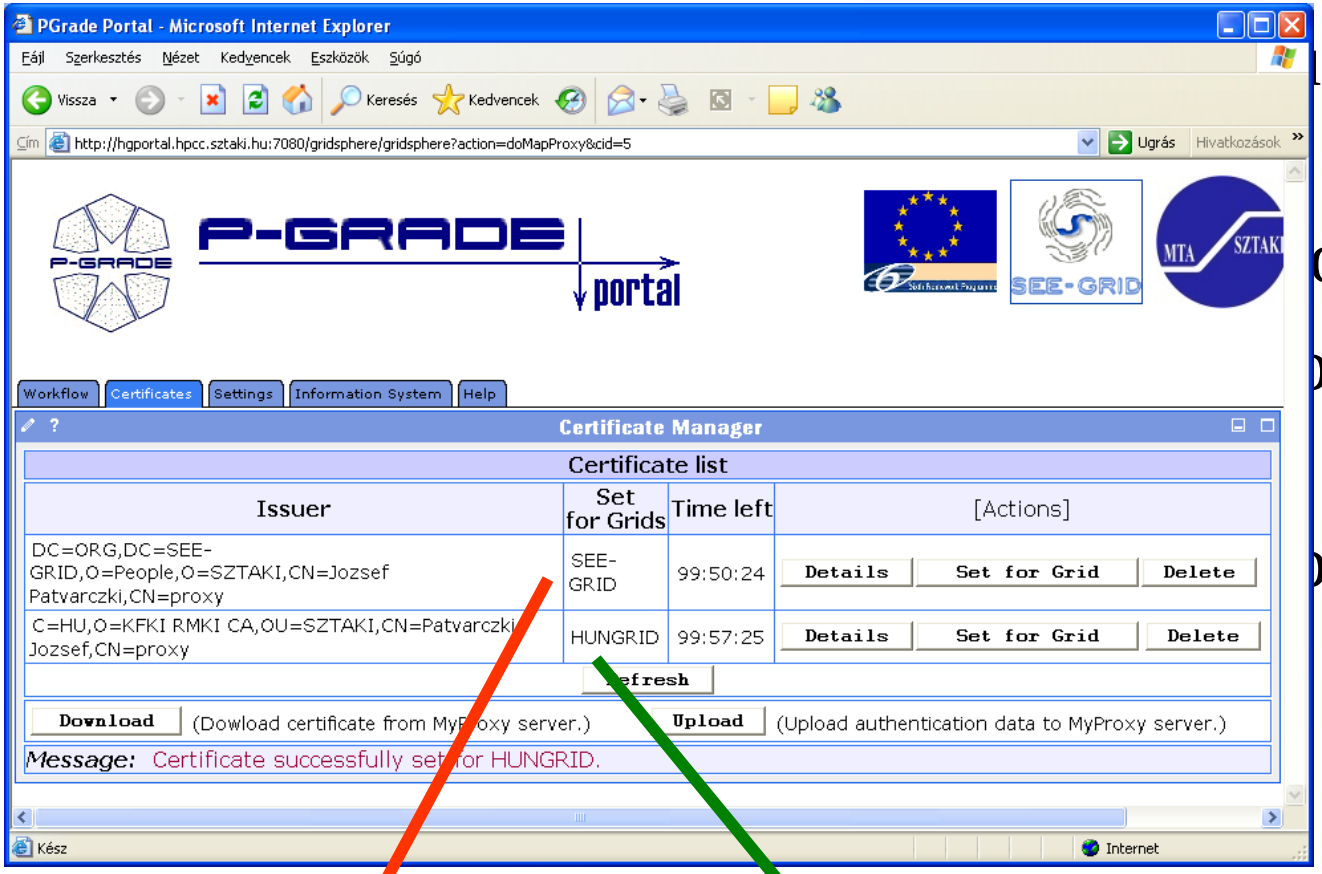
- **Portal administrator can**
  - connect the portal to several grids
  - register the basic resources of the connected grids

Settings Portlet



User can customize the connected grids by adding and removing resources

Certificate and proxy management Portlet



SEE-GRID access

HUNGRID access

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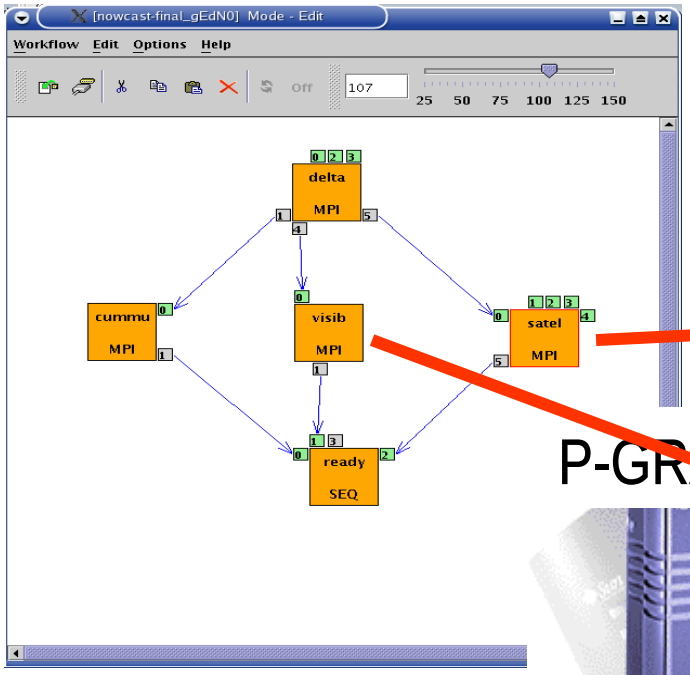
Solving Grid interoperation by P-GRADE Portal



