



P-GRADE Portal and Developer Alliance

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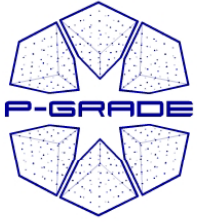
MTA SZTAKI
Hungarian Academy of Sciences

portal.p-grade.hu



Agenda

- **P-GRADE Portal and Developer Alliance status**
 - P-GRADE Portal goes open source!
- **Capabilities of P-GRADE Portal 2.5**
 - Workflow support
 - Parametric study support
 - Middleware compatibility
- **Presentations from Alliance members**
 - Tamas Kiss, University of Westminster
 - Onur Temizsoylu, Turkish Academic Network (presentation on behalf of Middle East Technical University)
- **Support services and roadmap**
 - From P-GRADE to gUSE
- **Discussion**



P-GRADE Portal goes open source!

- At the end of the session we would like to hear your opinion on
 - Open source strategy
 - Licensing
 - Directions of future development
 - ...
- But first see what is available now...



Motivations to P-GRADE Portal

- 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 WMS → WMPProxy), 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 (file management)
 - Computation services (job submission)
 - Security services (proxy based single sign-on)
 - Brokers (not in every middleware, but e.g. in gLite - WMS)
- **Provide an easy to use environment for the management of grid services and applications**



P-GRADE Portal in a nutshell

- General purpose grid user environment
- Based on GridSphere web portal framework
- Development started in 2003
- Tool that helps you develop and execute workflows and workflow based parametric studies
- A Grid orchestration environment. Supported services:

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

Solves Grid interoperability problem at the workflow level



Portal Developer Alliance

- Core development by **MTA SZTAKI, Budapest:**
P-GRADE Portal 2.5
Application specific Supplier Chain Portal
- Support for legacy codes and code repositories by **University of Westminster, London:**
GEMLCA P-GRADE Portal 2.4.1
Application specific Rendering Portal
Application specific Traffic Simulator Portal
- File manager and credential manager portlet by **Middle East Technical University, Ankara**
Portlets used in Turkish National Grid Portal
- Alternative job scheduling component by **Eötvös Loránd University, Budapest**
Under development
- Monte Carlo simulation support library portlet by **Rudjer Boskovic Institute, Zagreb**
Under development





Related projects

Development and support services of P-GRADE are supported by the following projects:

- **SEE-GRID** www.see-grid.eu
portal development
grid application development
- **Coregrid** www.coregrid.net
Research & development
- **EGEE** www.eu-egee.org
grid end user training
grid application development
- **ICEAGE** www.iceage-eu.org
Grid end user training, conceptual training





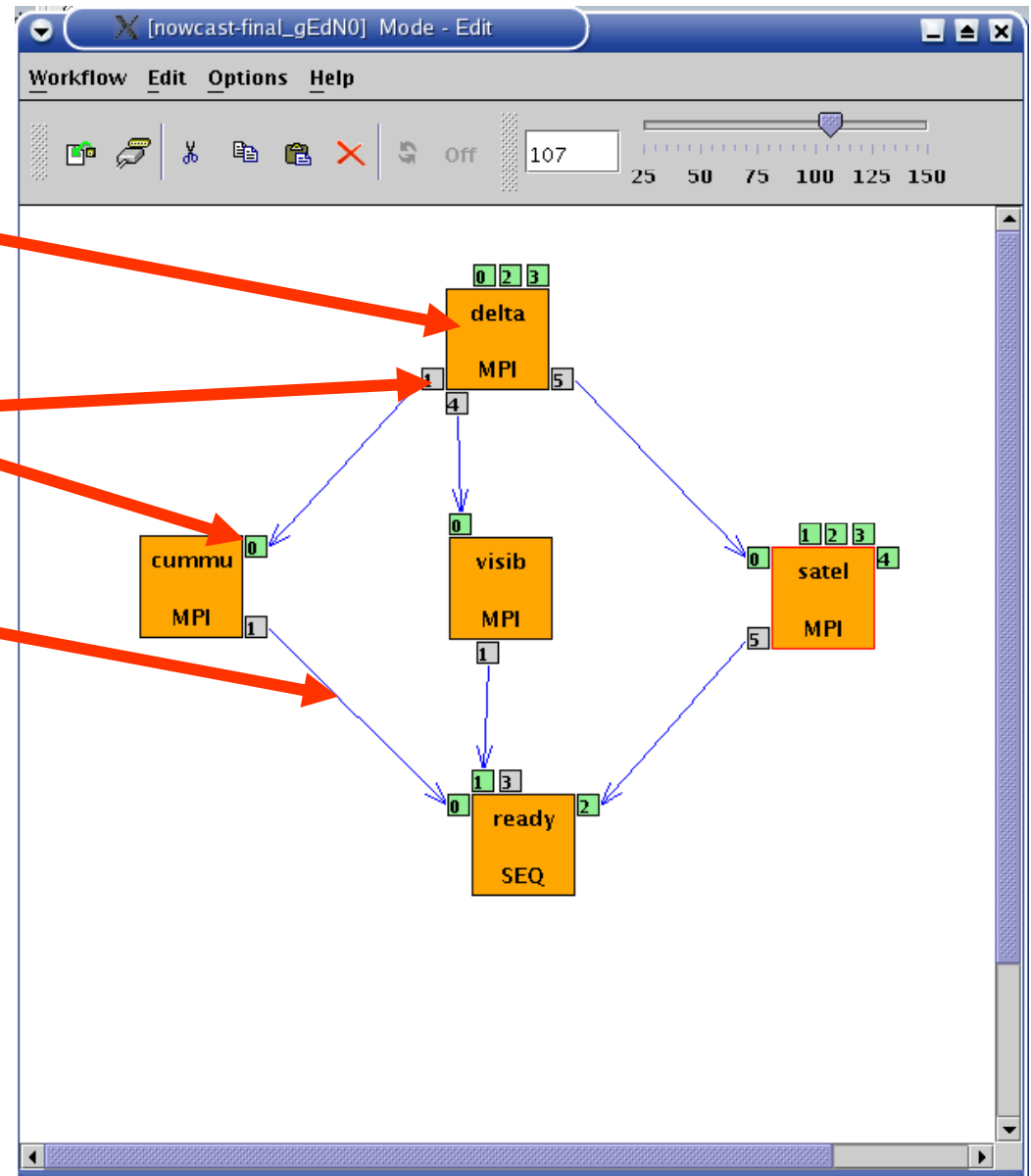
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Elements of a P-Grade Portal 2.5 application

