



Porting applications to the NGS, using the P-GRADE portal and GEMMLCA



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Hands-on with the P-GRADE/GEMMLCA Portal

1. Login to the Portal

- 1.1 Go to the URL:
`https://gngs-portal.cpc.wmin.ac.uk:8080/gridsphere/gridsphere`
- 1.2 Use your account and password to login

2. Upload your private key file (userkey.pem) and certificate file (usercert.pem) into the MyProxy server.

Note: If the files are already in MyProxy then go to 3.

- 2.1 Hit the "Certificates" tab
- 2.2 Click on the "Upload" button
- 2.3 With the "browse" button find userkey.pem and hit OK
- 2.4 Specify the passphrase of your private key (XXXXXXXX)
- 2.4 With the "browse" button find usercert.pem and hit OK
- 2.5 Submit the upload form with the following data:
Hostname: node40.cluster.cpc.wmin.ac.uk
Port: 7512
Login: userXX
Password: XXXXXXXX
Lifetime: 100

3. Download a short-term proxy credential from the MyProxy server into the Portal server. The proxy will be used by the workflow manager during workflow execution.

- 3.1 Hit the "Certificates" tab
- 3.2 Click on the "Download" button
- 3.3 Submit the download form with the following data:
Hostname: node40.cluster.cpc.wmin.ac.uk
Port: 7512
Login: ***
Password: ***
Lifetime: 10
Description: <optional>
- 3.4 If download is successful then set your proxy for the "NGS" Grid

4. Use the "Settings" tab to view available resources.

- 4.1 Available Grids are listed here as it was set by the portal administrator. Hit the resources button besides the Grid and view available resources.
- 4.2 You can load default resources specified by the portal administrator by hitting the "Load default" button.
- 4.3 You can also load resources from the MDS2 information system.

4.4 Your training certificate enables you to submit jobs to Rutherford(rl), Oxford (ox), Manchester (man) and Westminster (wmin). Only these resources will be used during this tutorial. Delete all the other resources from your resource list.

5. Define a matrix multiplication workflow

Note: The "Matrix operations" program will be used in most parts of the hands-on to demonstrate scientific workflows. Please read the description of this program now (see attached sheet for description)!

5.1 On the "Workflow" tab click on the "Workflow editor" button

Warning: because the browser needs a java plugin to run the Workflow Editor, it may ask for an application to open the downloaded jnlp file. If this happens please locate "javaws" on your computer or ask for help!

5.2 Define a matrix multiplication workflow using your locally available matrix_operations, INPUT1 and INPUT2 files:

5.2.1 Define a job with the following parameters:

Name: <any>
Job type: SEQ
Job executable: <path of matrix_operations file>
Attributes: M V
Grid: NGS
Resource: RL, Oxford, Manchester or UoW

5.2.2 Define a port for the job with the following parameters:

Port Name: 0
Type: In
File type: Local
File: <path of INPUT1 file>
Internal File Name: INPUT1

5.2.3 Define another port to the job with the following parameters:

Port Name: 1
Type: In
File type: Local
File: <path of INPUT2 file>
Internal File Name: INPUT2

5.2.4 Define a third port to the job with the following parameters:

Port Name: 2
Type: Out
File type: Local
Internal File Name: OUTPUT
File storage type: Permanent

5.3 Save your workflow (e.g. as multiplication)

5.4 Submit your workflow:

5.4.1 Go back to the browser and click on the "Refresh" button on the "Workflow" tab

5.4.2 Submit the workflow by the "Submit" button

- Monitor the execution from the workflow editor
- Monitor and visualize the progress of execution on the "Workflow" tab (Click on "Details" then on "Visualize")

5.4.3 Download and unzip the result file

6. Define a workflow which solves the following computational problem:

$AB[* , 0]^T * AB[* , 1]$

Hint: The "Matrix operations" program generates and expects similar files. Connect the "Matrix operations" program 4 times to one of your existing workflows. (See Figure 1)

Set the jobs to perform the following operations:

- *Multip* - AB
- *Column0* - $AB[* , 0]$
- *Column1* - $AB[* , 1]$
- *Transpose* - $AB[* , 0]^T$
- *Multip.2* - $AB[* , 0]^T * AB[* , 1]$

