SHIWA Portal tutorial
Submission Service version, 21/05/2014
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Contents

Goals of the tutorials and definitions

The aim of this tutorial is to introduce the basic features provided by the SHIWA Simulation Platform.

The following features will be covered by the tutorials:

1. Creating, configuring and submitting a WS-PGRADE workflow, consisting of a single native job.
   - Exporting this WS-PGRADE workflow to the SHIWA Repository, and importing it back to the SHIWA Portal.
2. Creating, configuring and submitting a meta-workflow, consisting of both native and non-native workflows.

Native workflows

For the purpose of this tutorial, the term *native workflows* will refer to a standard job in a WS-PGRADE workflow which executes an executable uploaded to the portal during configuration of the WS-PGRADE workflow. In this tutorial the executables used will be a Bash shell script. Native workflows do not make use of any repository.

Non-native workflows

For the purpose of this tutorial, the term *non-native workflow* will refer to a job in a WS-PGRADE workflow, which executes a workflow of some workflow engine, is selected from a SHIWA Repository and submitted using the Submission Service.

Meta-workflow

For the purpose of this tutorial, the term *meta-workflow* will refer to a WS-PGRADE workflow which consists of several other workflows. These embedded workflows may be native, non-native or a mixture.

The figure below is of the meta-workflow from the second tutorial. The job *Taverna* is a non-native job, which executes the Taverna 2.4 workflow in the graphic.
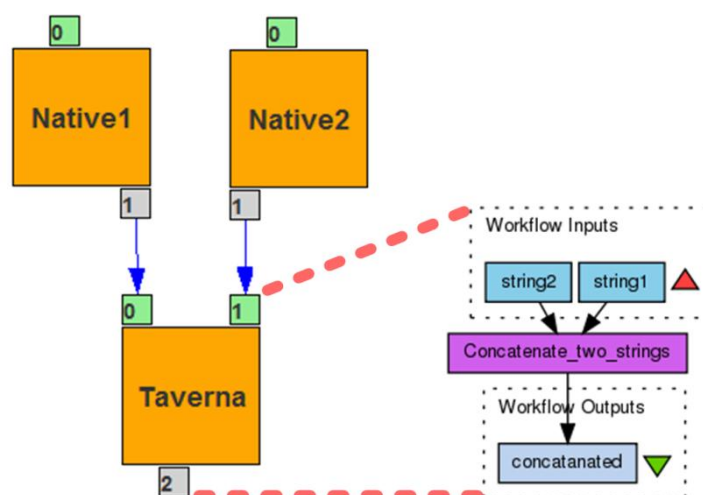
Usage of the SHIWA 2 Portal

The Prototype SHIWA 2 Portal is available at this address:

http://ssp.shiwa-workflow.eu/

If you own an account, then you can use it to log in. Otherwise, the next subsection will explain how you can create one.

i.   Creation of a portal account

On the **Welcome page** of the portal, click on **Sign In** located at the top right of the page to open the **login page**.

Then, click on **Create Account** for accessing to the **account creation page**.

Fill all required field and click on **Save** to validate your account.

A default password will be automatically attributed to your account for your first connection and sent to your email address.

You will be able to change it after validating *Terms of Use*.

Your account is created then, and you can start using the SHIWA Portal as a normal user.

ii.   Certificate management

Once you are logged in the SHIWA Portal, you can get a certificate to allow workflow execution on a specific resource.