- A directed acyclic graph where
 - Nodes represent batch jobs to be submitted to a job queue (WMS, SE or GRAM)
 - Ports represent input/output files the jobs require or produce
 - Arcs represent file transfer operations and dependencies among jobs
- semantics of the workflow:
 - A job can be executed if all of its input files are available
 - Responsibility of the built-in workflow manager





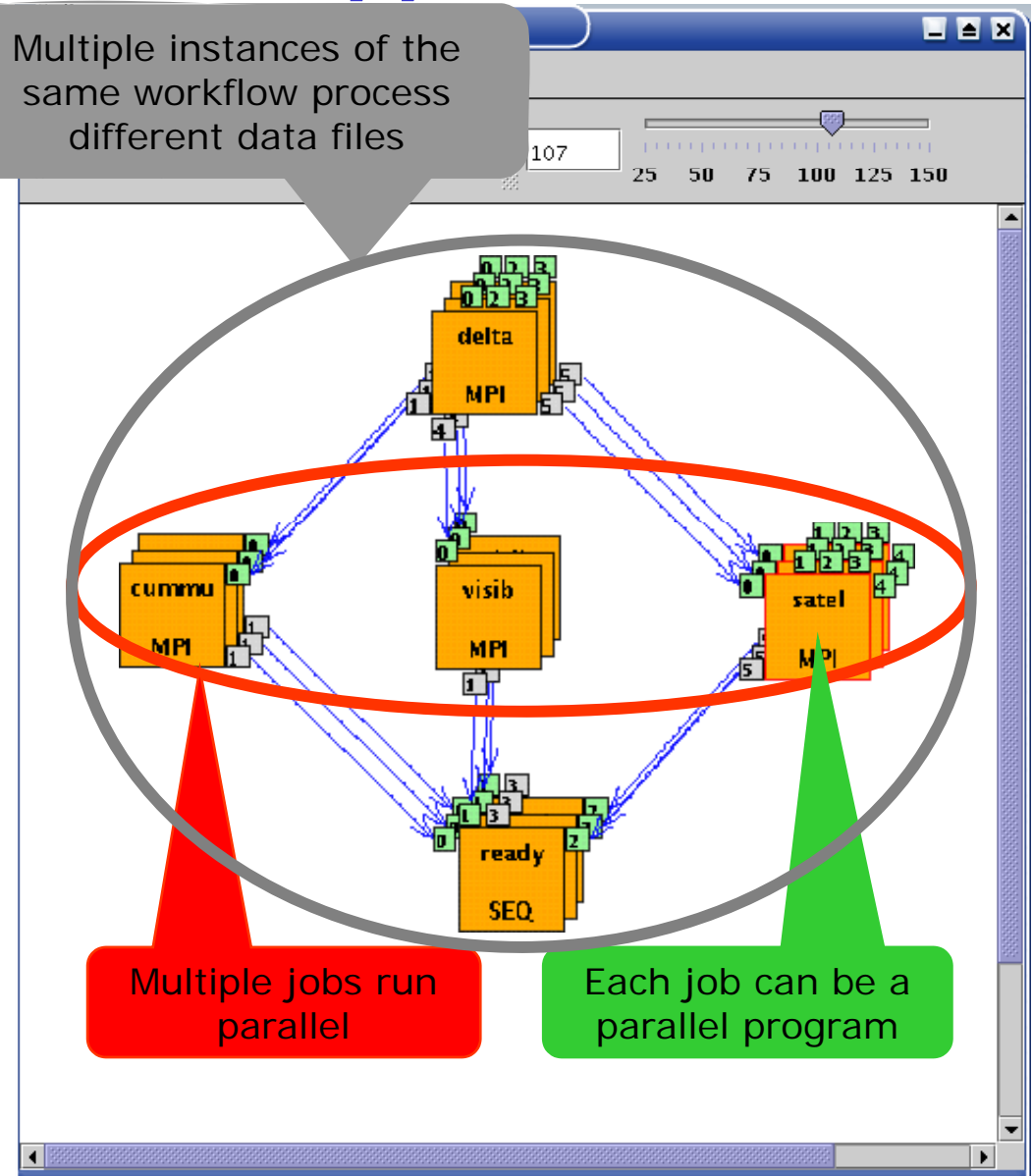
Parallel execution by a P-GRADE Portal application

– Parallel execution inside
a workflow node
(MPI job as workflow
component)

– Parallel execution among
workflow nodes
(different jobs on different
clusters)

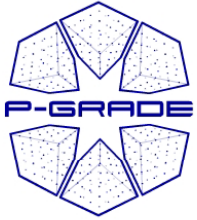
– Parameter study execution
of the workflow (Single
instruction Multiple Data)