EGEE Grid

P-GRADE-Portal

Different jobs can be parallel executed in different grids

UK NGS

London

Rome

Athens

Interoperation vs. Interoperability

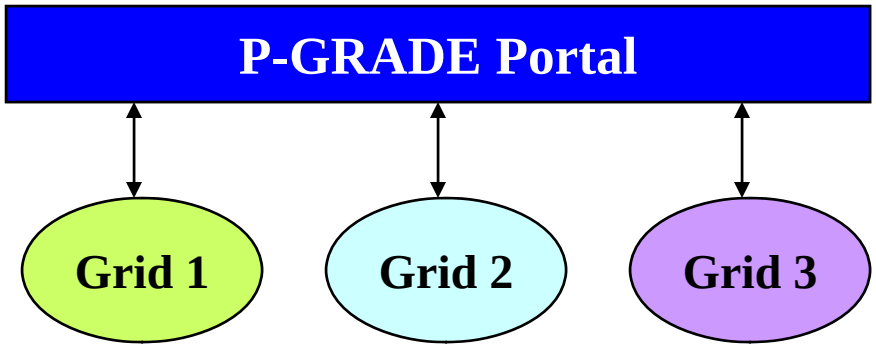
As defined by the **GIN** (Grid Interoperation Now)
CG (Community Group) of the **OGF** (Open Grid Forum)

Interoperation:

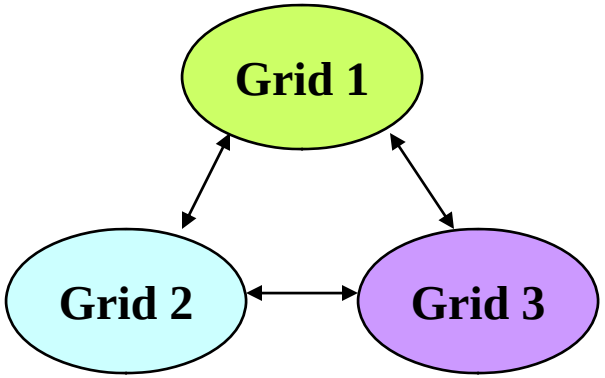
- short term solution that defines what needs to be done to achieve interoperation between current production grids using **existing technologies**

Interoperability:

- native ability of Grids and Grid middleware to interact directly via common **open standards**

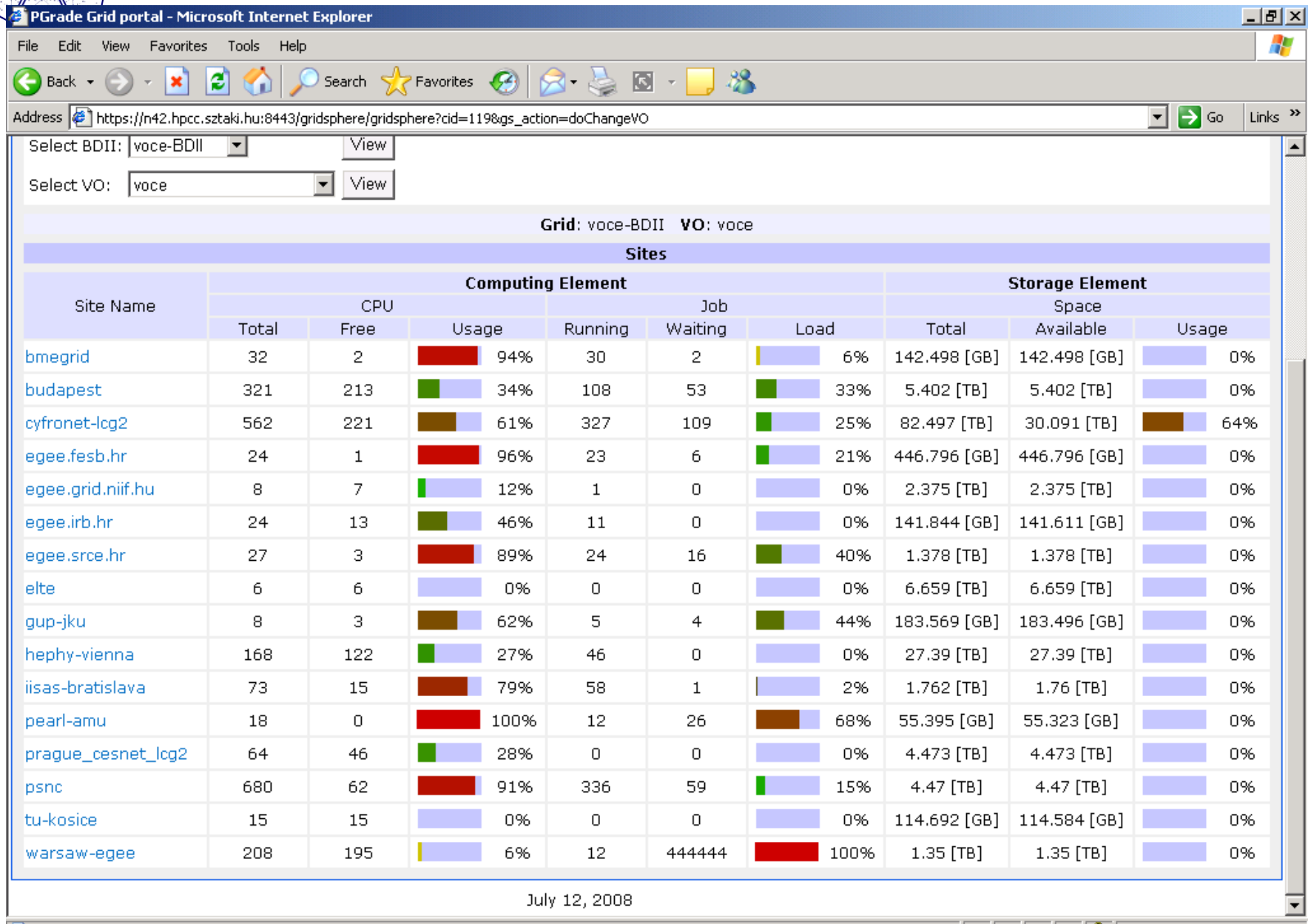


Interoperation



Interoperability

Information system Portlet



PGrade Grid portal - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites

Address https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=119&gs_action=doChangeVO Go Links

