



# ***P-GRADE Portal tutorial at EGEE'09***

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**EGEE Training and Induction  
EGEE Application Porting Support**

**[www.lpds.sztaki.hu/gasuc](http://www.lpds.sztaki.hu/gasuc)  
[www.portal.p-grade.hu](http://www.portal.p-grade.hu)**



# *Agenda of the morning*

- Introduction to workflow concept
- Workflow hands-on

## ~ **Break**

- Parameter studies
- Parameter study hands-on
  
- Further information and next steps



# Workflow

*The automation of a **business process**, in whole or part, during which documents, information or tasks are passed from one participant to another for action, according to a set of procedural rules to achieve, or contribute to, an overall business goal.*

*Workflow Reference Model, 19/11/1998*



WORKFLOW MANAGEMENT COALITION

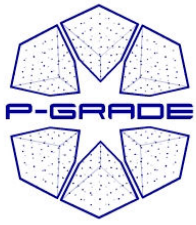
[www.wfmc.org](http://www.wfmc.org)

- Workflow management system (WFMS) is the software that does it



# *Why use workflows in Grid?*

- Build distributed applications through orchestration of multiple services
  - A single job or a single service is good for nothing...
- Integration of multiple teams involved
  - Collaborative work
- Unit of reusage
  - (E-)science requires traceable, repeatable analysis
- (Typically) ease of use grids
  - Graphical representation



# *Grid Workflow definition examples*

*Grid workflow can be defined as the composition of grid application services which execute on heterogeneous and distributed resources in a well-defined order to accomplish a specific goal.*

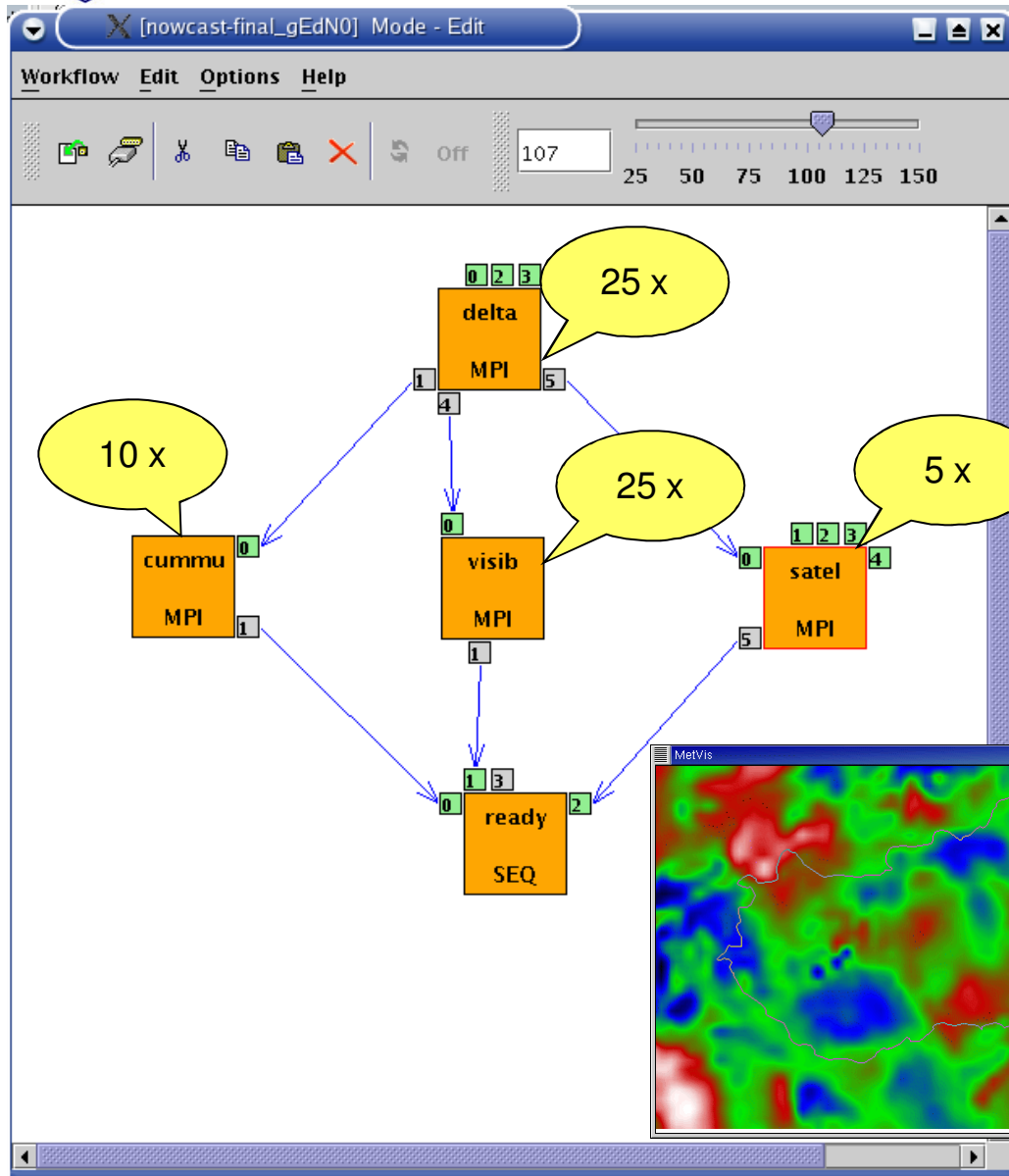
*R. Buyya*

*The automation of the processes, which involves the orchestration of a set of Grid services, agents and actors that must be combined together to solve a problem or to define a new service.*

*Geoffrey Fox [GGF 10]*



# Example: Ultra-short range weather forecast with P-GRADE Portal



Forecasting dangerous weather situations (storms, fog, etc.), crucial task in the protection of life and property

Processed information:  
surface level measurements, high-altitude measurements, radar, satellite, lightning, results of previous computed models

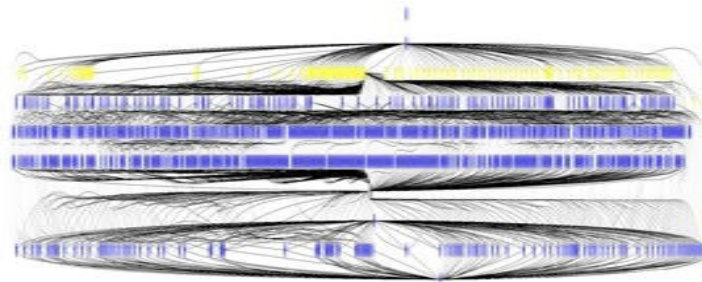
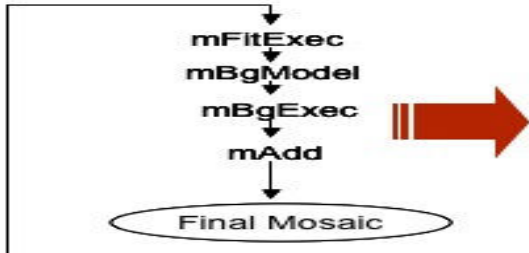
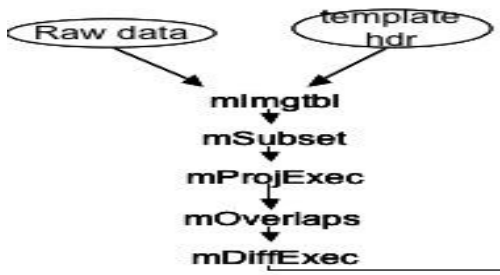
Requirements:

- Execution time < 10 min
- High resolution (1km)

Execution on a GT2 based Hungarian Grid



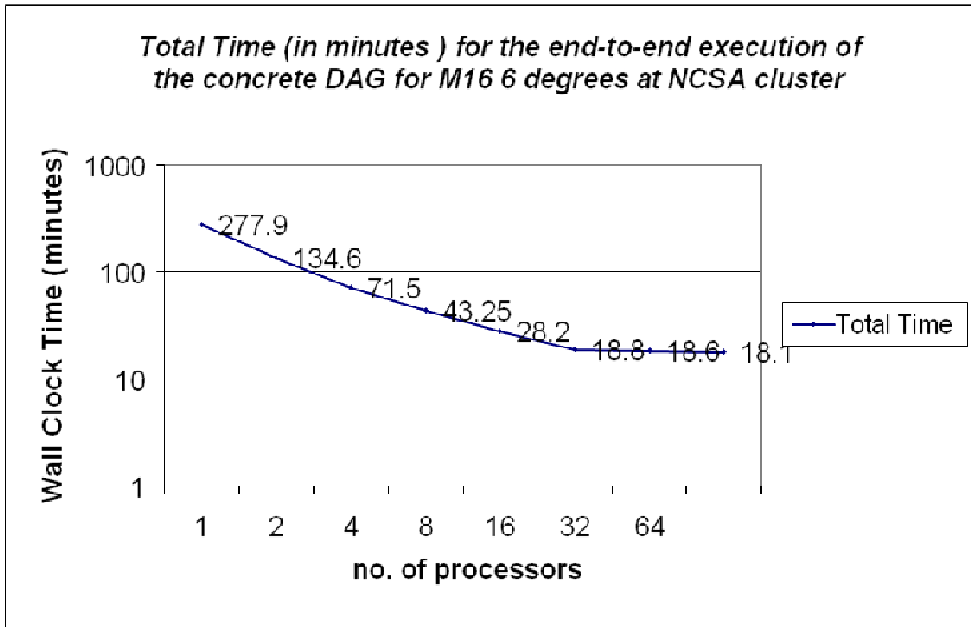
# Example: Montage workflow with Pegasus (and DAGMan)



*Tasks run on NSF's TeraGrid*

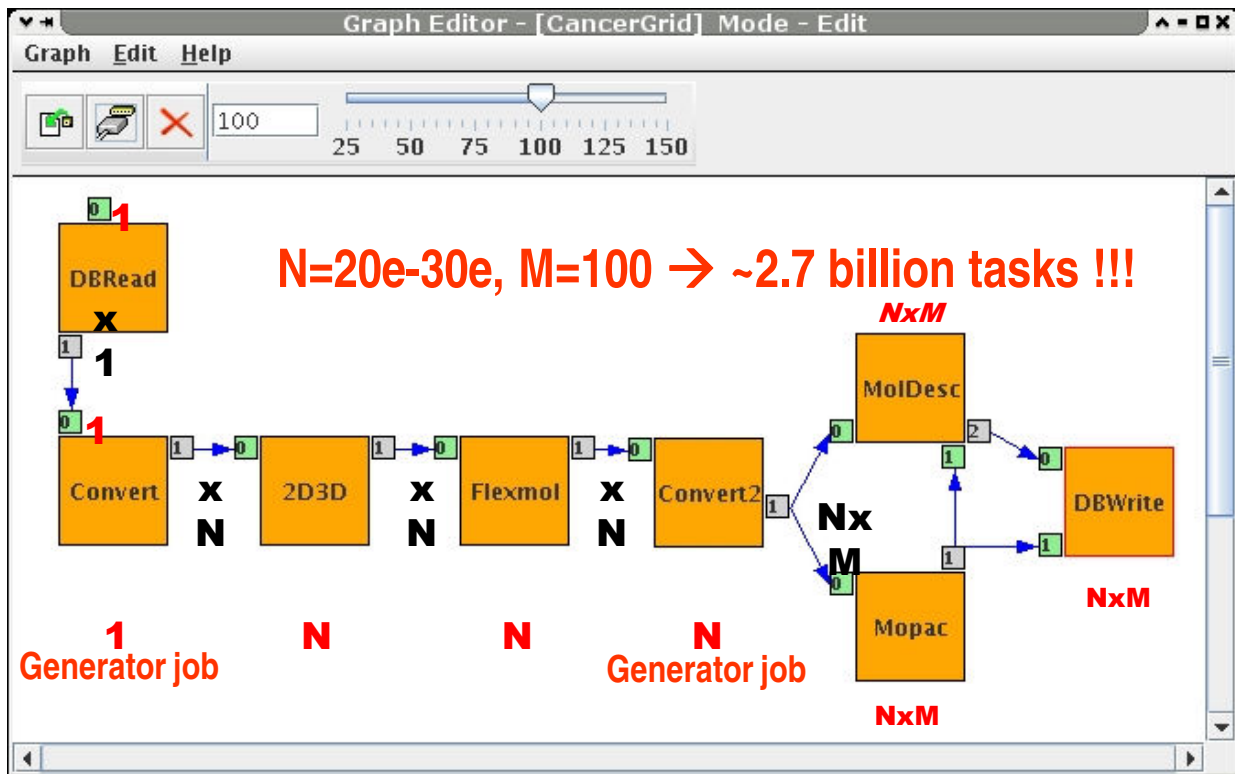
## Montage application

- ~7,000 compute jobs in instance*
- ~10,000 nodes in the executable workflow*
- same number of clusters as processors*
- speedup of ~15 on 32 processors*

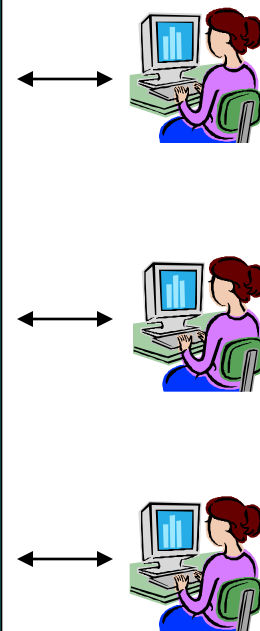
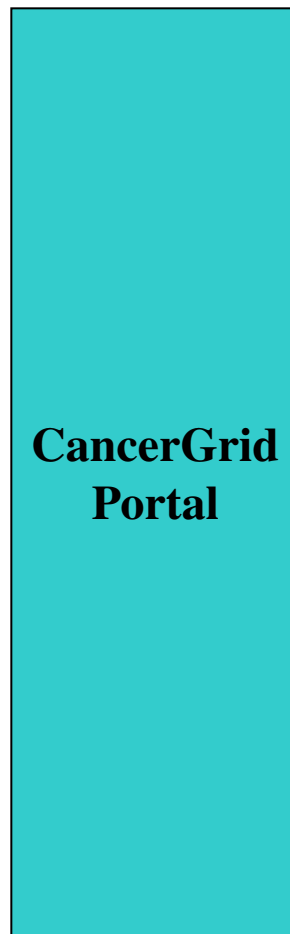




# Example: CancerGrid workflow with gUSE (and WS-PGRADE)



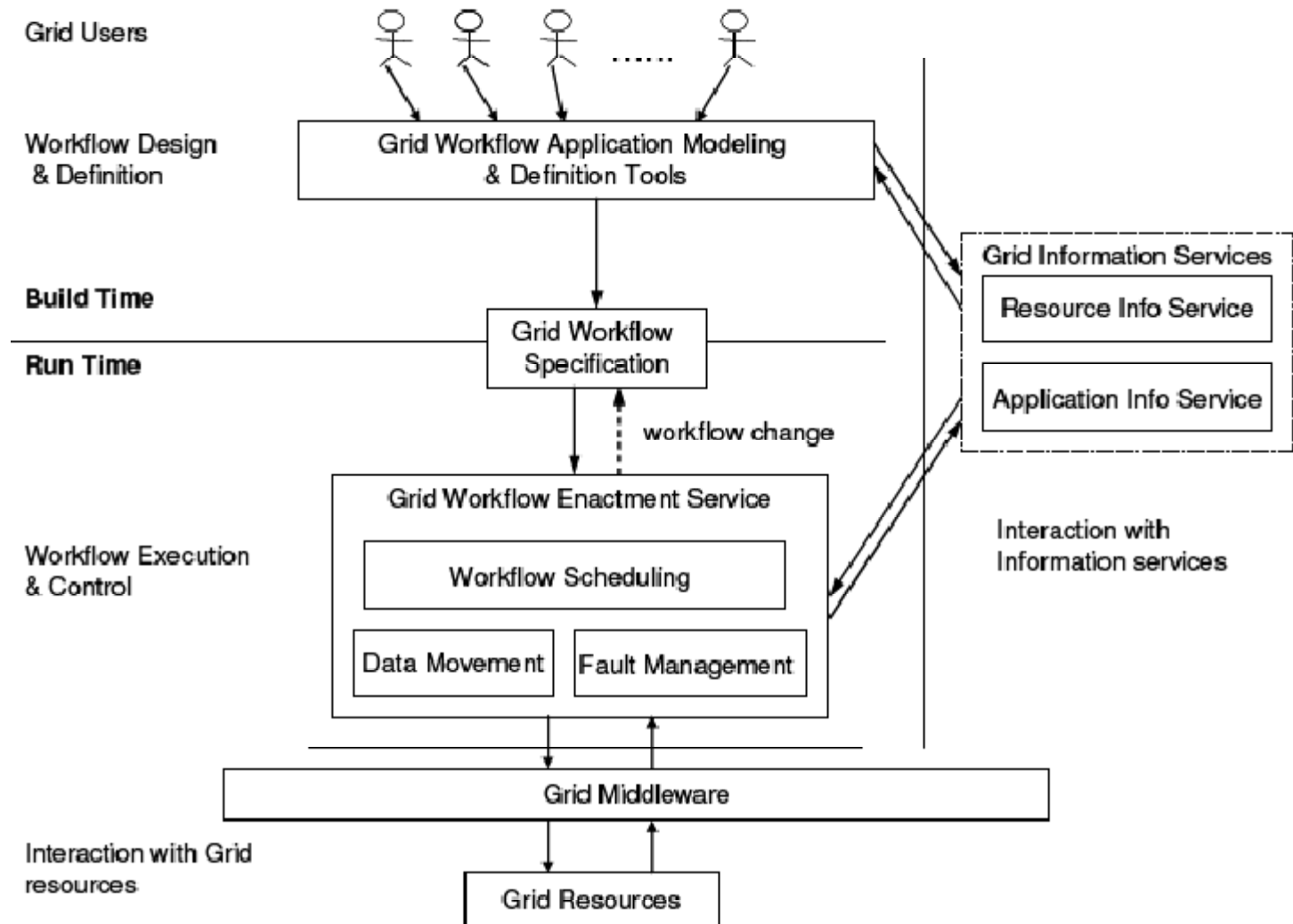
*Workflow is hidden from end users  
Tasks run on Desktop Grids and RDBMS*