Multiple instances of the
same workflow process
different data files



Multiple jobs run
parallel

Each job can be a
parallel program



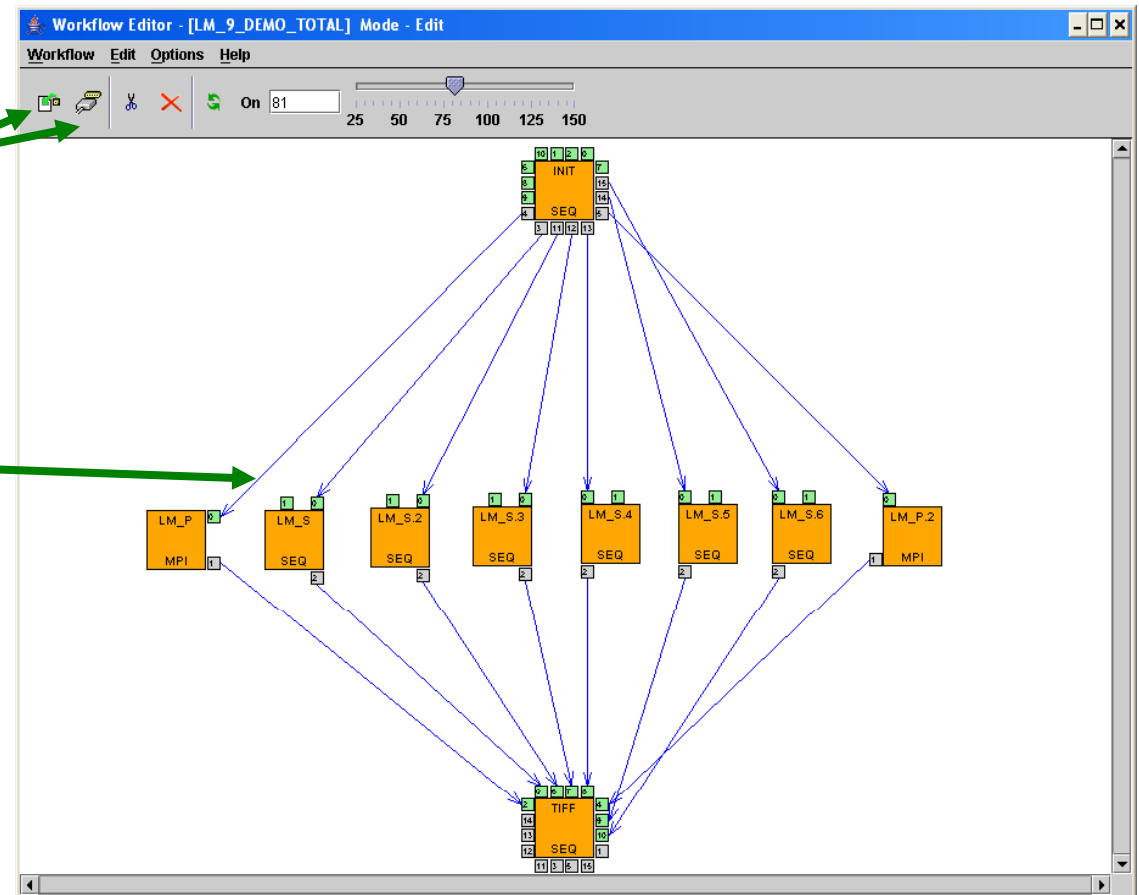
Defining a grid application

Define a Directed Acyclic Graph (*DAG*) of jobs:

1. **Drag & drop components:** nodes and ports
2. **Define component properties** (double click)
3. **Connect ports by channels**
(no cycles, no loops, no conditions...)

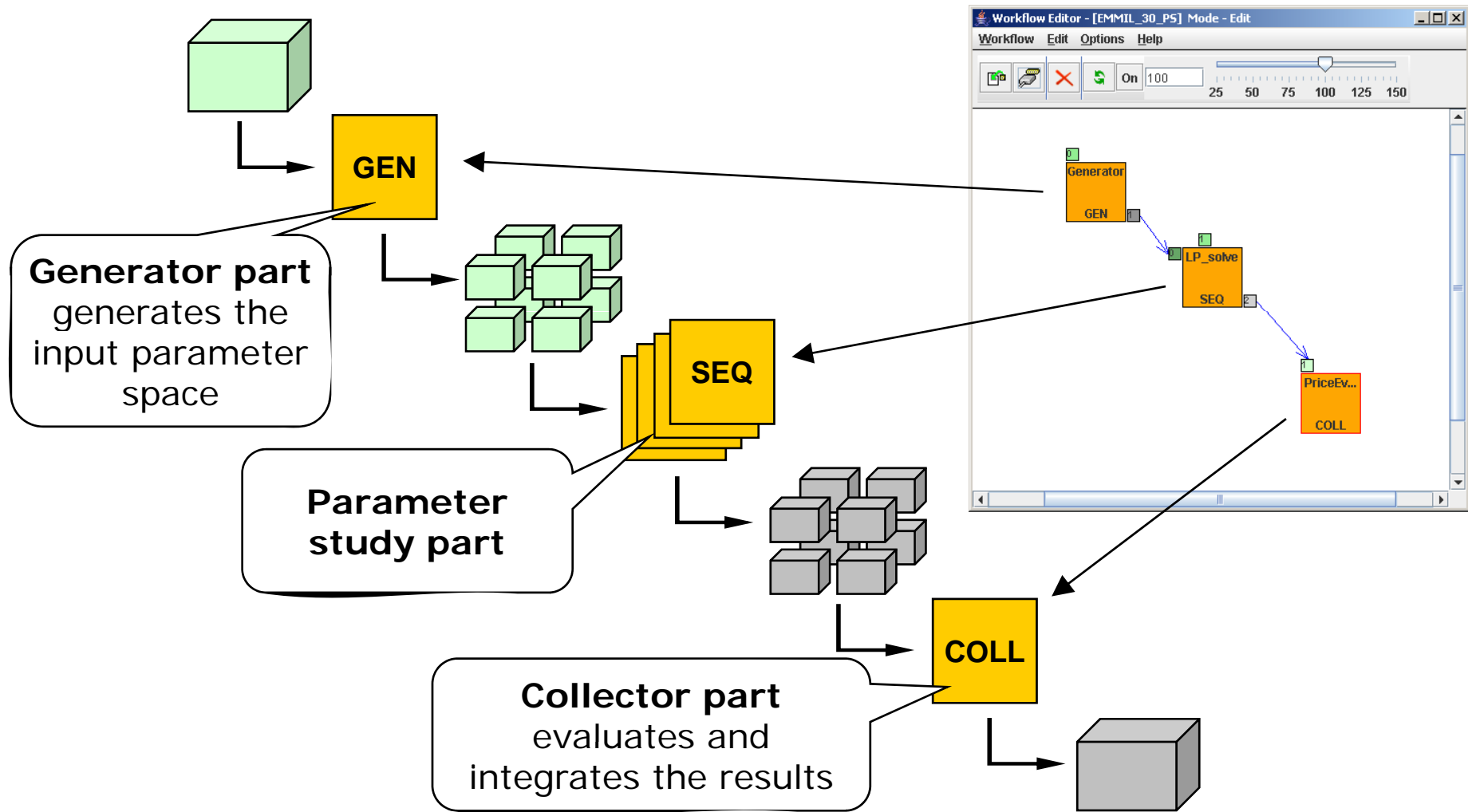
Extend the workflow to a parameter study:

1. **Add pre-defined or custom generator components**
2. **Add collector components**





Concept of parameter study workflows





Graphical User Interfaces in a nutshell

Proxy management

Workflow Certificates Settings Demo Help

Certificate Manager

Used certificate

| | |
|------------------|---------------------------------------------------------------------|
| Downloaded from: | albert.lpds.sztaki.hu |
| Issued by: | O=HunGrid,O=SZTAKI HPCC,OU=lpds.sztaki.hu,CN=Hermann Gabor,CN=proxy |
| Timeleft: | 40:0:56 |
| Description: | proxy for the demo |

Certificate list

| Issuer | Time Left | Status | [Actions] |
|---------------------------------------------------------------------|-----------|--------|------------------------------------------------------------------------------|
| O=HunGrid,O=SZTAKI HPCC,OU=lpds.sztaki.hu,CN=Hermann Gabor,CN=proxy | 40:0:56 | [used] | <input type="button" value="Details"/> <input type="button" value="Delete"/> |

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

Message: Download successful.



Graphical User Interfaces in a nutshell

Proxy management
Grid, VO and Grid
resource management

Globus resources

| URL | Job manager | [Actions] |
|--------------------------|-----------------|-----------|
| fs0.das2.cs.vu.nl | jobmanager-fork | Delete |
| hitcross.lrz.muenchen.de | jobmanager-fork | Delete |
| litchi.zib.de | jobmanager-fork | Delete |
| parsifal.cpc.wmin.ac.uk | jobmanager-fork | Delete |
| peyote.aei.mpq.de | jobmanager-fork | Delete |
| skirit.ics.muni.cz | jobmanager-fork | Delete |
| sr8000.lrz-muenchen.de | jobmanager-fork | Delete |

Contact string: Job manager:

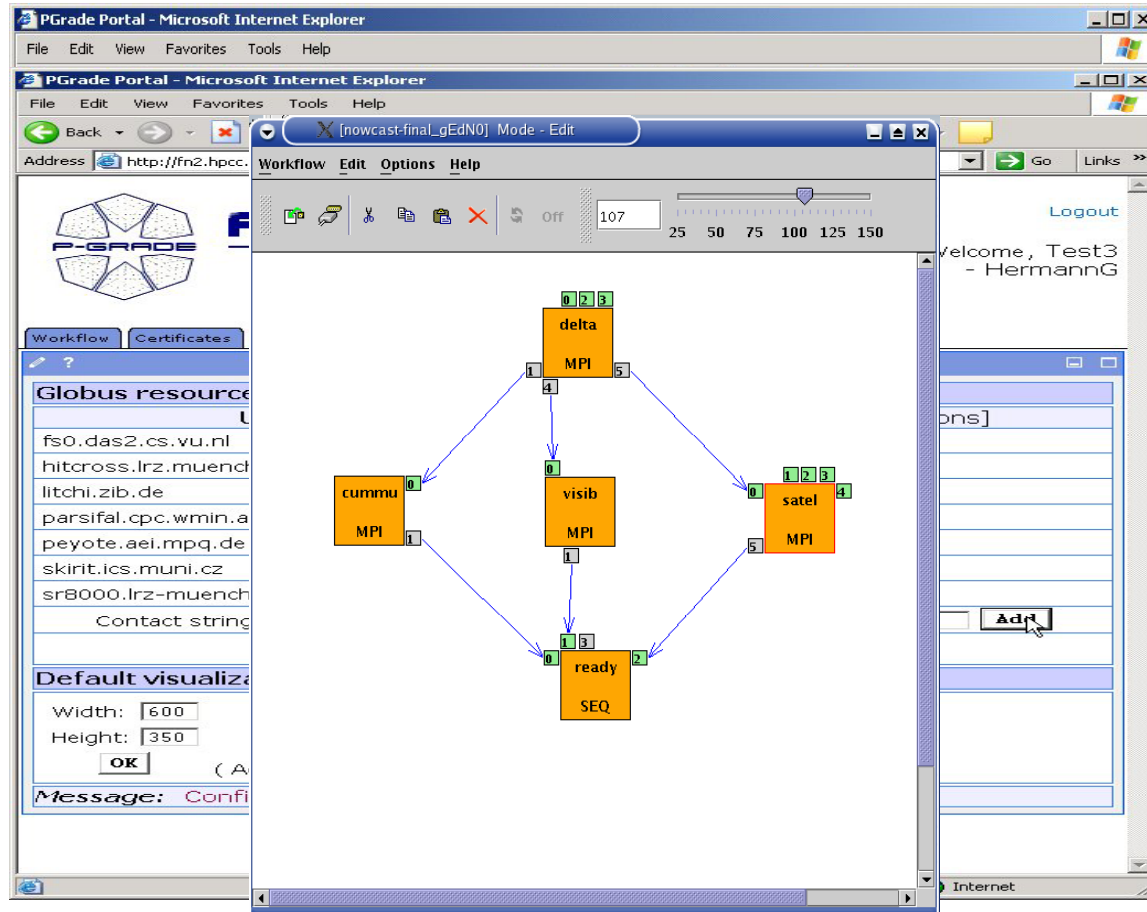
Default visualization size

Width:
Height:
 (Accept values between 150-1000.)

Message: Configuration successfully deleted.