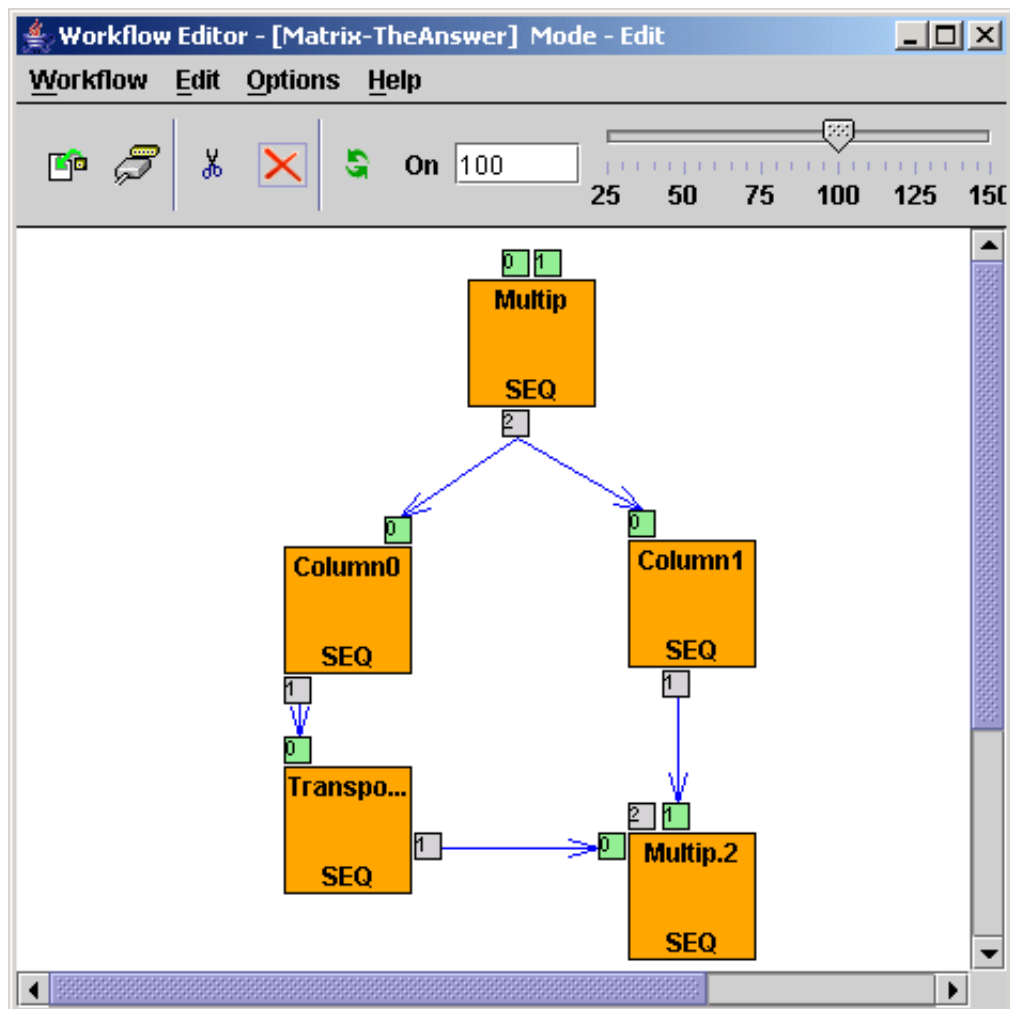


Figure 1. Matrix workflow to compute $AB[* , 0]^T * AB[* , 1]$

6. Create a traffic simulation workflow using the GEMLCA repository.

You can utilize already published legacy codes in your workflows from the GEMLCA repository. The executables of these programs are already uploaded, you only have to specify actual parameter values.

- 6.1. Create a new job in the workflow editor. Go into properties by right-clicking on the job and set job type as "GEMLCA job".
- 6.2. Double click on the job and go into job properties. Define a job with the following parameters:

Name: Manhattan
Grid: NGS
Resource: RL, Oxford, Manchester or UoW
Legacy code: Manhattan road network generator

Parameters with default values and ports are created automatically.

6.3. Define two more jobs with the following parameters:

Name: Sim1 and Sim2 (respectively)

Grid: NGS

Resource: RL, Oxford, Manchester or UoW

Legacy code: MadCity traffic simulator

Change the parameter value "starting car density" in one on the simulators from 14 to another value.

6.3. Define a 4th job with the following parameters:

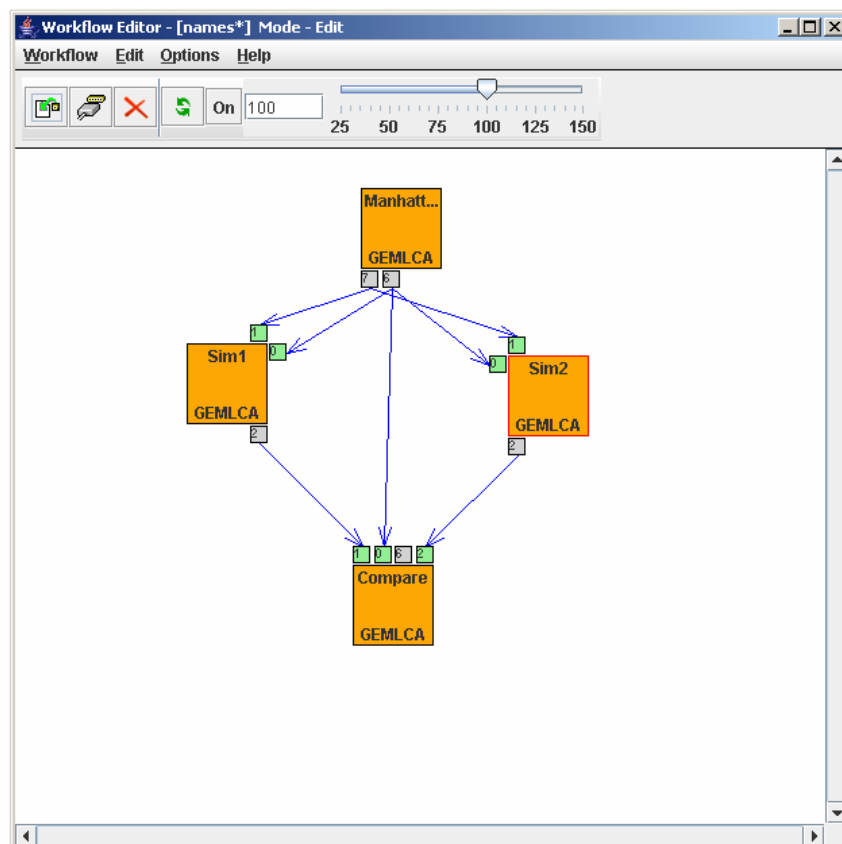
Name: Compare

Grid: NGS

Resource: RL, Oxford, Manchester or UoW

Legacy code: Trace compare

6.3. Draw the workflow graph as follows:



6.4. Save the workflow, submit it, visualize execution, and download results.