GEMLCA / P-GRADE: A workflow-oriented portal and application hosting environment

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www.portal.p-grade.hu
www.cpc.wmin.ac.uk/gemlca

Contents

- Motivation of creating the tools portal
- P-GRADE Portal and GEMLCA in a nutshell
- Multi-grid capabilities
- Lifecycle of GEMLCA / P-GRADE applications
- Services for application developers

- Introduction of the hands-on
- Hands-on

- Roadmap of the NGS GEMLCA portal
- Further steps

Context

Graphical interface

Middleware independent services of P-GRADE Portal and GEMLCA

Middleware specific clients

Grid middleware services

Current situation and trends in Grid computing

- Fast evolution of Grid systems and middleware:
  - **GT2, OGSA, GT3 (OGSI), GT4 (WSRF), LCG-2, gLite, …**
- Many production Grid systems are built with them
  - EGEE (LCG-2 → gLite), UK NGS (GT2), Open Science Grid (GT2 → GT4), NorduGrid (~GT2)
- Although **the same set of core services** are available everywhere, they **are implemented in different ways**
  - Data services
  - Computation services
  - Security services (single sign-on)
  - (Brokers)

E-scientists' concerns

- How to concentrate own **my own research** if the tool I would like to use is in continuous change?
- How can I learn and understand **the usage of the Grid**?
- How can I **develop Grid applications**?
- How can I **execute grid applications**?
- How to **tackle performance issues**?
- How to **use several Grids at the same time**?
- How to **migrate my application** from one grid to another?
- How can I **collaborate with fellow researchers**?

The GEMLCA / P-GRADE Portal give you the answers!

P-GRADE Portal in a nutshell

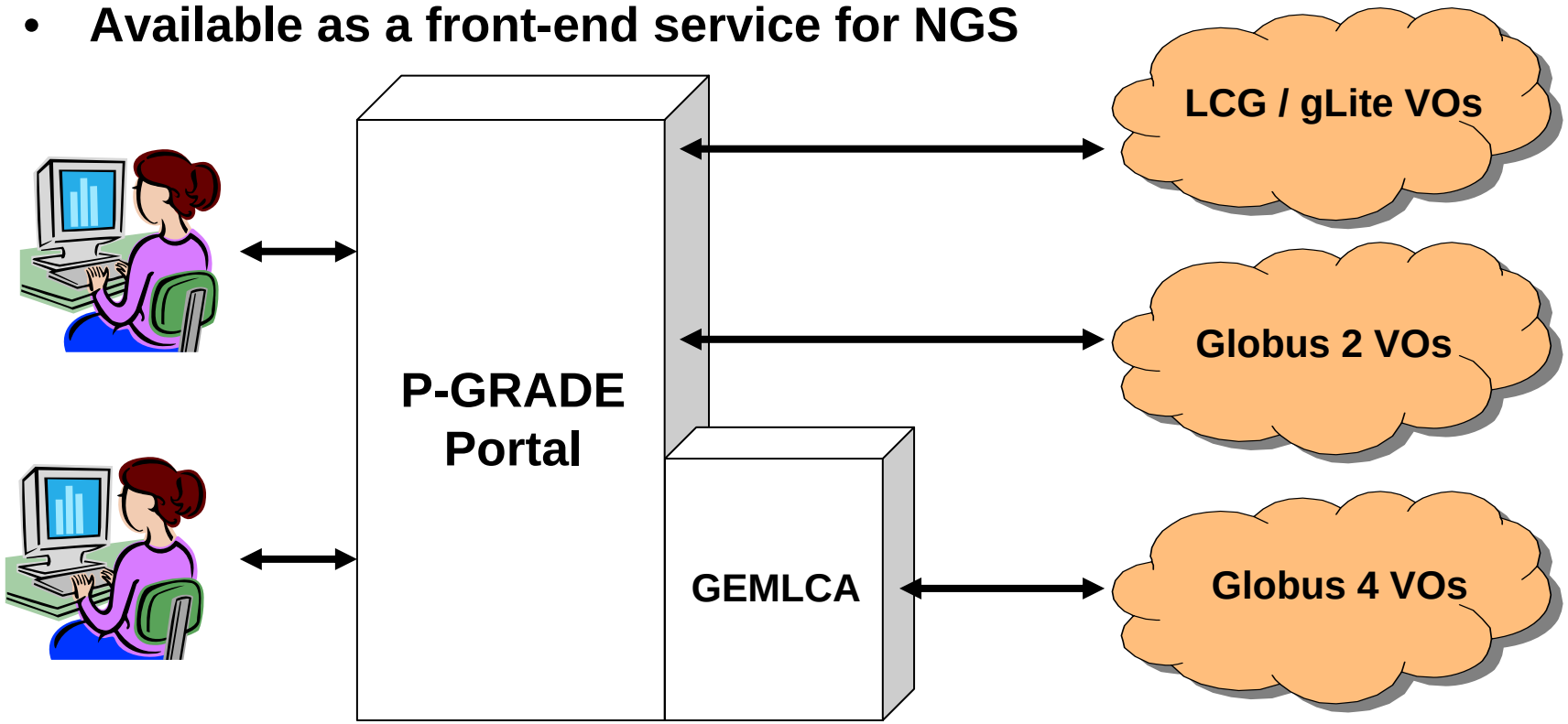
- **General purpose**, **workflow-oriented computational Grid portal**. Supports the development and execution of workflow-based Grid applications – **a tool for Grid orchestration**
- Based on **GridSphere-2**
  - Easy to expand with new portlets (e.g. application-specific portlets)
  - Easy to tailor to end-user needs
- Developed by SZTAKI
- **Grid services** supported by the portal:

Service	EGEE grids (LCG/gLite)	Globus 2 grids
Job execution	Computing Element	GRAM
File storage	Storage Element	GridFTP server
Certificate management	MyProxy	
Information system	BDII	MDS-2, MDS-4
Brokering	Workload Management System	(GTbroker)
Job monitoring	Mercury	
Workflow & job visualization	PROVE	

Solves Grid interoperability problem at the workflow level

GEMLCA / P-GRADE Portal in a nutshell

- P-GRADE Portal extended with GEMLCA back-end
  - Sharing jobs and legacy codes as workflow components
  - GEMLCA is a grid service implemented by UoW
- A step towards collaborative e-Science
- Support for Globus 4 grids (besides GT2 and EGEE)
- Available as a front-end service for NGS

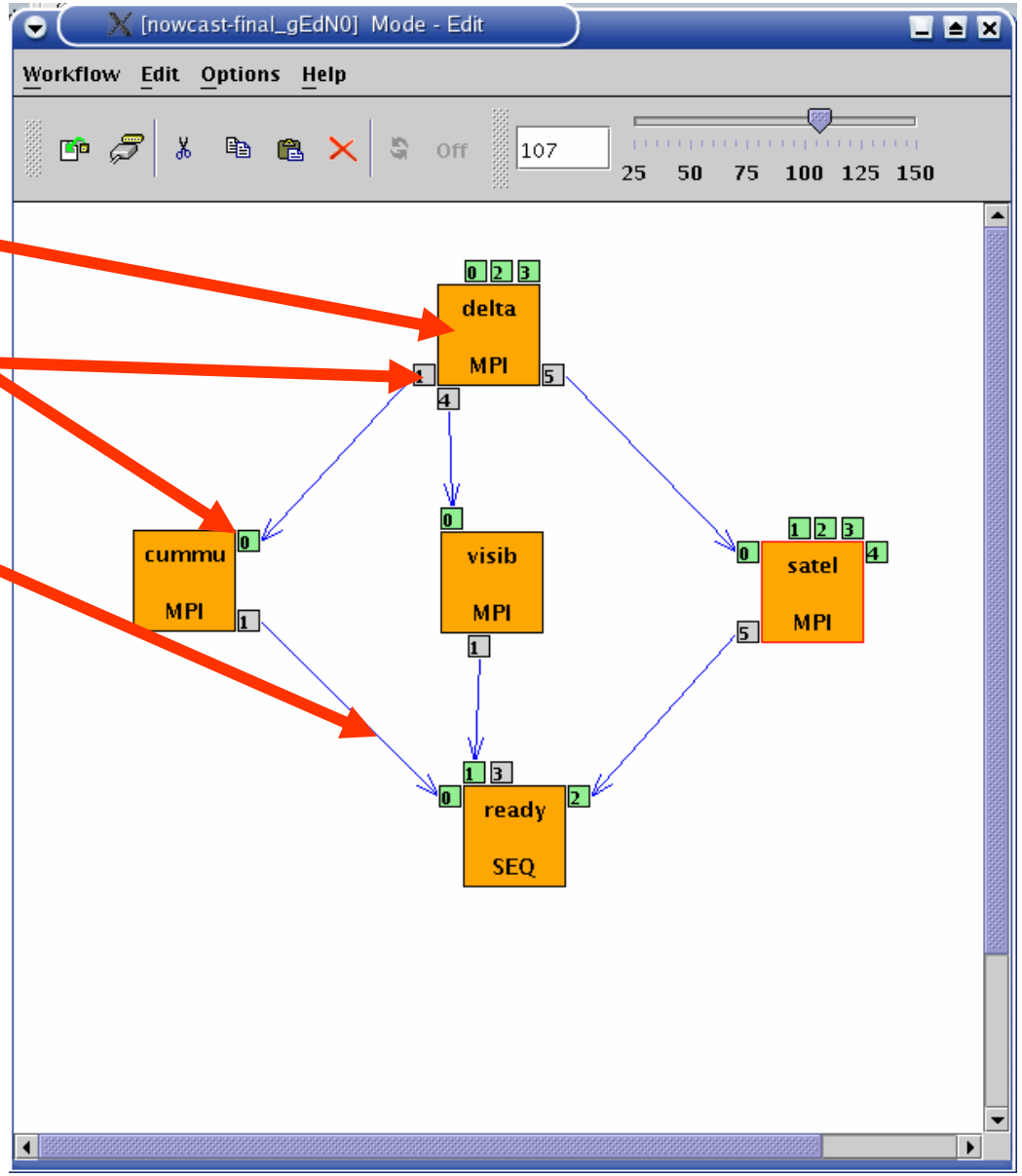


Related projects

- The development, operation and training of P-GRADE Portal and GEMLCA is supported by the following projects:
  - **SEE-GRID** *www.see-grid.eu*
    Development, application support
  - **Coregrid** *www.coregrid.net*
    Research, development
  - **EGEE** *www.eu-egee.org*
    LCG and gLite training, application development
  - **ICEAGE** *www.iceage-eu.org*
    Grid training and education

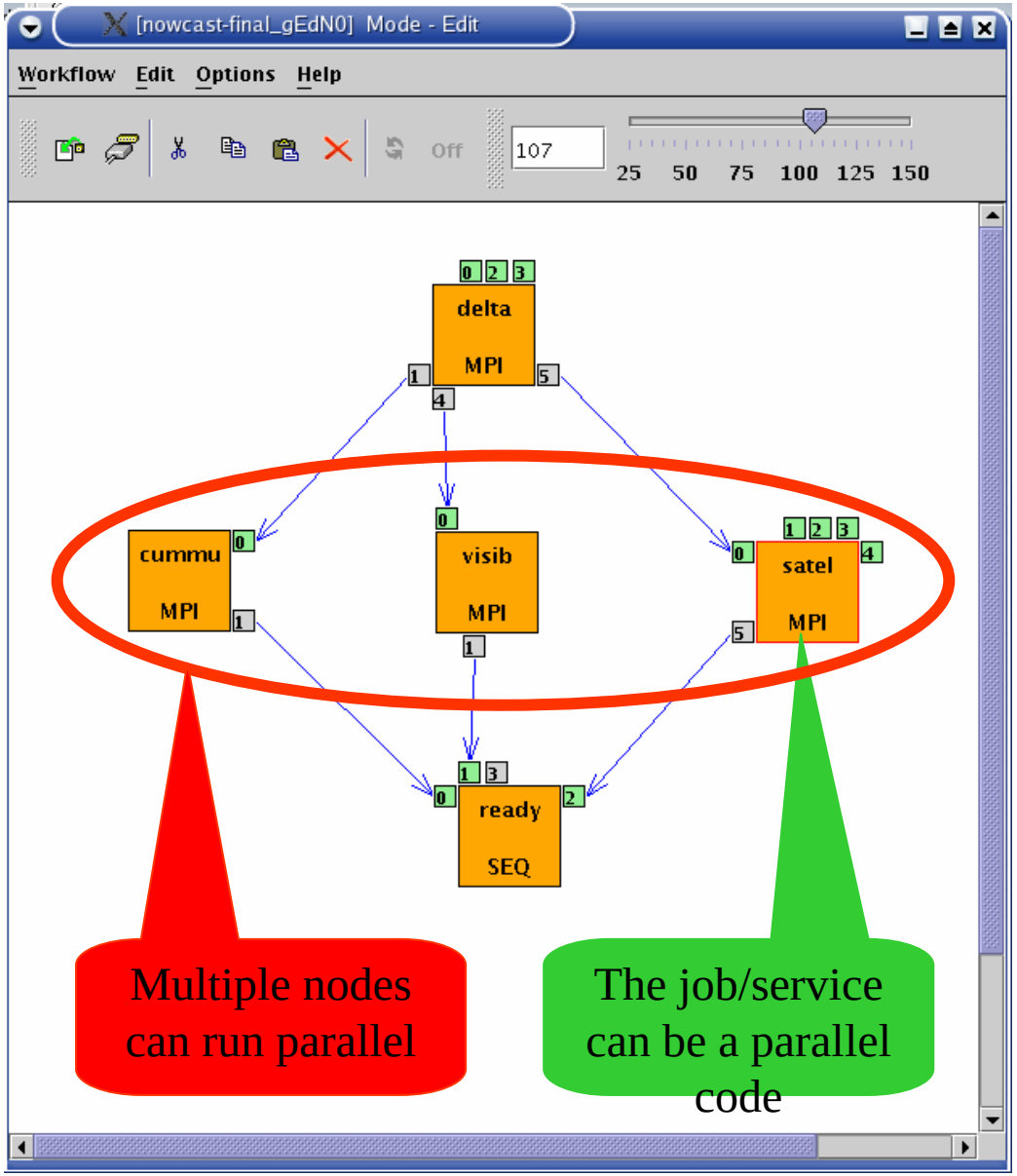
What is a GEMLCA / P-GRADE Portal workflow?