Click on the *Security -> Certificate tab* to open the *Certificate page*.
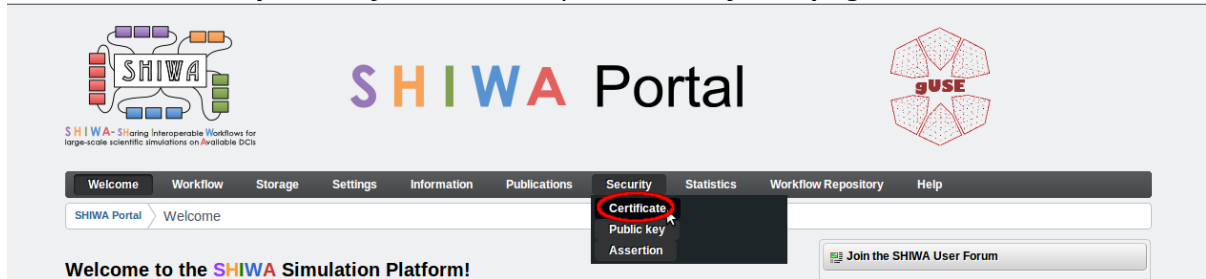
On the *Certificate page*, click on the *Download button* to open the *Download certificate page*.
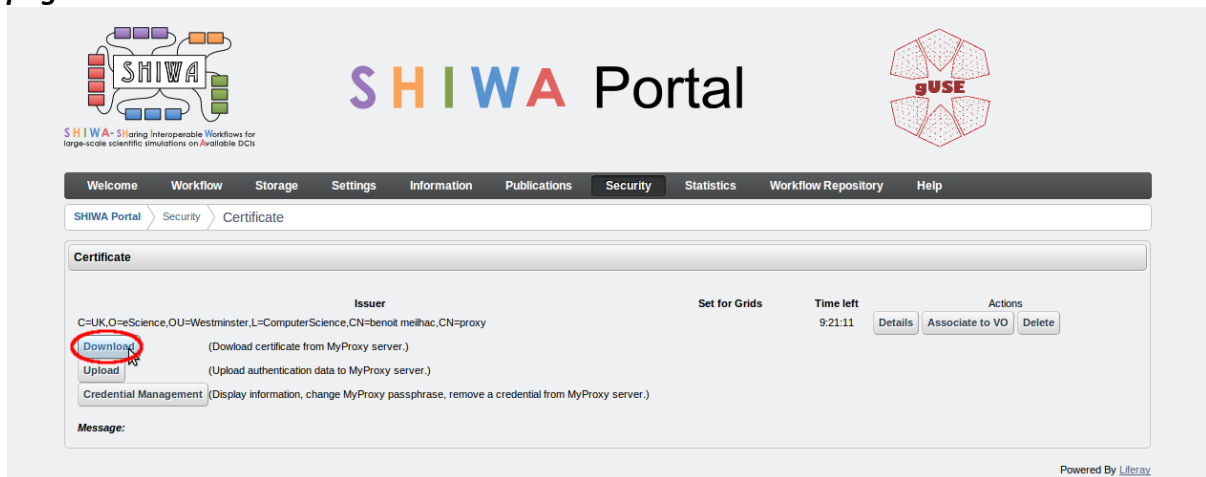
On the *Download certificate page*, specify the following parameters:

Hostname: **myproxy.ngs.ac.uk**
Login: **SHIWAtraining2014**
Password: **shiwa12345**

The above credentials are only effective for the duration of the *SHIWA Technology hackathon at EGI Community Forum 2014* event.

Click on the *Download button* to download your certificate on the SHIWA Portal.

Then, you have to associate the certificate with a *Virtual Organization* in order to be able to submit workflows.

By clicking on the **Associate to VO button**, you open the **Setting Certificate for Grid page**.

Select **WestFocus** and then click on the OK button to move the **Confirm certificate page**.

On the **Confirm certificate page**, click on the **Yes button** to finalize the certificate download and association with a Grid.

The portal returns to the **Certificate page** where your certificate is displayed and you can check its details by clicking on the **Details button**.

In order to configure and execute non-native workflows on the SHIWA Portal, you need to associate your certificate with the resource the job will be submitted to.

Tutorial 1: Creation and execution of a single native workflow

In this tutorial, the creation, configuration and execution of the "*helloyou*" job will be described. Then the workflow will be exported to the SHIWA Repository, using the export functionality. Finally, the workflow will be imported back from the SHIWA Repository.