# Grid WFMS



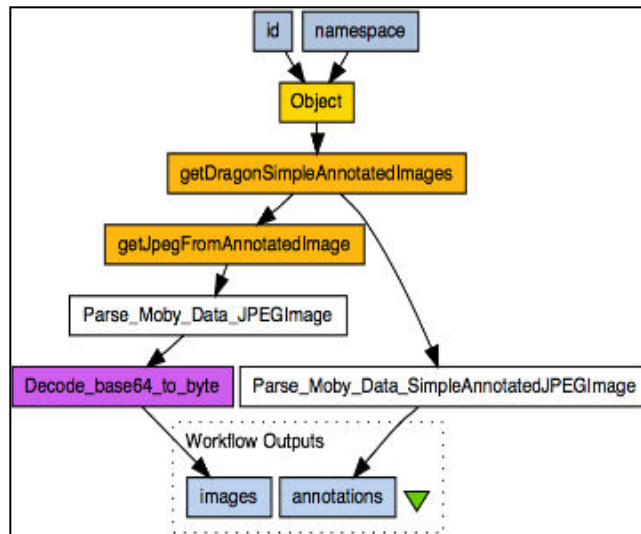
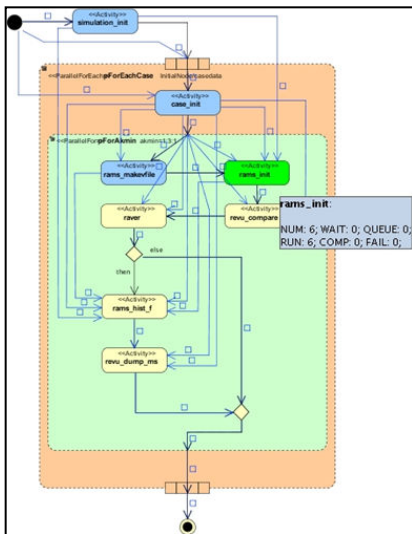
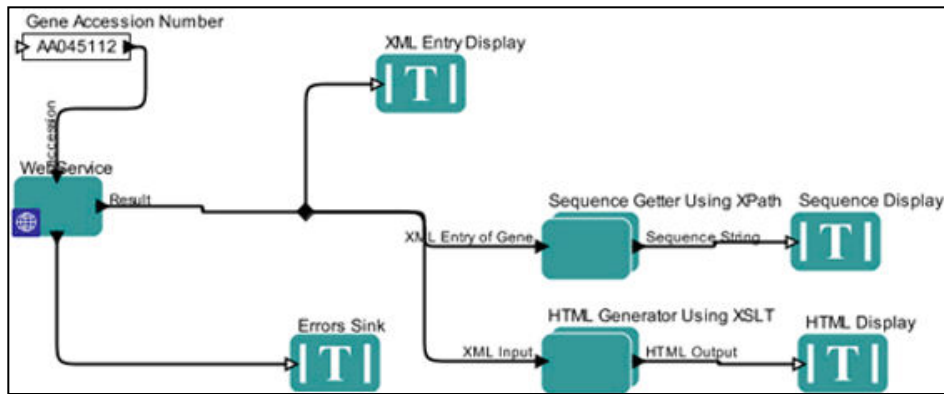
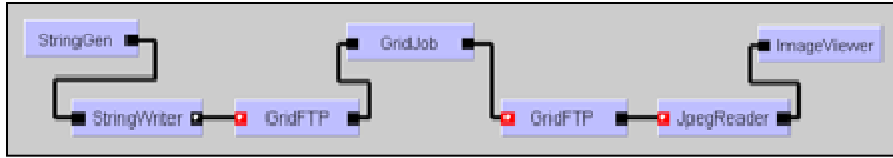


# *What does a typical Grid WFMS provide?*

- A level of abstraction above grid processes
  - gridftp, lcg-cr, lfc-mkdir, ...
  - condor-submit, globus-job-run, glite-wms-job-submit, ...
  - lcg-infosites, ...
- A level of abstraction above „legacy processes”
  - SQL read/write
  - HTTP file transfer
  - ...
- Automated mapping and execution of tasks grid resources
  - Submission of jobs
  - Invocation of (Web) services
  - Manage data
  - Catalog intermediate and final data products
- Improve successful application execution
- Improve application performance
- Provide provenance tracking capabilities



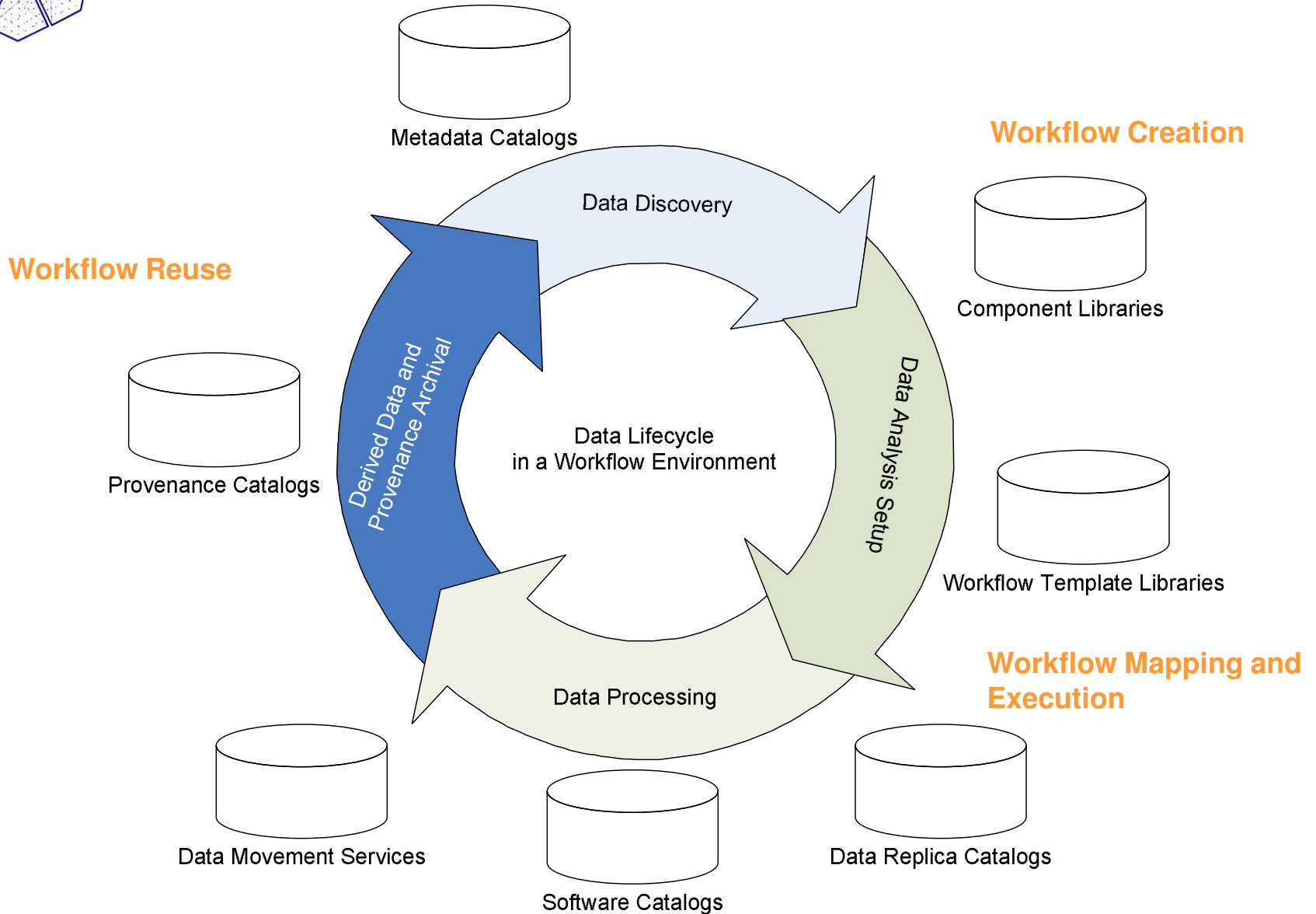
# What does a typical grid workflow consist of?



- Dataflow graph
- Activities
  - Definition of Jobs
  - Specification of services
- Data channels
  - Data transfer
  - Coordination
- Cyclic (DAG) /acyclic
- Conditional statements

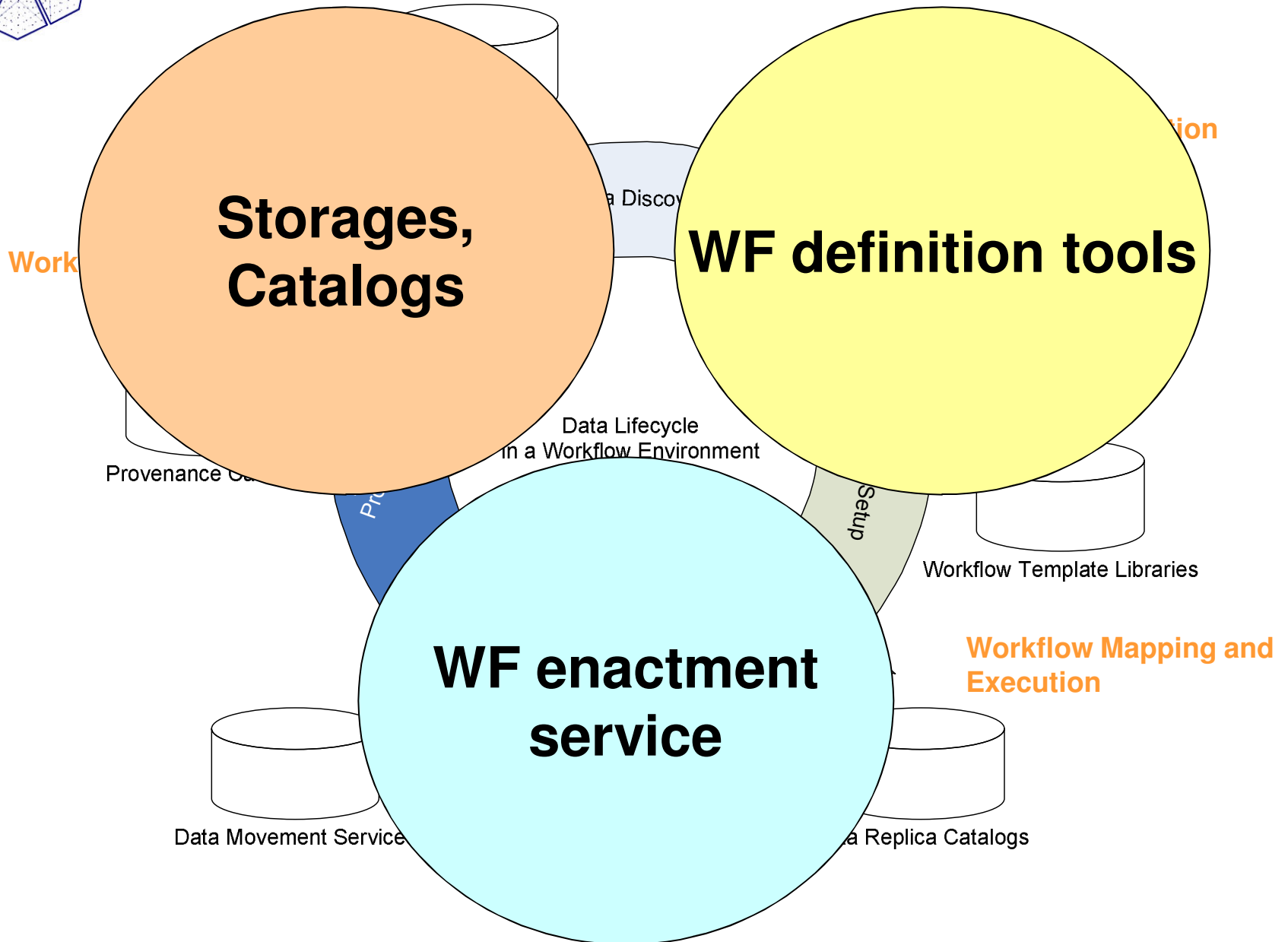


# Data lifecycle in workflows





# User interaction



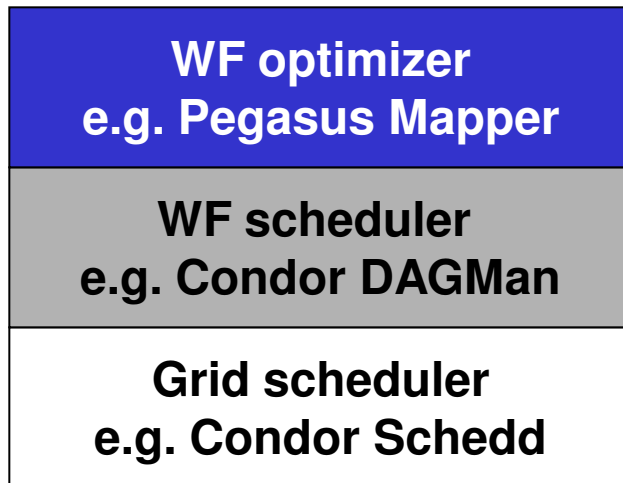


# Layered architecture of WFMS

Abstract Workflow



Results



A decision system that develops strategies for reliable and efficient execution in a variety of environments

Reliable and scalable execution of *dependent* tasks

Reliable, scalable execution of *independent* tasks (locally, across the network), priorities, scheduling

Cyberinfrastructure: Cluster, Condor pool, OSG, EGEE, TeraGrid



# *(Some of the) available grid workflow systems*

<http://www.gridworkflow.org>

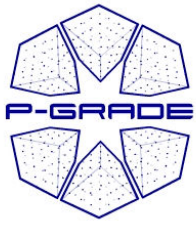


## Categories for

- Composition tools
- Description languages
  - Scientific
  - Industrial
  - Formalism
- Engines

## Some relevant tools for ARC, gLite, Globus, UNICORE grid users

- Condor DAGMan
  - Used as an enactor in P-GRADE Portal, Pegasus, ...
  - Uses DAGMan WF language (DAG = Directed Acyclic Graph)
- MOTEUR
  - Interfaced with “pilot job” framework on EGEE (pull style job execution)
  - Uses SCUFL WF language
- gLite WMS
  - Describe workflows in JDL
  - Share Input-Output sandboxes with multiple jobs
- Taverna
  - Mainly for cluster computing
  - ARC interface is available by Lubeck University
- ...

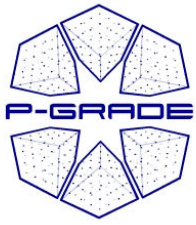


# ***P-GRADE Portal***

A Grid WFMS

[www.portal.p-grade.hu](http://www.portal.p-grade.hu)





# *Short History of P-GRADE portal*

- **P**arallel **G**rid **A**pplication **D**evelopment **E**nvironment
- Initial development started in the Hungarian SuperComputing Grid project in 2003
- It has been continuously developed since 2003
  - Around 30 manyear development + training + user support
- Detailed information: <http://portal.p-grade.hu/>
- Open Source community development since January 2008:  
<https://sourceforge.net/projects/pgportal/>
- Current version: 2.8



# *Current P-GRADE Portal related projects*

- **GGF GIN** (Since 2006)
  - Providing the GIN Resource Testing portal
- **EU EGEE-II, EGEE-III** (2006-2010)
  - Tool recommended for application development
  - Intensively used in new users' training
- **EU SEE-GRID-SCI** (2008-2010)
  - Interfacing to DSpace-based workflow storage
  - Infrastructure testing workflows
- **EU CancerGrid** (2007-2009)
  - Development of new generation P-GRADE (gUSE and WS-PGRADE)
  - Integration with desktop grids
- **EU EDGeS** (2008-2009)
  - Transparent access to Desktop Grid systems



# Portal installations

## P-GRADE Portal services:

- SEE-GRID infrastructure
- Several VOs of EGEE:
  - Biomed, Astronomy, Central European, NA4,...
- GILDA: Training VO of EGEE
- Many national Grids (UK National Grid Service, HunGrid, Turkish Grid, etc.)
- US Open Science Grid, TeraGrid
- OGF Grid Interoperability Now (GIN) VO
- ...