Select BDII: voce-BDII View

Select VO: voce View

Grid: voce-BDII **VO**: voce

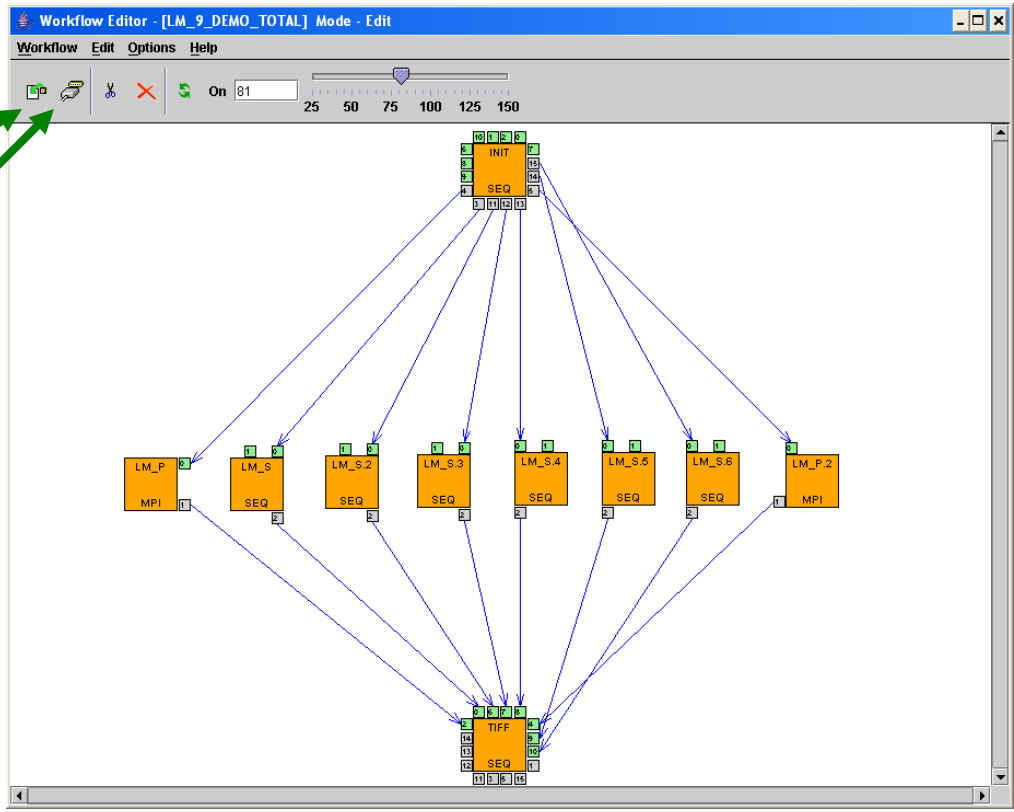
Sites

Site Name	Computing Element						Storage Element		
	CPU			Job			Space		
	Total	Free	Usage	Running	Waiting	Load	Total	Available	Usage
bmegrid	32	2	94%	30	2	6%	142.498 [GB]	142.498 [GB]	0%
budapest	321	213	34%	108	53	33%	5.402 [TB]	5.402 [TB]	0%
cyfronet-lcg2	562	221	61%	327	109	25%	82.497 [TB]	30.091 [TB]	64%
egee.fesb.hr	24	1	96%	23	6	21%	446.796 [GB]	446.796 [GB]	0%
egee.grid.niif.hu	8	7	12%	1	0	0%	2.375 [TB]	2.375 [TB]	0%
egee.irb.hr	24	13	46%	11	0	0%	141.844 [GB]	141.611 [GB]	0%
egee.srce.hr	27	3	89%	24	16	40%	1.378 [TB]	1.378 [TB]	0%
elte	6	6	0%	0	0	0%	6.659 [TB]	6.659 [TB]	0%
gup-jku	8	3	62%	5	4	44%	183.569 [GB]	183.496 [GB]	0%
hephy-vienna	168	122	27%	46	0	0%	27.39 [TB]	27.39 [TB]	0%
iisas-bratislava	73	15	79%	58	1	2%	1.762 [TB]	1.76 [TB]	0%
pearl-amu	18	0	100%	12	26	68%	55.395 [GB]	55.323 [GB]	0%
prague_cesnet_lcg2	64	46	28%	0	0	0%	4.473 [TB]	4.473 [TB]	0%
psnc	680	62	91%	336	59	15%	4.47 [TB]	4.47 [TB]	0%
tu-kosice	15	15	0%	0	0	0%	114.692 [GB]	114.584 [GB]	0%
warsaw-egee	208	195	6%	12	444444	100%	1.35 [TB]	1.35 [TB]	0%