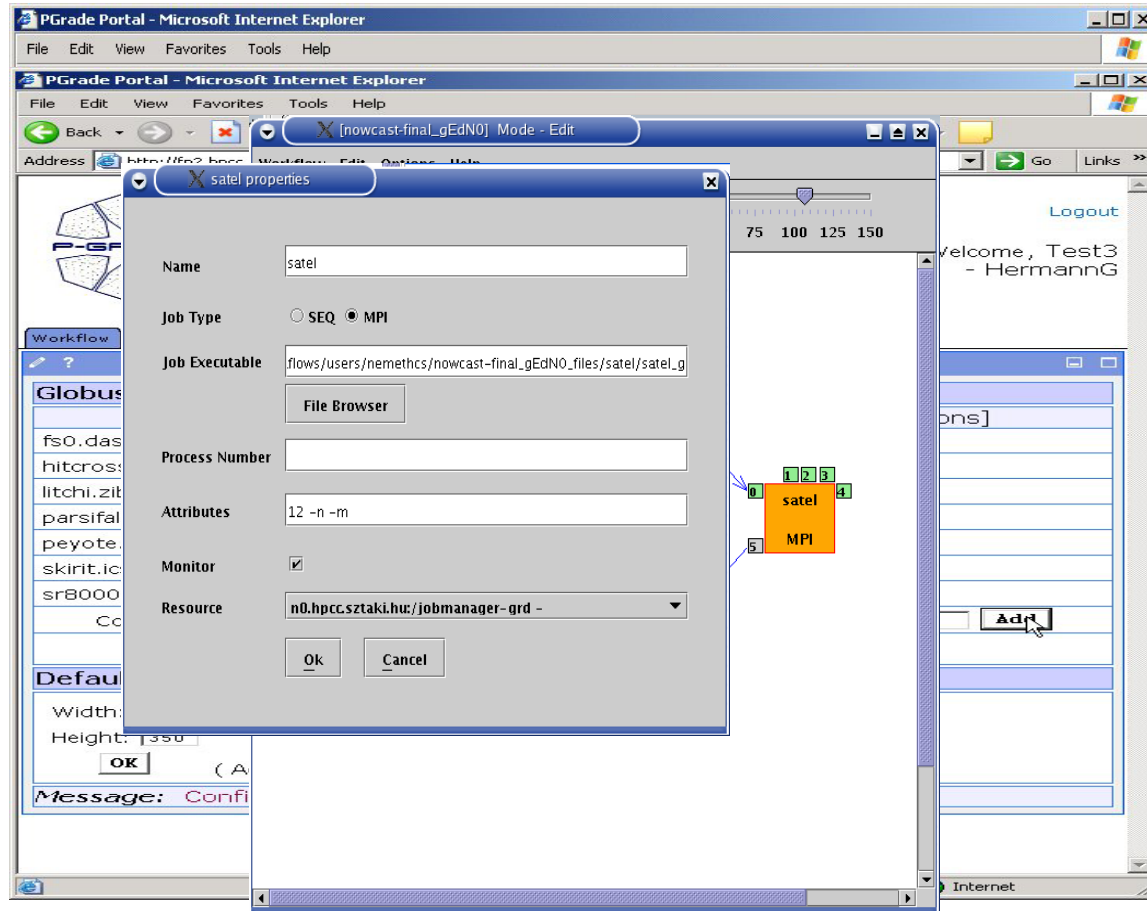
Graphical User Interfaces in a nutshell



- Proxy management
- Grid, VO and Grid resource management
- Graphical editor for workflow creation



Graphical User Interfaces in a nutshell



Proxy management

Grid, VO and Grid resource management

Graphical editor for workflow creation

Mapping job to Grids and Grid resources



Graphical User Interfaces in a nutshell

PS workflow details of 'Ax_EQUAL_B_seeGRID_broker__PS'

| Statistics | | | | | | Logs |
|------------|------|-----------|--------|-------|----------|------|
| Total | Init | Submitted | Rescue | Error | Finished | - |
| 6 | 2 | 4 | 0 | 0 | 0 | |

eWorkflow list

| Workflow | Status | [Output] | [View] | [Action] |
|---------------------------------|-----------|------------|----------|------------|
| Ax_EQUAL_B_seeGRID_broker__PS.1 | submitted | N/A | Details | Abort |
| Ax_EQUAL_B_seeGRID_broker__PS.2 | submitted | N/A | Details | Abort |
| Ax_EQUAL_B_seeGRID_broker__PS.3 | submitted | N/A | Details | Abort |
| Ax_EQUAL_B_seeGRID_broker__PS.4 | submitted | N/A | Details | Abort |
| Ax_EQUAL_B_seeGRID_broker__PS.5 | init | N/A | Details | Abort |

Message: The list refreshed.