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

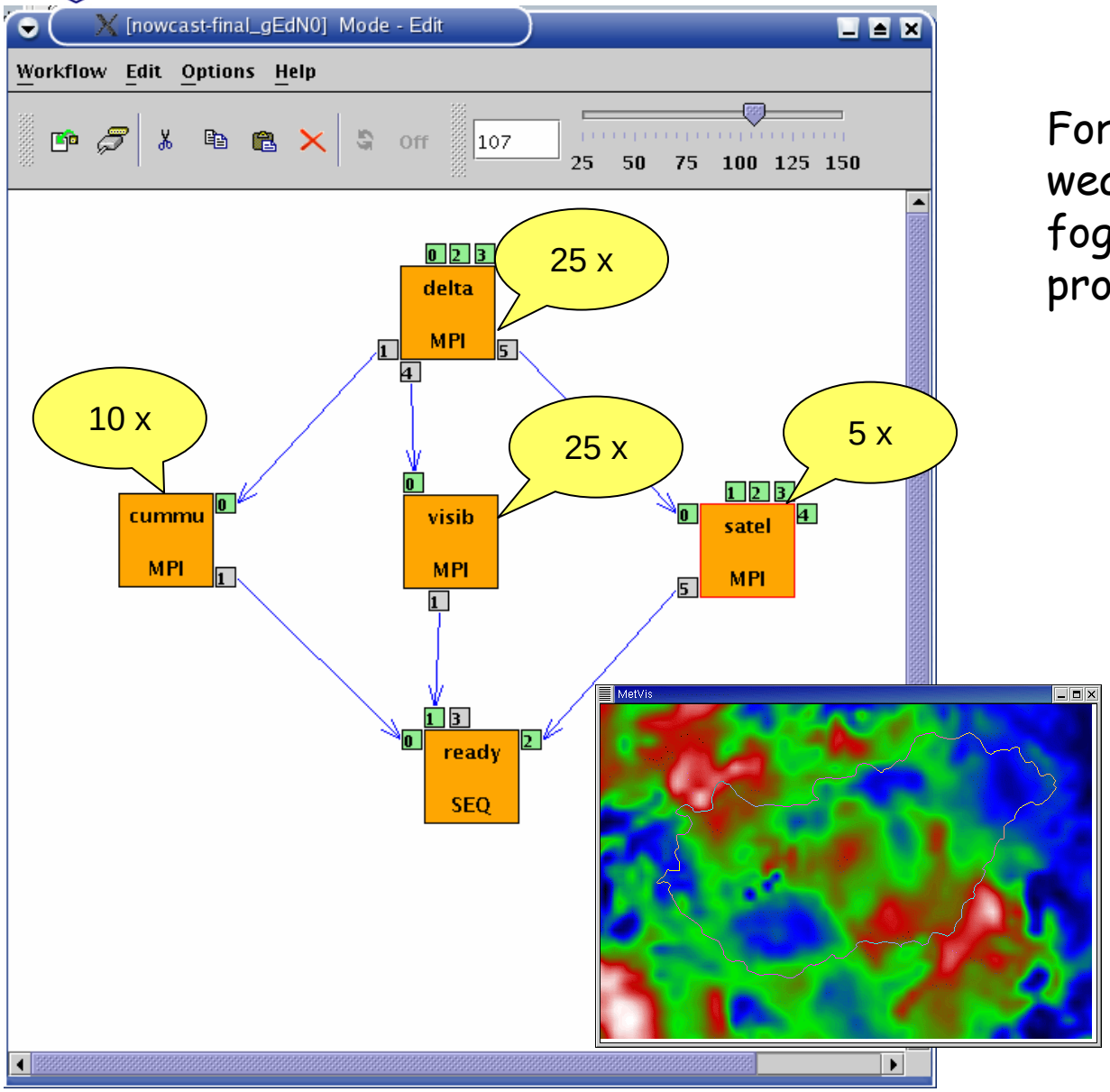


Two levels of parallelism within a workflow

- The workflow concept of the GEMLCA/ P-GRADE Portal enables the efficient parallelization of complex problems
- Semantics of the workflow enables two levels of parallelism:
  - Parallel execution inside a workflow node
  - Parallel execution among workflow nodes



Ultra-short range weather forecast (Hungarian Meteorology Service)



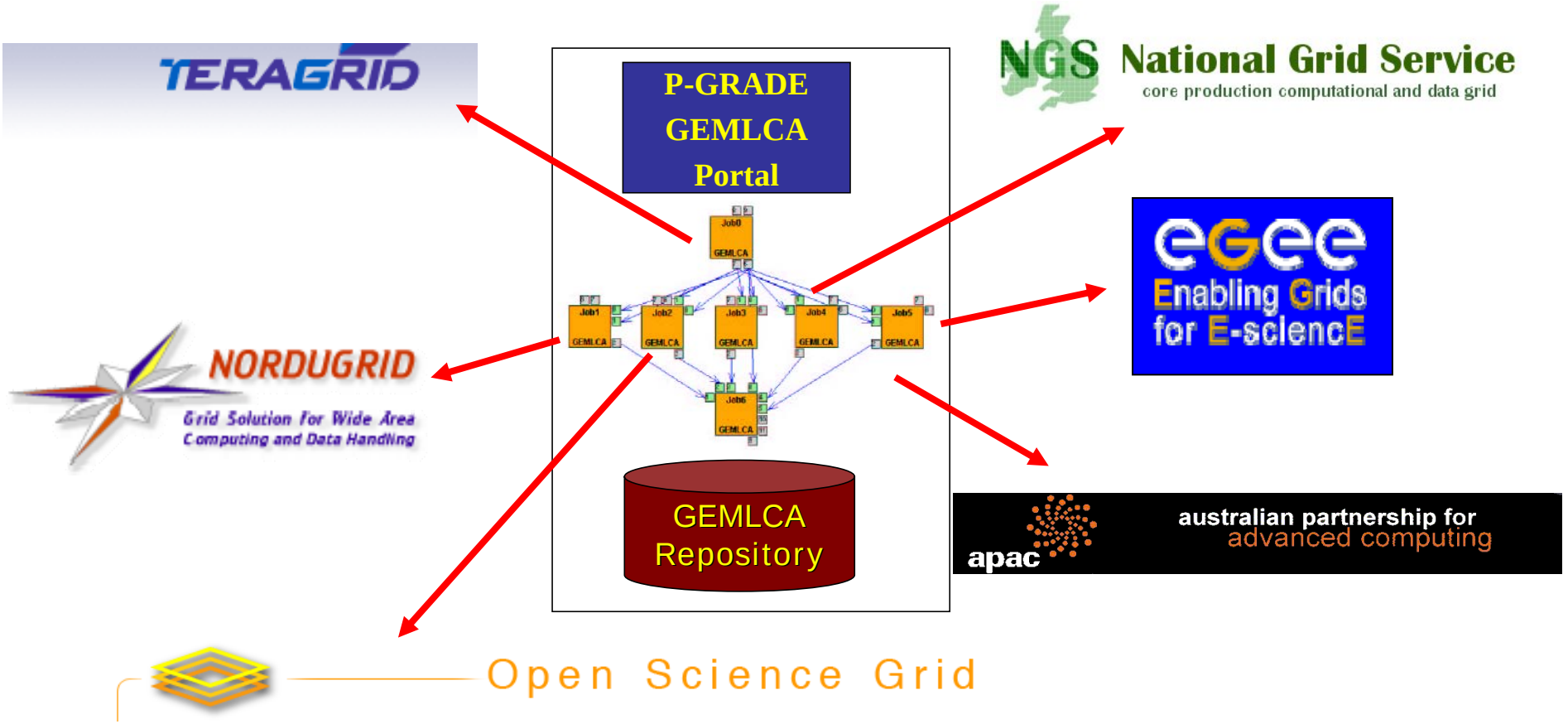
Forecasting dangerous weather situations (storms, fog, etc.), crucial task in the protection of life and property

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

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

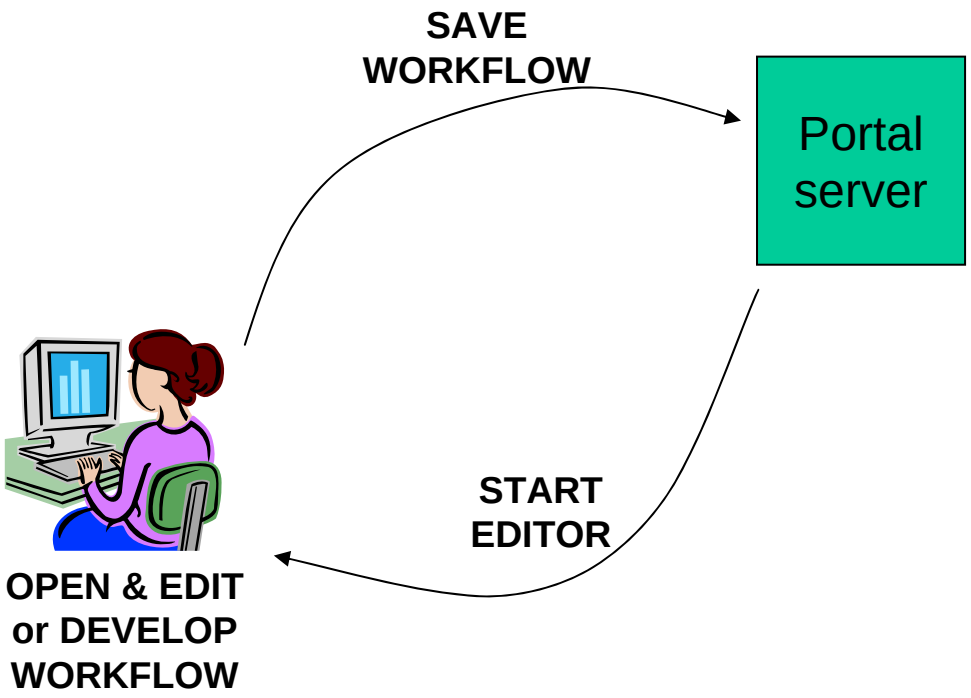
Workflow-level Grid interoperability: The GIN Resource Testing portal

OGF effort to demonstrate workflow level grid interoperability between major production Grids and to monitor OGF GIN VO resources



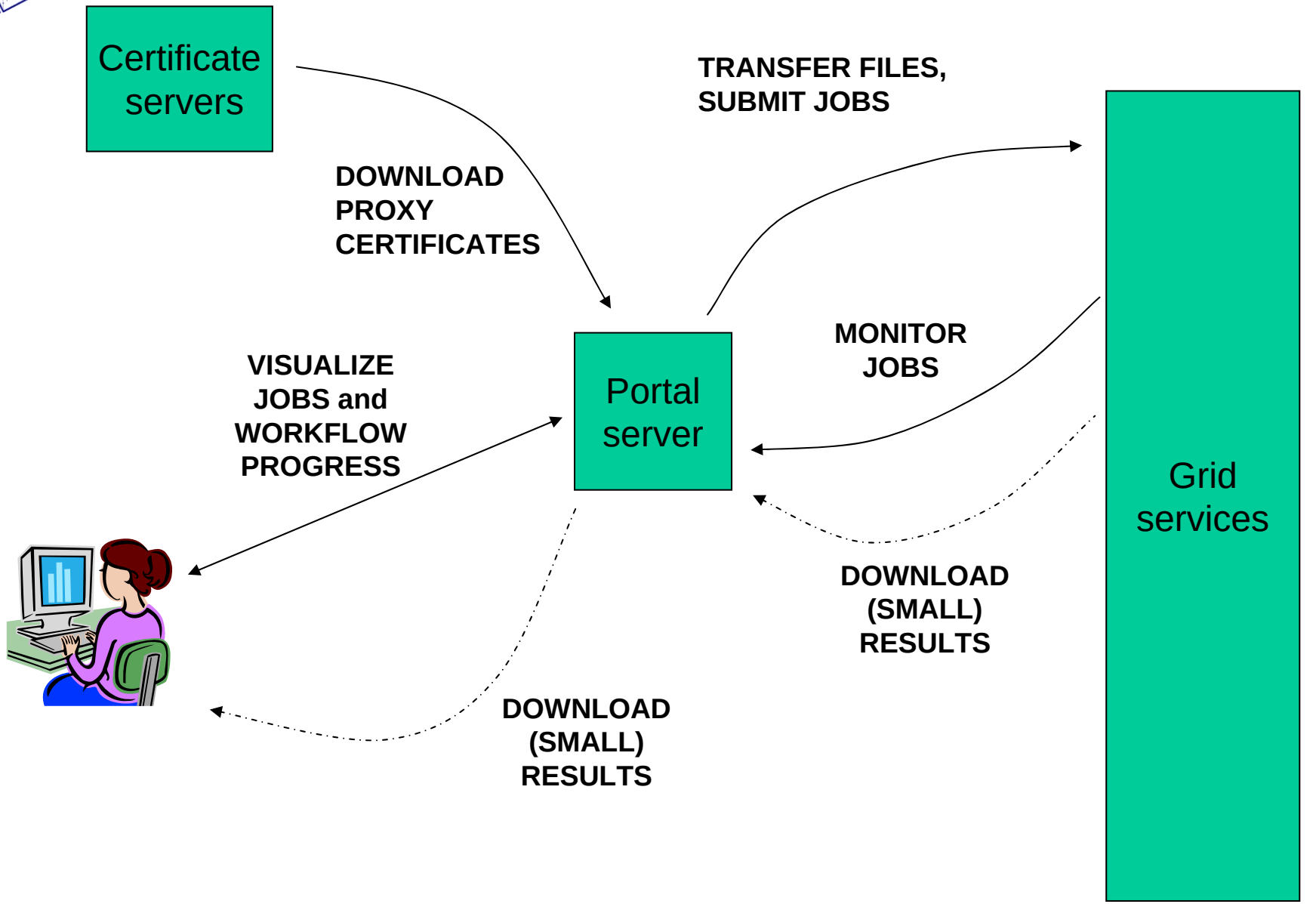
The typical user scenario
Part 1 - development phase