July 12, 2008

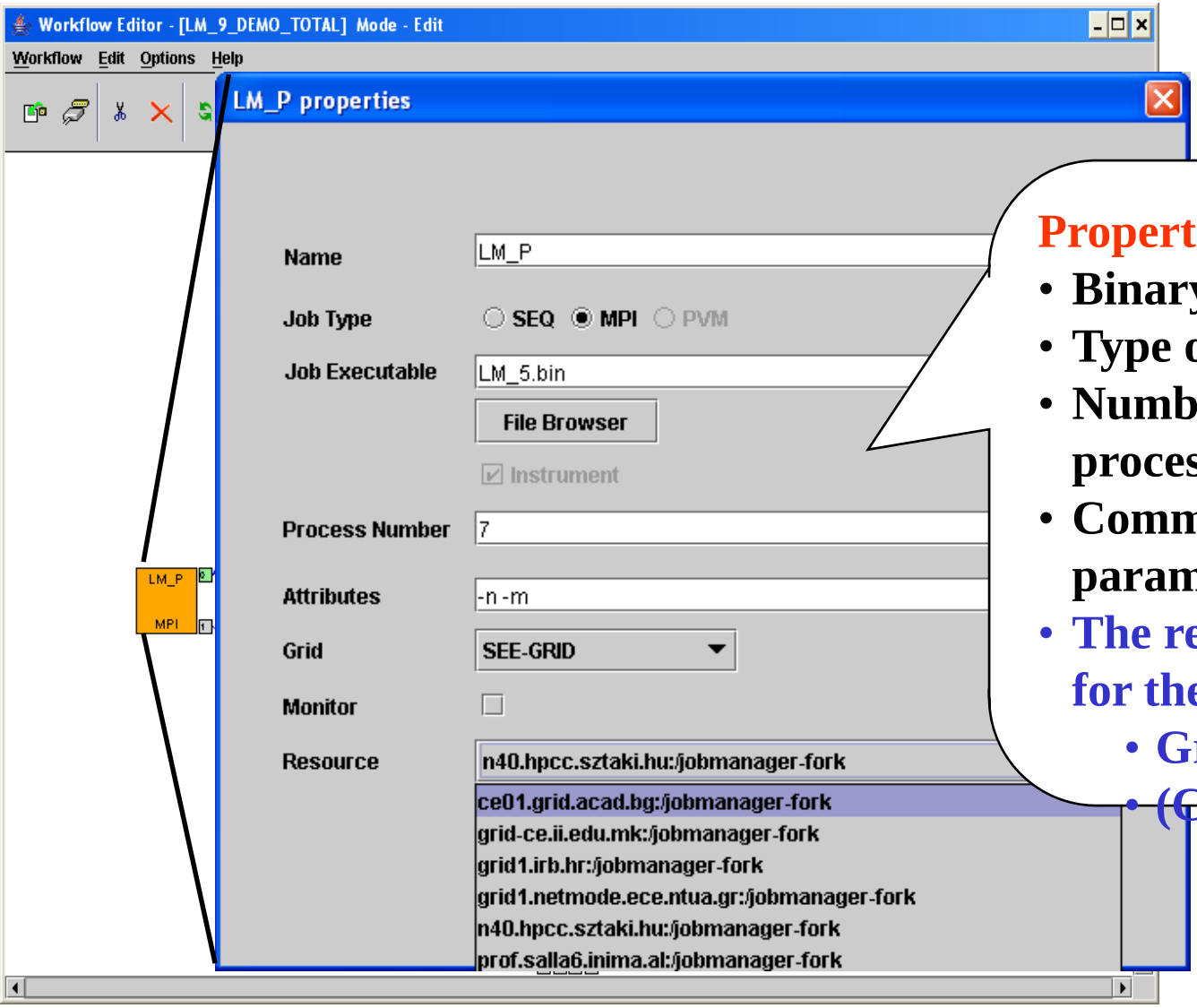
Graphical workflow editing

- The aim is to define a DAG of batch jobs:
  1. **Drag & drop components:** jobs and ports
  2. **Define their properties**
  3. **Connect ports by channels** (no cycles, no loops, no conditions)
  4. Automatically generates JDL file



