Parameter study practical with the P-GRADE Portal

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Developing and executing a parameter study workflow

This part of the practical demonstrates the parameter study services of P-GRADE Portal 2.5.
The GILDA P-GRADE Portal 2.5 installation is used for this purpose.

1. **Login to the GILDA P-GRADE Portal**

   1.1 Go to the URL:
          http://portal.p-grade.hu/gilda
   1.2 Login with the following account and password:
          user***XX***
          user***XX***

2. **Download a short-term proxy credential into the Portal server. This proxy will be used by the workflow manager to access GILDA resources.**

   2.1 Hit the "Certificates" tab
   2.2 Click on the "Download" button
   2.3 Submit the download form with the following data:
         Hostname: *grid001.ct.infn.it*
         Port: 7512
         Login: bpuser***XX***
         Password: bpuser***XX***
         Lifetime: 10
         Description: *<optional>*
   2.4 Set your certificate to be used with the ***gilda_LCG_2_BROKER*** Grid.
   2.5 Set your certificate to be used with the ***gilda_GLITE_BROKER*** Grid.

3. **Create a "Matrix multiplication" workflow**

   This workflow will be later executed on many parameters as a parameter study. The same "MatrixDemo" binary is used in the workflow here that was used earlier today during the GEMLCA / P-GRADE workflow practical. The workflow consists of only one job which multiplies two matrixes provided in two different input files.

   Download the binary executable with two sample input matrixes onto your desktop from this page:
   http://portal.p-grade.hu/tutorials/induction/Matrix_operations_program_description.htm

   ### 3.1. Create a job workflow using the "matrix_operations" executable

   Click on the "Workflow" tab, then on the "Workflow manager" button. Open the workflow editor.

   3.1.1 Create a new standard job in the workflow editor. Go into properties by right-clicking the job and set job type as "Standard job". Set the following parameters:
         Name: multiply
         Job type: SEQ
         Job executable: *<Path of the downloaded "matrix_operations" file>*
         Attributes: M V

Grid: *<gilda_LCG_2_BROKER> or <gilda_GLITE_BROKER>*
Resource: *<default>*

Open the JDL editor of the job and:
- Set "Retry count" to 3 on the "Job" tab.
- Define the following variables on the "Environment" tab:
  (They should be familiar from the data management practical)

> LCG_CATALOG_TYPE = lfc
> LFC_HOST = lfc-gilda.ct.infn.it
> LCG_GFAL_INFOSYS = grid004.ct.infn.it:2170

3.1.2 Define a port for the job with the following parameters:
     Port Name: 0
     Type: in
     File type: local
     File: *<Path of the downloaded "INPUT1" file>*
     Internal File Name: INPUT1   *(case sensitive)*

3.1.3 Define a second port to the job with the following parameters:
     Port Name: 1
     Type: in
     File type: local
     File: *<Path of the downloaded "INPUT2" file>*
     Internal File Name: INPUT2   *(case sensitive)*

3.1.4 Define a third port to the job with the following parameters:
     Port Name: 2
     Type: out
     File type: local
     Internal File Name: OUTPUT   *(case sensitive)*
     File storage type: permanent

The workflow could be executed in its current form. However that would result one matrix: INPUT1 * INPUT2. What we need are 3 matrixes: $INPUT1_{version-1}$ * INPUT2; $INPUT1_{version-2}$ * INPUT2; $INPUT1_{version-3}$ * INPUT2. For that the workflow has to be turned into a parameter study.

3.2 Extend the workflow with an auto input generator and configure it for PS execution

Switch Port 0 of the multiplicator job to "PS" by right clicking on the Port.

Add a new job to the workflow and turn it first to a "generator" by right clicking on the component then into an "auto generator" by another right click.

Set the properties of the generator:
     Job name: Matrix1Gen
     Input file text:

```
3 3
1 2 3
4 5 6
7 8 <X>
```
Click on **"Parse"**, then double click on **"X"** in the "Keys" window
Set the range values:
```
From: 9
To: 15
Step: 3
```
Click on **"Generate"** → Parameter space is displayed in "Generated items"

Set the properties of the PS output port of the generator:

        Directory: `/grid/gilda/training/riodejaneiro/MatrixPS-`***XX***

        (Do not put a "/" to the end of the name!)

        Internal file name: `Matrix1`

Open the property window of the generator and set the following on the Attributes Editor:

        Environment:

            LCG_CATALOG_TYPE = lfc

            LFC_HOST = lfc-gilda.ct.infn.it

            LCG_GFAL_INFOSYS = grid004.ct.infn.it:2170

        Output data:

            Output SE: **choose one from the list below**

            (output of `lcg-infosites --vo gilda se`)

                      aliserv6.ct.infn.it

                      trigrid-ce01.unime.it

                      se-nano-38.to.infn.it

                      gilda04.ihep.ac.cn

                      dgt02.ui.savba.sk

                      gilda-se-01.pd.infn.it

                      grid—5.iucc.ac.il

                      gn0.hpcc.sztaki.hu

                      grid-se.bio.dist.unige.it

Open the PS property window in the "Workflow" menu of the editor. Set the following:

        Grid: *<gilda_LCG_2_BROKER>*

        LCG Catalog Type: lfc

        LFC Host: lfc-gilda.ct.infn.it

        Output **Directory**: `/grid/gilda/training/riodejaneiro/MatrixPS-`***XX/results***

        (Do not put a "/" to the end of the name!)