Certificate servers



Grid services

The typical user scenario
Part 2 - execution phase



The typical user scenario
Part 3 - collaborative phase

Certificate servers

Share workflow components az GEMLCA jobs with other users of the same portal

Portal server

Export and share workflows with users of the same, or another portal

Grid services

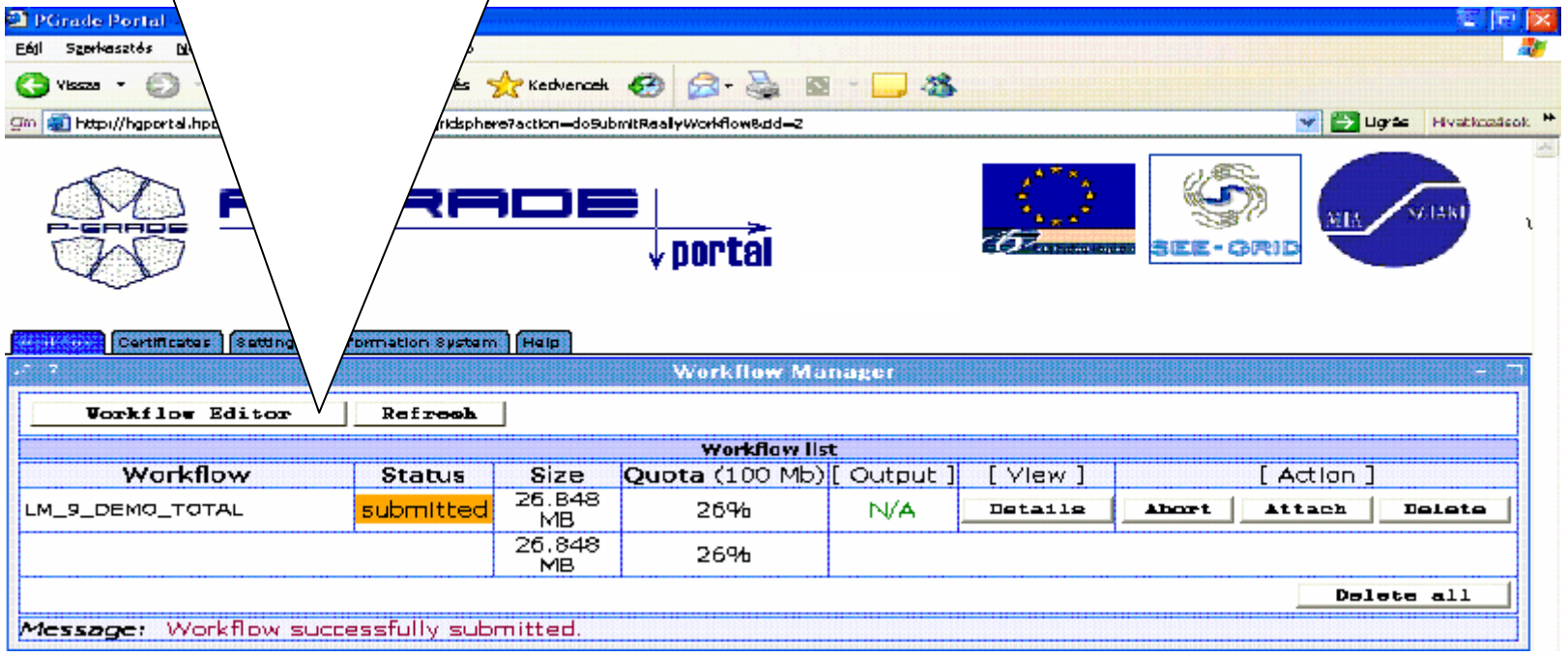
Workflow development

Opening the workflow editor

The editor is a Java Webstart application

↓

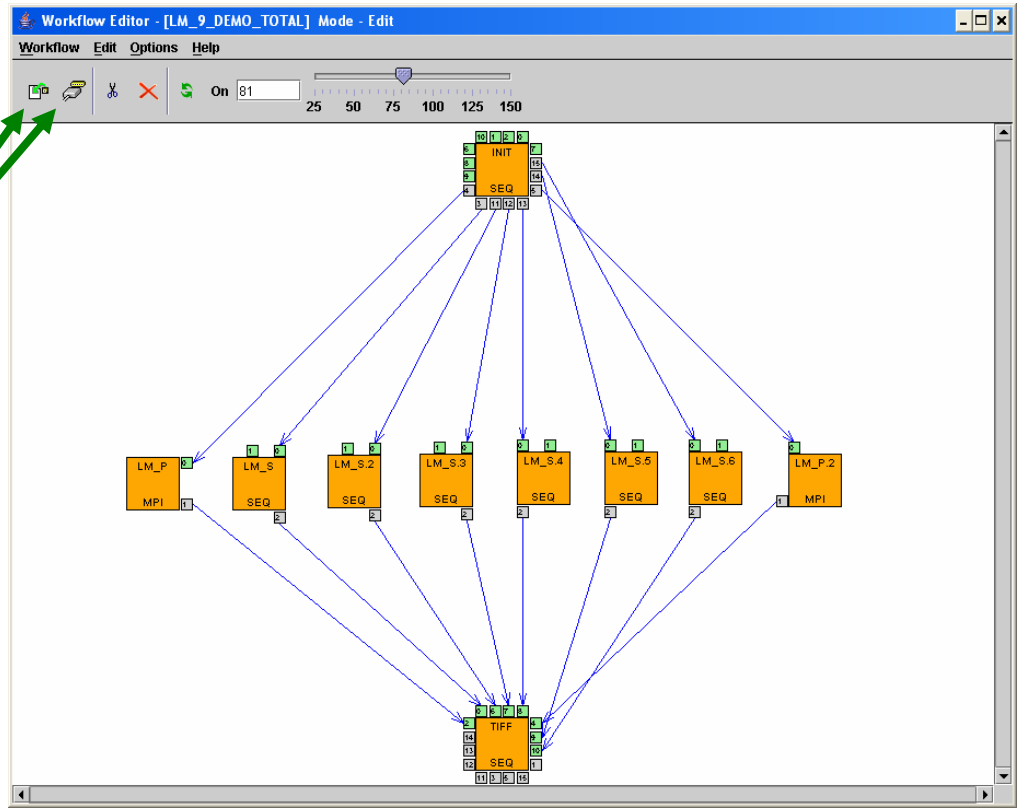
download and installation is only one click!



Workflow Editor

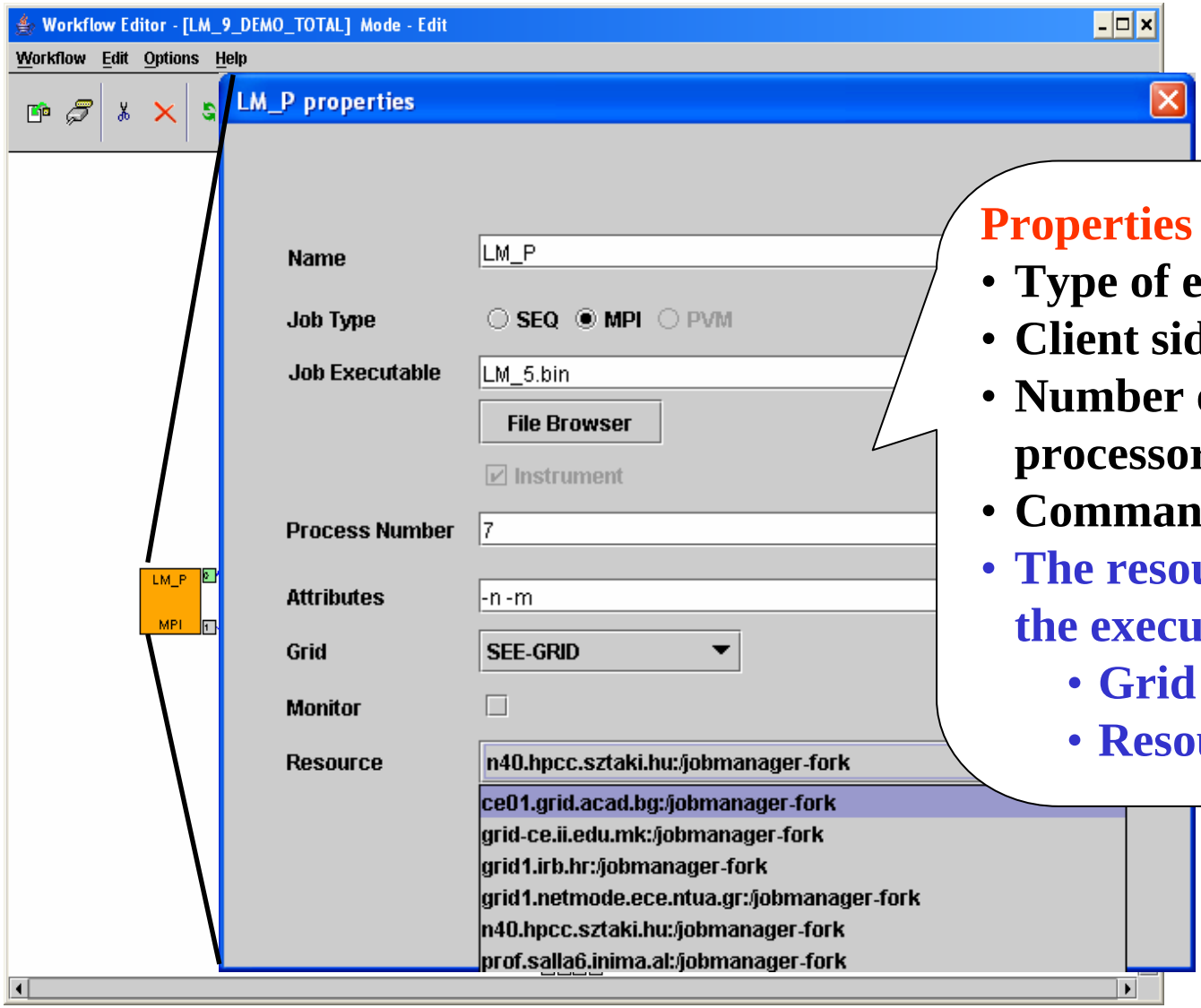
Defining the graph

- The aim is to define a DAG of jobs and services (GEMLCA jobs):
  1. **Drag & drop components:** nodes and ports
  2. **Define their properties**
  3. **Connect ports by channels** (no cycles, no loops, no conditions)



Workflow Editor

Properties of a job component

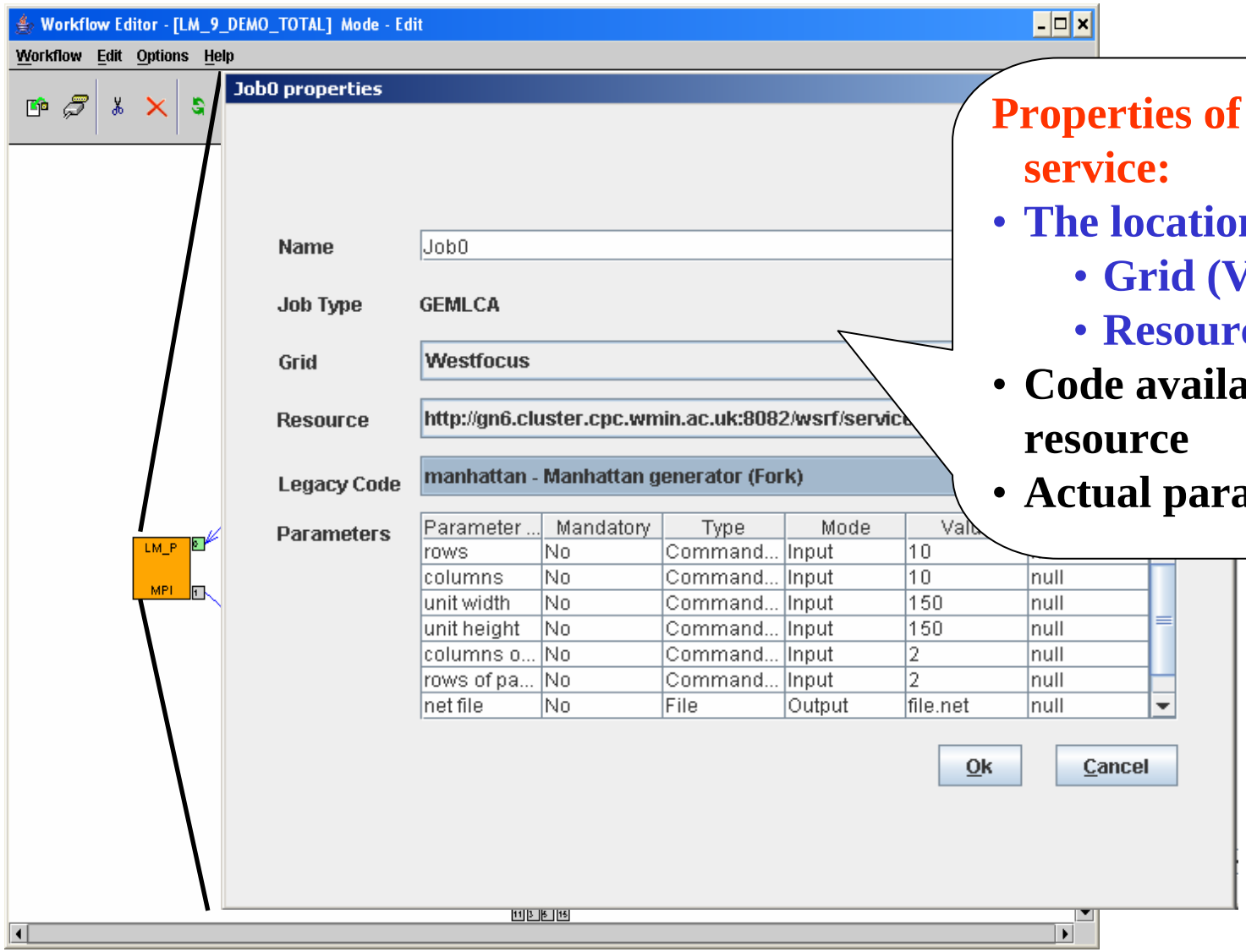


Properties of a job:

- **Type of executable**
- **Client side location of binary**
- **Number of required processors**
- **Command line parameters**
- **The resource to be used for the execution:**
  - **Grid (VO)**
  - **Resource / broker**