## Portal services and account request:

<http://portal.p-grade.hu/index.php?m=3&s=0>

Account request form on portal login page





# Multi-Grid portal installation:

## [www.lpds.sztaki.hu/multi-grid](http://www.lpds.sztaki.hu/multi-grid)

PGrade Grid portal - Microsoft Internet Explorer

Address: <https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=99>

Settings

### GRID configurations

Name	Information System			BaseDn	[Actions]
	Type	Host	Port		
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



# ***Design principles of P-GRADE portal***

- **P-GRADE Portal is not only a user interface**, it is a
  - General purpose
  - Workflow-level
  - Multi-Grid
  - Application Development and Execution Environment
- **P-GRADE Portal includes a high-level middleware layer** for orchestrating jobs on grid resources
  - inside a grid
  - among several different grids (and several VOs)
- **P-GRADE Portal is grid-neutral**:
  - Unlike many existing grid portals it is not tailored to any particular grid type
  - Can be connected to various grids based on different grid middleware
    - LCG-2, gLite, GT2, GT4, ARC, Unicore, etc.
  - Implements the high-level grid middleware services on top of the existing grid middleware services
  - The workflow interface is the same no matter which type of grid is connected to it



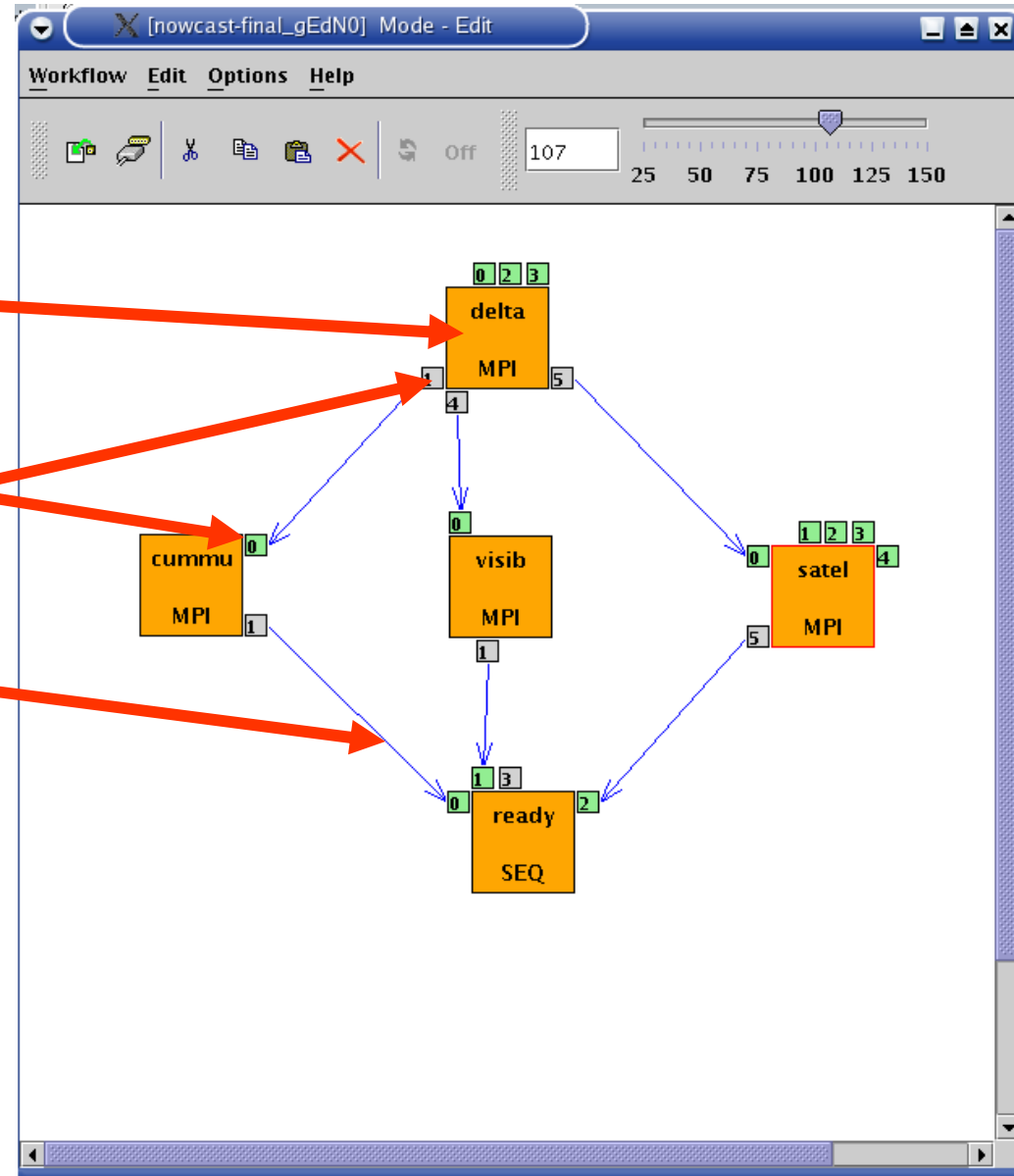
# What is a P-GRADE Portal workflow?

- **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





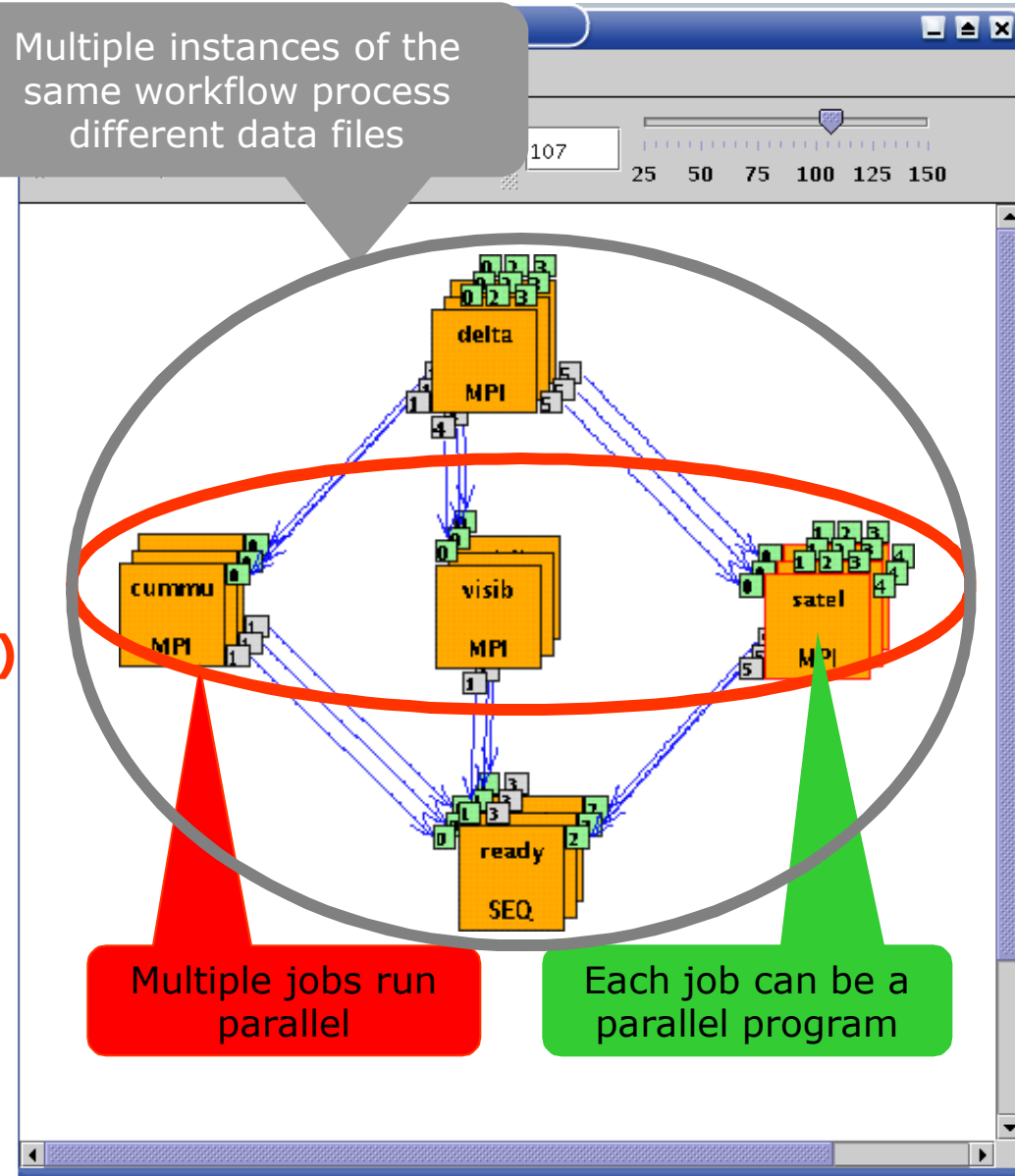
# Three levels of parallelism

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

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

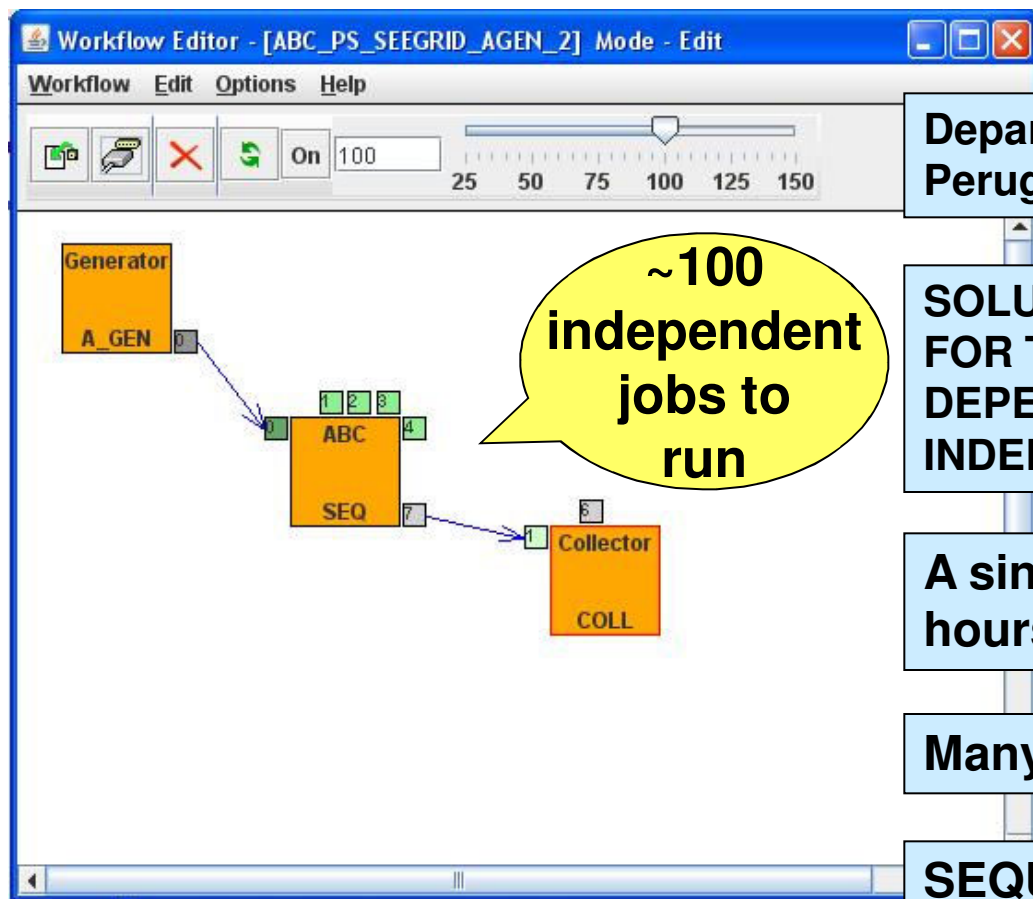
– **PS workflow level: Parameter study execution of the workflow**

Multiple instances of the same workflow process different data files





# Example: Computational Chemistry



Department of Chemistry, University of Perugia

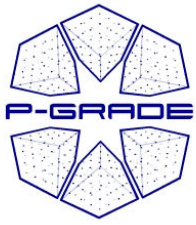
SOLUTION OF SCHRODINGER EQUATION FOR TRIATOMIC SYSTEMS USING TIME-DEPENDENT (RWAVEPR) OR TIME INDEPENDENT (ABC) METHOD

A single execution can be between 5 hours and 10 hours

Many simulations at the same time

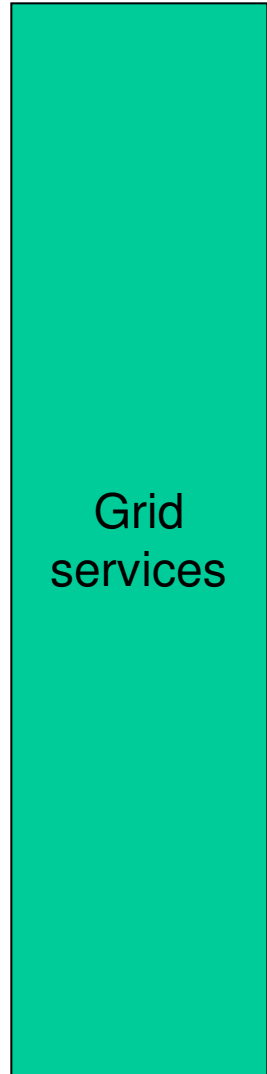
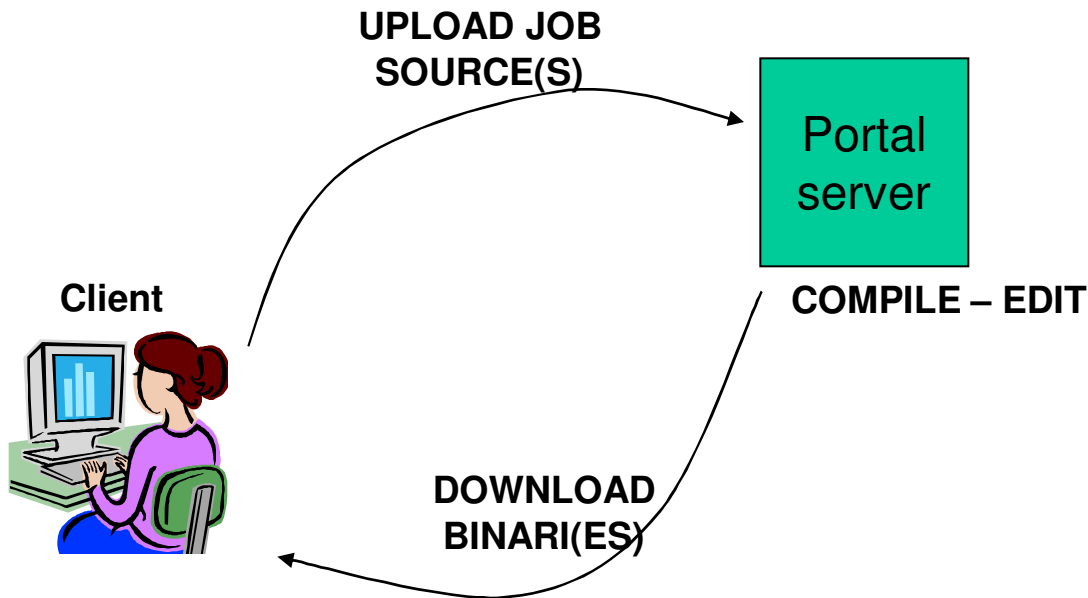
SEQUENTIAL FORTRAN 90