The *"helloyou"* job is a simple shell script named helloyou.sh, which returns a greeting including what the input file contained, and the command line argument. This output is then redirected to an output file. For your convenience the code of this shell script is provided below:

```
#! /bin/bash
echo "Hello " `cat input` " , "$* > output
echo "   This greeting was generated by a native shell script" >> output
cat output
```

You can download this file from this link

You are free to use your own bash shell script. To follow this tutorial the script should use a single input file named *input*, and a single output file named *output*.

1.1 Creation and execution of a single native workflow

1.1.1 Accessing workflow graph editor

Click on the ***Workflow tab -> Graph*** to open the ***Graph page***.
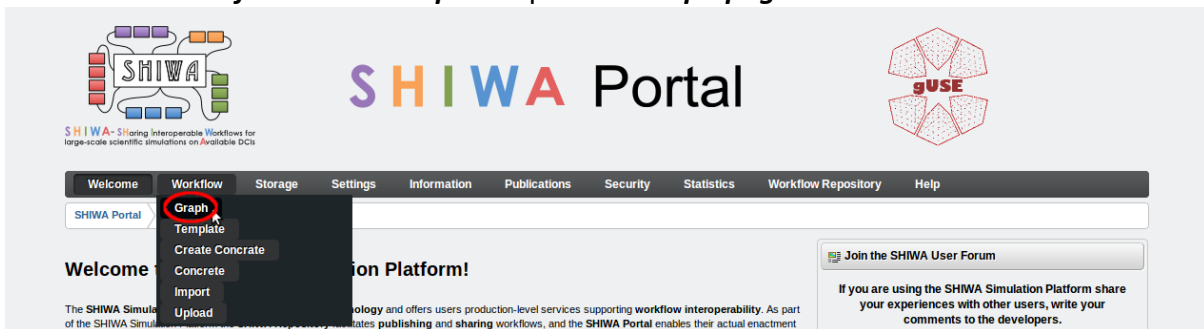
Click on the ***Graph Editor button*** to start the Java Web Start based workflow editor to be able to create the workflow graph.

1.1.2 Creating the abstract workflow

Click on the New Job and New Port buttons to produce the graph below.

Click on the Job icon to specify the name of job.

Click on the two Port icons to specify the ports as being input or output, and their details.

To specify an output port, double click on the desired port and change the input to output.

Create the following graph:
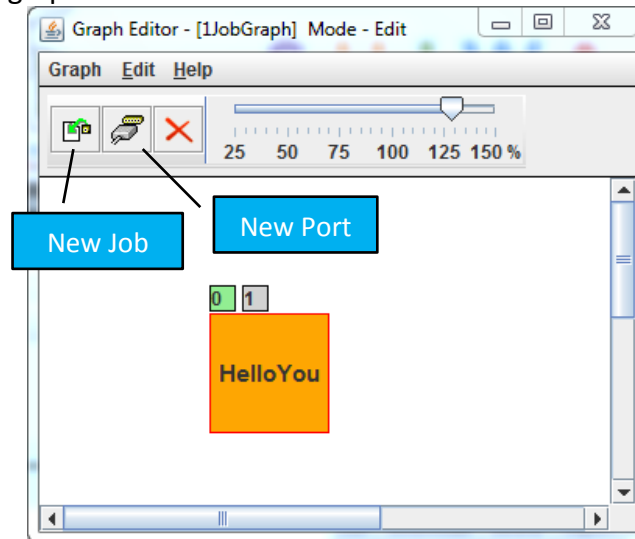
- 1 job, there is no need to change the name of this job.
    - 1 input port, change the name of the port to : input
    - 1 output port, change the name of the port to : output
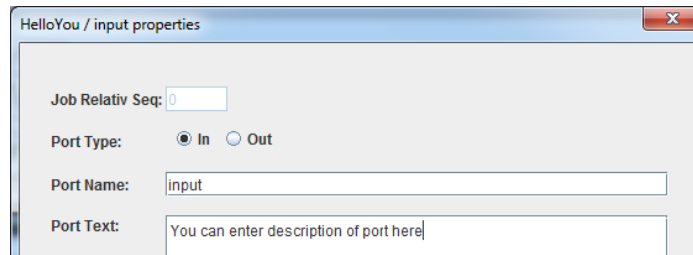
After reproducing the graph corresponding to the "helloyou" job, save it by clicking on the **Graph tab** and selecting the **Save option**.