Workflow Editor

Properties of a GEMLCA service component

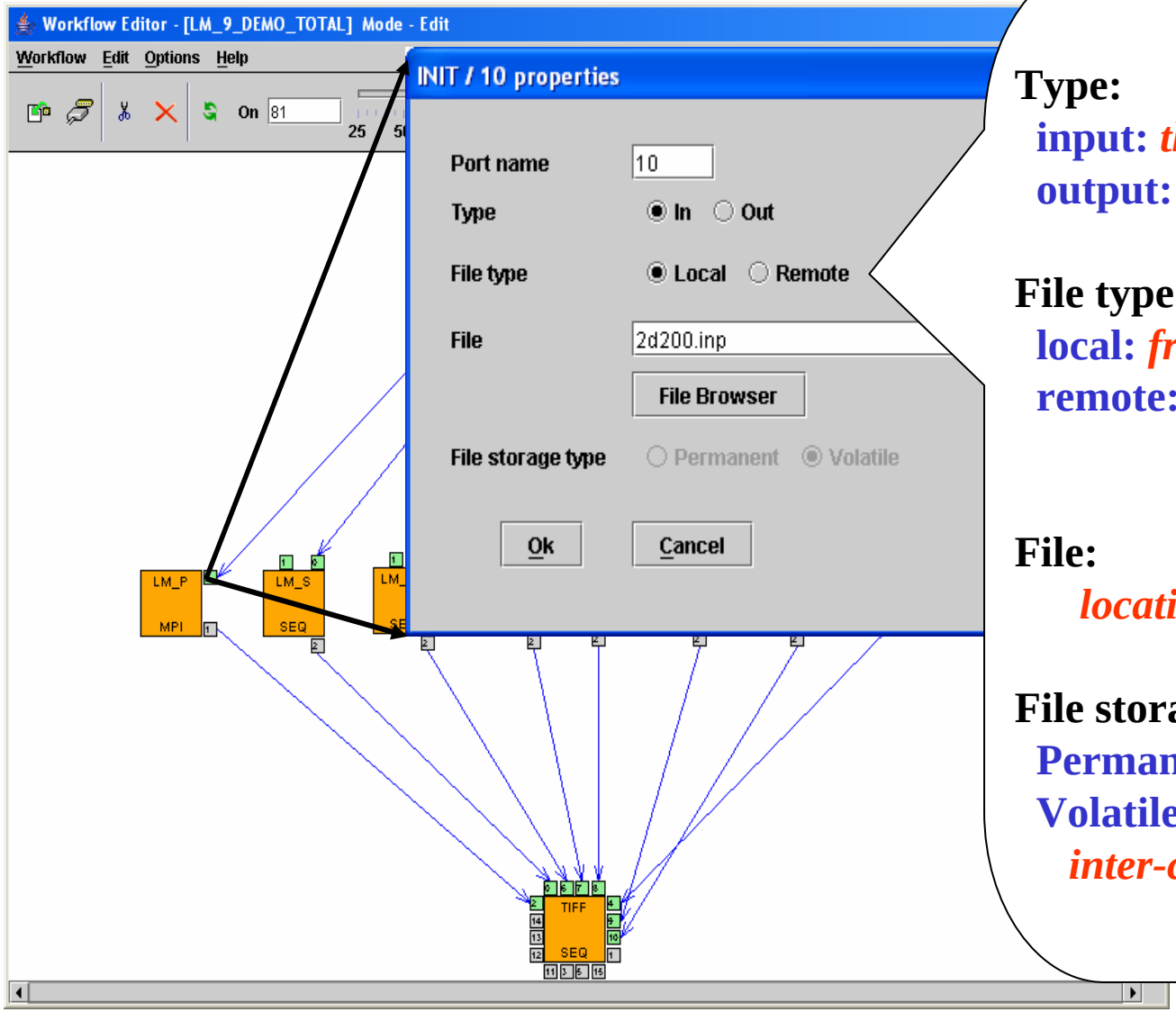


Properties of a GEMLCA service:

- **The location of the service:**
  - **Grid (VO)**
  - **Resource / broker**
- **Code available for that resource**
- **Actual parameter values**

Workflow Editor

Defining job / service input-output data



File properties

Type:

input: *the component requires*

output: *the component produces*

File type:

local: *from/to my desktop*

remote: *from/to a storage resource*

File:

location of the file

File storage type (for outputs only):