September 9, 2006

Proxy management

Grid, VO and Grid resource management

Graphical editor for workflow creation

Mapping job to Grids and Grid resources

Workflow management



Graphical User Interfaces in a nutshell

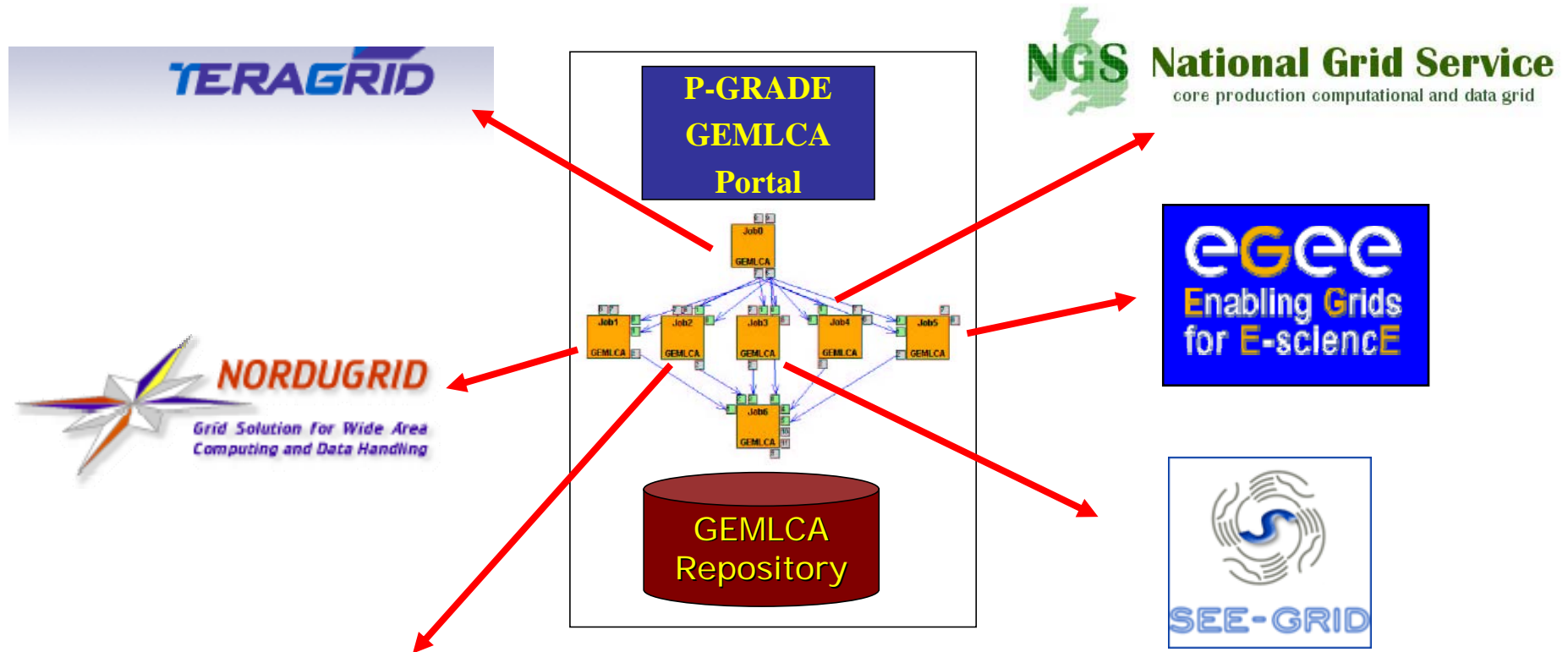
| Workflow | Job | Hostname | Status | [Logs] | [Output] | [Action] |
|-----------------------|-------|-------------------|------------|----------|------------|-----------------|
| nowcast-final_gEdN0_b | cummu | n0.hpcc.sztaki.hu | 3_finished | Out | - | Attach Delete |
| | delta | n0.hpcc.sztaki.hu | 3_finished | Out | Err | |
| | ready | n0.hpcc.sztaki.hu | 3_finished | - | Err | |
| | satel | n0.hpcc.sztaki.hu | 3_finished | - | - | |
| | visib | n0.hpcc.sztaki.hu | 3_finished | Out | - | |

The 'Tracefile visualization' section shows a Gantt chart for the workflow 'nowcast-final_gEdN0_b'. The chart displays the execution timeline for jobs: visib, delta, ready, satel, and cummu. The x-axis represents time in milliseconds (0s to 6m0s). The y-axis lists the jobs and their hostnames. The jobs are connected by arrows, indicating dependencies and the flow of the workflow.

- Proxy management
- Grid, VO and Grid resource management
- Graphical editor for workflow creation
- Mapping job to Grids and Grid resources
- Workflow management
- Execution visualization