1.1.3 Creating the concrete workflow

Click on the *Workflow tab -> Create concrete* to open the *Create concrete page*.
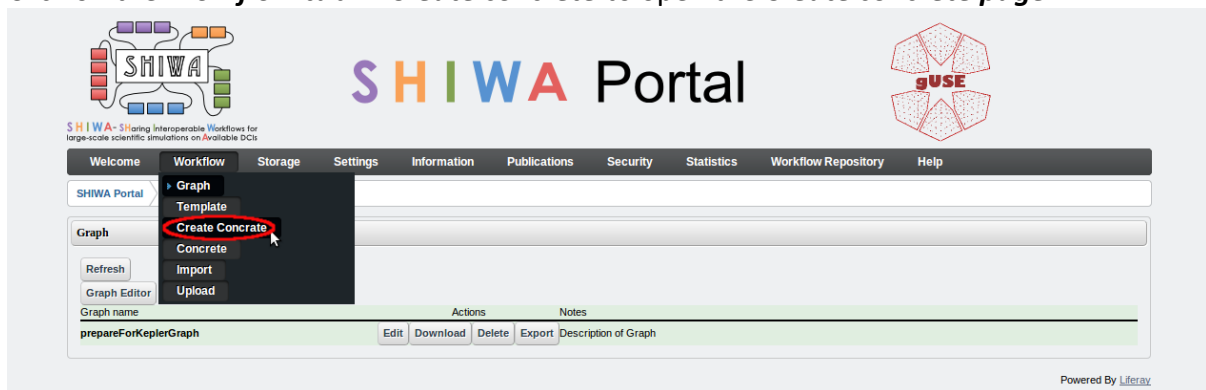
Select the previously created graph to be used to create the concrete workflow, define its name and then press the **OK button**.

Please specify a name unique to yourself, such as "*HelloYou_Peter*", this will enable exporting to the Repository later, as there is a workflow names on the Repository must be unique.
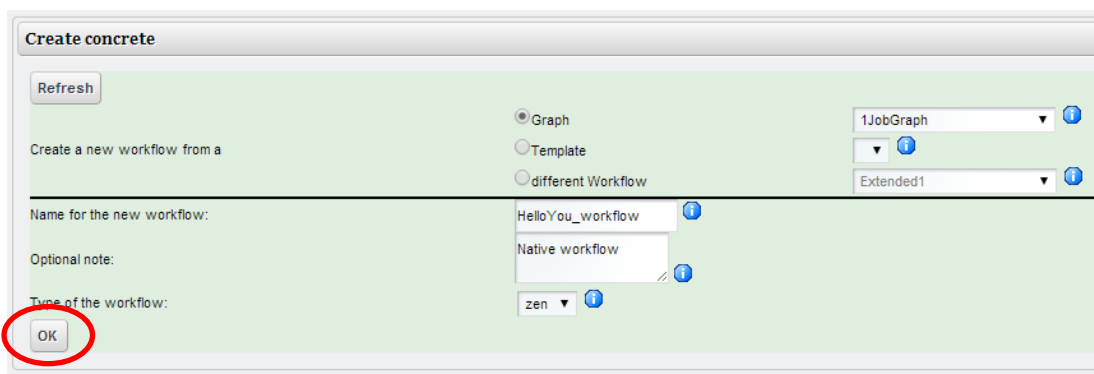
1.1.4 Configuring the concrete workflow