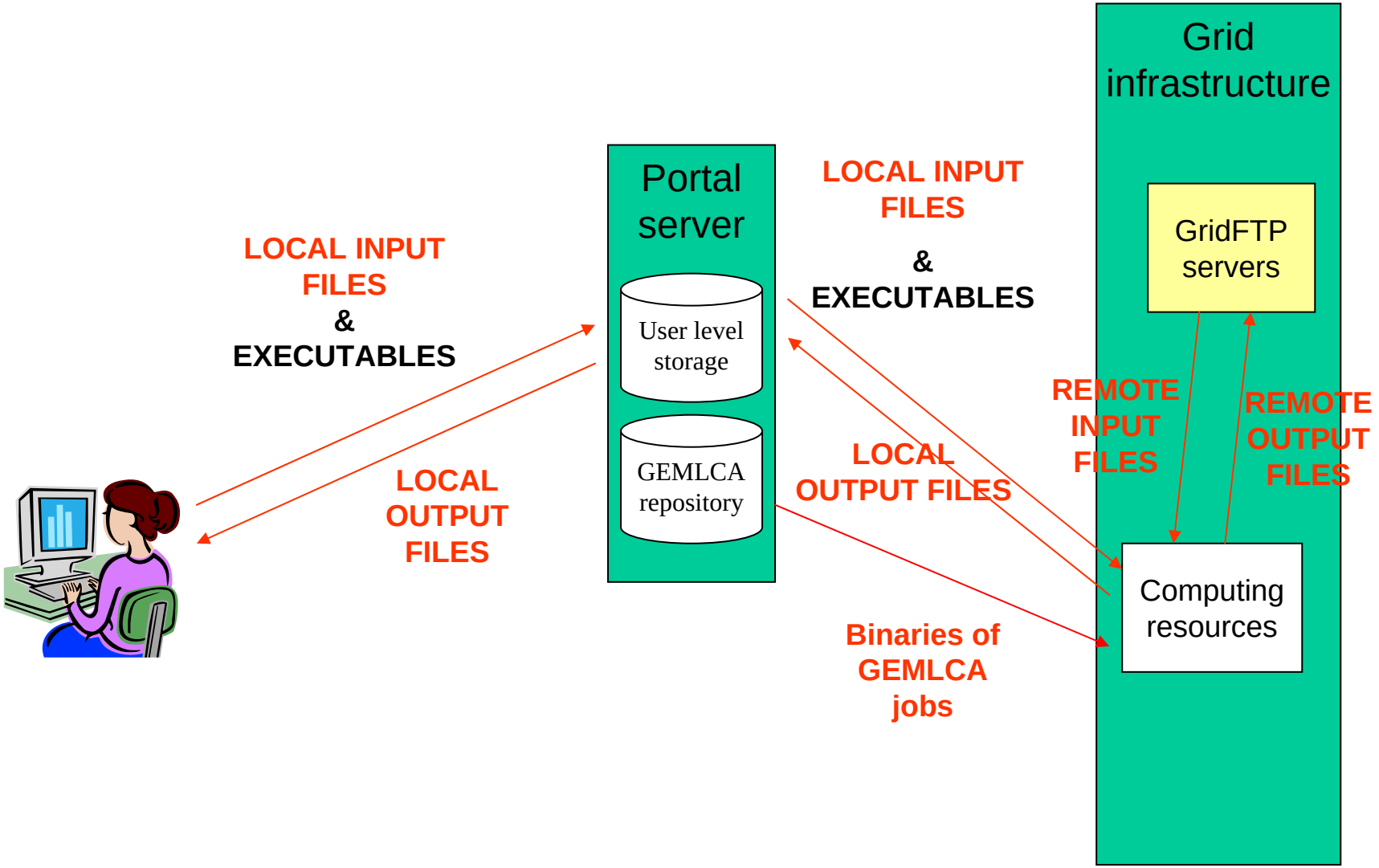
Permanent: *final result*

Volatile: *used only for inter-component data transfer*

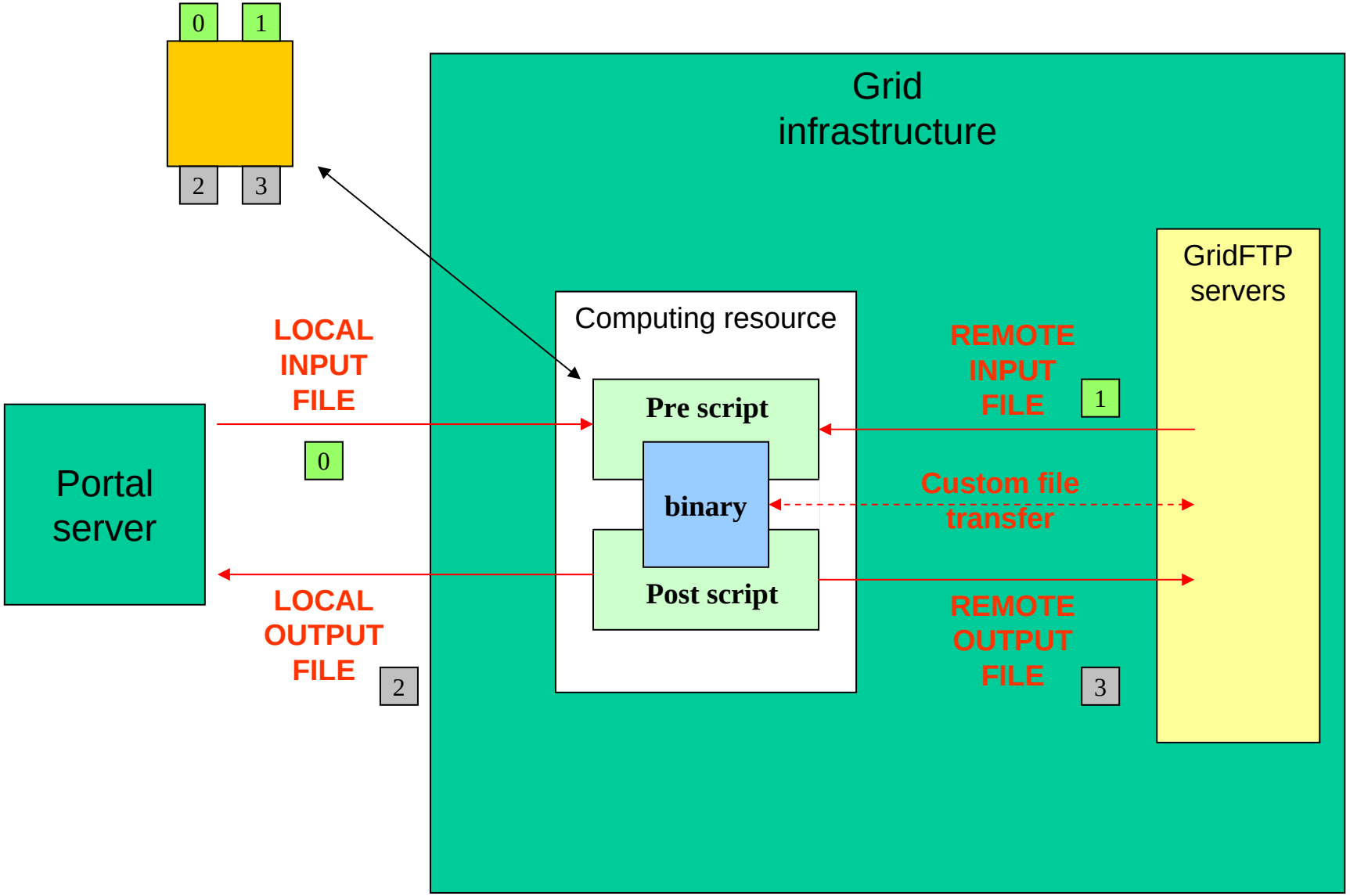
Possible file references

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

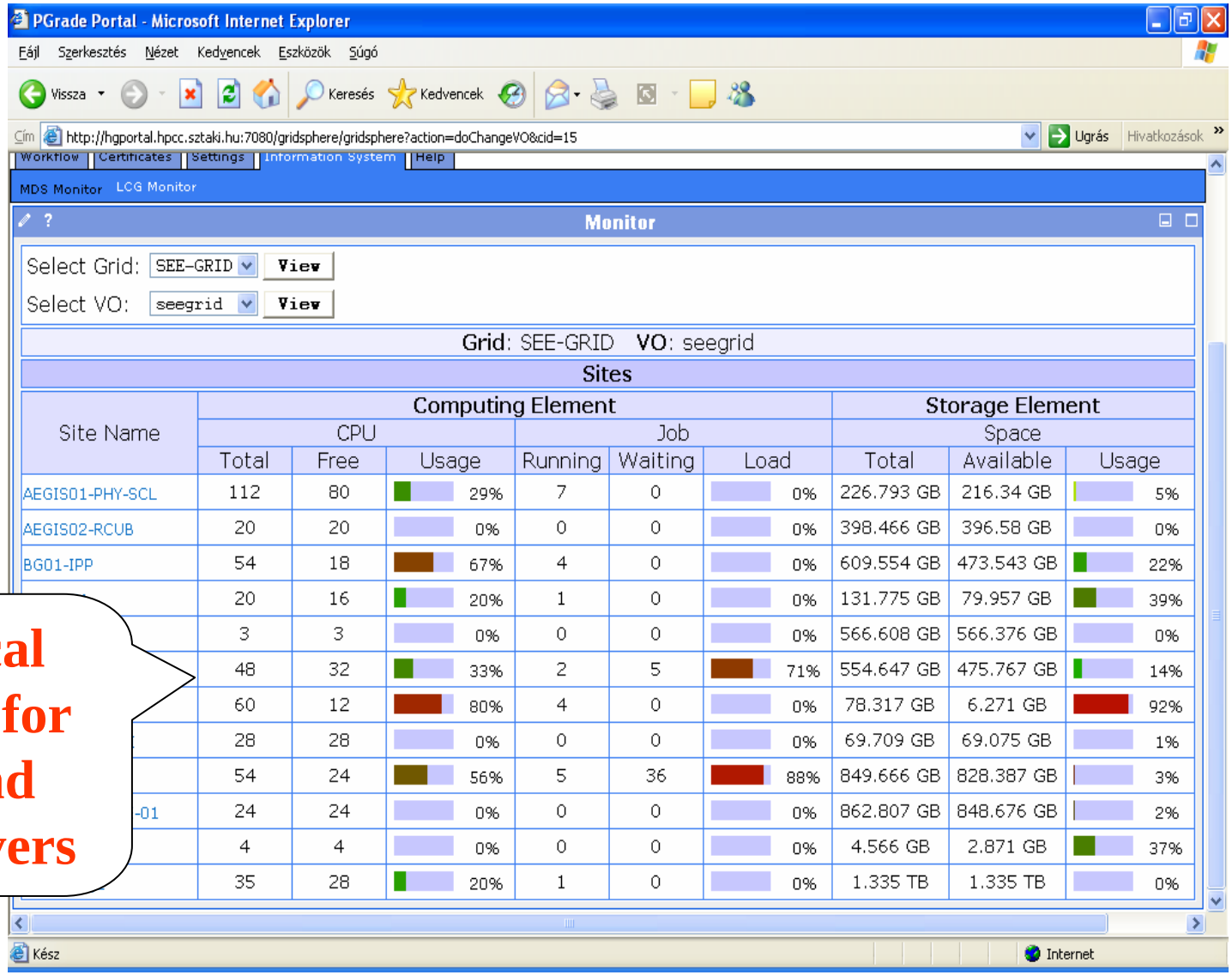
Workflow level file transfer



Job / service level file transfer



Browsing computing resources by the information system portlet



Graphical interface for GIIS and BDII servers

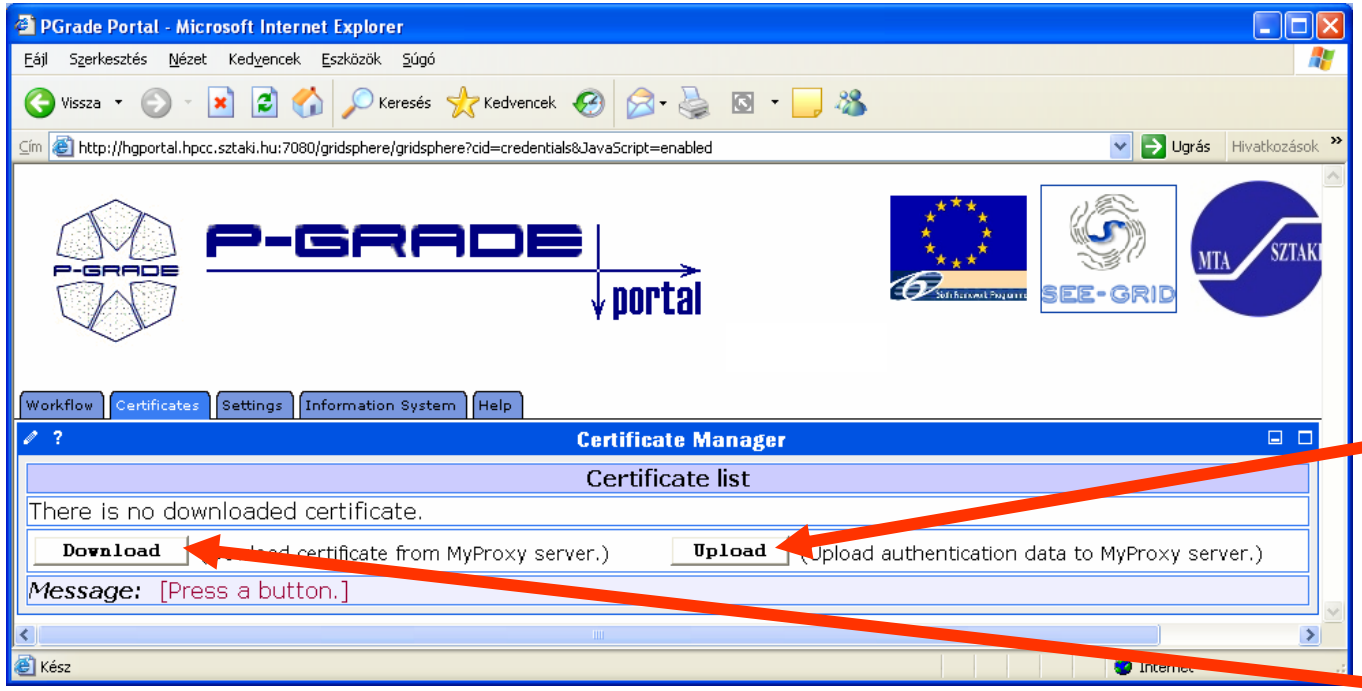
Executing workflows

Main steps

1. Download proxies
2. Submit workflow
3. Observe workflow progress
4. If some error occurs correct the graph
5. Download result

Certificate Manager

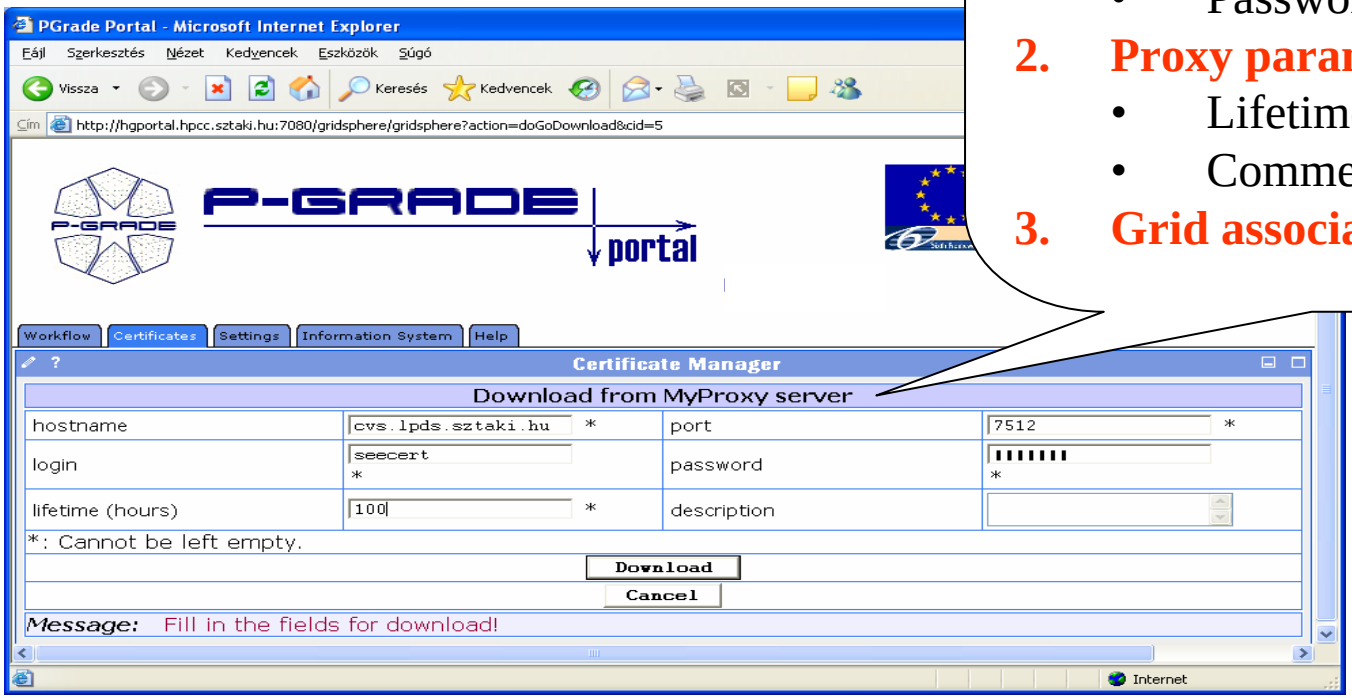
Certificates portlet



- To access GSI-based Grids the portal server application needs proxy certificates
- "Certificates" portlet:
  - to upload X.509 certificates into MyProxy servers
  - to download short-term proxy credentials into the portal server application

Certificate Manager

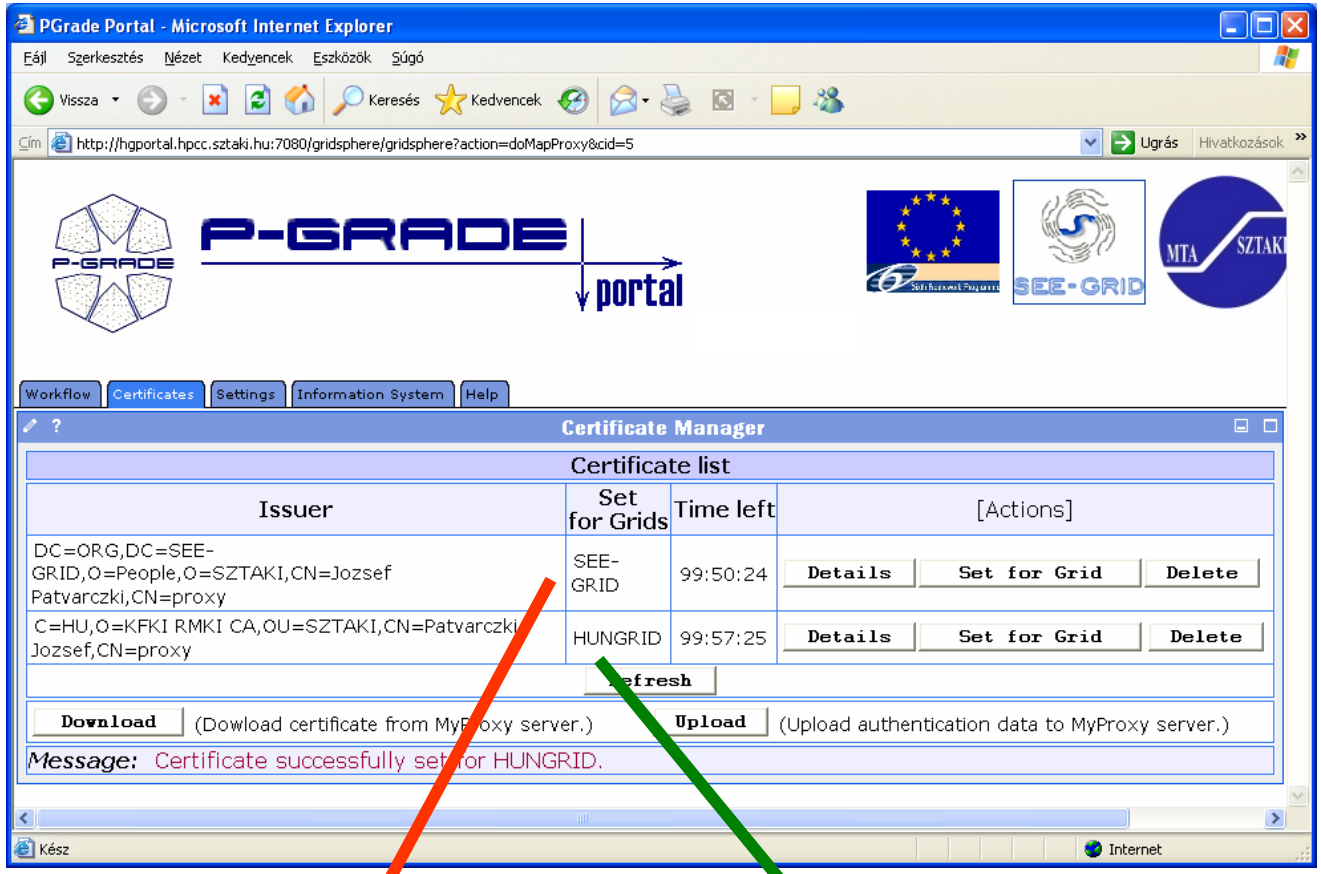
Downloading a proxy



1. **MyProxy server access details:**
   - Hostname
   - Port number
   - User name (from upload)
   - Password (from upload)
2. **Proxy parameters:**
   - Lifetime
   - Comment
3. **Grid association**

Certificate Manager

Multi-grid → Multi-proxy



SEE-GRID CEs and SEs

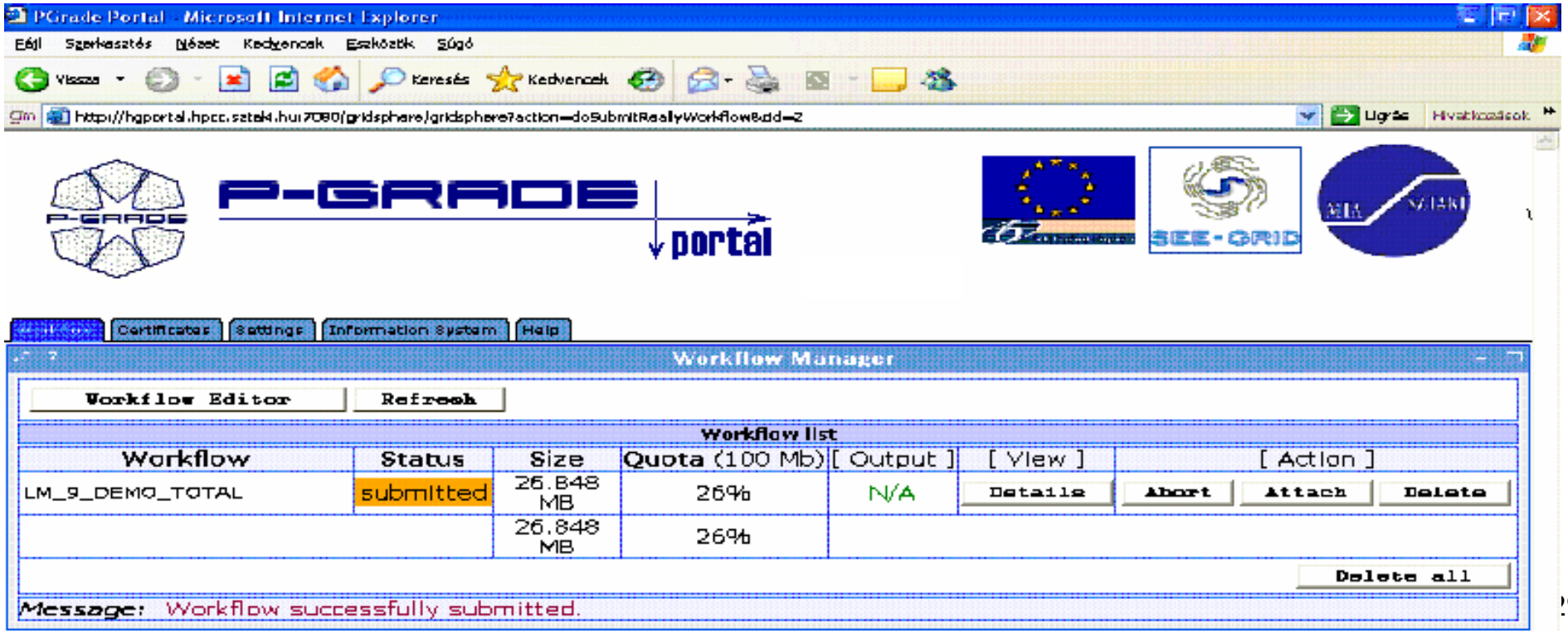
HUNGRID CEs and SEs

Multiple proxies can be available on the portal server at the same time!