Middleware interoperability: Multi-grid workflows

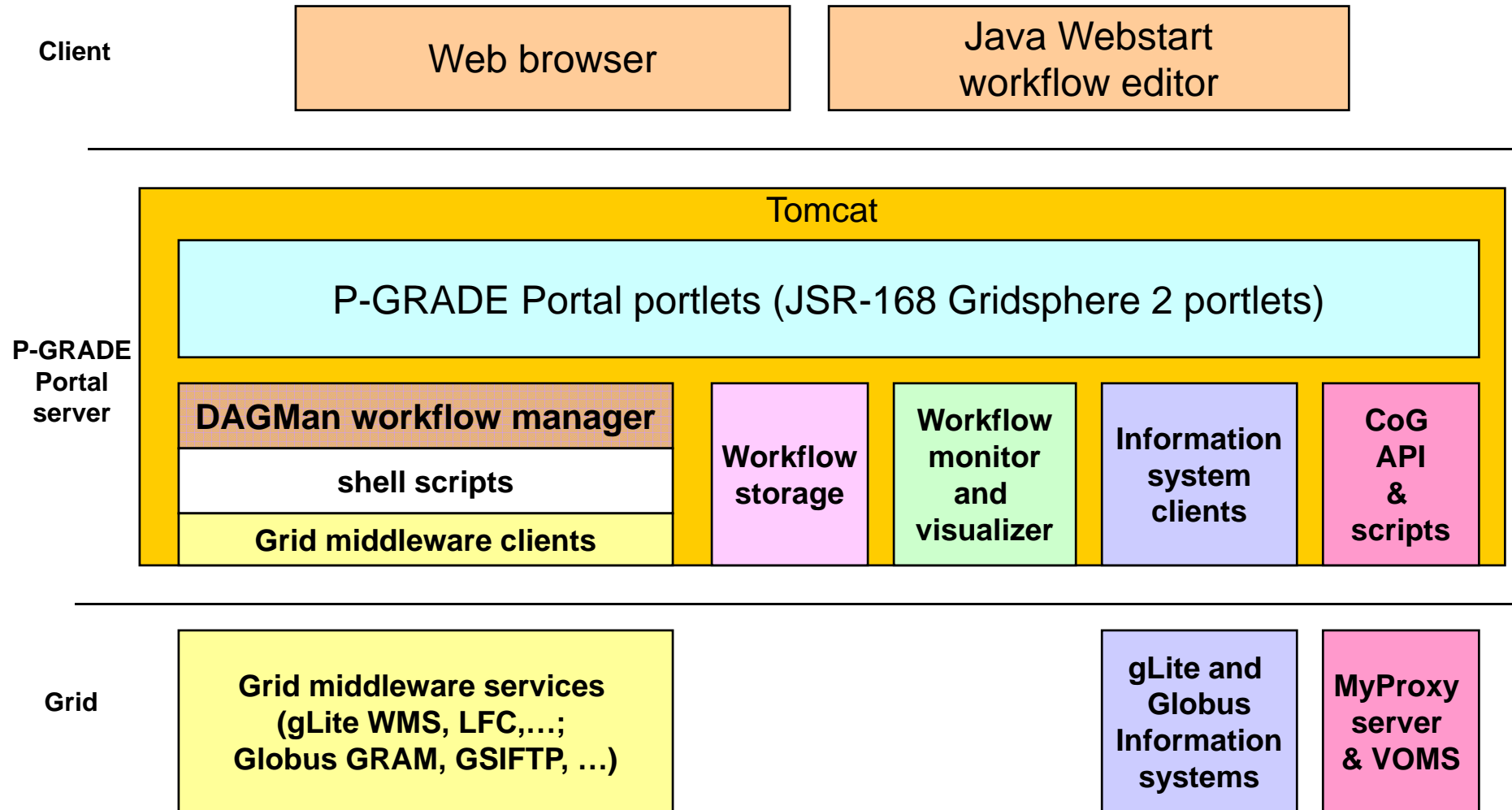


 Open Science Grid

OGF GIN VO



Implementation overview





Typical P-GRADE Use Case

- Develop and test the workflow
 - Workflow editor, certificate manager, workflow manager, Information system portlets
- Scale up to a parameter study
 - Input file generator
 - Output file collector
- Develop an application specific portlet to hide workflow and application logic from real end users:

Separate grid experts from end users



Some applications gridified with P-GRADE 2.5 by SZTAKI

- Ultra short range weather forecast (MEANDER): **workflow** that integrates 4 meteorological algorithms and one visualizer component
- Road traffic simulation: predict the density of cars on the roads of Manchester. **Workflow** that integrates 4 simulator components
- Minimizing operational cost of factories and logistic service providers (EMMIL): **Parametric workflow** resulting thousands of short running jobs (job clustering)
- Molecular Dynamics Study of Water Penetration (CHARMM): **Parametric workflow** resulting hundreds of long running jobs
- Studying oscillons and magnetic monopole configurations: **Parametric workflow** resulting hundreds of short running jobs



Portal installations

- **P-GRADE Portal service available:**
 - **SEE-GRID infrastructure**
 - **Central European VO of EGEE**
 - **GILDA: Training VO of EGEE**
 - **Many national Grids (UK National Grid Service, HunGrid, Turkish Grid, etc.)**
 - **US Open Science Grid, TeraGrid**
 - **Economy-Grid, Swiss BioGrid, Bio and Biomed EGEE VOs, BalticGrid**
 - **OGF Grid Interoperability Now (GIN) VO**
 - portal.p-grade.hu/index.php?m=5&s=0





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Support services **<http://portal.p-grade.hu>**

- User and admin documentation
- Test portal based on the GILDA VO
- User forum
- Training events, trainer community support (email list pgrade-training@lpds.sztaki.hu)
- Team to serve installation requests
- Grid Application Porting Support:
Not only with P-GRADE!
<http://www.lpds.sztaki.hu/gasuc> (Hungary)
<http://wgrass.wmin.ac.uk> (UK)



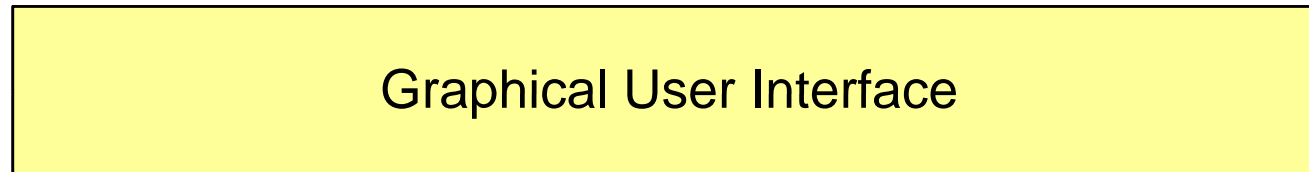
From P-GRADE to gUSE

gUSE: Grid User Support Environment

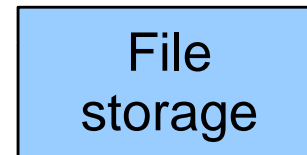
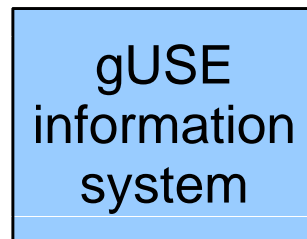
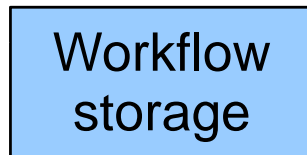
- **Architectural features: Expose P-GRADE services as Web Services**
 - Scalable
 - Flexible
 - Extendable
 - Autonomous
 - Replaceable, customizable
- **New functionalities**
 - Loops at workflow level
 - If-then structures at workflow level
 - Nested workflows
- Open source gUSE release for SC'07



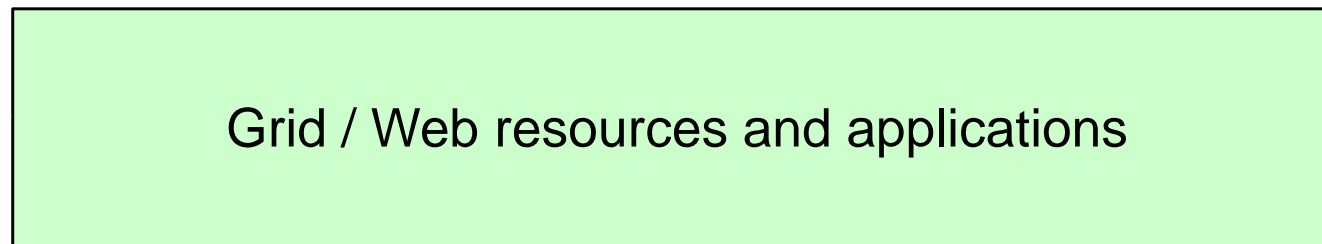
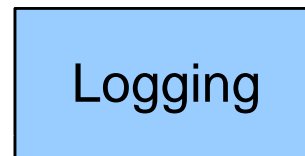
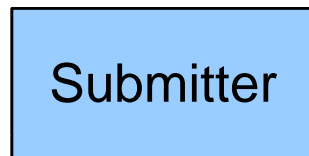
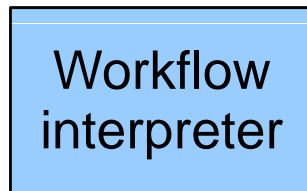
Services in gUSE