Connect the output port of the generator to the PS input of the Matrix job

3.1.5 Save and submit the workflow. Monitor and visualize the progress of execution.

Notice the difference in the Workflow portlet for normal and PS workflows: generators and real jobs are separated. (Collectors too but currently we do not have any.)

Check the existence of the parameter files:

Login with ssh to the GILDA UI machine

Execute the following:

- `voms-proxy-init –voms gilda` (passphrase RIODEJANEIRO)
- `lfc-ls /grid/gilda/training/riodejaneiro/MatrixPS-`***XX***
- `lcg-cp --vo gilda`
  `lfn:/grid/gilda/training/riodejaneiro/MatrixPS-`***XX***`/Matrix1.0`
  `file://`\`pwd\`/Matrix-local.0`

3.1.6 Download and unzip the result file.

Part III: *Turn a matrix operations workflow into a parameter study*

In this exercise you should turn a workflow into a multi-dimensional parameter study. The workflow computes the following matrix expression, where A and B represent the input matrixes:

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

The workflow is presented in the figure below, its jobs result the following formulas:
- Multip: A*B
- Column0: A*B[*, 0]
- Column1: A*B[*, 1]
- Transpose: A*B[*, 0]T
- Multip.2: A*B[*, 0]T * A*B[*, 1] → *Final result, represented by Port 2 of "Multip.2"*

Please download the workflow from here
http://portal.p-grade.hu/tutorials/induction/workflows/Matrix-operations-workflow.tar.gz

Import it into your portal account like this:
- Click on the Workflow portlet, then onto "Upload"
- Select the previously downloaded archive from your computer and click OK.
- Open the workflow in the workflow editor. (Workflow/Open menu)

Add to two auto input generators to the graph in a way that the workflow should be executed 4 times on the combination of 2 different INPUT1 and 2 different INPUT2 matrixes.
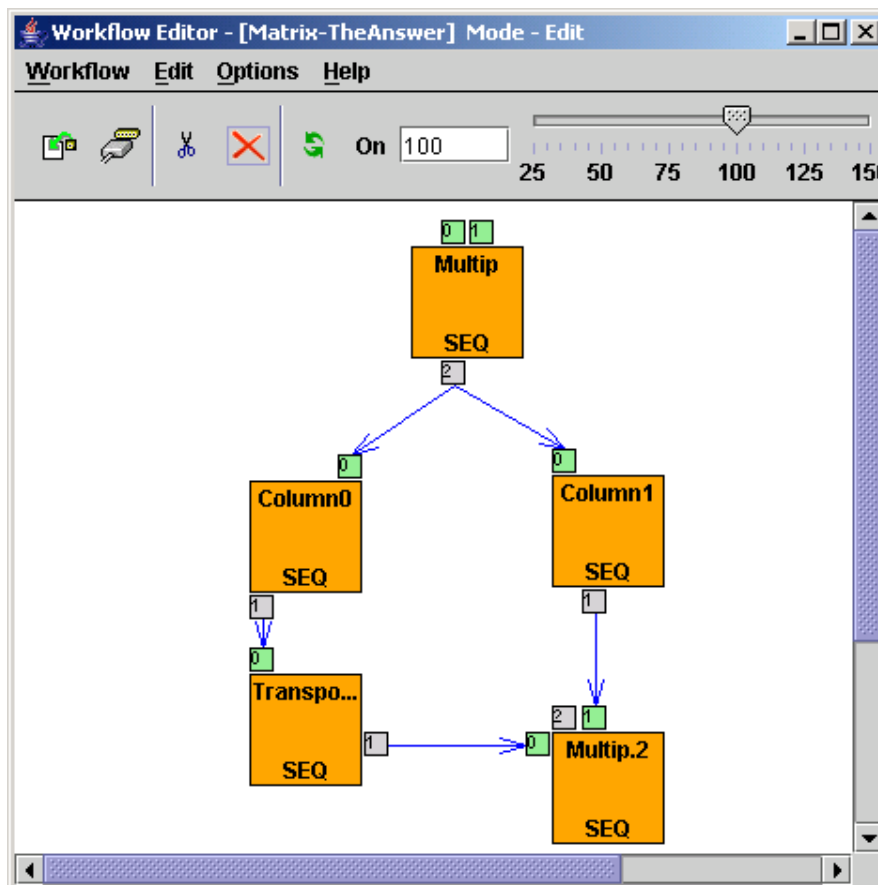
Workflow to compute AB[*, 0]T * AB[*, 1] matrix expression