Workflow Management

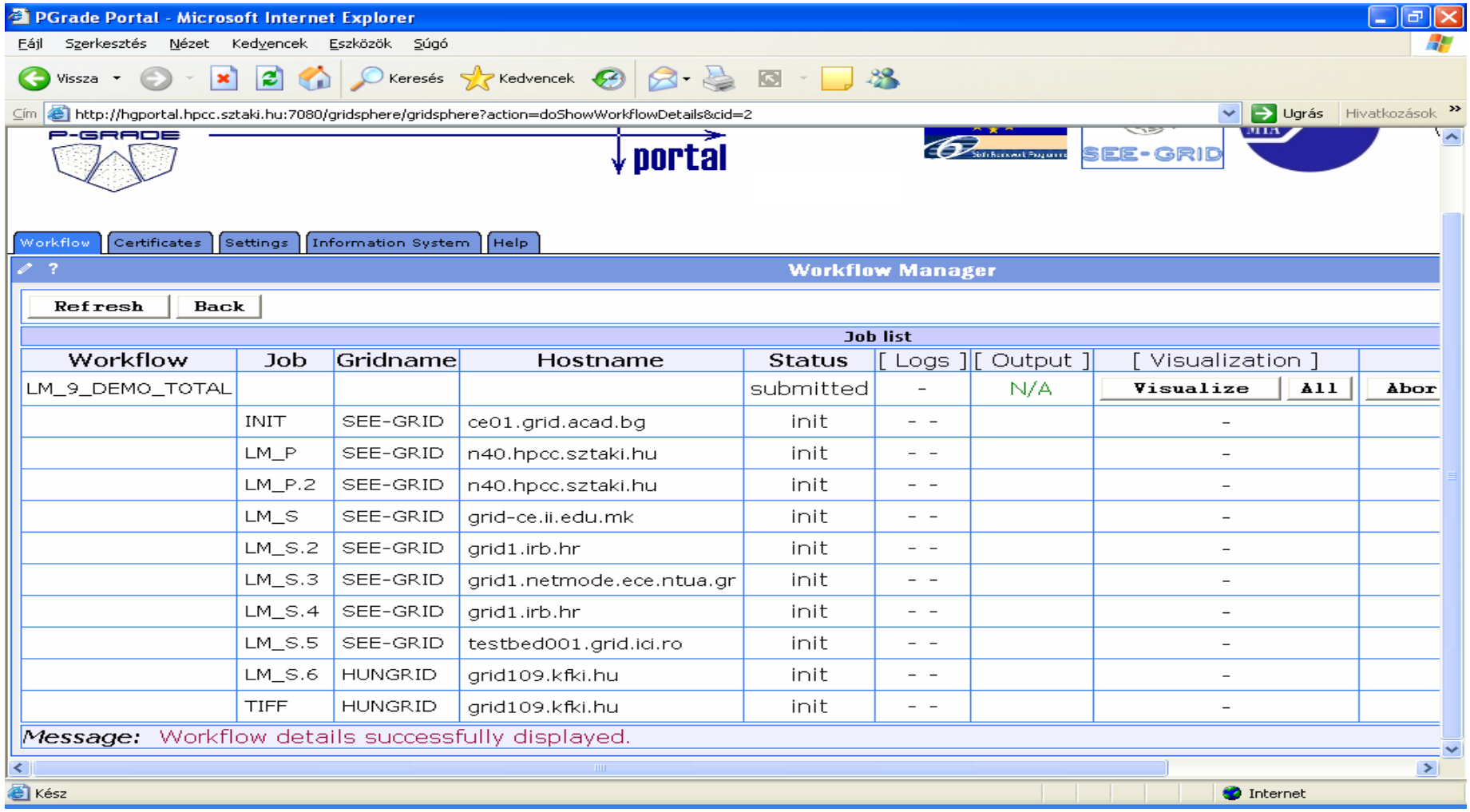
(workflow portlet)

- The portlet presents the status, size and output of the available workflow in the "**Workflow**" list
- It has a Quota manager to control the users' storage space on the server
- The portlet also contains the "**Abort**", "**Attach**", "**Details**", "**Delete**" and "**Delete all**" buttons to handle execution of workflows
- The "**Attach**" button opens the workflow in the Workflow Editor
- The "**Details**" button gives an overview about the jobs of the workflow



Workflow Execution

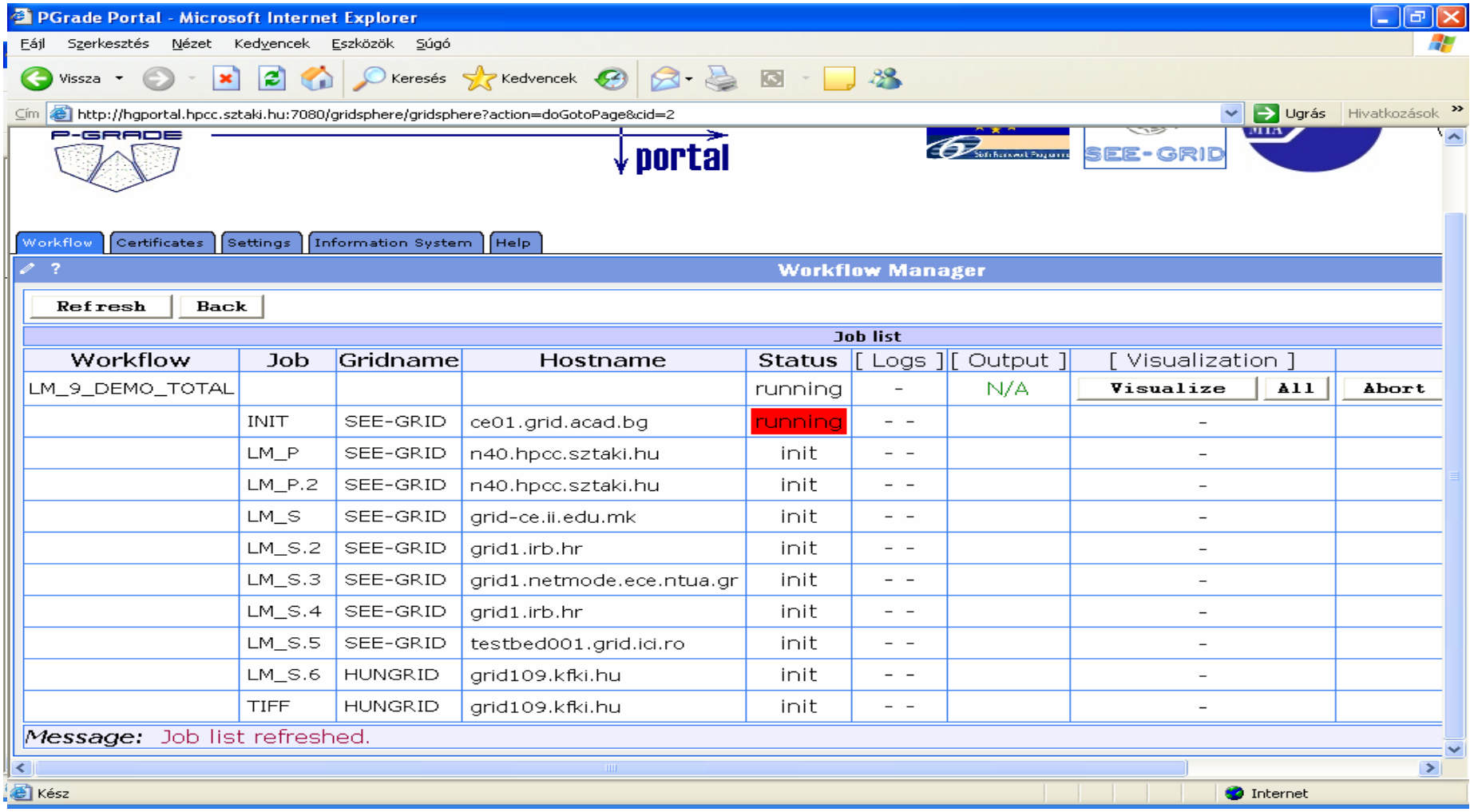
(observation by the workflow portlet)



White/Red/Green color means the job is initial/running/finished state

Workflow Execution

(observation by the workflow portlet)



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Workflow Execution

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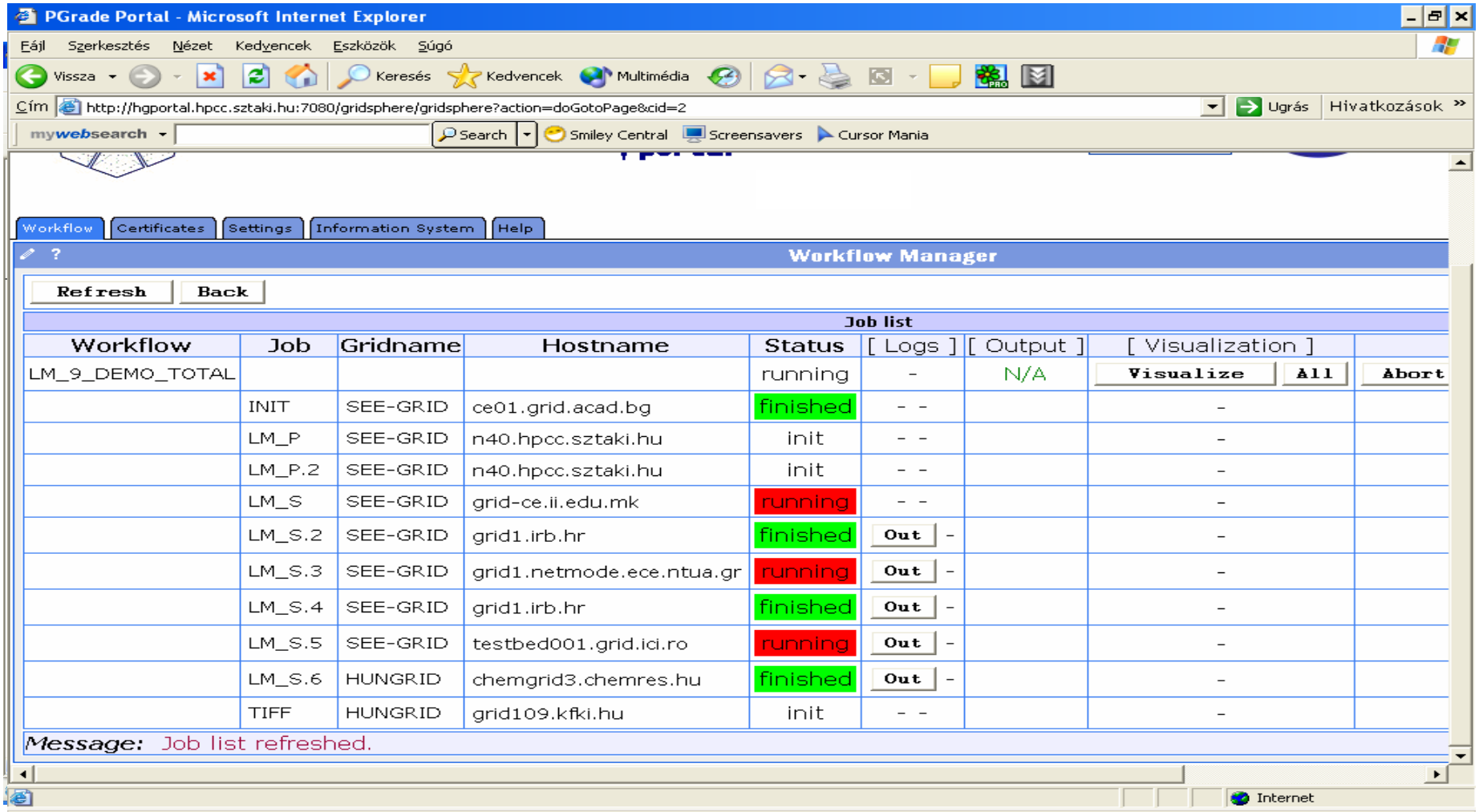

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Workflow Execution

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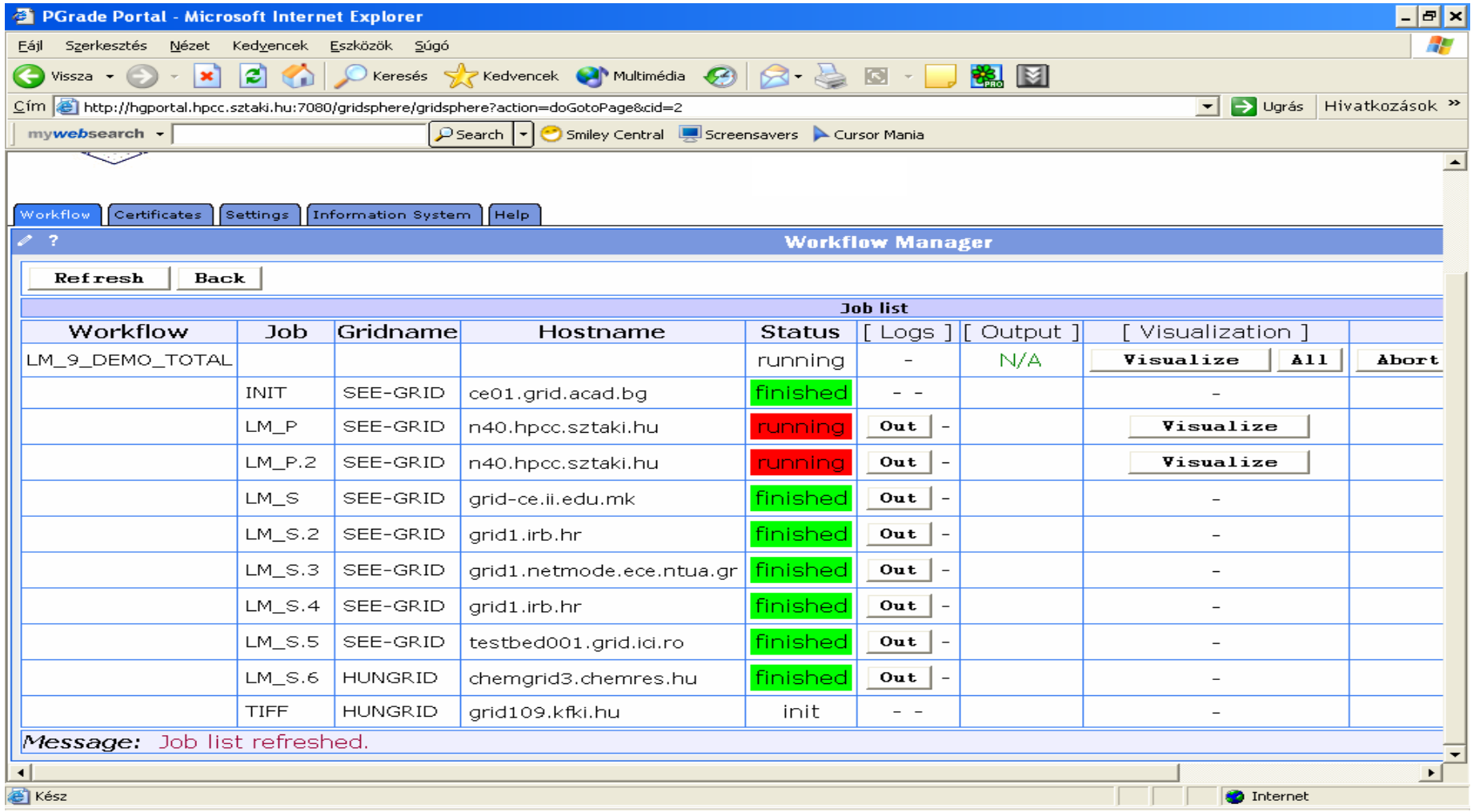

