

P-GRADE Portal tutorial part 1.: Managing workflow applications on EGEE

Miklos Kozlovszky MTA SZTAKI <u>m.kozlovszky@sztaki.hu</u>

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







- P-GRADE Portal in a nutshell
- Workflow development with P-GRADE Portal
- Workflow execution with P-GRADE Portal

Family of P-GRADE Portal products

- P-GRADE portal
 - Creating (basic) workflows and parameter sweeps for service grids
 - <u>www.portal.p-grade.hu</u>
- P-GRADE/GEMLCA portal (University of Westminster)
 - To wrap legacy applications into Grid Services
 - To add legacy code services to P-GRADE Portal workflows
 - <u>http://www.cpc.wmin.ac.uk/cpcsite/gemlca</u>
- WS-PGRADE
 - Creating complex workflow and parameter sweeps for clusters, service grids and desktop grids
 - Creating complex applications using embedded workflows, legacy codes and community components from workflow repository
 - www.wspgrade.hu

References and P-GRADE installations

- P-GRADE Portal service is available for
 - SEE-GRID-SCI infrastructure
 - Central European VO of EGEE
 - GILDA: Training VO of EGEE
 - Many national Grids (UK National Grid Service, GridIreland, Turkish Grid, Croatian Grid, etc.)
 - US Open Science Grid
 - Economy-Grid, Swiss BioGrid, Bio and Biomed EGEE VOs, BioInfoGrid, BalticGrid
 - GIN VO of OGF
 - EGEE Respect program tool
 - Total:
 - 12 community installations, connection to ~20 grids
 - ~1200 additional downloads from Sourceforge
 - Developers from: UK, Turkey, Croatia, Italy, France
 - http://portal.p-grade.hu/?m=installations&s=0









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NGS



Some applications/services based on P-GRADE Portal

- Molecular Dynamics Study of Water Penetration (CHARMM): Parametric workflow resulting hundreds of long running jobs
 - http://wgrass.wmin.ac.uk/index.php/W-Grass:autodock
- R: Patient Readmission Analysis
 - http://wgrass.wmin.ac.uk/index.php/W-Grass:r
- In Silico Modelling using Autodock
 - http://wgrass.wmin.ac.uk/index.php/W-Grass:autodock
- MultiBayes DNA sequence analyzer application
- GAMESS-UK ab initio molecule structure analyzer application
- Minimizing operational cost of factories and logistic service providers (EMMIL): Parametric workflow resulting thousands of short running jobs
- Studying oscillons and magnetic monopole configurations: Parametric workflow resulting hundreds of short running jobs
- Ultra short range weather forecast (MEANDER): workflow that integrates 4 meteorological algorithms and one visualizer component











Application Specific Portals

The Rendering Portal



Application Specific Portals (contd.)

Supplier chain portal: EMMIL P-GRADE Procurement Portal

Application Specific Portals (contd.) EMMIL P-GRADE Procurement Portal

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- **Supplier**
- Supplier
- **3PL plac**

EMMIL

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EMMIL P-Grade P

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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)

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:

Service	EGEE grids	Globus grids
Job execution	Computing Element	GRAM
File storage	Storage Element	GridFTP server
Certificate management	MyF	roxy
Information system	BDII	MDS-2, MDS-4
Brokering	Workload Management System	GTbroker
Job monitoring	Mer	cury
Workflow & job visualization	PR	OVE

Solves Grid interoperability problem at the workflow level

The typical user scenario Part 2 - execution phase

Defining workflow with the P-GRADE Portal

Main steps

- 1. Define workflow structure
- 2. Define binaries & setup parameters and properties (JDL)
- 3. Define resource selection
- 4. Setup In/Outputs
- 5. Create or upload file/directory structure on SE (optional)
- 6. Name & Save the workflow (Upload binaries, and other files)

What is a P-GRADE Portal workflow?

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

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, highaltitude measurements, radar, satellite, lightning, results of previous computed models

> > Requirements:

Execution time < 10 min

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•High resolution (1km)

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The typical user scenario Development phase:

Workflow development

Opening the workflow editor

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Defining the graph

- 🗆 🗙 Workflow Editor - [LM 9 DEMO TOTAL] Mode - Edit Workflow Edit Options Help 📭 🐬 🐰 🗙 😫 On 81 25 50 75 100 125 150 The aim is to define a DAG of batch jobs: 1. Drag & drop components: jobs and ports LM_S.4 LM_S.5 I D LM_P.2 SEQ SEQ SEQ 2. Define their properties 3. Connect ports by channels (no cycles, no loops, no conditions)

Properties of a job

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Direct resource selection:

Which computing element to use?