# Typical user scenario

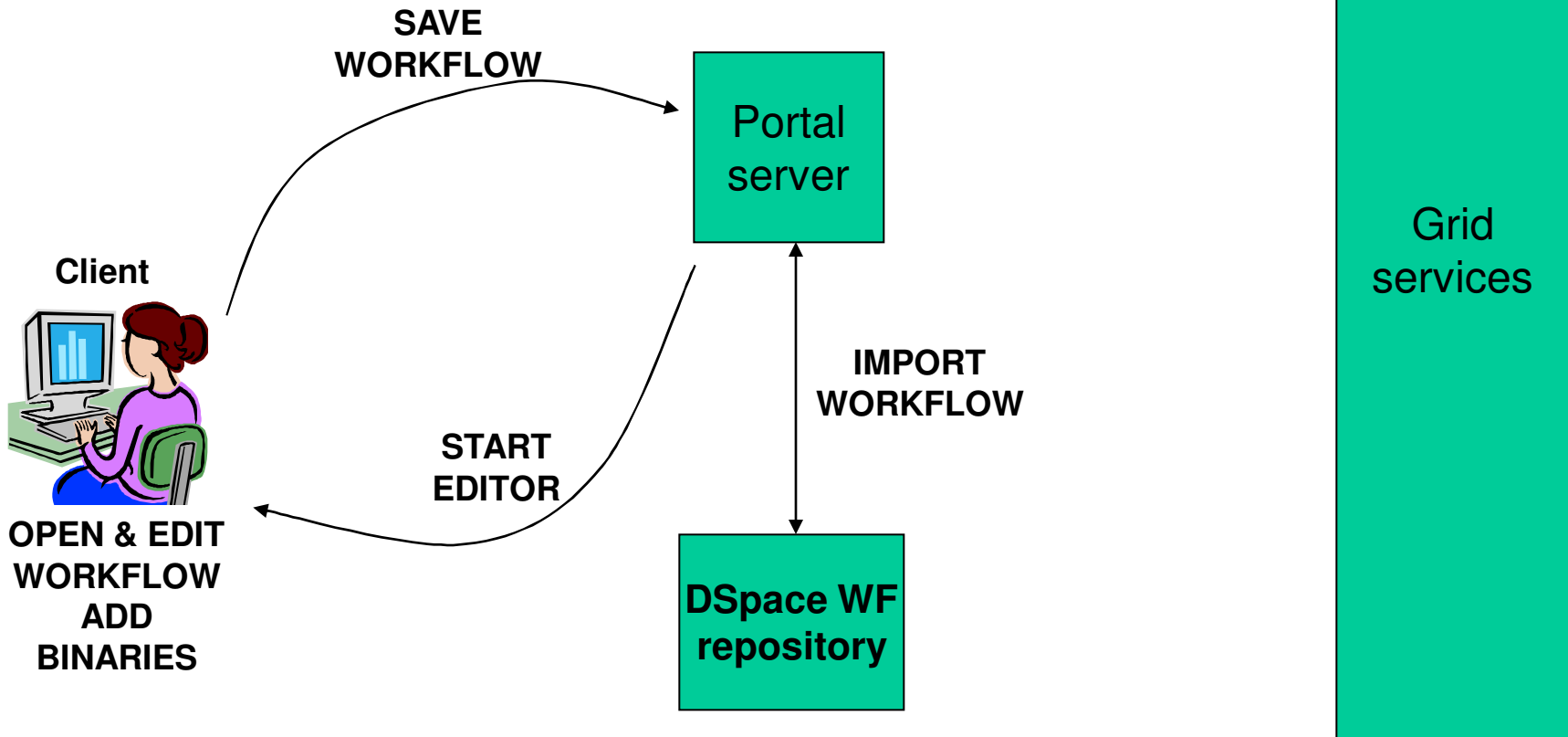
## Job compilation phase





# Typical user scenario

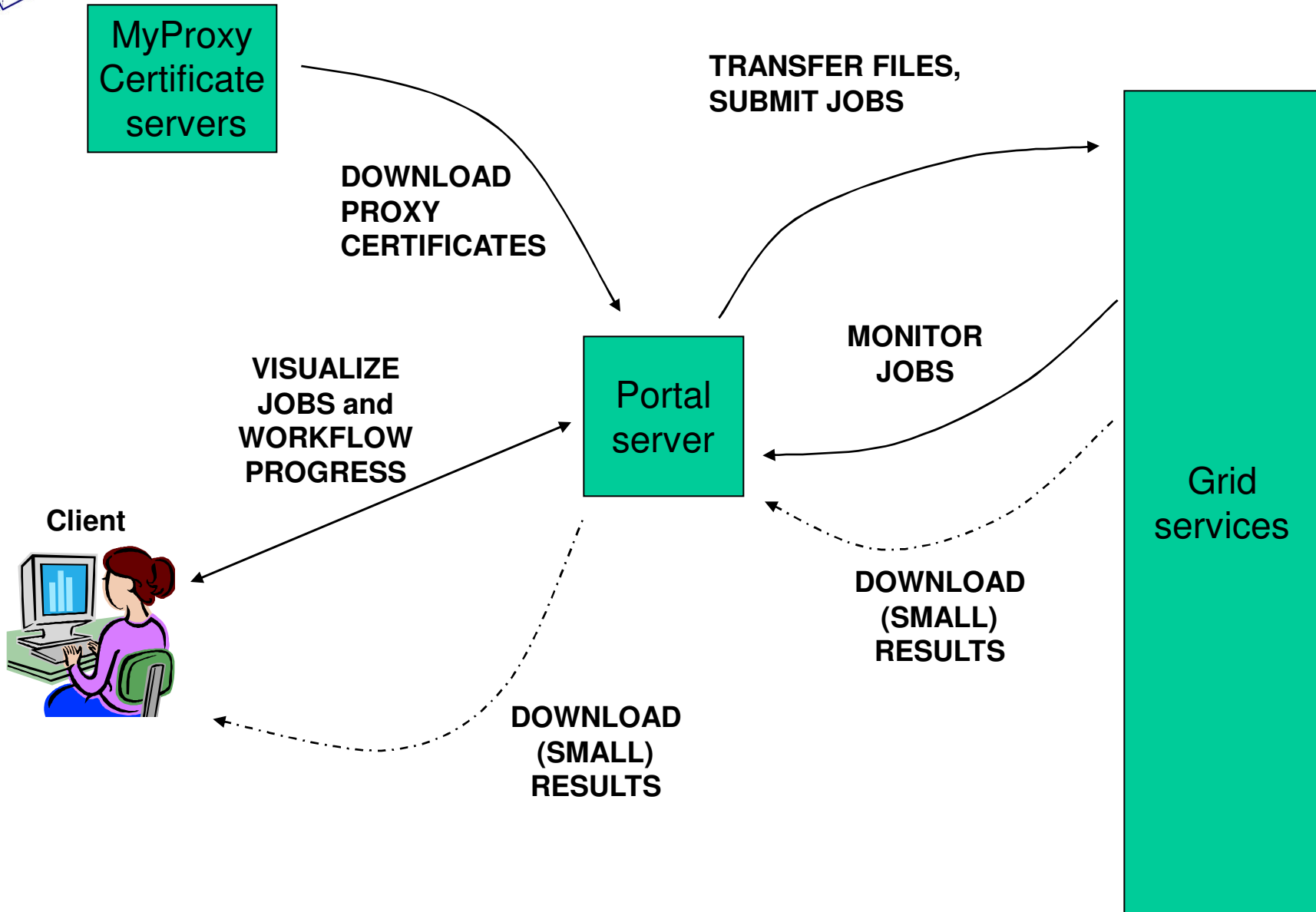
## Workflow development phase





# Typical user scenarios

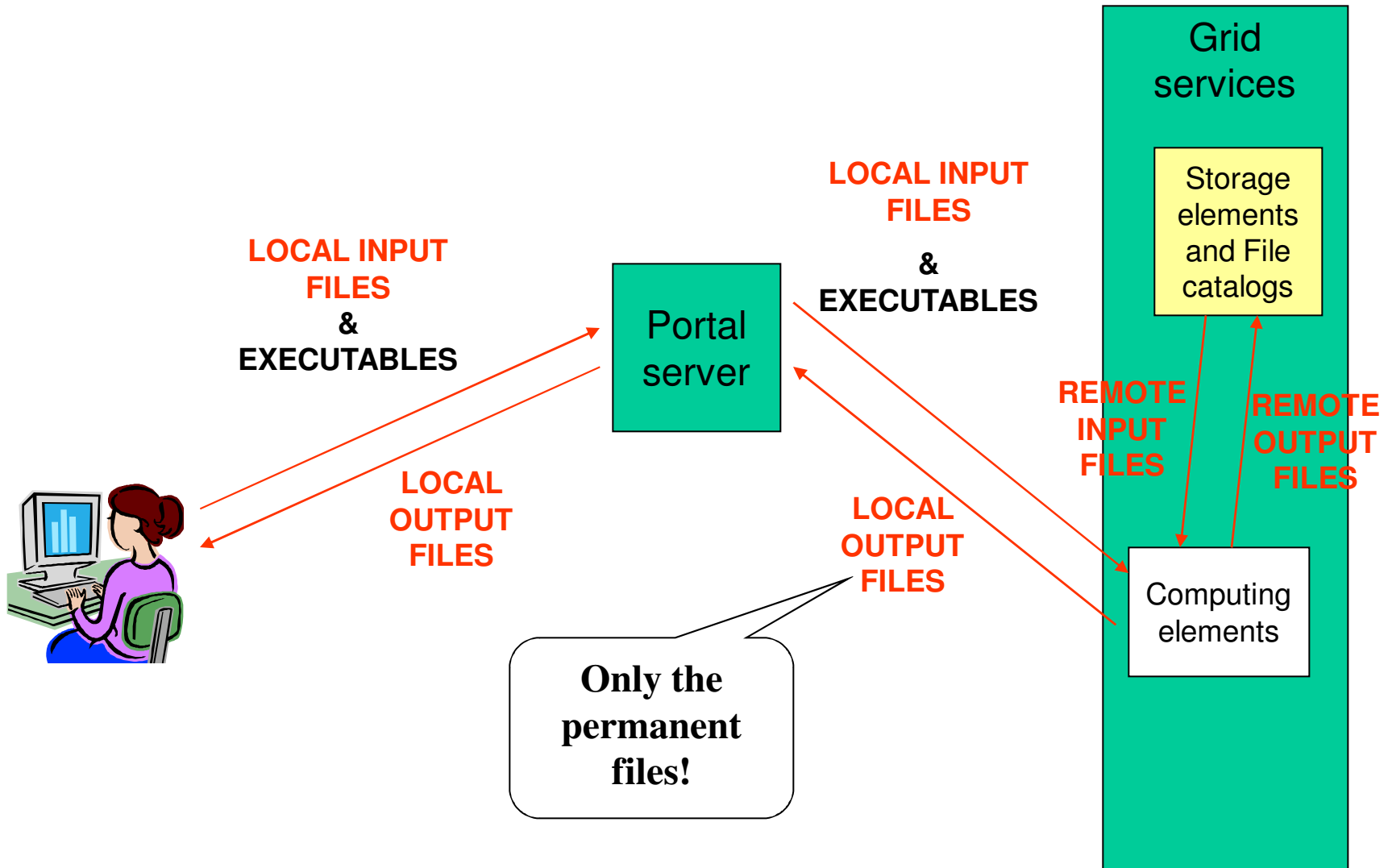
## Workflow execution phase





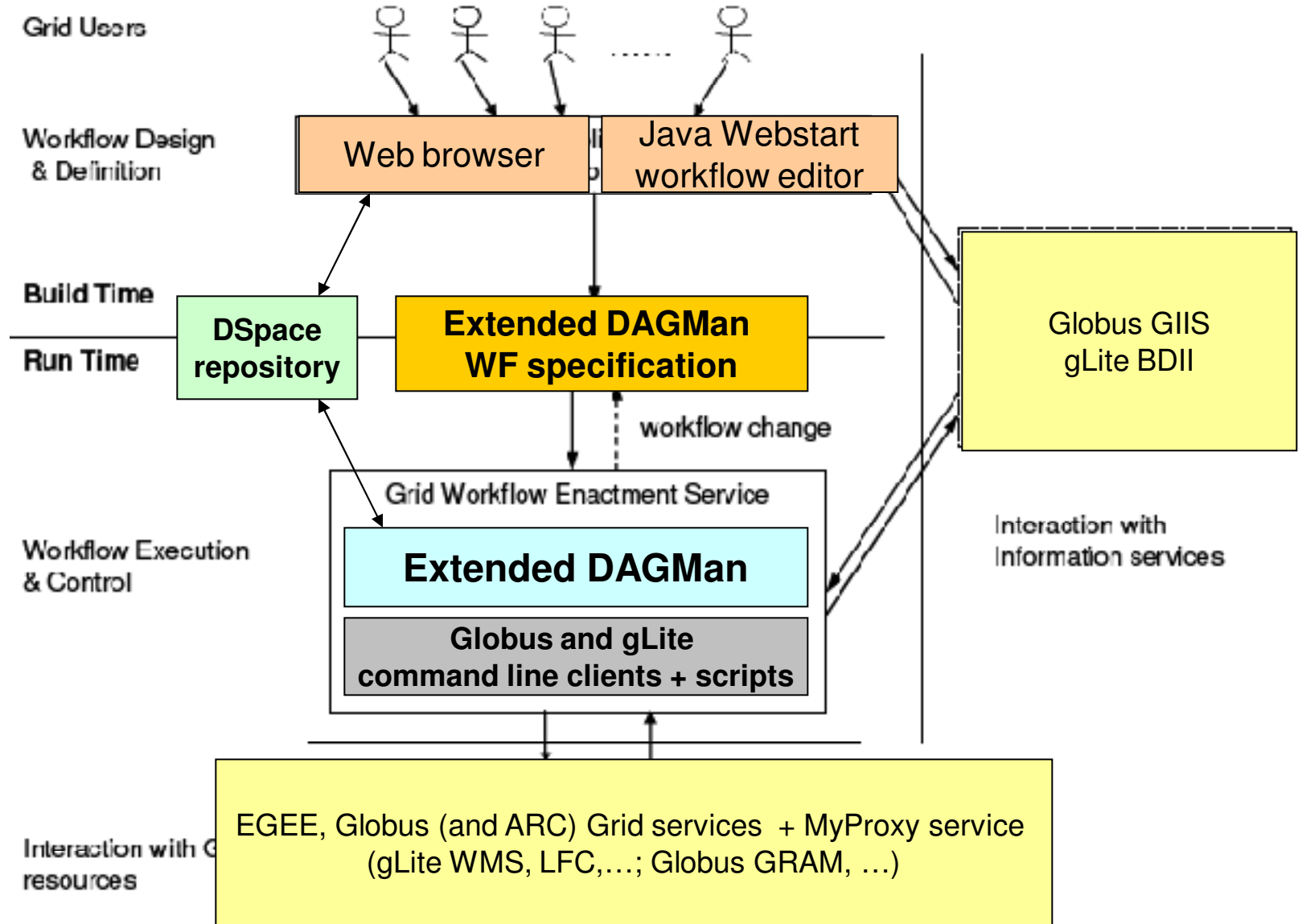
# Accessing local and remote files

Use legacy executables with Grid files without touching the code





# P-GRADE Portal structural overview





# Web interface - Portlets

PGrade Grid portal - Windows Internet Explorer



RELEASE 2.7



Welcome Workflow Certificates Settings Information System File Management Compiler Portlet Help

Settings Layout

?