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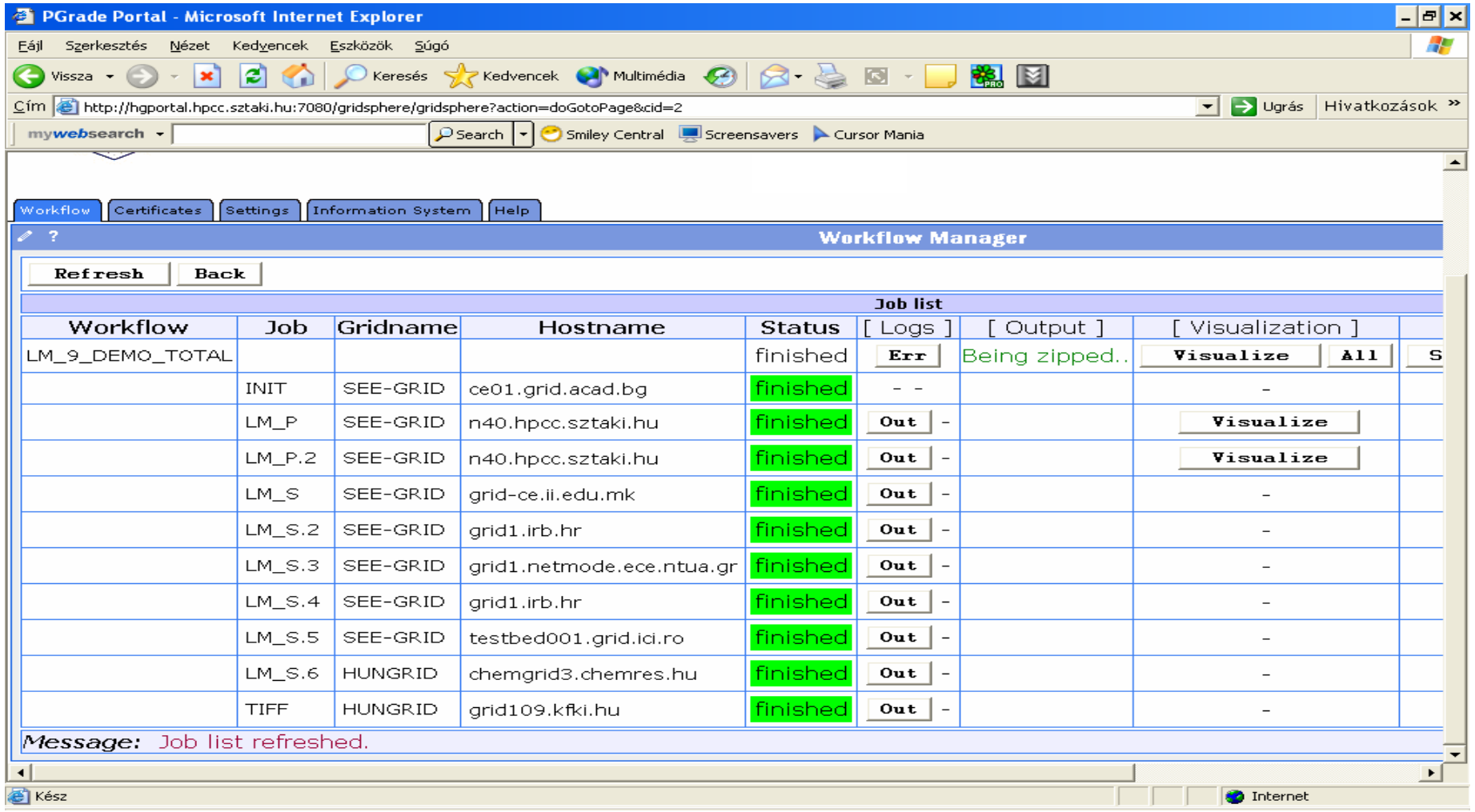
Workflow Execution

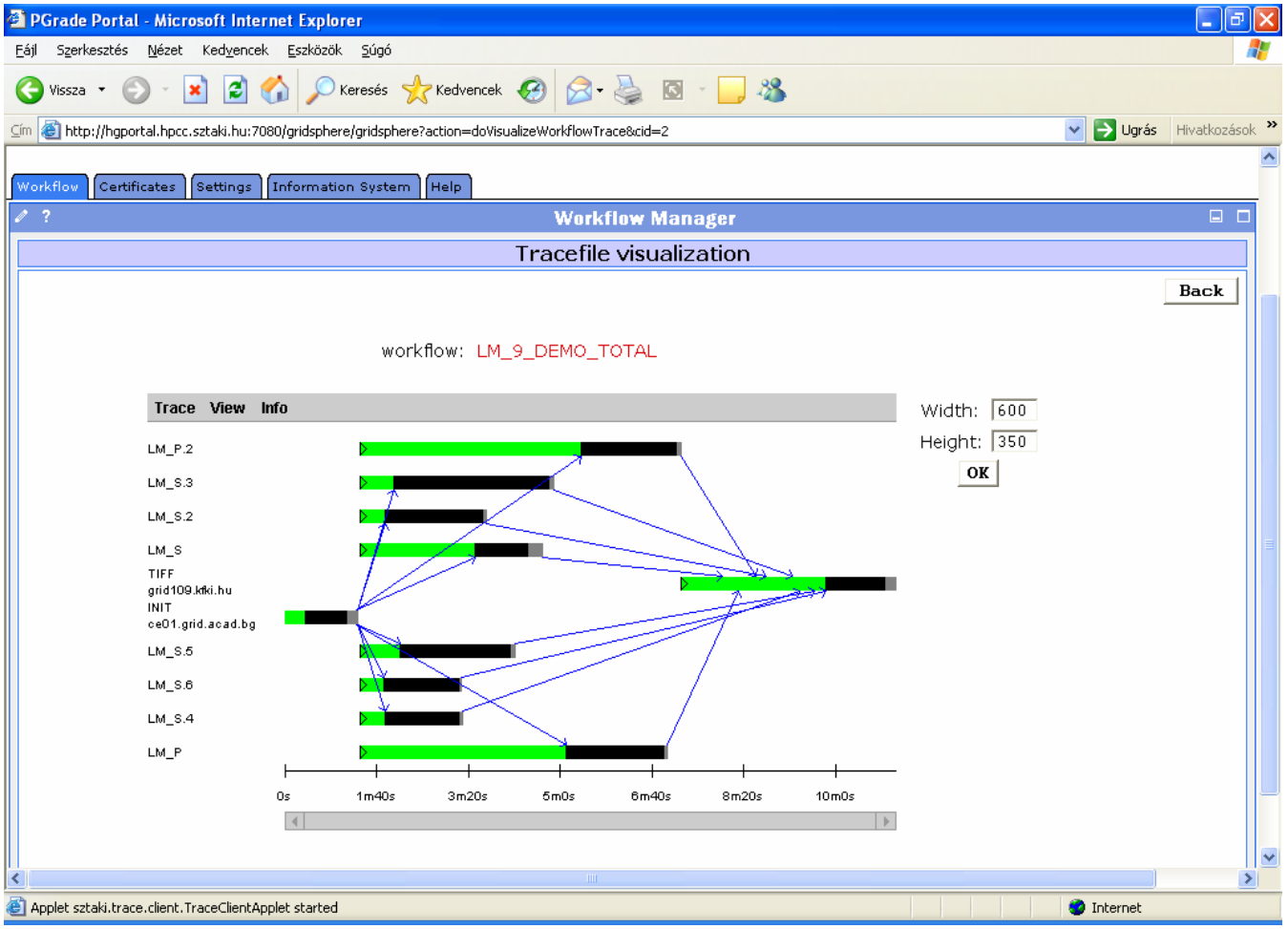
(observation by the workflow portlet)



Workflow	Job	Gridname	Hostname	Status	[Logs]	[Output]	[Visualization]
LM_9_DEMO_TOTAL				finished	Err	Being zipped..	Visualize All S
	INIT	SEE-GRID	ce01.grid.acad.bg	finished	- -		-
	LM_P	SEE-GRID	n40.hpcc.sztaki.hu	finished	Out -		Visualize
	LM_P.2	SEE-GRID	n40.hpcc.sztaki.hu	finished	Out -		Visualize
	LM_S	SEE-GRID	grid-ce.ii.edu.mk	finished	Out -		-
	LM_S.2	SEE-GRID	grid1.irb.hr	finished	Out -		-
	LM_S.3	SEE-GRID	grid1.netmode.ece.ntua.gr	finished	Out -		-
	LM_S.4	SEE-GRID	grid1.irb.hr	finished	Out -		-
	LM_S.5	SEE-GRID	testbed001.grid.ici.ro	finished	Out -		-
	LM_S.6	HUNGRID	chemgrid3.chemres.hu	finished	Out -		-
	TIFF	HUNGRID	grid109.kfki.hu	finished	Out -		-

White/Red/Green color means the job is initialised/running/finished

On-Line Monitoring both at the workflow and job levels *(workflow portlet)*

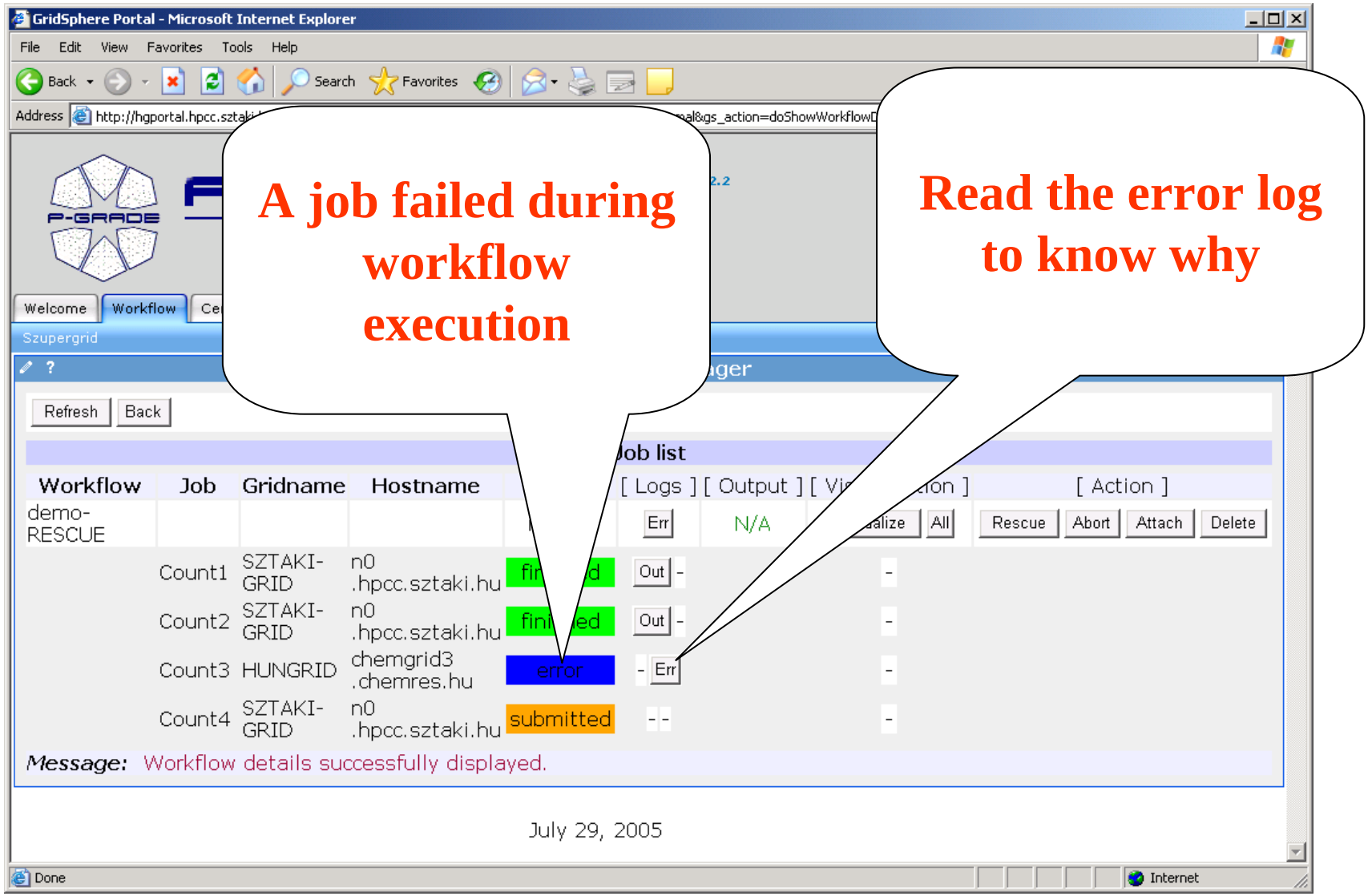


- The portal monitors and visualizes workflow progress

On-Line Monitoring both at the workflow and job levels *(workflow portlet)*

- **The portal monitors and visualizes parallel jobs**
  (if they are prepared for Mercury monitor)

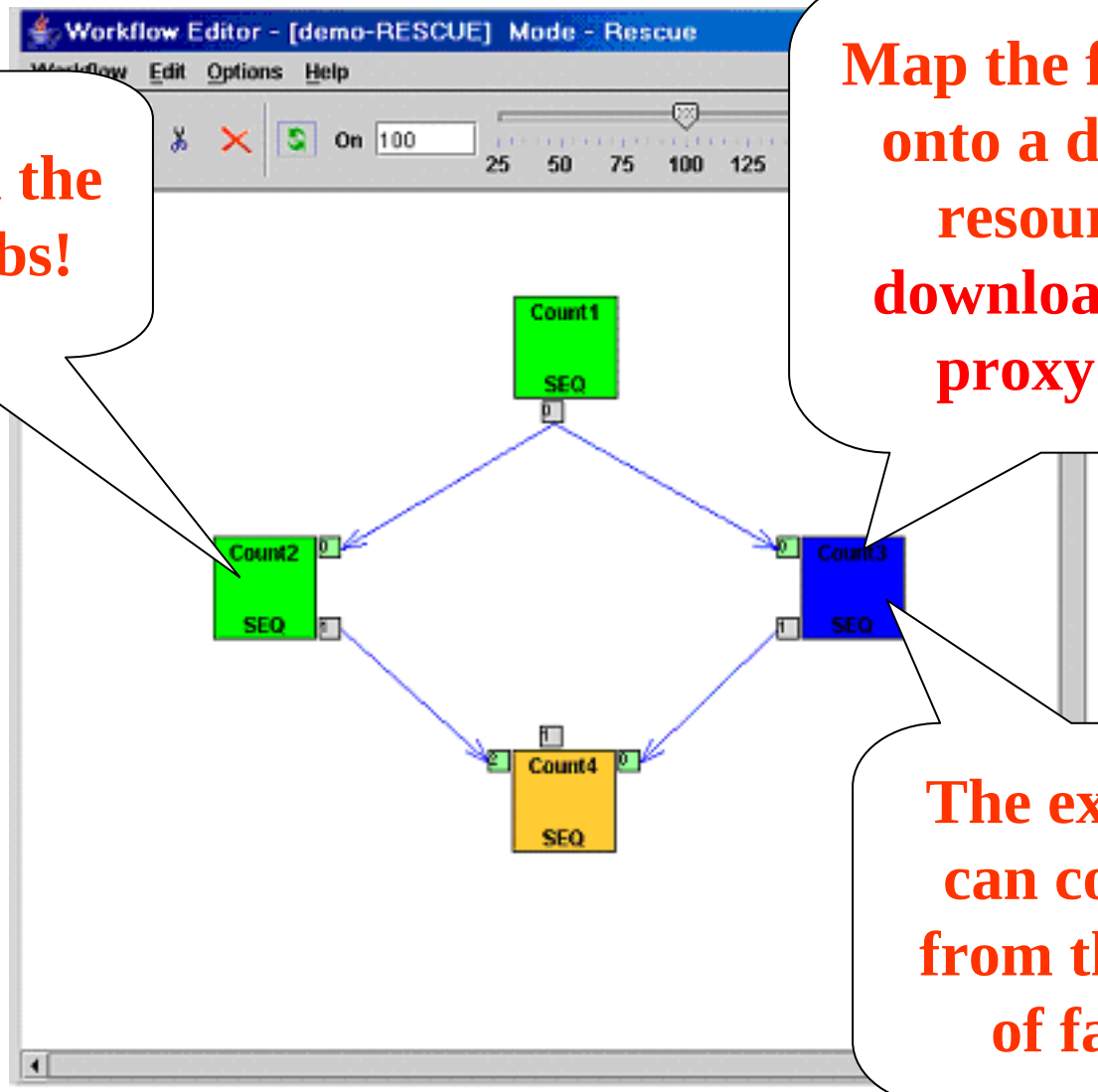
Rescuing a failed workflow 1.