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BG02-IM	20	16	20%	1	0		0%	131.775 GB	79.957 GB	39
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- Select a broker Grid/VO for the job (e.g. GILDA_LCG2_broker/GILDA_gLite_broker)
- 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!

Defining broker jobs

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	Job Type SEQ MPI	
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Built-in JDL editor

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JDL \rightarrow look at the gLite Users' manual!

Defining input-output files

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File properties Type: input: the job reads output: the job generates File type: local: comes from my desktop remote: comes from an SE File: location of the file nternal file name: Executable reads the file in this name – fopen("file.in", ...) File storage type (output files) only): Permanent: final result Volatile: only data channel

▼

How to refer to an I/O file?

Input file	Output file
Local	file
Client side location: c:\experiments\11-04.dat	Client side location: result.dat
LFC logical file name Ifn:/grid/gilda/kozlovszky/11-04.dat	 LFC logical file name Ifn:/grid/gilda/kozlovszky/11-04result.dat
Remot	e file

Job level file transfer in EGEE VOs

Miklos Kozlovszky - EGEE and EDGeS Summer School on Grid Application Support '09 June 29-04 July 2009

Reminder: Grid files and JDL

Your executable does not have to know any grid protocol if it is used in P-GRADE Portal

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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

MyProxy interaction in P-GRADE: Certificate Manager

Certificates portlet

- To start your session on the Grid you must create a proxy certificate on the portal server
- "Certificates" portlet:
 - to upload a proxy into
 MyProxy servers
 - to download a proxy from MyProxy into the portal server

Certificate Manager

Downloading a proxy

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Certificates, proxies with gLite VOs:

Certificate Manager

Associating the proxy with a grid

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Certificate Manager

browsing proxies

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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

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(observation by the workflow portlet)

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

(observation by the workflow portlet)

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		LM_S.4	SEE-GRID	grid1.irb.hr	init			-			
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White/Red/Green color means the job is initial/running/finished state

(observation by the workflow portlet)

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

(observation by the workflow portlet)

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

(observation by the workflow portlet)

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	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 -		_				
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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

Rescuing a failed workflow 1.

Rescuing a failed workflow 2.

Rescuing a failed workflow 3.

Rescuing a failed workflow 4.

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	Count4	SZTAKI- GRID	n0 .hpcc.sztaki.hu	submitted		-			
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Logs provided for each job

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Analysis of the log

- 2008.01.09 09:32:19 Proxy with VOMS extensions created for VO "voce" with accounting group "".
- 2008.01.09 09:32:19 Job submission in progress...
- 2008.01.09 09:32:23 Job has been submitted successfully!
- 2008.01.09 09:32:23 Job identifier is:
- "https://skurut1.cesnet.cz:9000/mD_8VzPhm8AmIToTJKtigg"
- 2008.01.09 09:32:26 EGEE job's status has changed to "Waiting" (host is).
- 2008.01.09 09:33:00 EGEE job's status has changed to "Ready" (host is ce1egee.srce.hr).
- 2008.01.09 09:35:46 EGEE job's status has changed to "Waiting" (host is egeece.grid.niif.hu).
- 2008.01.09 09:36:19 EGEE job's status has changed to "Ready" (host is ce.cyf-kr.edu.pl).
- 2008.01.09 09:36:53 EGEE job's status has changed to "Waiting" (host is
- ce.cyf-kr.edu.pl).
- 2008.01.09 09:37:26 EGEE job's status has changed to "Done" (host is
- egee-ce.grid.niif.hu).
- 2008.01.09 09:37:26 Job found to be finished. Checking again if this is
- really the case.
- 2008.01.09 09:38:03 EGEE job's status has changed to "Ready" (host is
- egee-ce1.gup.uni-linz.ac.at).