Workflow Editor

Properties of a job

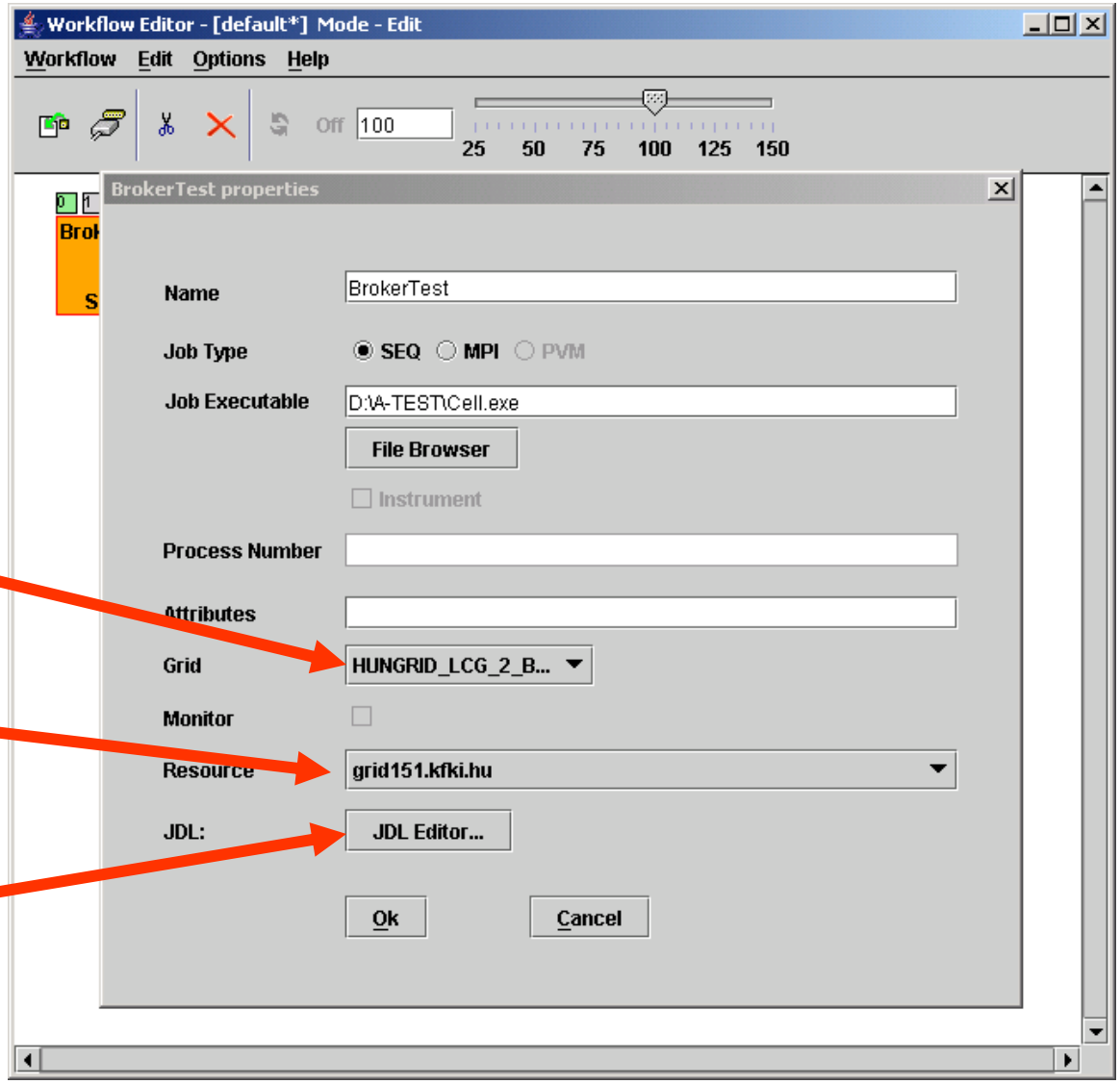


Properties of a job:

- **Binary executable**
- **Type of executable**
- **Number of required processors**
- **Command line parameters**
- **The resource to be used for the execution:**
  - **Grid/VO**
  - **(Computing element)**

Workflow Editor

Defining broker jobs



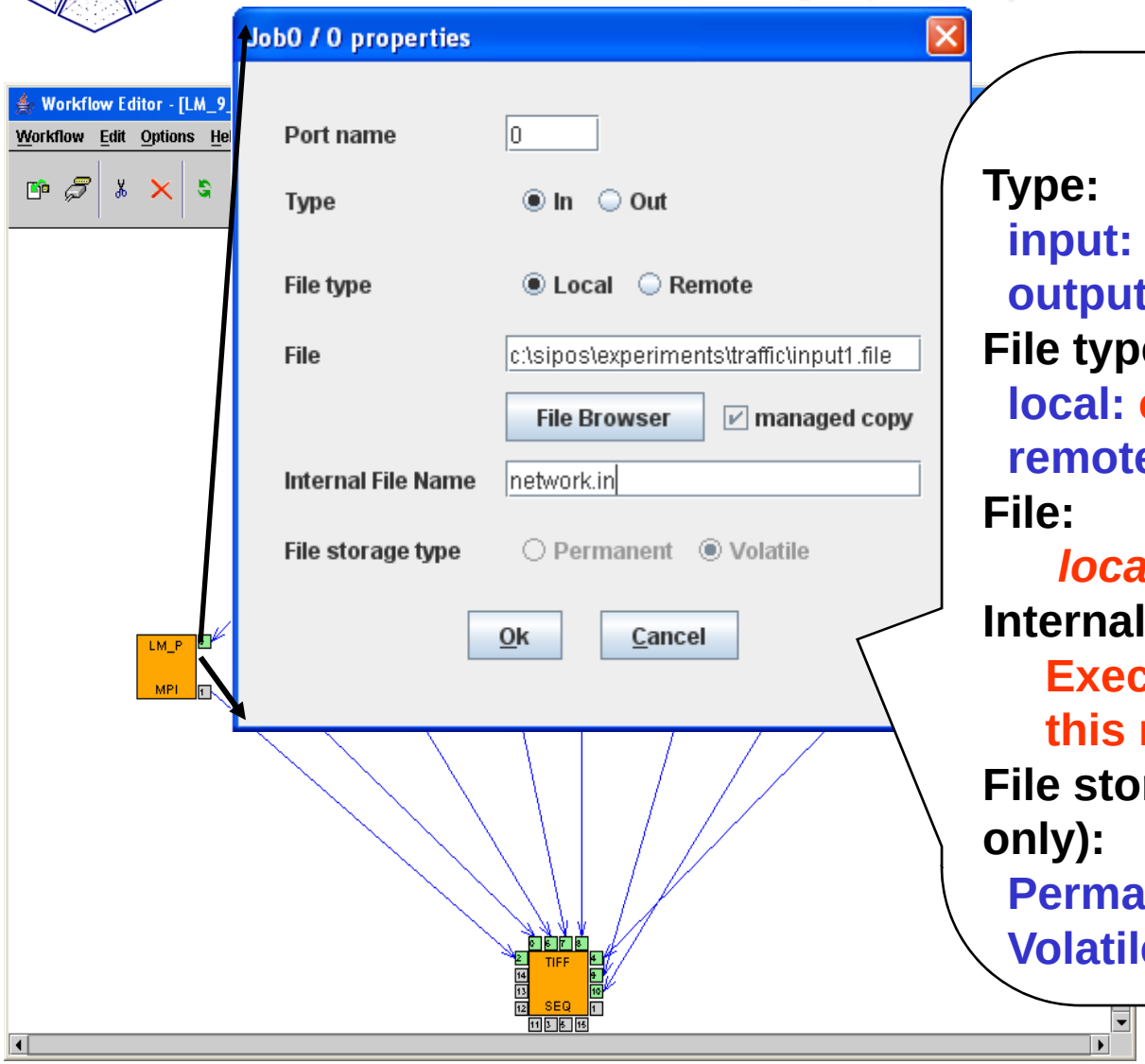
Select a Grid with broker! (*_BROKER)

Ignore the resource field!

If default JDL is not sufficient use the built-in JDL editor!