A job failed during workflow execution

Read the error log to know why

Rescuing a failed workflow 2.

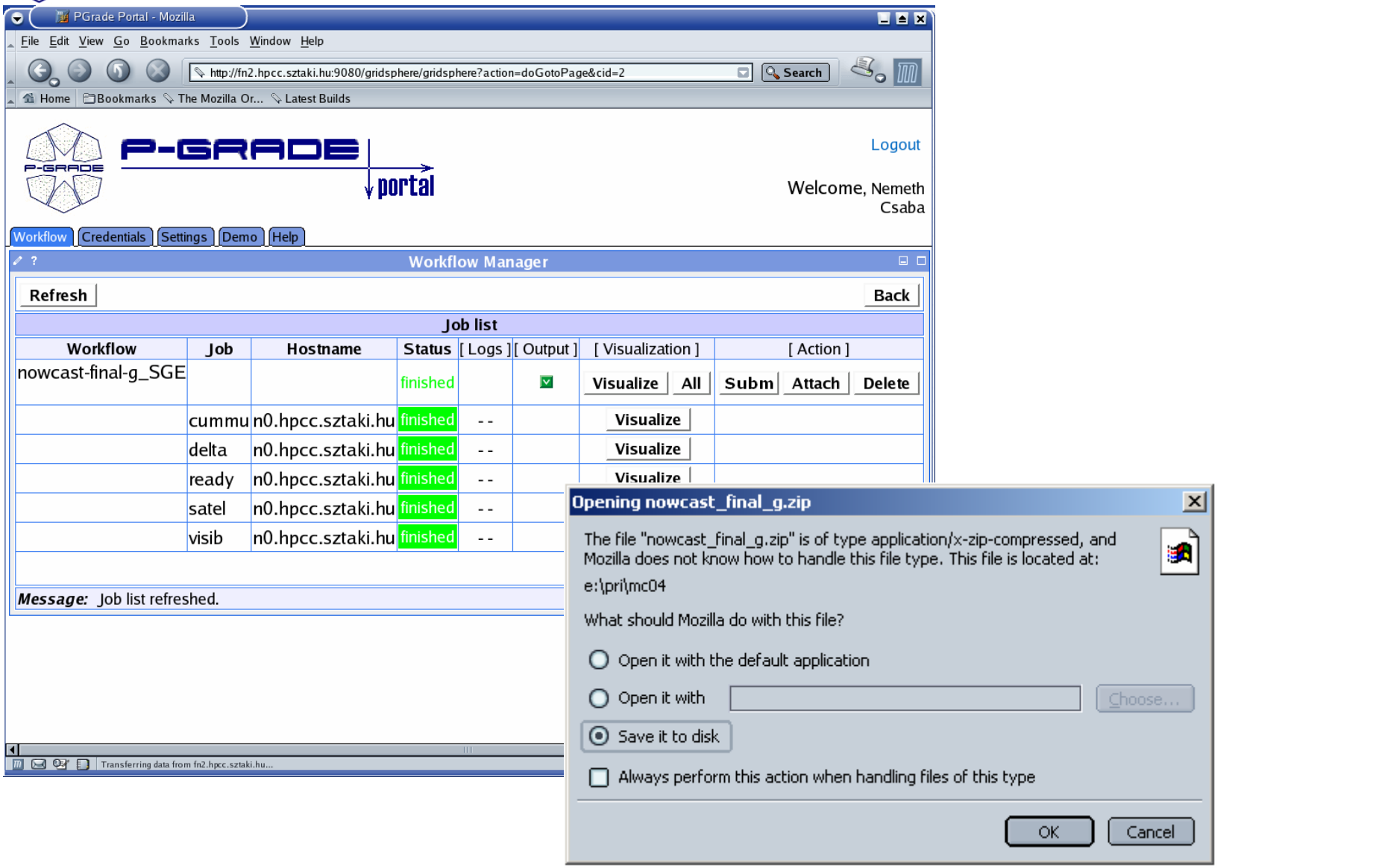


Don't touch the finished jobs!

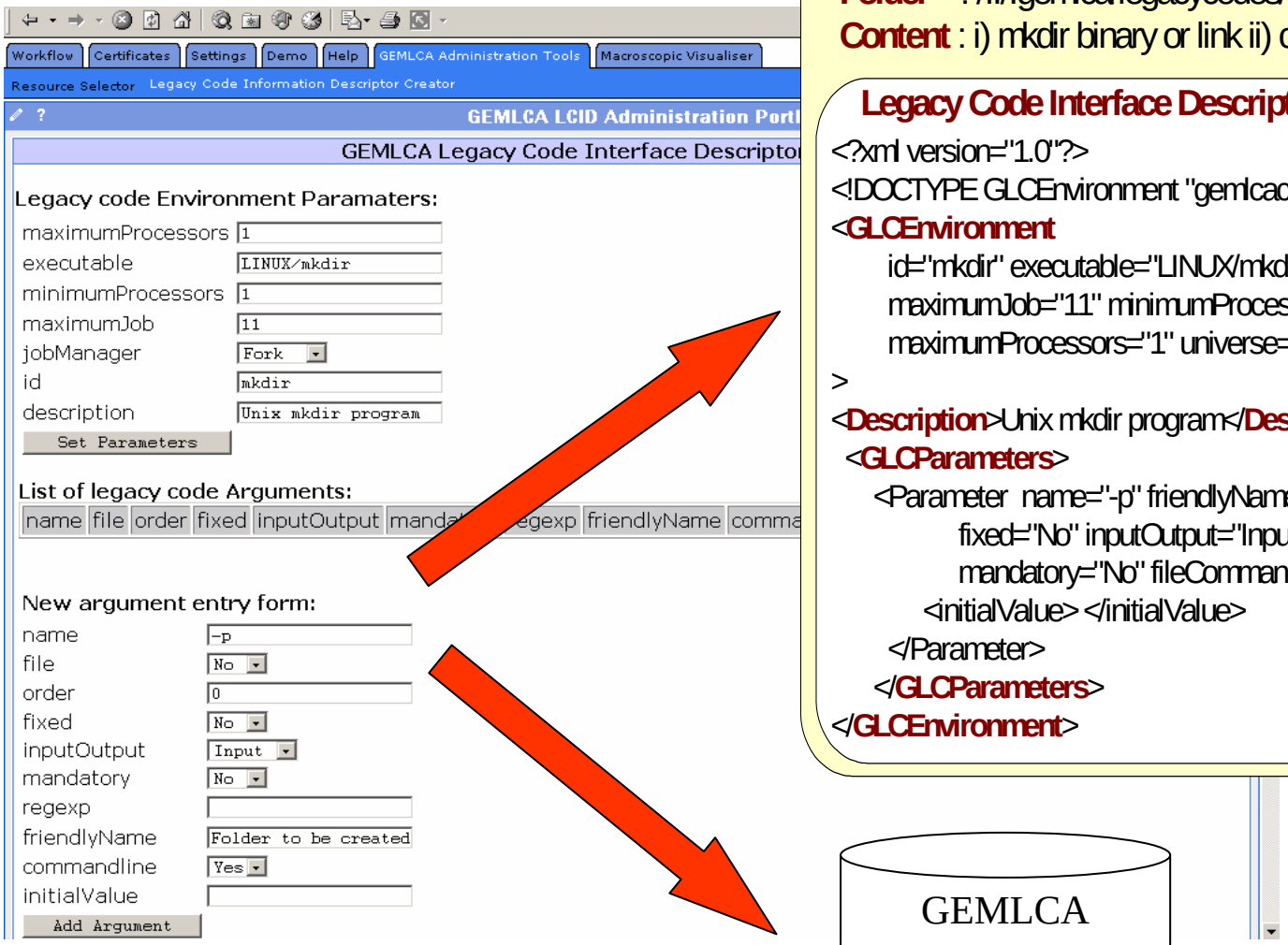
Map the failed job onto a different resource or download a new proxy for it

The execution can continue from the point of failure

Downloading the results…



Putting a successfully finished job into the GEMLCA repository



Mkdir Legacy Code exposed as a Grid Service

Folder : /../.gemlca/legacycodes/mkdir

Content : i) mkdir binary or link ii) config.xml

Legacy Code Interface Description File: config.xml

```
<?xml version="1.0"?>
<!DOCTYPE GLCEnvironment "gemlcaconfig.dtd">
<GLCEnvironment
      id="mkdir" executable="LINUX/mkdir" jobManager="Fork"
      maximumJob="11" minimumProcessors="1"
      maximumProcessors="1" universe="PVM"
>
<Description>Unix mkdir program</Description>
 <GLCParameters>
    <Parameter  name="-p" friendlyName="Folder to be created"
          fixed="No" inputOutput="Input" order="0"
          mandatory="No" fileCommandline="Commandline">
        <initialValue> </initialValue>
    </Parameter>
   </GLCParameters>
</GLCEnvironment>
```

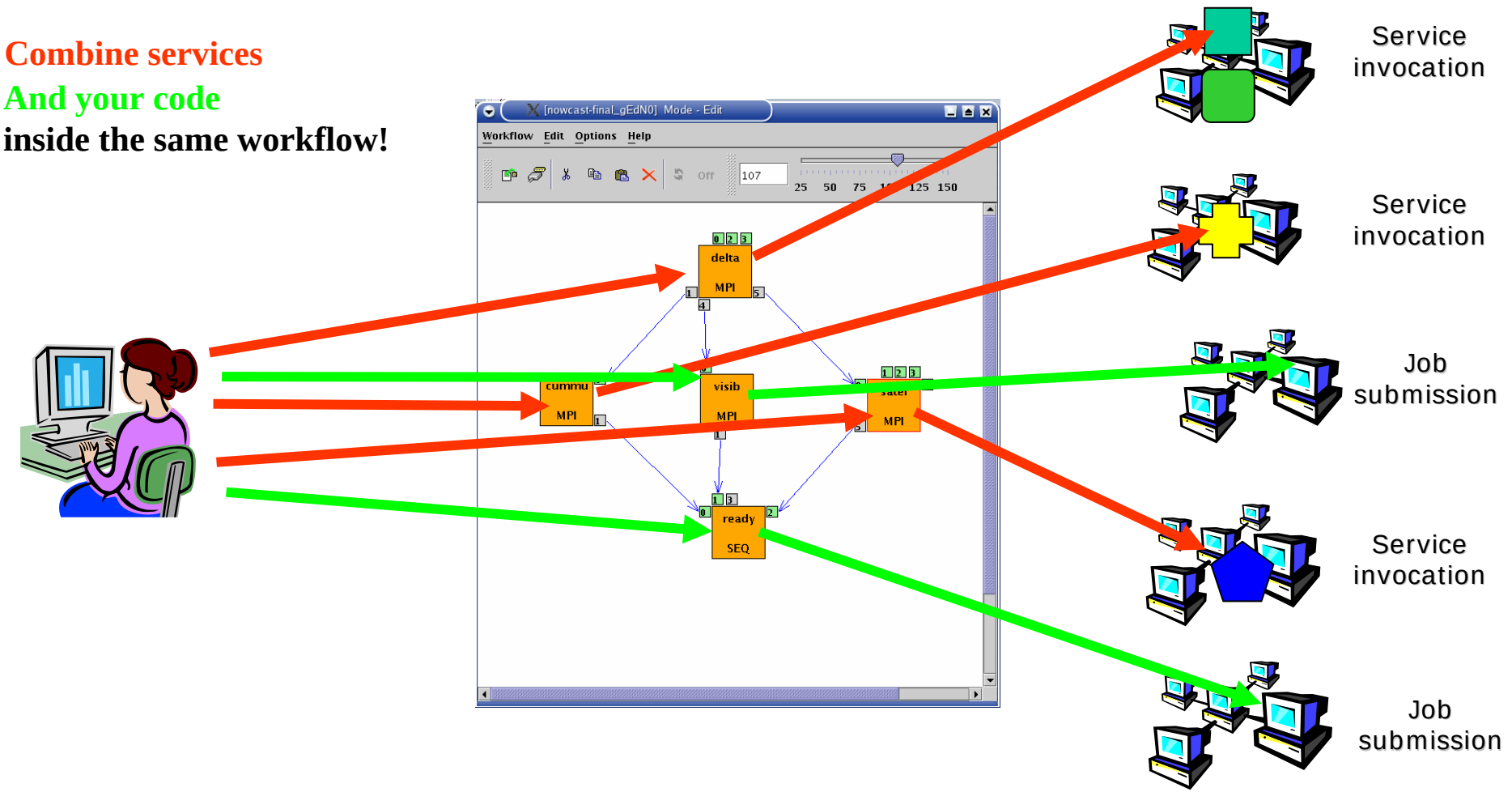
GEMLCA repository

Collaborative applications

Combine services

And your code

inside the same workflow!



GEMLCA / P-GRADE on the UK NGS:
P-GRADE NGS GEMLCA Portal

- **Information website:** http://www.cpc.wmin.ac.uk/ngsportal/
- Interface for NGS GT2 sites
- Interface for GT4 Westminster site
- Interface for EGEE GILDA sites
- Open for the NGS and EGEE communities

Other P-GRADE Portal installations

- P-GRADE Portal service is available for
  - SEE-GRID infrastructure
  - Central European VO of EGEE
  - GILDA: Training VO of EGEE
  - US Open Science Grid, TeraGrid
  - Economy-Grid, Swiss BioGrid, Bio and Biomed EGEE VOs, BioInfoGrid, BalticGrid
  - OGF GIN VO (also connected to NGS)

Hands-on slides