Fault-tolerance by P-GRADE portal

- 09:33: the broker assigned the job to a site: **ce1-egee.srce.hr**
- 09:35: The broker moved the job to another site: **egee-ce.grid.niif.hu**
- 09:36: Again the broker moved the job to another site: **ce.cyf-kr.edu.pl**
- 09:37: The broker indicated that the job is **Done**, but .
- 09:38: ... It turned out that the job was not finished (Done Failed status), only it was moved to another site: egee-ce1.gup.uni-linz.ac.at
- 09:39: Again the broker moved the job to another site: ares02.cyfkr.edu.pl
- 09:39: Again the broker moved the job to another site: **ce.cyf-kr.edu.pl**
- 09:40: After trying 10 different sites the VOCE broker gave it up and aborted the job (the Shallow RetryCount was set for 10):
- 2008.01.09 09:40:16 The job has been aborted!

Fault-tolerance by P-GRADE portal

- Our fault-tolerant portal did not give it up:
- 2008.01.09 09:40:16 The job can be submitted again (try 1 out of 3,
- excluding host(s): ce.cyf-kr.edu.pl)
- 2008.01.09 09:40:17 Proxy with VOMS extensions created for VO "voce" with
- accounting group "".
- 2008.01.09 09:40:17 Job submission in progress...
- 2008.01.09 09:40:27 Job has been submitted successfully!
- 2008.01.09 09:40:27 Job identifier is:
- "https://skurut1.cesnet.cz:9000/o22BTVqQsvwzj2wn5KP8_A"
- 2008.01.09 09:40:30 EGEE job's status has changed to "Waiting" (host is).
- 2008.01.09 09:41:04 EGEE job's status has changed to "Ready" (host is
- eszakigrid66.inf.elte.hu).

Fault-tolerance by P-GRADE portal

- 2008.01.09 09:41:37 EGEE job's status has changed to "Scheduled" (host is
- eszakigrid66.inf.elte.hu).
- 2008.01.09 09:44:57 EGEE job's status has changed to "Done" (host is
- eszakigrid66.inf.elte.hu).
- 2008.01.09 09:44:57 Job found to be finished. Checking again if this is
- really the case.
- 2008.01.09 09:45:34 EGEE job's status has changed to "Waiting" (host is
- eszakigrid66.inf.elte.hu).
- 2008.01.09 10:06:06 The job's status hasn't changed for 20 minutes,
- resubmitting...

It is a quite frequently occurring problem in EGEE-like grids that the broker leaves jobs stuck in CEs. queues.) In such case the portal automatically kills the job on this site and resubmits it to the broker.

- 2008.01.09 10:06:06 Proxy with VOMS extensions created for VO "voce" with accounting group "".
- 2008.01.09 10:06:06 Job submission in progress...
- 2008.01.09 10:06:12 Job has been submitted successfully!
- 10:10: The job successfully finished with exit code 0 on site: ce.ui.savba.sk

The typical user scenario

Downloading the results...

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File management portlet

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- POSIX-TEST-10485-24626	
- POSIX-TEST-11134-23067 - POSIX-TEST-12464-3948 Change Directory	
- POSIX-TEST-16138-5559	
- POSIX-TEST-17957-20543	
- POSIX-TEST-24498-25005	
- POSIX-IES1-24/76-20792	
- POSIX-TEST-29926-26667	
- POSIX-TEST-6451-13508	
- POSIX-TEST-7730-2/146 + SAM	
- SE-lcg-cr-cluster1.csk.kg.ac.yu-temp-1177332816	
Current Path: /grid/seegrid	
Download	
Message: LFC name server directory/file entries listed	

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- Pros.
 - Easy-to-use workflow system with graphical editor
 - Easy-to-use parameter sweep concept at workflow level
 - Multi-grid / multi-VO access mechanism: job submission to LCG, gLite and GT2
 - Intelligent handling of grid errors
 - Open source community on Sourceforge
 - Reliable, production *installations* for several Grid, EGEE VOs
 - Part of EGEE <u>RESPECT programme</u>
 - ...
 - Features can serve most grid scenarios

To become a user of P-GRADE Portal

- Become user of EGEE
- Select a portal installation: http://portal.p-grade.hu

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To become a user of P-GRADE Portal

contd.

Thank you

Miklos Kozlovszky m.kozlovszky@sztaki.hu

www.lpds.sztaki.hu