Workflow Editor

Defining input-output files



File properties

Type:

input: ***the job reads***

output: ***the job generates***

File type:

local: **comes *from my desktop***

remote: ***comes from an SE***

File:

location of the file

Internal file name:

Executable reads the file in this name – fopen(“file.in”, …)

File storage type (output files only):

Permanent: ***final result***

Volatile: ***only data channel***

How to refer to an I/O file?

Input file

Output file

Local file

- Client side location:
  c:\experiments\11-04.dat

- Client side location:
  result.dat

- LFC logical file name
  (LFC file catalog is required – EGEE VOs)
  lfn:/grid/gilda/sipos/11-04.dat

- GridFTP address (in Globus Grids):
  gsiftp://somengshost.ac.uk/mydir/11-04.dat

- LFC logical file name
  (LFC file catalog is required – EGEE VOs)
  lfn:/grid/gilda/sipos/11-04_-_result.dat

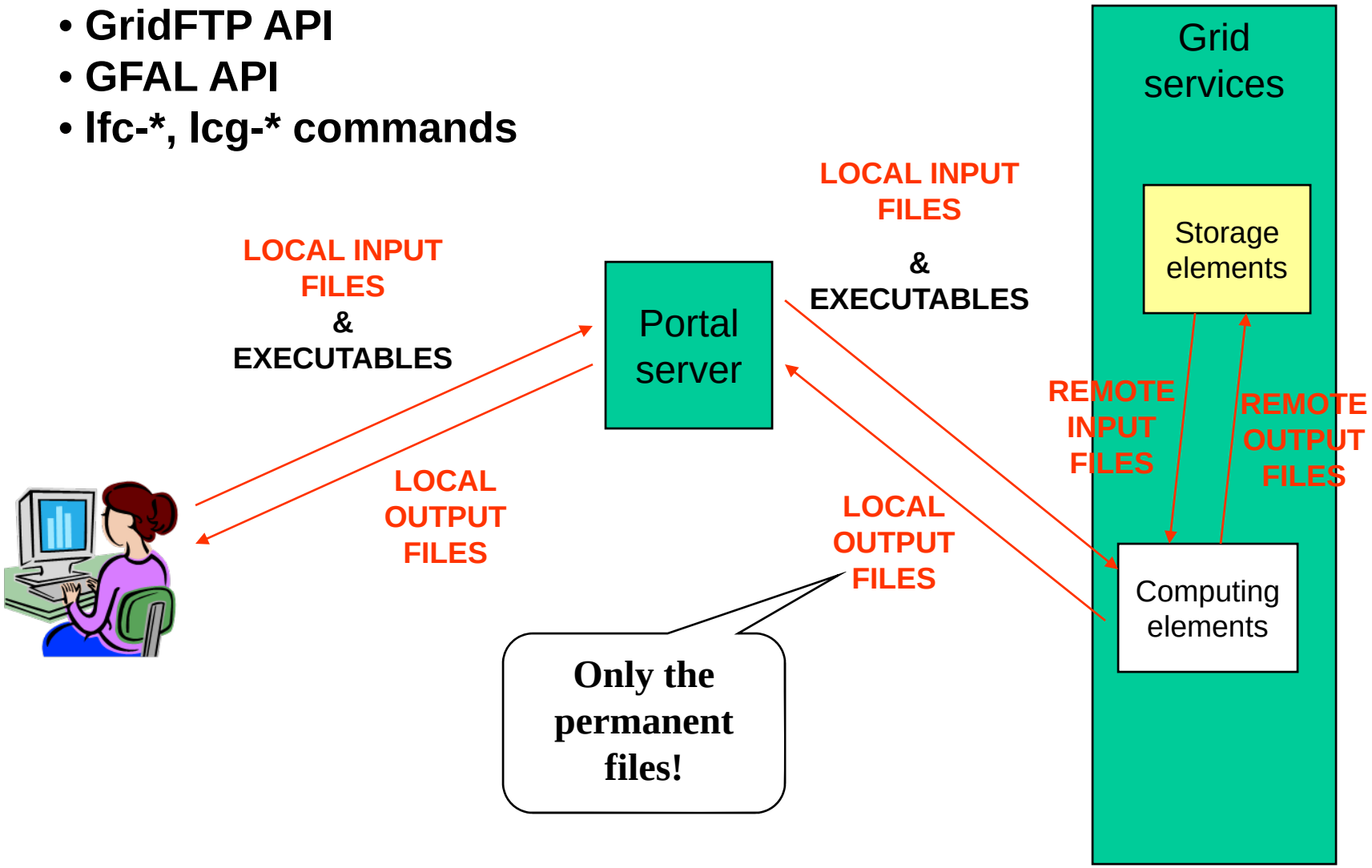
- GridFTP address (in Globus Grids):
  gsiftp://somengshost.ac.uk/mydir/result.dat