**Gridsphere
portlets**



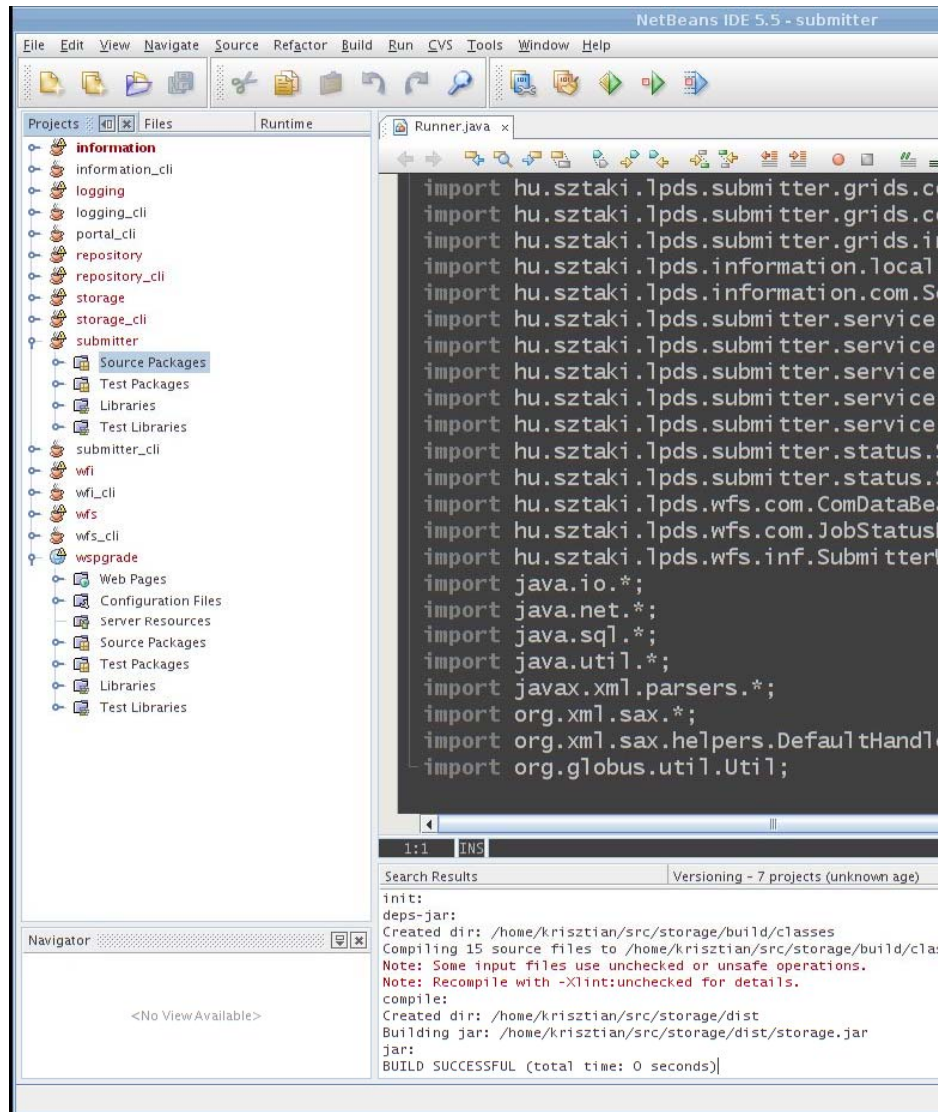
**Autonomous
Web
Services:
high level
middleware
service layer**



**gLite or Globus
or Web service:
low level
middleware
service layer**



gUSE packages



- Services of gUSE implemented as Web services
- Each service has a server and a client package
- Service communication protocols are pluggable
- Documented API for each service
- Any service can be re-implemented or replaced



New features and interfaces

The screenshot displays the P-Grade GUI interface. At the top, there are fields for 'Job's name:' (Separator) and 'Job's description:'. Below this is a tabbed interface with 'Job Executable', 'Job Inputs and Outputs', 'JDL/RSL', and 'Job Configuration'. The 'Job Inputs and Outputs' tab is active, showing 'Inputs' and '0: INPUT'. A 'Storage Upload Repository' section is visible. The main area shows a workflow graph with a red 'Separator' node at the top, connected to three yellow nodes: 'InvertA', 'MultiplB', and 'AmulX'. A 'Message:' field is at the bottom. An inset window shows a 'Parametric Input' dialog with fields for 'name:', 'description:', 'workflow graph:', and 'workflow template:'.

- Easily customizable GUI to grid applications
- Seamless change from local to remote execution environment
- Logic programming at workflow level
 - Loops
 - If-then
 - Nesting



Conclusions

Lessons learnt

- Workflows need parametric study support ✓
- Portals must be easily customizable for applications ✓
- Portals must be easily customizable for middleware **Next release**
- P-GRADE must be open source **Started**
- Workflows need loops, if-then-else structures **Next release**
- Job failure rate is sometimes high: failure management layer required **Future work**



Summary & conclusions

- **Benefits of being member of the user community**
 - Short learning curve → Swift uptake of grid technology
 - Graphical access → Protection against cmd line and API changes
 - High level, abstract tools → easy to perform complex operations (e.g. file transfer + LFC update)
 - Support services
- **Benefits of being member of the developer community**
 - Customizable to certain user communities
 - Customizable to certain applications
 - Customizable to certain middleware releases
- **Benefits of keeping your eyes on P-GRADE activities**
 - Regular releases in the last 4 years
 - Broadening developer community
 - Broadening user community



Learn once, use everywhere
Develop once, execute anywhere

Questions & discussion

portal.p-grade.hu
pgportal@lpds.sztaki.hu



Topics

- **Open source strategy**
 - Alliance based vs Open Source code sharing
- **Licensing**
 - Which one?
- **Directions of development**
 - What new features to add and why?
- **Support services**
 - How to improve?
 - How to get more partners involved?