## Profile Manager

Organization: MTA SZTAKI  
Roles: USER  
timezone: Europe/Budapest  
Europe/Chisinau  
Europe/Copenhagen  
Europe/Dublin  
Europe/Gibraltar  
Europe/Guernsey

Save

Update password  
Enter original password:   
Password:   
Confirm password:

Save

Configure group membership  
Groups: Group Description:  
 szupergrid szupergrid desc

Save

Done

Internet

100%



# Email notifications

PGrade Grid portal - Windows Internet Explorer

https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=notify

RELEASE 2.7

Kijelentkezés  
Üdvözöllek!, user14

**NOTIFY**

Üdvözöllek | Workflow | Certificates | **Settings** | Information System | File Management | Compiler Portlet | Help

Workflow Manager | Storage | Upload | Notify

### Notifications

**Email Settings:**

Enabled: Yes

Email Address: sipos@sztaki.hu

Email Subject: P-GRADE Portal workflow state change

**Workflow Change Settings:**

Enabled: Yes

Message:

```
Time: #now#  
P-GRADE Portal account: #user#  
P-GRADE Portal installation: #portal#  
Workflow name: #workflow#  
Old status: #oldstatus#  
New status: #newstatus#  
Details: #details#
```

key list:  
#now#  
#user#  
#portal#  
#workflow#  
#oldstatus#  
#newstatus#  
#details#



# Workflow portlet

PGrade Grid portal - Windows Internet Explorer

https://pgrade-portal.sztaki.hu/gridsphere/gridsphere?cid=71

PGrade Grid portal

RELEASE 2.7

**P-GRADE** portal

Logout  
Welcome, Sipos Gergely

Welcome Workflow Certificates Settings Information System File Management Compiler Portlet Help

Workflow Manager Storage Upload Notify

**Workflow Manager**

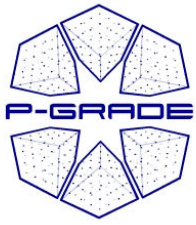
Workflow Editor Refresh

Workflow	Status	Size	Quota (100 Mb)	[ Output ]	[ View ]	[ Action ]
080225_fem25d_ps_gen_coll_ha	incomplete	1.911 [MB]	1.91%	N/A	PS Details	Attach Delete
080225_fem25d_ps_gen_coll_ha_farkasz	init	616.352 [KB]	0.60%	N/A	PS Details	Submit Attach Delete
080225_fem25d_ps_gen_coll_ha_totha	init	616.731 [KB]	0.60%	N/A	PS Details	Submit Attach Delete
0_Rod_Traffic-simulation_workflow	incomplete	956.896 [KB]	0.93%	N/A	Details	Attach Delete
1_det2x2	init	204.702 [KB]	0.20%	N/A	Details	Submit Attach Delete
2_Matrix_27_hatvany	init	122.137 [KB]	0.12%	N/A	Details	Submit Attach Delete

https://pgrade-portal.sztaki.hu/gridsphere/gridsphere?cid=77&gs\_action=doDeleteWorkflow

Internet 100%

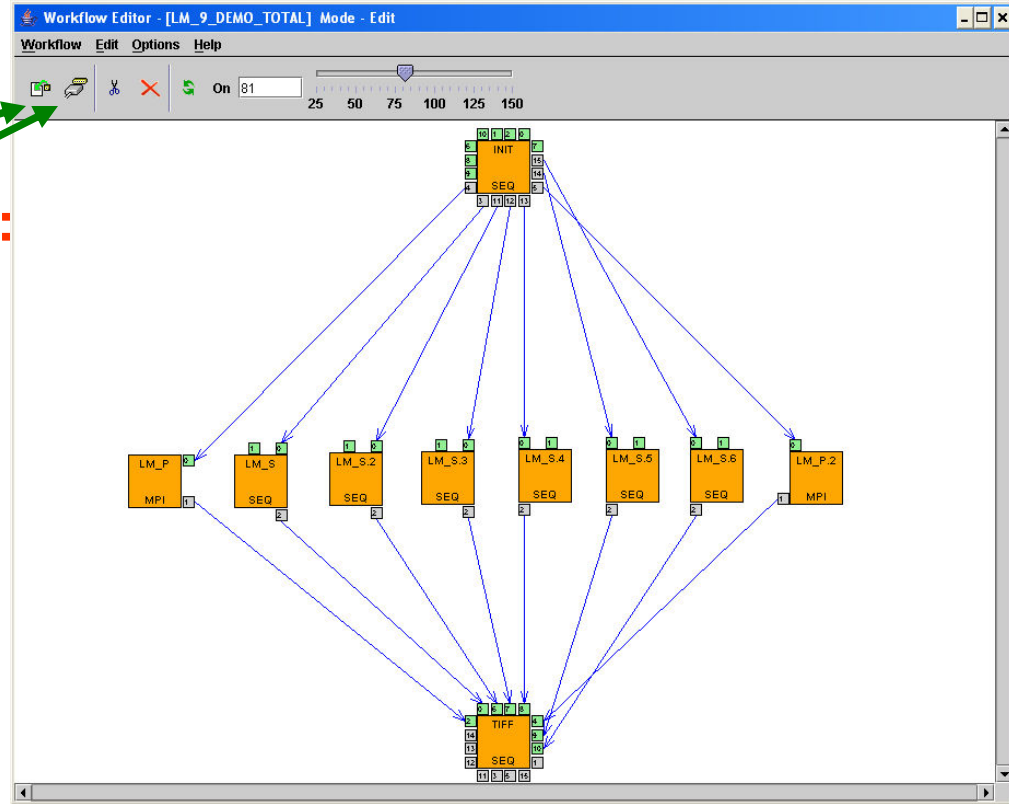




# Graphical workflow editing

- To define a graph:
  1. **Drag & drop components:**  
jobs and ports
  2. **Define their properties**
  3. **Connect ports by channels**  
(no cycles, no loops)

System generates JDL for each job automatically





# Workflow Editor

## Properties of a job

Workflow Editor - [LM\_9\_DEMO\_TOTAL] Mode - Edit

Workflow Edit Options Help

LM\_P properties

Name: LM\_P

Job Type:  SEQ  MPI  PVM

Job Executable: LM\_5.bin

File Browser

Instrument

Process Number: 7

Attributes: -n -m

Grid: SEE-GRID

Monitor:

Resource: n40.hpcc.sztaki.hu:jobmanager-fork  
ce01.grid.acad.bg:jobmanager-fork  
grid-ce.ii.edu.mk:jobmanager-fork  
grid1.irb.hr:jobmanager-fork  
grid1.netmode.ece.ntua.gr:jobmanager-fork  
n40.hpcc.sztaki.hu:jobmanager-fork  
prof.salla6.inima.al:jobmanager-fork

### Properties of a job:

- Executable file
- Type of executable (Sequential / Parallel)
- Command line parameters
- Which resource to use?
  - Which VO?
  - Broker or Computing element?



# Workflow Editor

## Defining input-output files

Job0 / 0 properties

Port name

Type  In  Out

File type  Local  Remote

File   
  managed copy

Internal File Name

File storage type  Permanent  Volatile

### File properties

#### Type:

**input:** *the executable reads*  
**output:** *the executable generates*

#### File type:

**local:** *comes from my desktop*  
**remote:** *comes from an SE*

#### File:

*location of the file*

#### Internal file name:

**Executable uses this**  
**e.g. fopen("file.in", ...)**

#### File storage type (output files only):

**Permanent:** *final result*

**Volatile:** *temp. 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`

- 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/11-04.dat`

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

### Remote file

# Upload a workflow from client side or from FTP server



PGrade Grid portal - Windows Internet Explorer

https://pgrade-portal.sztaki.hu/gridsphere/gridsphere?cid=pgradeupload

RELEASE 2.7

**P-GRADE** portal

Logout  
Welcome, Sipos Gergely

Welcome Workflow **Upload** Certificates Settings Information System File Management Compiler Portlet Help

Workflow Manager Storage Upload Notify

**Upload**

Workflow archive:  Browse... OK

Equation solver : gilda gLite broker  
 Equation solver : gilda LCG2 broker  
 Equation solver : voce direct  
 Equation solver Parameter Study : seegrid gLite broker  
 Equation solver single input : voce gLite broker  
 Equation solver : seegrid direct  
 Matrix op : hungrid direct  
 Matrix op : hungrid broker

Demo Workflows  Equation solver single input : seegrid gLite broker OK  
 Equation solver : seegrid gLite broker  
 MPI job with on line translation : gilda gLite broker  
 Equation solver : voce gLite broker  
 Equation solver Parameter Study : gilda gLite broker  
 Equation solver Parameter Study : voce gLite broker  
 Site test : gilda gLite broker  
 JavaDemoThirdPower : voce gLite broker  
 JavaDemoThirdPower : seegrid gLite broker

Upload all

**STORED on FTP server**

Internet 100%



# Importing an application

PGrade Grid portal - Windows Internet Explorer

https://pgrade-portal.sztaki.hu/gridsphere/gridsphere?cid=77&gs\_action=doRefreshList

PGrade Grid portal

RELEASE 2.7

**P-GRADE** portal

MTA SZTAKI

Logout  
Welcome, user01

Welcome Workflow Certificates Settings Information System File Management Compiler Portlet Help

Workflow Manager Storage Upload Notify

Workflow Manager

Workflow Editor Refresh

Workflow	Status	Size	Quota (100 Mb)	[ Output ]	[ View ]	[ Action ]
Traffic-simulation	incomplete	915.018 [KB]	0.89%	N/A	Details	Attach Delete
<b>Overall used quota:</b>		915.018 [KB]	0.89%			

**INCOMPLETE WORKFLOW → Open it in editor and save it again** Delete all Submit All

February 26, 2009

Internet 100%



# Import a workflow from DSpace repository

RELEASE 2.8

**P-GRADE** portal

Logout  
Welcome, Sipos Gergely

MTA SZTAKI

Welcome | Workflow | Certificates | Settings | Information System | File Management | Compiler Portlet | **DSpace Repository** | Help

Download/DSpaceView Upload

**Download**

Download Workflow  
**NO HANDLE ENTERED**  
DSpace Handle:   Browse to a workflow below to find its handle (e.g. dspace/1)

**DSpace View**

**DSpace™** About DSpace Software

**P-GRADE** Workflow repository portal

**Search DSpace**  
   
[Advanced Search](#)  
[Home](#)

**Browse**  
[Communities & Collections](#)  
[Issue Date](#)  
[Author](#)  
[Title](#)  
[Subject](#)

**Sign on to:**  
[Receive email updates](#)  
[My DSpace](#) authorized users  
[Edit Profile](#)  
[Help](#)

DSpace on P-Grade Portal >

**DSpace is Live**  
Welcome to our digital repository for the P-Grade Portal!

**Search**  
Enter some text in the box below to search DSpace.

**Communities in DSpace**  
Choose a community to browse its collections.  
[P-Grade Portal Repository](#)

**Welcome to the Workflow Repository on the P-Grade Portal.**  
The aim of the repository is to facilitate collaborative development and information dissemination among P-Grade Portal users. This is accomplished by allowing users to browse, search, download, and upload application

https://pgrade-dspace.sztaki.hu/jspui/handle/dspace/43

Internet 100%



# External access to DSpace

## <http://pgrade-dspace.sztaki.hu>

DSpace on P-GRADE Portal: Home - Windows Internet Explorer

https://pgrade-dspace.sztaki.hu/jspui/

DSpace on P-GRADE Portal: Home

**DSpace™** **P-GRADE** Workflow repository portal

About DSpace Software

**Search DSpace**

[Advanced Search](#)

[Home](#)

**Browse**

- [Communities & Collections](#)
- [Issue Date](#)
- [Author](#)
- [Title](#)
- [Subject](#)

**Sign on to:**

- [Receive email updates](#)
- [My DSpace authorized users](#)
- [Edit Profile](#)
- [Help](#)
- [About DSpace](#)

DSpace on P-GRADE Portal >

**DSpace is Live**

Welcome to our digital repository for the P-GRADE Portal!

**Search**

Enter some text in the box below to search DSpace.

**Communities in DSpace**

Choose a community to browse its collections.

[P-GRADE Portal Repository](#)

**Welcome to the Workflow Repository on the P-GRADE Portal.**

The aim of the repository is to facilitate collaborative development and information dissemination among P-GRADE Portal users. This is accomplished by allowing users to browse, search, download, and upload application workflows and other files to/from their local machine or Portal storage space.

[DSpace Software](#) Copyright © 2002-2008 The DSpace Foundation - [Feedback](#)

https://pgrade-dspace.sztaki.hu/jspui/handle/dspace/43

Internet 100%






# Certificate and proxy management Portlet


PGrade Grid portal - Windows Internet Explorer

https://pgrade-portal.sztaki.hu/gridsphere/gridsphere?cid=103&gs\_action=doMapProxy

PGrade Grid portal

RELEASE 2.7

 **P-GRADE** portal



Logout  
Welcome, Sipos Gergely

Welcome Workflow **Certificates** Settings Information System File Management Compiler Portlet Help

Certificates

Certificate Manager

Certificate list

Issuer	Set for Grids	Time left	[Actions]
C=IT,O=GILDA,OU=Personal Certificate,L=CATANIA,CN=CATANIA01,CN=proxy	gilda_GLITE_BROKER	99:59:54	Details Set for Grid Delete

Refresh

Download (Download certificate from MyProxy server.) Upload (Upload authentication data to MyProxy server.)

Credential Management (Display information, change MyProxy passphrase, remove a credential from MyProxy server.)

**Message:** Certificate successfully set for gilda\_GLITE\_BROKER.

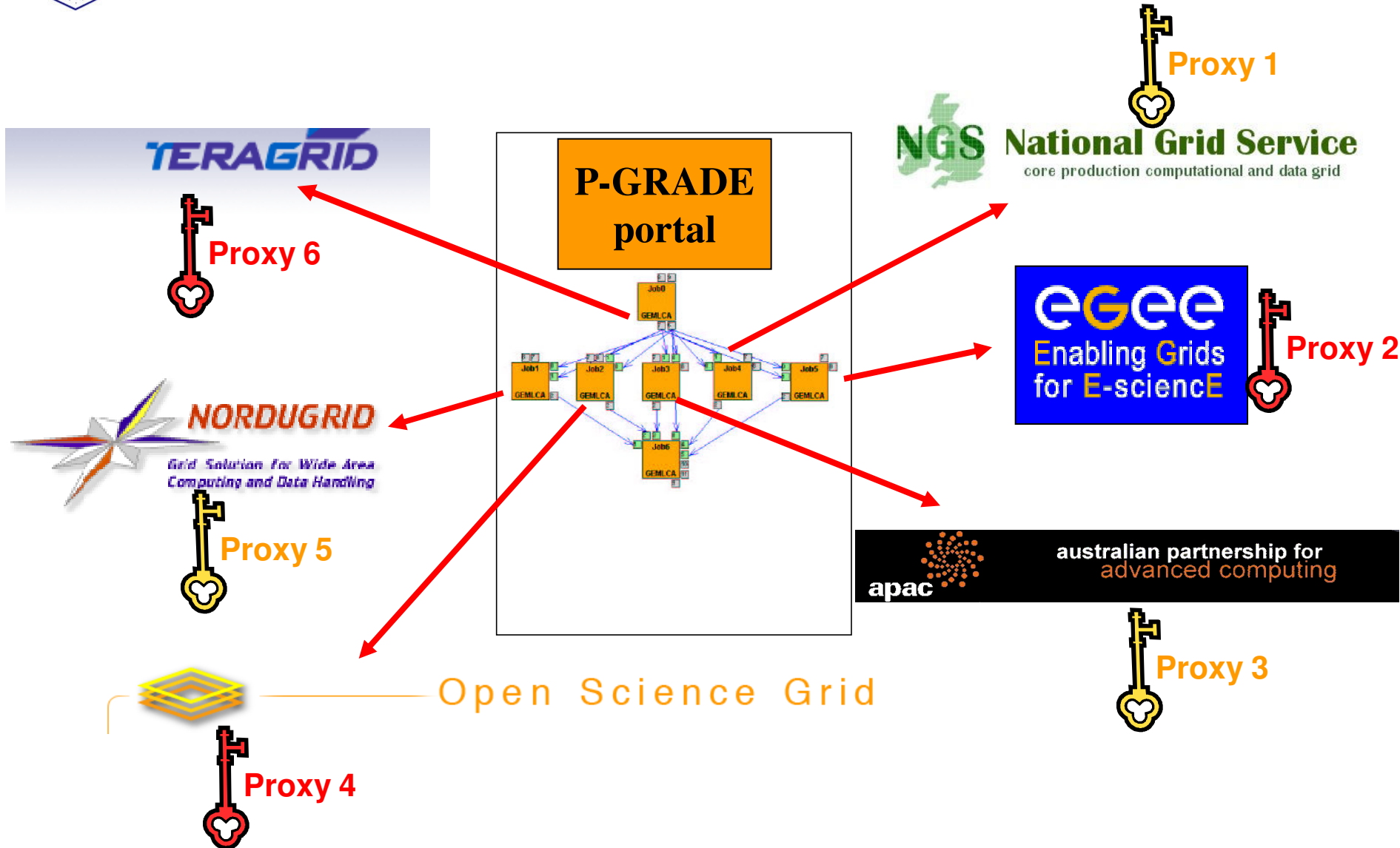
February 26, 2009

Internet 100%



# OGF GIN interoperability portal by P-GRADE

Accessing Globus, gLite and ARC based grids/VOs simultaneously





# Application execution

PGrade Grid portal - Windows Internet Explorer

https://pgrade-portal.sztaki.hu/gridsphere/gridsphere?cid=77&gs\_action=doShowWorkflowDetails

non-techies

PGrade Grid portal

RELEASE 2.7

**P-GRADE** portal

Logout  
Welcome, user01

Welcome Workflow Certificates Settings Information System File Management Compiler Portlet Help

Workflow Manager Storage Upload Notify

Workflow Manager

Refresh Back

Job list								
Workflow	Job	Gridname	Hostname	Status	[ Logs ]	[ Output ]	[ Visualization ]	[ Action ]
Traffic-simulation				finished	-	✓	Visualize All	Submit Attach Delete
	Job0	gilda_GLITE_BROKER	iceage-ce-01 .ct.infn.it	finished	Out - Log	✓		-
	Job1	gilda_GLITE_BROKER	iceage-ce-01 .ct.infn.it	finished	Out - Log	✓		-
	Job2	gilda_GLITE_BROKER	iceage-ce-01 .ct.infn.it	finished	Out - Log	✓		-
	Job3	gilda_GLITE_BROKER	vega-ce.ct.infn.it	finished	Out - Log	✓		-

**Message:** Workflow details successfully displayed.

February 26, 2009

Internet 100%



# ***Fault-tolerant execution***

- 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



# Information system visualization

PGrade Grid portal - Microsoft Internet Explorer

Address: https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=119&gs\_action=doChangeVO