Remote file

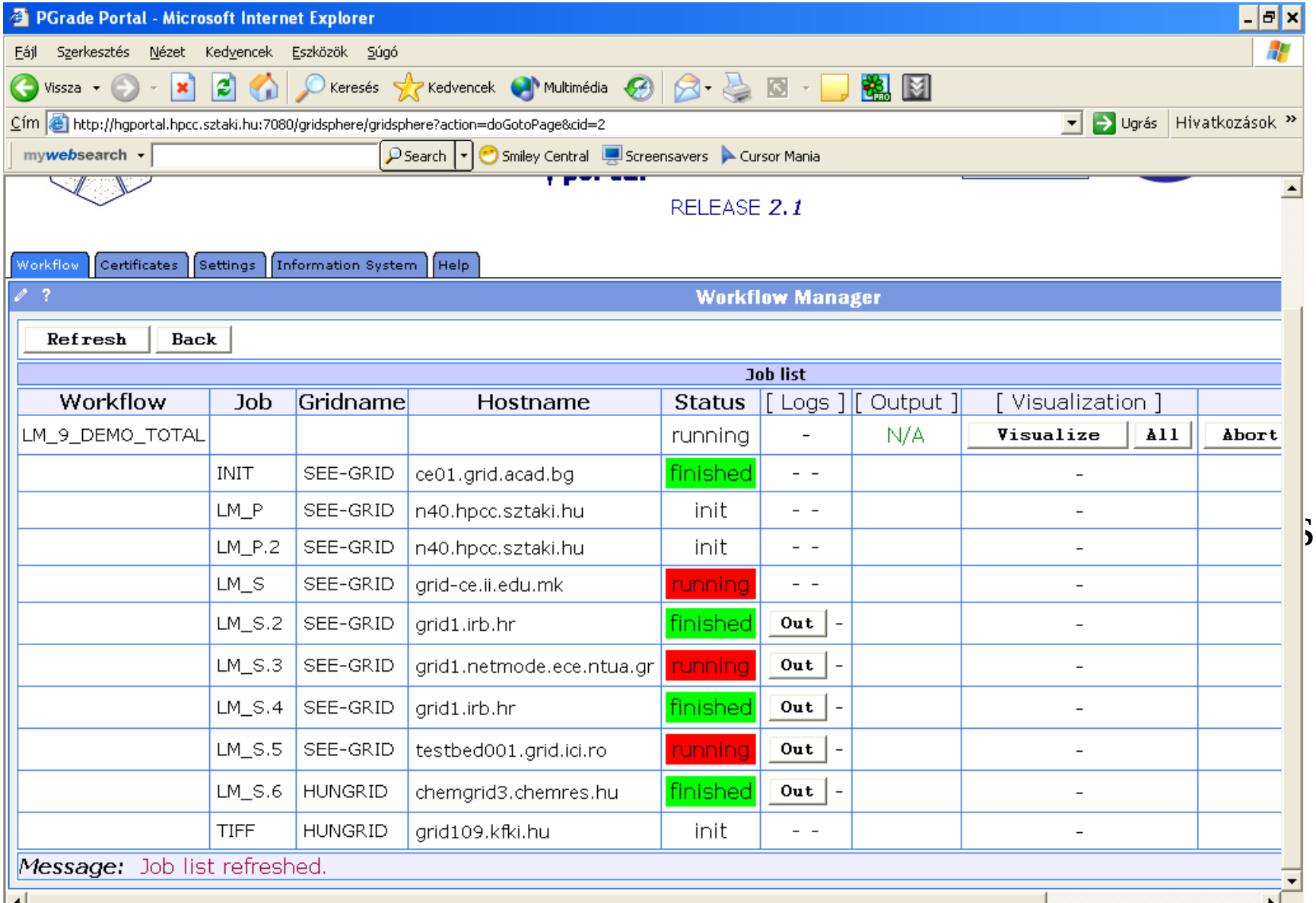
Local vs. remote files

Your binary can access data services directly too

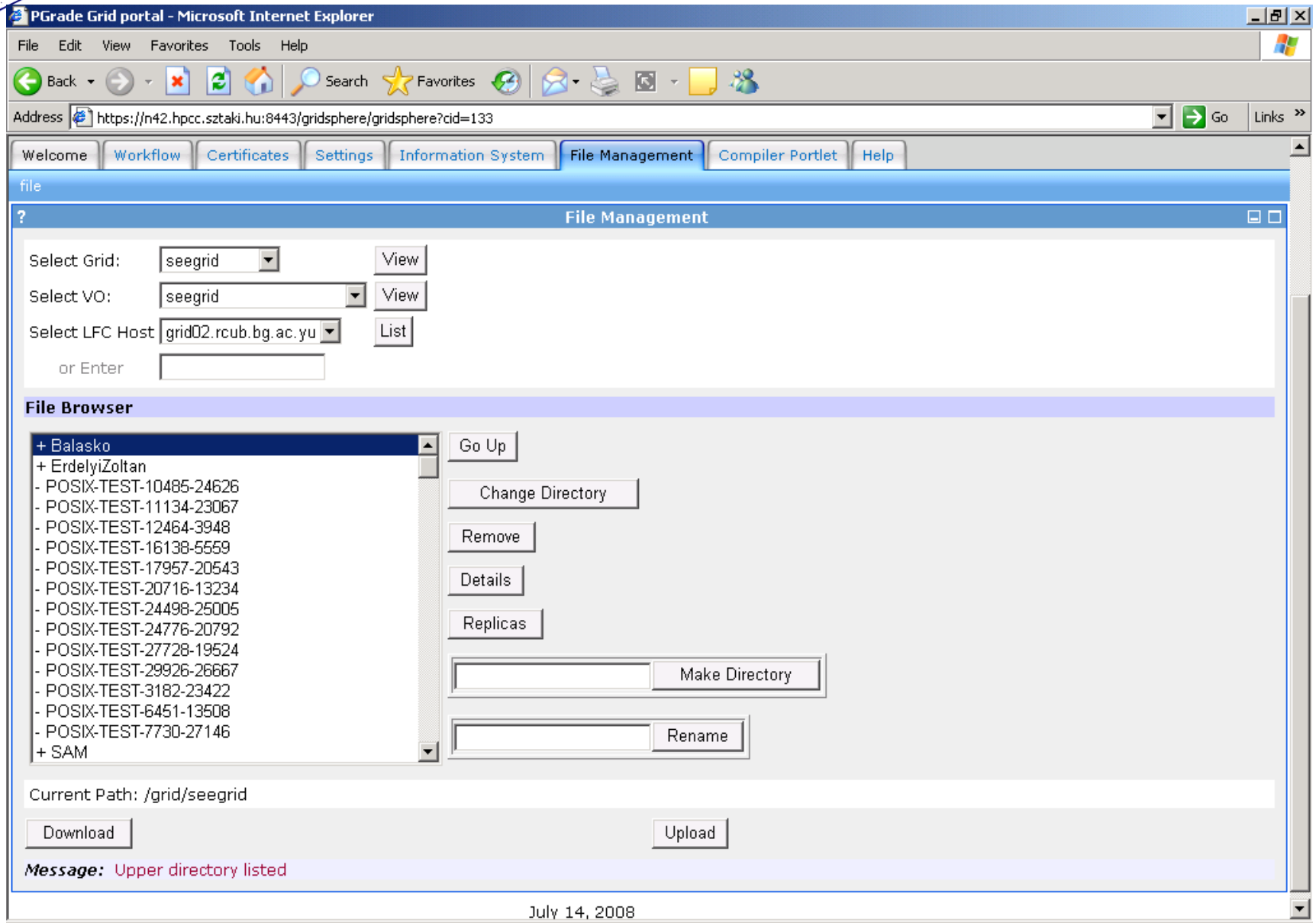
- **GridFTP API**
- **GFAL API**
- **lfc-*, lcg-* commands**



