Grid application support by the P-GRADE Portal

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Contents

• Motivation of creating P-GRADE portal
• P-GRADE Portal in a nutshell
• Application development with the Portal
• Application execution with the Portal
Context

Application

Application toolkits, standards

Higher-level grid services (brokering, …)

Basic Grid services:
AA, job submission, info, …

Graphical interface
P-GRADE Portal and GEMLCA
Command line tools
Grid middleware
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 P-GRADE Grid Portal gives 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
- **Grid services** supported by the portal:

<table>
<thead>
<tr>
<th>Service</th>
<th>EGEE grids</th>
<th>Globus grids</th>
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<tbody>
<tr>
<td>Job execution</td>
<td>Computing Element</td>
<td>GRAM</td>
</tr>
<tr>
<td>File storage</td>
<td>Storage Element</td>
<td>GridFTP server</td>
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<tr>
<td>Certificate management</td>
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<td>MyProxy</td>
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<tr>
<td>Information system</td>
<td>BDII</td>
<td>MDS-2, MDS-4</td>
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<td>Brokering</td>
<td>Workload Management System</td>
<td>GTbroker</td>
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<td>Job monitoring</td>
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<td>Mercury</td>
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<tr>
<td>Workflow &amp; job visualization</td>
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<td>PROVE</td>
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</table>

Solves Grid interoperability problem at the workflow level
The development and education of P-GRADE Portal is supported by several projects:

- **SEE-GRID** [www.see-grid.eu](http://www.see-grid.eu)
  Development, application support

- **Coregrid** [www.coregrid.net](http://www.coregrid.net)
  Research, development

- **EGEE** [www.eu-egee.org](http://www.eu-egee.org)
  LCG and gLite training, application development

- **ICEAGE** [www.iceage-eu.org](http://www.iceage-eu.org)
  Grid training and education
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
Two levels of parallelism by a workflow

- The workflow concept of the 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

Multiple jobs can run parallel
The job can be a parallel program
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)
The typical user scenario
Part 1 - development phase

Certificate servers

Portal server

Grid services

START
EDITOR

OPEN & EDIT or DEVELOP WORKFLOW

SAVE WORKFLOW
The typical user scenario

Part 2 - execution phase

Certificate servers

TRANSFER FILES, SUBMIT JOBS

DOWNLOAD PROXY CERTIFICATES

Download (small) results

Portal server

VISUALIZE JOBS and WORKFLOW PROGRESS

Grid services

MONITOR JOBS

DOWNLOAD (small) RESULTS
The typical user scenario

Development phase:

Certificate servers

Portal server

Grid services

Open & Edit or Develop or Import Workflow

Save Workflow

Start Editor
Workflow development

Opening the workflow editor

The editor is a Java Webstart application

download and installation is only one click!
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)
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)
Direct resource selection: Which computing element to use?

I still don’t know which resource to use!

The information system portlet queries BDII and GIIS servers.
Automatic resource selection

1. Select a broker Grid/VO for the job (e.g. GILDA)

2. (Describe the ranks & requirements of the job in JDL)

3. The portal will use the broker to find the best resource for the job!
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
Built-in JDL editor

JDL ➔ look at the LCG-2 Users’ manual!
Defining ports

**Type:**
- **input:** the job requires
- **output:** the job produces

**File type:**
- **local:** from/to my desktop
- **remote:** from/to a storage resource

**File:**
- location of the file

**File storage type:**
- **Permanent:** belongs to the final results of the WF
- **Volatile:** used only for inter-job data transfer
Possible file reference values

Input file

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

- LFC logical file name
  *(LFC file catalog is required – eGrid, Hungrid)*
  lfn:/grid/egrid/sipos/11-04.dat

- GridFTP address (in Globus Grids):
  gsiftp://myhost.com/11-04.dat

Output file

- Client side location:
  result.dat

- LFC logical file name
  *(LFC file catalog is required – eGrid, Hungrid)*
  lfn:/grid/egrid/sipos/11-04_-_result.dat

- GridFTP address (in Globus Grids):
  gsiftp://myhost.com/11-04_-_result.dat

Local file

Remote file
Your jobs can access storage files directly too!

Only the permanent files!
Workflow Editor

Saving the workflow

Workflow is defined!
Let’s execute it!
Executing workflows with the P-GRADE Portal

Main steps

1. Download proxies
2. Submit workflow
3. Observe workflow progress
4. If some error occurs correct the graph
5. Download result
The typical user scenario
Execution phase – step 1:

Certificate servers → Portal server

DOWNLOAD PROXY CERTIFICATES

Grid services
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
1. **MyProxy server access details:**
   - Hostname
   - Port number
   - User name (from upload)
   - Password (from upload)

1. **Proxy parameters:**
   - Lifetime
   - Comment
Certificate Manager
associating the proxy with a grid

This operation displays the details of the certificate and the list of available Grids (defined by portal administrator)
Multiple proxies can be available on the portal server at the same time!
The typical user scenario

Execution phase - step 2:

Certificate servers

TRANSFER FILES, SUBMIT JOBS

Portal server

Grid services
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)

<table>
<thead>
<tr>
<th>Workflow</th>
<th>Job</th>
<th>Gridname</th>
<th>Hostname</th>
<th>Status</th>
<th>Logs</th>
<th>Output</th>
<th>Visualization</th>
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<tbody>
<tr>
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Message: Workflow details successfully displayed.