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	
<a href="#">bmegrid</a>	32	2	94%	30	2	6%	142.498 [GB]	142.498 [GB]	0%	
<a href="#">budapest</a>	321	213	34%	108	53	33%	5.402 [TB]	5.402 [TB]	0%	
<a href="#">cyfronet-icg2</a>	562	221	61%	327	109	25%	82.497 [TB]	30.091 [TB]	64%	
<a href="#">egee.fesb.hr</a>	24	1	96%	23	6	21%	446.796 [GB]	446.796 [GB]	0%	
<a href="#">egee.grid.niif.hu</a>	8	7	12%	1	0	0%	2.375 [TB]	2.375 [TB]	0%	
<a href="#">egee.irb.hr</a>	24	13	46%	11	0	0%	141.844 [GB]	141.611 [GB]	0%	
<a href="#">egee.srce.hr</a>	27	3	89%	24	16	40%	1.378 [TB]	1.378 [TB]	0%	
<a href="#">elte</a>	6	6	0%	0	0	0%	6.659 [TB]	6.659 [TB]	0%	
<a href="#">gup-jku</a>	8	3	62%	5	4	44%	183.569 [GB]	183.496 [GB]	0%	
<a href="#">hephy-vienna</a>	168	122	27%	46	0	0%	27.39 [TB]	27.39 [TB]	0%	
<a href="#">iisas-bratislava</a>	73	15	79%	58	1	2%	1.762 [TB]	1.76 [TB]	0%	
<a href="#">pearl-amu</a>	18	0	100%	12	26	68%	55.395 [GB]	55.323 [GB]	0%	
<a href="#">prague_cesnet_icg2</a>	64	46	28%	0	0	0%	4.473 [TB]	4.473 [TB]	0%	
<a href="#">psnc</a>	680	62	91%	336	59	15%	4.47 [TB]	4.47 [TB]	0%	
<a href="#">tu-kosice</a>	15	15	0%	0	0	0%	114.692 [GB]	114.584 [GB]	0%	
<a href="#">warsaw-egee</a>	208	195	6%	12	444444	100%	1.35 [TB]	1.35 [TB]	0%	



# LFC-SE file browser portlet

PGrade Grid portal - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Mail Print Share

Address <https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=133> Go Links >>

Welcome Workflow Certificates Settings Information System **File Management** Compiler Portlet Help

file

? File Management

Select Grid:  View

Select VO:  View

Select LFC Host:  List

or Enter

**File Browser**

- + Balasko
- + ErdelyiZoltan
  - POSIX-TEST-10485-24626
  - POSIX-TEST-11134-23067
  - POSIX-TEST-12464-3948
  - POSIX-TEST-16138-5559
  - POSIX-TEST-17957-20543
  - POSIX-TEST-20716-13234
  - POSIX-TEST-24498-25005
  - POSIX-TEST-24776-20792
  - POSIX-TEST-27728-19524
  - POSIX-TEST-29926-26667
  - POSIX-TEST-3182-23422
  - POSIX-TEST-6451-13508
  - POSIX-TEST-7730-27146
- + SAM

Go Up

Change Directory

Remove

Details

Replicas

Make Directory

Rename

Current Path: /grid/seegrid

Download Upload

**Message:** Upper directory listed

July 14, 2008



# Compilation support


PGrade Grid portal - Microsoft Internet Explorer


File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites

Address <https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=Compiler+Portlet> Go Links

RELEASE 2.7

 **P-GRADE** | **portal**

 **Logout**  
Welcome, Gabor Hermann

Welcome Workflow Certificates Settings Information System File Management **Compiler Portlet** Help

Compiler

**Compiler Portlet**

File:  /

Name:

Name	Size	Last modified / Type
<input type="button" value="Copy"/>	<input type="button" value="Move"/>	<input type="button" value="Delete"/> <input type="button" value="Download"/>

File:  /

Name:

Name	Size	Last modified / Type
<input type="button" value="Copy"/>	<input type="button" value="Move"/>	<input type="button" value="Delete"/> <input type="button" value="Download"/>