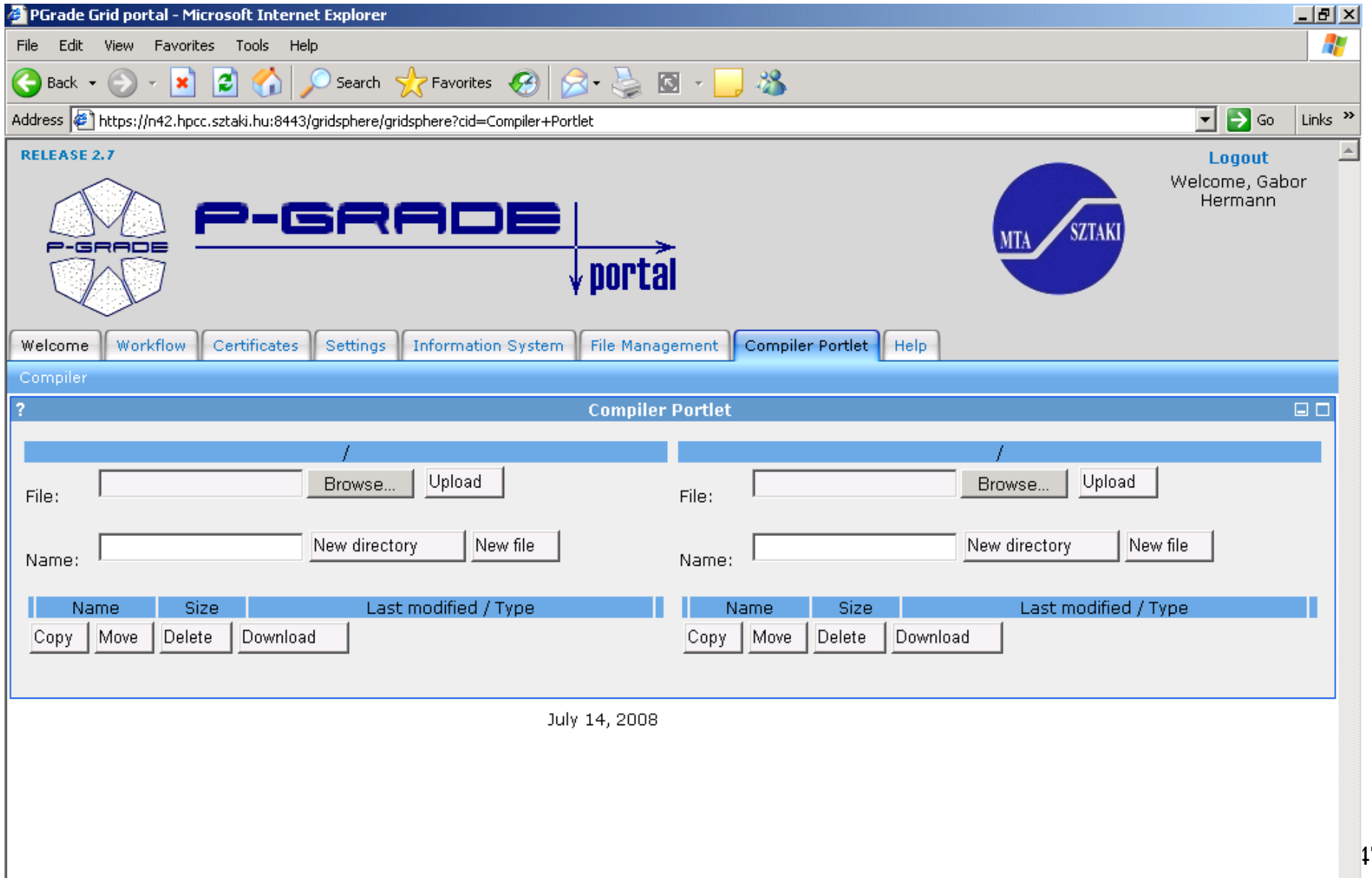
Workflow manager



LFC (EGEE) file management



Compilation support



Fault-tolerant Grid applications

- Utilizing
  - Condor DAGMan's rescue mechanism
  - EGEE job resubmission mechanism of WMS
- If the EGEE broker leaves a job stuck in a CEs' queue, the portal automatically
  - kills the job on this site and
  - resubmits the job to the broker by prohibiting this site.
- As a result
  - the portal guarantees the correct submission of a job as long as there exists at least one matching resource
  - job submission is reliable even in an unreliable grid

Lessons learnt

- **P-GRADE portal provides**
  - Easy-to-use but powerful workflow system (graphical editor, wf manager, etc.)
  - Three levels of parallelism
    - MPI job level
    - Workflow branch level
    - Parameter sweep at workflow level
  - Multi-grid/multi-VO access mechanism for various grids (LCG-2, gLite and GT2)
    - Simultaneous access
    - Transparent access
    - Migrating a workflow from one grid to another requires no modification in the workflow

Learn once, use everywhere
Develop once, execute anywhere

Thank you!

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