*White/Red/Green color means the job is initial/running/finished state*
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(observation by the workflow portlet)

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( observation by the workflow portlet )

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</table>

Message: Job list refreshed.

White/Red/Green color means the job is initialised/running/finished
What about data transfers?
The typical user scenario
Execution phase – step 3:

Certificate servers

Portal server

VISUALIZE JOBS and WORKFLOW PROGRESS

MONITOR JOBS

Grid services
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)

Workflow/job: LM_9_DEMO_TOTAL/LM_P

- 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.

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

Don’t touch the finished jobs!

The execution can continue from the point of failure!
The typical user scenario
Execution phase – step 5

The typical user scenario
Execution phase – step 5

Portal server

Download (small) results

Certificate servers

Download (small) results

Grid services
Downloading the results...
Additional features

• Workflows and traces can be exported from the portal server onto your client machine

• Workflows and traces can be imported into the Portal

  • Share your workflows or results with other researchers!
  • Migrate your application from one portal into another!
Workflow/trace export/import

- To export a workflow from the portal onto your machine.
- To delete every unnecessary files of the workflow.
- To delete trace/output of the workflow (if any).
• P-GRADE Portal service is available for
  – SEE-GRID infrastructure
  – Central European VO of EGEE
  – GILDA: Training VO of EGEE
  – Many national Grids (UK National Grid Service, HunGrid, etc.)
  – US Open Science Grid, TeraGrid
  – Economy-Grid, Swiss BioGrid, Bio and Biomed EGEE VOs, BioInfoGrid, BalticGrid
  – GIN VO
Parameter study extension of the portal

• Users want parameter study (PS) support at workflow level

• It means:
  – If the user has an existing workflow in a repository, he would like to run
    • the same workflow (without any change)
    • with many different parameters
Introducing three levels of parallelism

- Parallel execution inside a workflow node (SIMD/MIMD/MISD)
- Parallel execution among workflow nodes (SIMD/MIMD/MISD)
- Parameter study execution of the workflow (SIMD)
Parameter sweep (PS) workflow execution in P-GRADE portal

1 PS workflow execution

4 x 3 normal workflow execution

PS port: 4 instances of the input file

PS port: 3 instances of the input file

This provides the 3rd level of parallelism resulting a very large demand for Grid resources
Steps of creating a PS-workflow
1. Start from a tested Workflow
2. Define the PS Port(s)

New feature: Input Port can be defined as PS_port
3. Define Subdirectory of Inputs

Subdirectory of a Grid File Catalogue must be defined.
4. Define Subdirectory for the results

[Diagram of workflow editor with labels and connections]

- **Output Directory**: /grid/seegrid/hermann/PS_EQUATION_OUTP
- **Grid**: seegrid_LCG_2_BROKER
5. **PS Workflow ready to Submit**
Progress of submissions in PS
detailed view

Total = Init + Submitted + Rescue + Error + Finished
Conclusions: E-scientists’ concerns are resolved!

- The P-GRADE Portal hides the complexity and differences of Grids
  - Globus X – LCG2 – gLite Grid interoperability at the workflow level
  - Switching between Grid technologies will be transparent to the end-user
  - Various components can be integrated into large Grid applications
    - Sequential codes
    - MPI codes
    - Legacy codes (with the GEMLCA-specific P-GRADE Portal)
  - You code does not have to include grid specific commands
  - Graphical tools for application development, execution and monitoring
  - Support for collaborative team work
    - Sharing workflows
    - Sharing jobs (components)
  - Built by standard portlet API → customizable to specific application areas, user groups
How to learn the P-GRADE portal?

- Take a look at www.lpds.sztaki.hu/pgportal (manuals, slide shows, installation procedure, etc.)
- Visit or request a training event! (event list also on homepage)
  - Lectures, demos, hands-on tutorials, application development support

- Get an account for one of its production installations:
  - VOCE portal - SZTAKI
  - SEEGRID portal – SZTAKI
  - GILDA portal – SZTAKI
  - NGS portal – University of Westminster

- If you are the administrator of a Grid/VO then contact SZTAKI to get your own P-GRADE Portal!
- If you know the administrator of a P-GRADE Portal you can ask him/her to give access to your Grid through his/her portal installation! (Multi-Grid portal)
Learn once, use everywhere
Develop once, execute anywhere

Thank you!

www.lpds.sztaki.hu/pgportal
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