July 14, 2008



# ***WORKFLOW HANDS-ON***



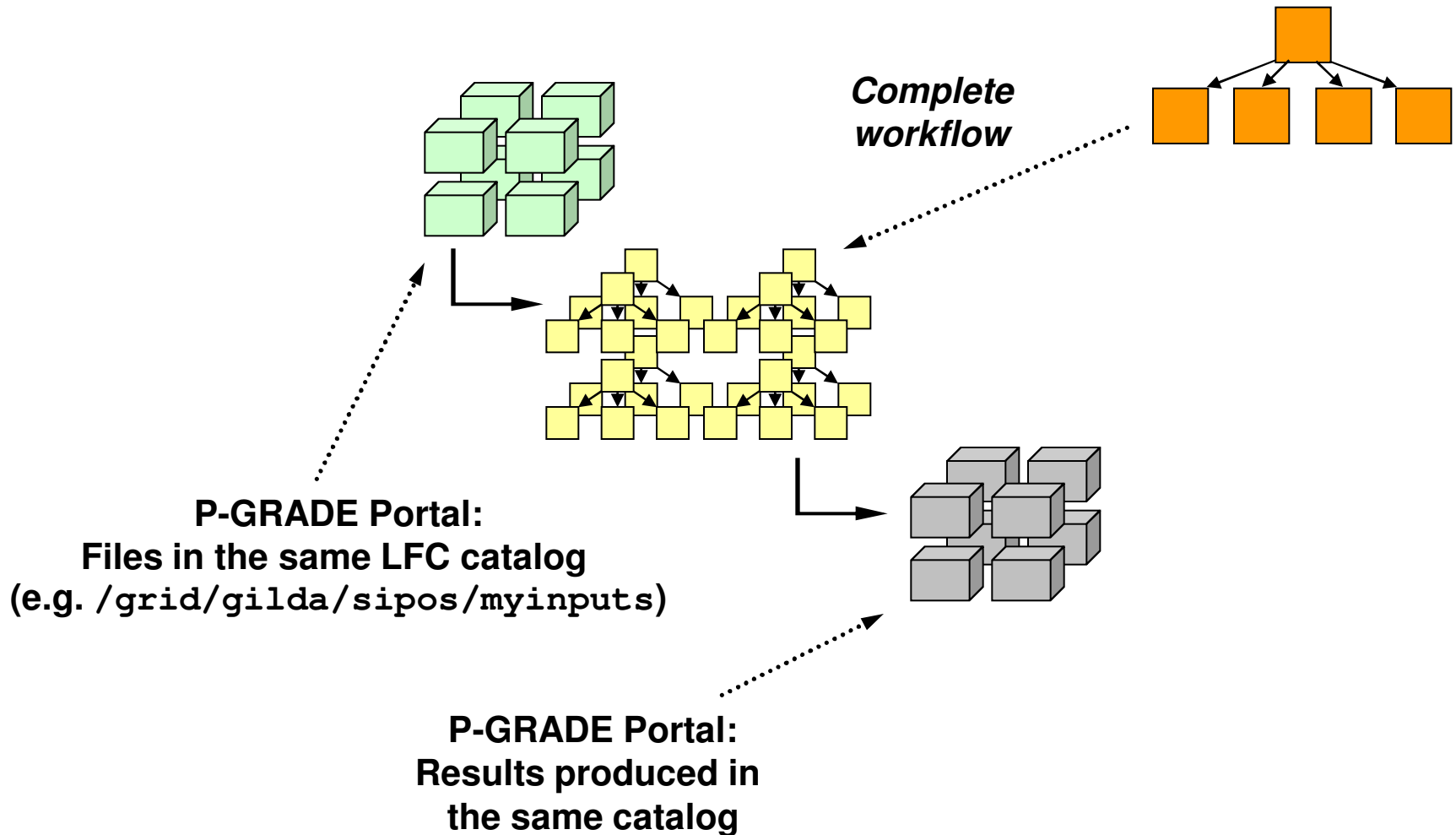


# ***From workflows to parameter studies***

Advanced execution patterns

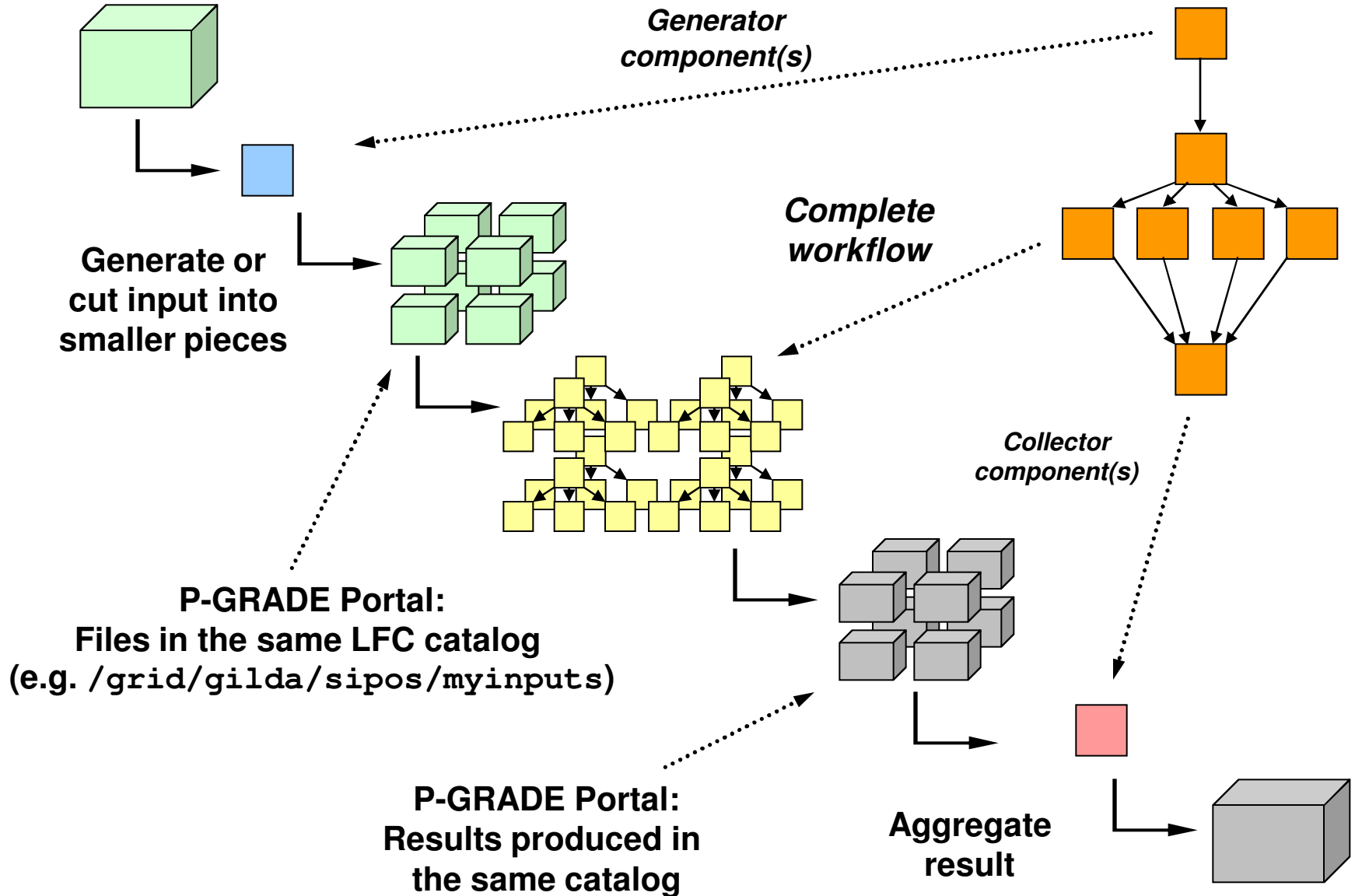


# Scaling up a workflow to a parameter study



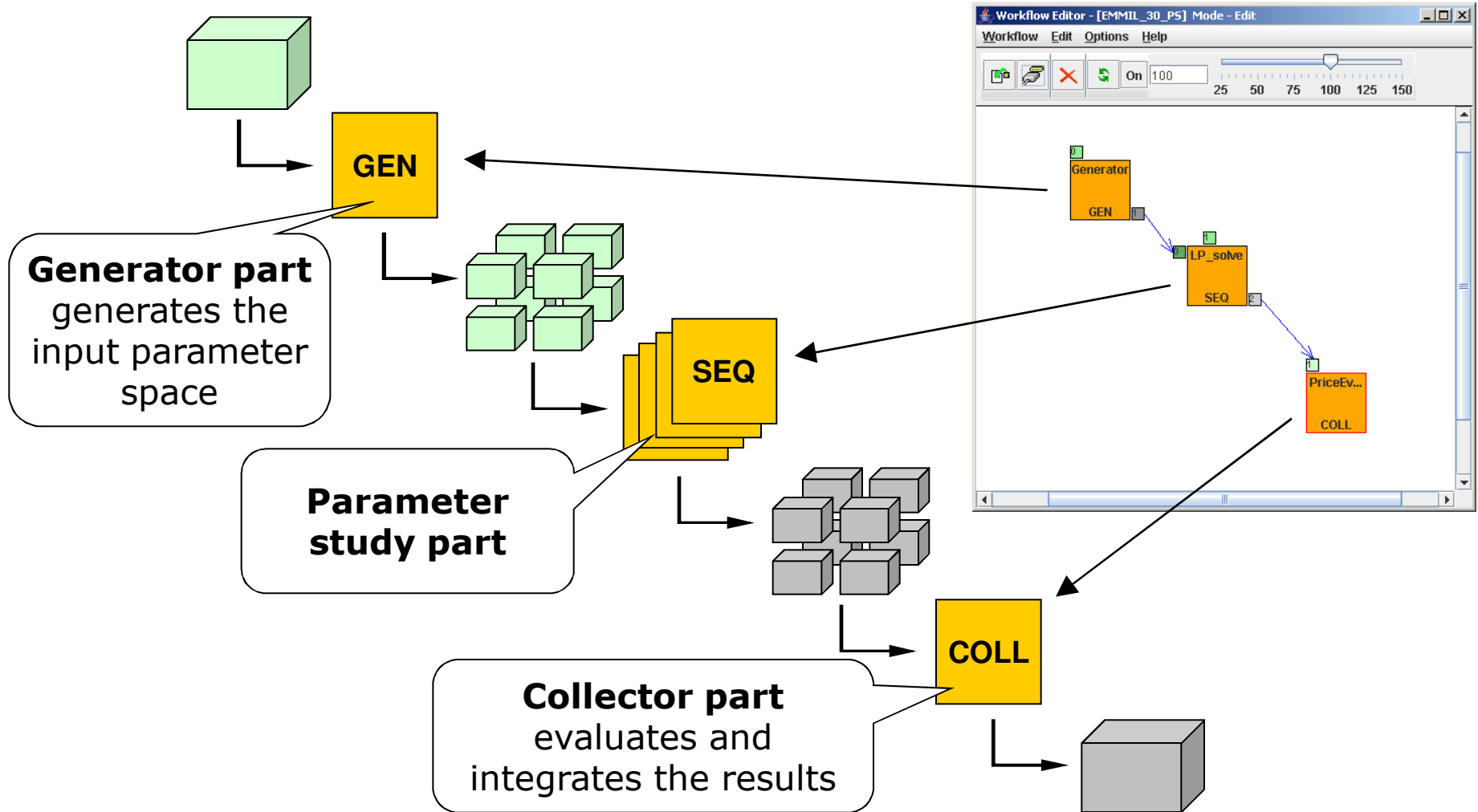


# Advanced parameter studies



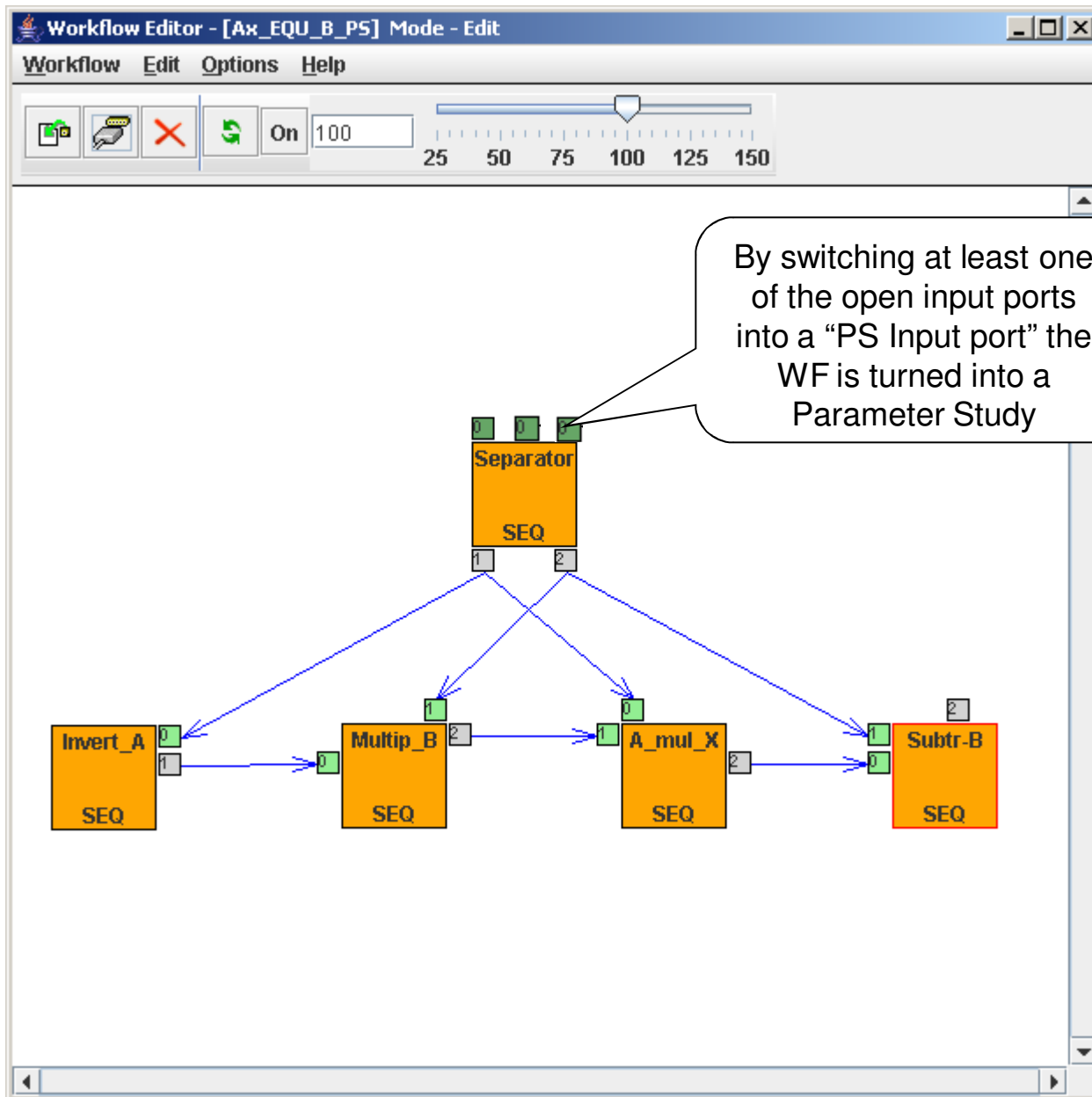


# Concept of parameter study workflows



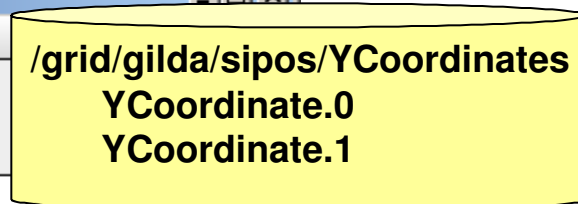
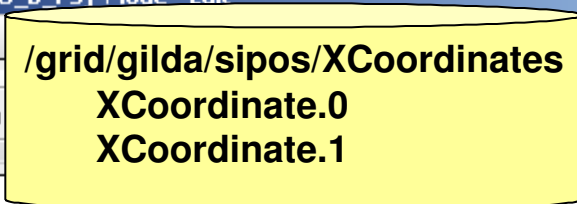
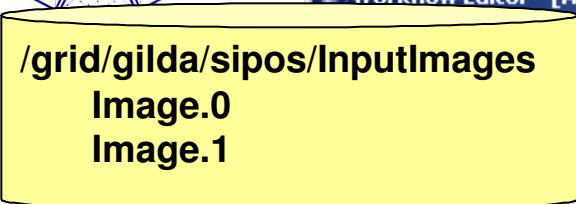


# Turning a WF into a parameter study



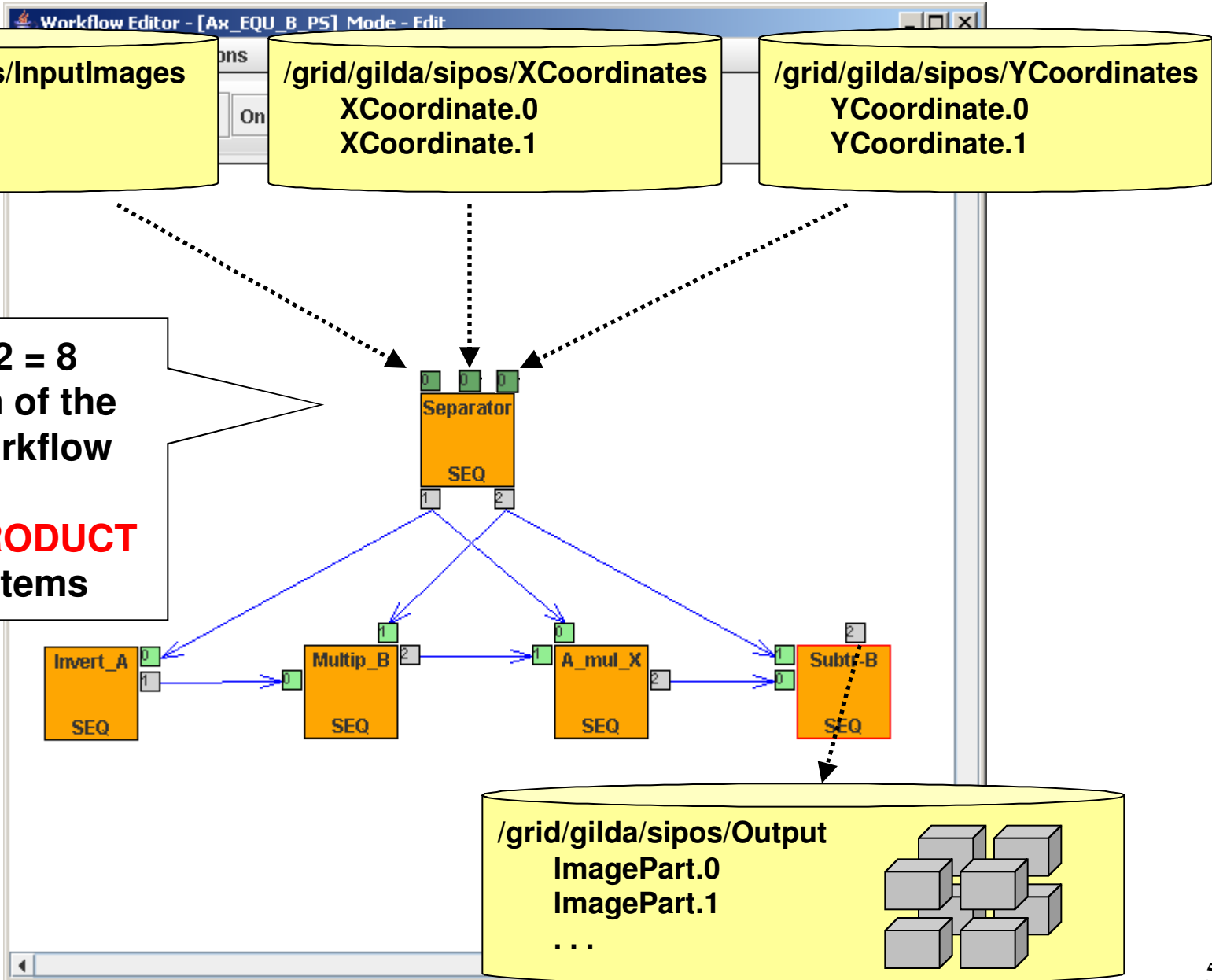


# Input-output files are stored in SEs



2 x 2 x 2 = 8  
execution of the  
whole workflow

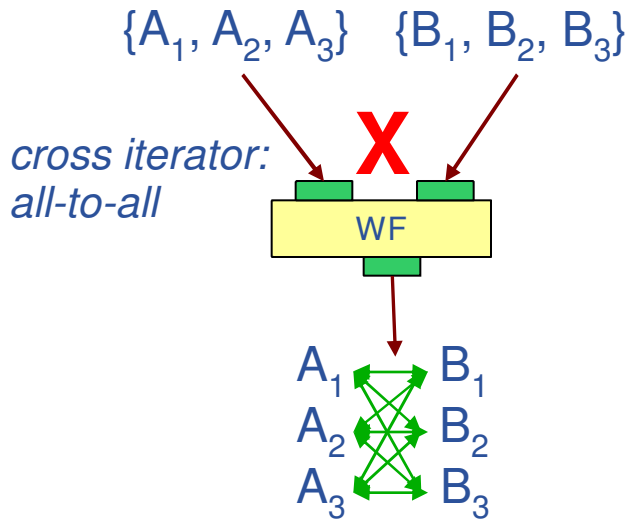
**CROSS PRODUCT**  
of data items





# Typical data-flow compositions

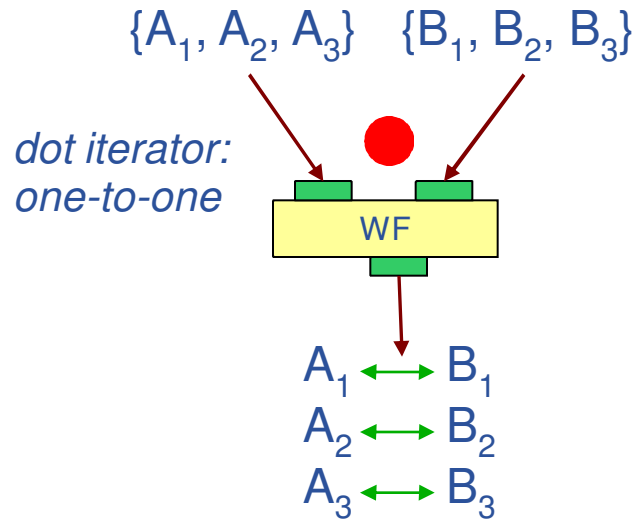
## CROSS ITERATOR



$A \times B$

*P-Grade Portal  
supports this*

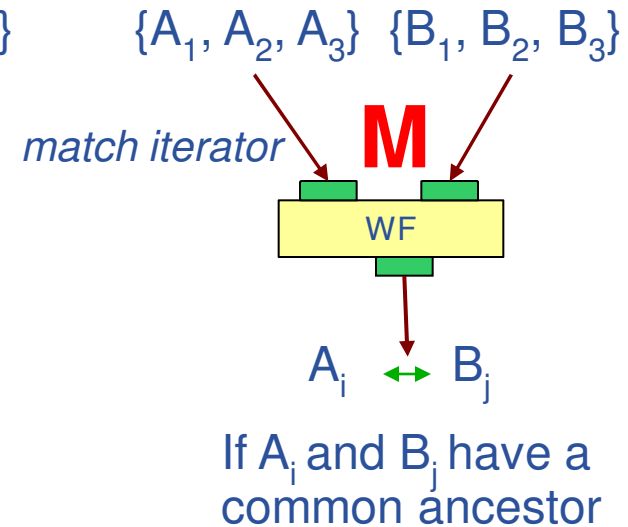
## DOT ITERATOR



$A \bullet B$

Find these in e.g. TAVERNA, MOTEUR

## MATCH ITERATOR



$A \text{ M } B$



# PS Input Port

The screenshot shows the Workflow Editor interface with a dialog box titled "Separator / 0 PS properties" open. The dialog box contains the following fields and options:

- PS Port name: [Empty text box]
- Type:  In  Out
- Directory type:  Local  Remote
- Directory: nann/PS/EQU\_AGEN\_11\_10/A\_GEN12
- File Browser: [Button]
- managed copy:
- Internal File Name: INPUT
- File storage type:  Permanent  Volatile
- Buttons: Ok, Cancel

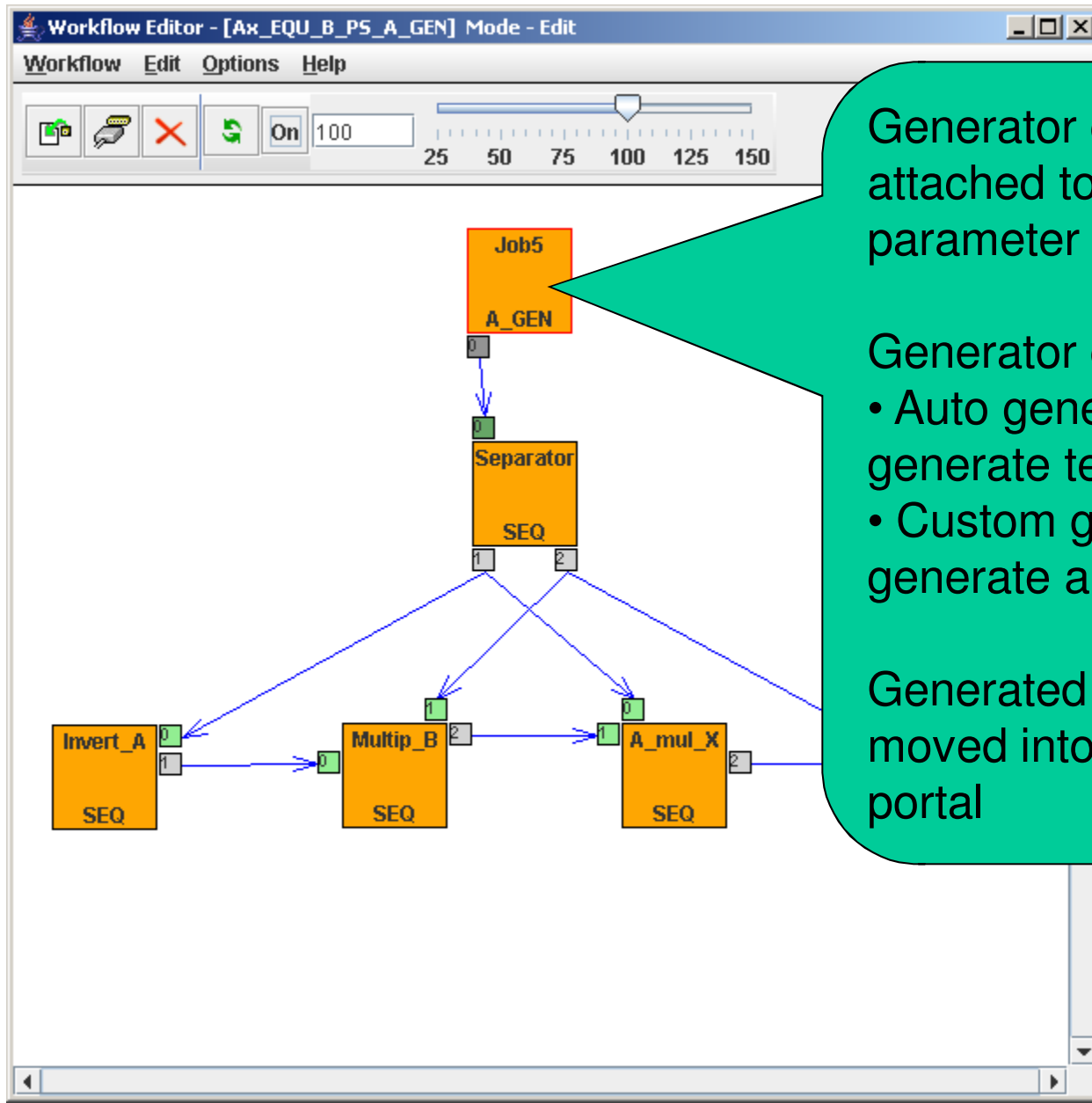
A green callout bubble points to the "Directory" field with the text: "Grid Directory instead of FILE reference".

In the background workflow, an "Invert\_A SEQ" block is connected to a "Multip. SEQ" block. The "Invert\_A" block has two output ports labeled "0" and "1". The "Multip." block has one input port labeled "0". Blue arrows indicate the flow of data from the "0" output of "Invert\_A" to the "0" input of "Multip.", and from the "1" output of "Invert\_A" to the "0" input of "Multip.".





# Parameter generator





# Definition Window of Auto Generator Job

Workflow Editor - [Ax\_EQU\_B\_PS\_A\_GEN] Mode - Edit

Workflow Edit Options Help

On 100 25 50 75 100 125 150

Job5 properties

Job name: Job5

Parametric key delimiter Left: < Right: >

Input file text:

```
5 5 10.0 9.0 8.0 7.0 6.0 30.0 8.0 7.0 5.0 9.0 40.0  
0 0.0 11.0 5.0 71.0 1.0 6.0 5.0 0.0 4.0 21.0 7.0  
4.0 8.0 0.0 #5 1 <Reals Of B>
```

Keys: Reals Of B

Load from File...

Grid: seegrid\_LCG\_2\_BROKER

Special attributes: Attributes editor...

Ok Cancel Parse

SEQ

User defines the template of the text file

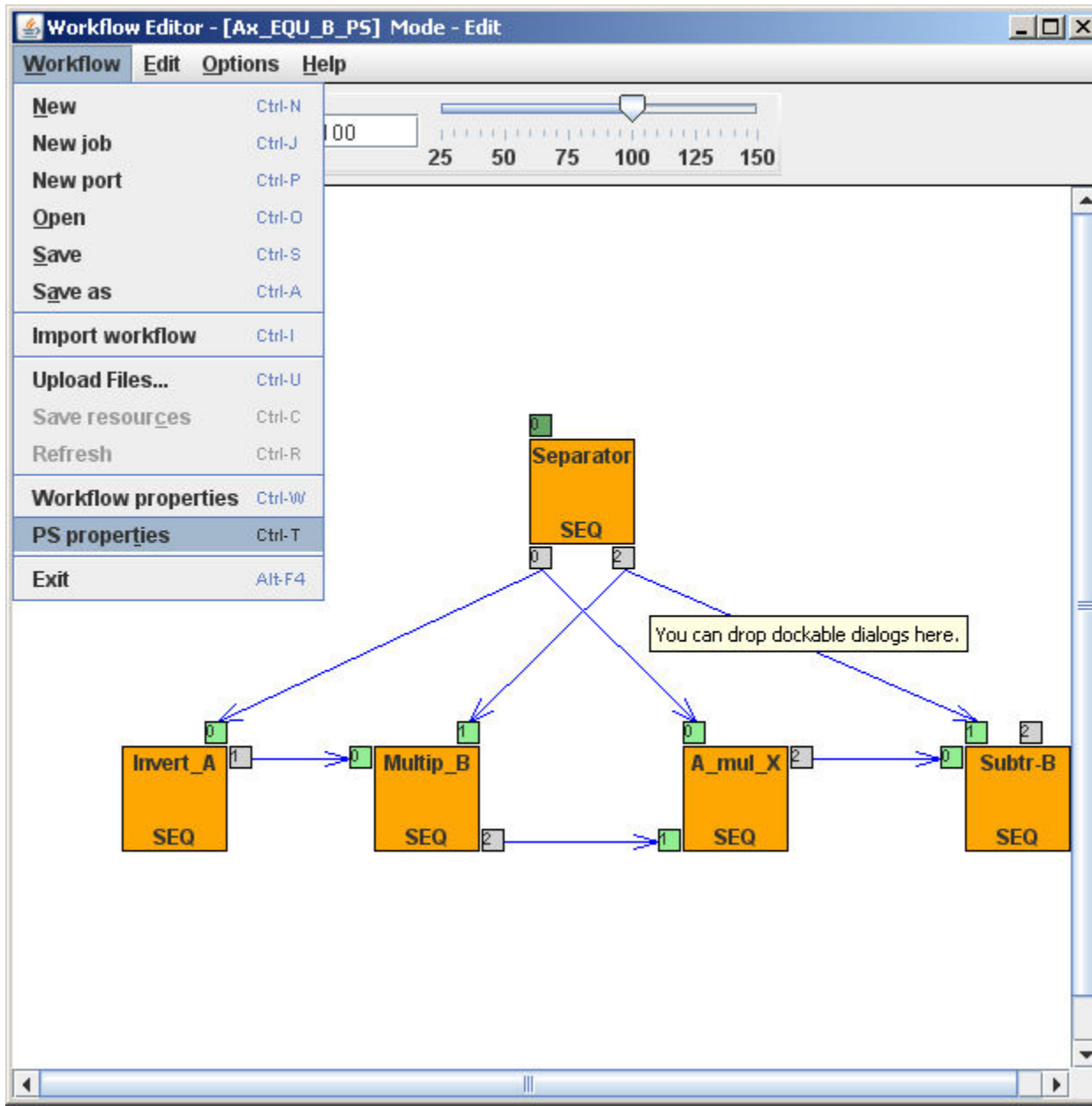
User puts key(s) into the template

User defines values for the key(s)

- Integer number
- Real number
- Custom set
- ...



# Placement of result





# Placement of result

The screenshot shows the 'Workflow Editor' window with the 'PS Properties' dialog box open. The dialog box contains the following fields:

- Output Directory: hermann/PS/EQU\_AGEN\_11\_10/RESULT\_12
- Grid: seegrid\_GLITE\_BROKER
- LCG Catalog Type:  lfc  edg
- LFC Host: grid02.rcub.bg.ac.yu
- SE: se.phy.bg.ac.yu

Below the dialog box, a workflow diagram is visible, consisting of four orange boxes labeled 'Invert\_A', 'Multip\_B', 'A\_mul\_X', and 'Subtr-B', each with 'SEQ' written below it. Blue arrows indicate the flow between these steps, with small green and white boxes at the connection points.

Will contain one compressed file for each execution of the workflow.

Use the default value!

Choose a „reliable” Storage Element



# Executing PS workflows

Job Name	Status	Size	Progress	Completion	Actions
Ax_EQUAL_B_PS_G_C_sztaki_fork	finished	253 KB	0.25%	✓	PS Details, Submit, Attach, Delete
Ax_EQU_B	init	112 KB	0.11%	N/A	Details, Submit, Attach, Delete
Ax_EQU_B_voce_PS	init	151 KB	0.15%	N/A	PS Details, Submit, Attach, Delete

PS Details for parameter sweep workflows applications



# Detailed view of a PS workflow

Workflow Manager

Refresh Back

PS workflow details					
PS Workflow	Status	[ Output ]	[ Logs ]	[ Action ]	
Ax_EQU_B_PS_A_GEN_Collector	submitted	N/A	-	Abort	Attach Delete

Jobs in generator phase					
Job	Status	Type	Gridname	Hostname	[ Logs ]
Job5	finished	auto-generator	seegrid_LCG_2_BROKER	Portal Server	Out

eWorkflow list Statistics					
Total	Init	Submitted	Rescue	Error	Finished
2	0	2	0	0	0

Workflow	Status	[ Output ]	[ View ]	[ Action ]	
Ax_EQU_B_PS_A_GEN_Collector.1	submitted	N/A	Details	Suspend	Abort
Ax_EQU_B_PS_A_GEN_Collector.2	submitted	N/A	Details	Suspend	Abort

Jobs in collector phase					
Job	Status	Type	Gridname	Hostname	[ Logs ]
Collector	init	collector	seegrid_LCG_2_BROKER	unknown	--

Message: eWorkflow list successfully shown.

November 13, 2006

Generator job(s)

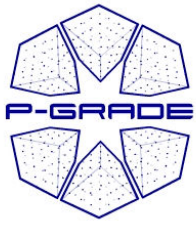
Overall statistics of workflow instances

Workflow instances

Collector job(s)



# ***PARAMETER STUDY HANDS-ON***



**Learn once, use everywhere**  
**Develop once, execute anywhere**

***Thank you!***

**[www.portal.p-grade.hu](http://www.portal.p-grade.hu)**  
**[pgportal@lpds.sztaki.hu](mailto:pgportal@lpds.sztaki.hu)**

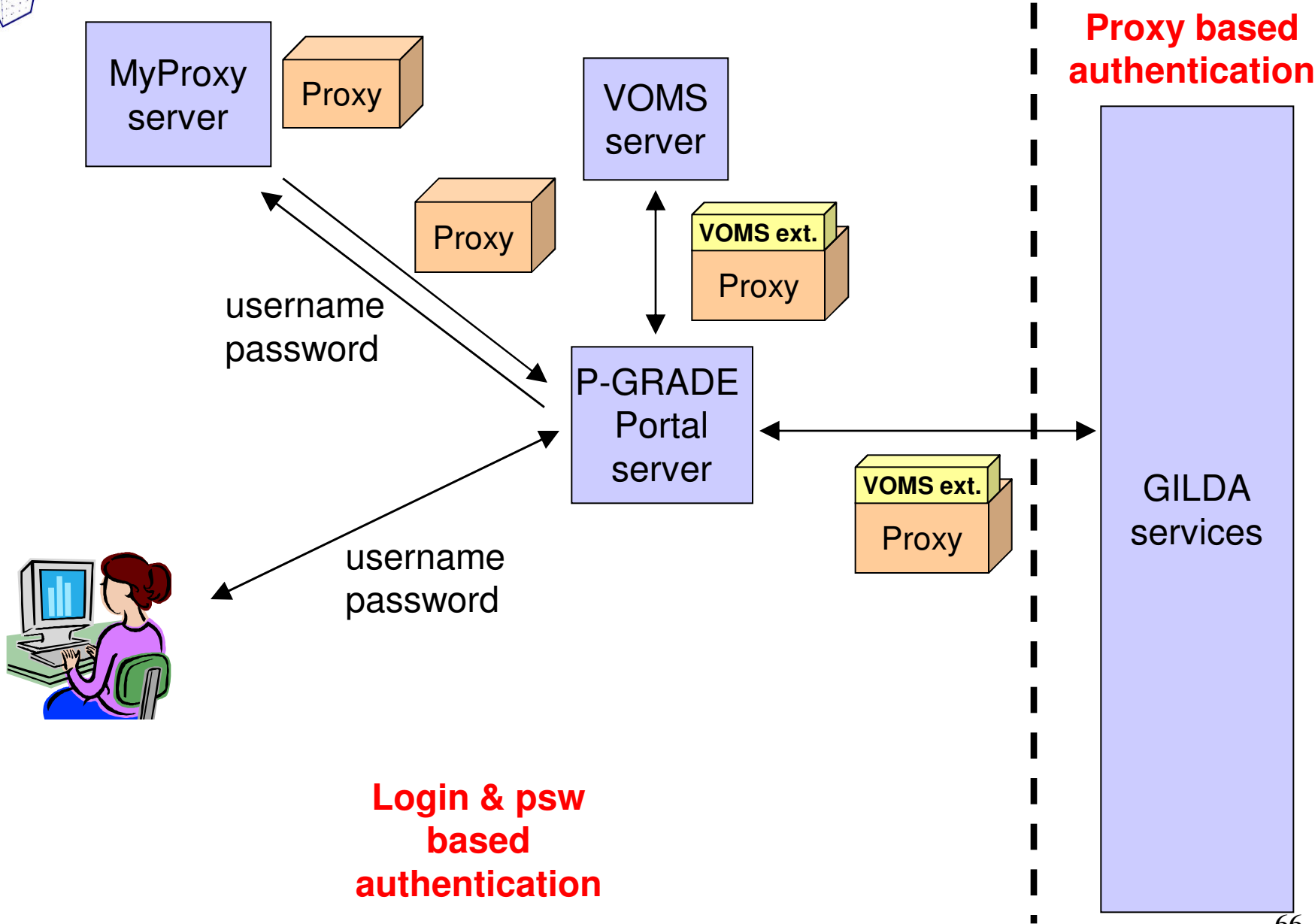




***Backup slides to answer  
questions***



# Proxy delegations





# Settings

PGrade Grid portal - Microsoft Internet Explorer

Address: https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=105

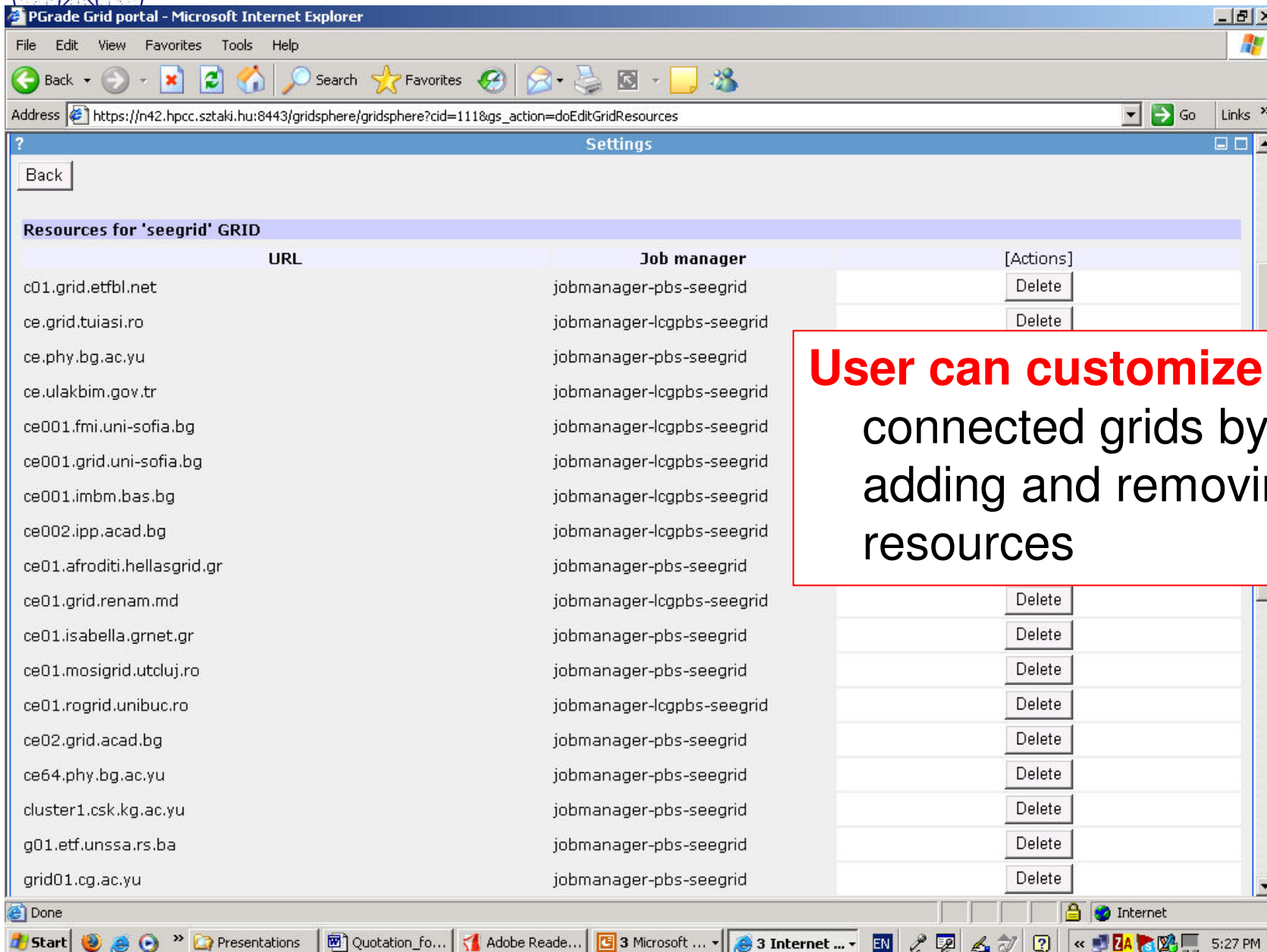
### Settings

Name	Information System			BaseDn	[Actions]
	Type	Host	Port		
biomed	LCG2	cclcgtopbdii02.in2p3.fr	2170	Mds-vo-name=local,o=grid	Resources
biomed_GLITE_BROKER			N/A		
biomed_LCG_2_BROKER			N/A		
compchem	LCG2	egee-bdii.cnaf.infn.it	2170	Mds-vo-name	
compchem_GLITE_BROKER			N/A		
compchem_LCG_2_BROKER			N/A		
gilda	LCG2	glite-rb.ct.infn.it	2170	mds-vo-name	
gilda_GLITE_BROKER			N/A		
gilda_LCG_2_BROKER			N/A		
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
voce	LCG2	bdii.cyf-kr.edu.pl	2170	mds-vo-name=local,o=grid	Resources
voce_GLITE_BROKER			N/A		Resources

**Portal administrator can**

- connect the portal to several grids
- register default resources of the connected grids

# Settings



PGrade Grid portal - Microsoft Internet Explorer

Address: https://n42.hpcc.sztaki.hu:8443/gridsphere/gridsphere?cid=111&gs\_action=doEditGridResources

### Settings

Back

#### Resources for 'seegrid' GRID

URL	Job manager	[Actions]
c01.grid.etfbl.net	jobmanager-pbs-seegrid	Delete
ce.grid.tuiasi.ro	jobmanager-lcgpbs-seegrid	Delete
ce.phy.bg.ac.yu	jobmanager-pbs-seegrid	
ce.ulakbim.gov.tr	jobmanager-lcgpbs-seegrid	
ce001.fmi.uni-sofia.bg	jobmanager-lcgpbs-seegrid	
ce001.grid.uni-sofia.bg	jobmanager-lcgpbs-seegrid	
ce001.imbm.bas.bg	jobmanager-lcgpbs-seegrid	
ce002.ipp.acad.bg	jobmanager-lcgpbs-seegrid	
ce01.afroditi.hellasgrid.gr	jobmanager-pbs-seegrid	
ce01.grid.renam.md	jobmanager-lcgpbs-seegrid	Delete
ce01.isabella.grnet.gr	jobmanager-pbs-seegrid	Delete
ce01.mosigrid.utdluj.ro	jobmanager-pbs-seegrid	Delete
ce01.rogrid.unibuc.ro	jobmanager-lcgpbs-seegrid	Delete
ce02.grid.acad.bg	jobmanager-pbs-seegrid	Delete
ce64.phy.bg.ac.yu	jobmanager-pbs-seegrid	Delete
cluster1.csk.kg.ac.yu	jobmanager-pbs-seegrid	Delete
g01.etf.unssa.rs.ba	jobmanager-pbs-seegrid	Delete
grid01.cg.ac.yu	jobmanager-pbs-seegrid	Delete

**User can customize the connected grids by adding and removing resources**

Done

Start Presentations Quotation\_fo... Adobe Reade... 3 Microsoft ... 3 Internet ... EN 5:27 PM