Click on the *Workflow tab -> Concrete* to open the *Concrete page*.
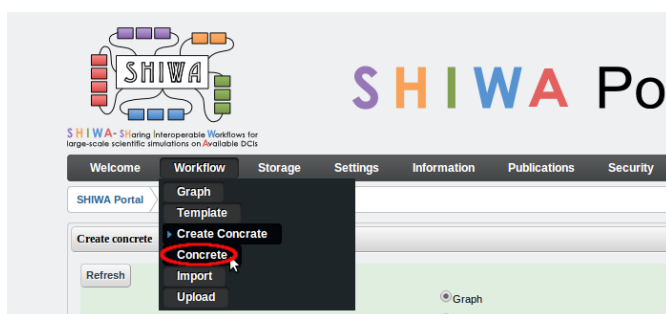
Select the concrete workflow corresponding to the *"helloyou"* job by clicking on the **Configure tab** of the created workflow.
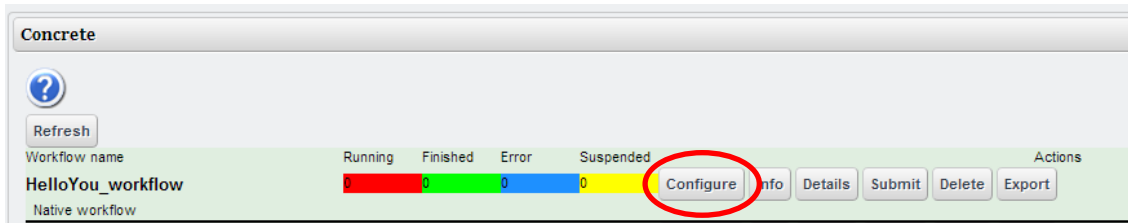
The portal displays the graph of the selected concrete workflow. To configure the workflow job, click on the job on the workflow graph.
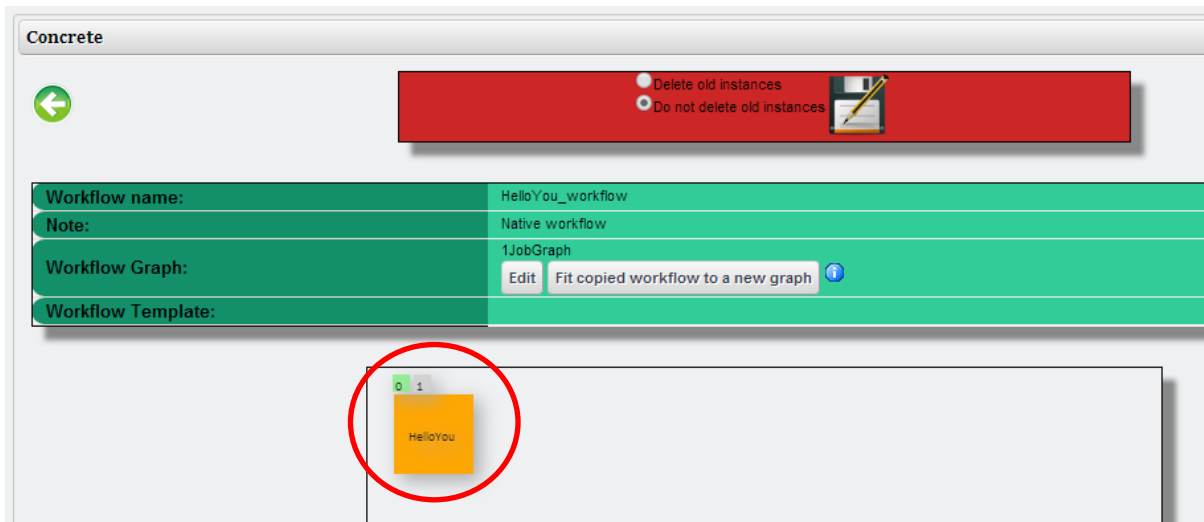
Specify both the job binary and input/output files and parameters. To specify job binaries, click on the **Job Executable tab** and set the following parameters:

Type:	gt4
Grid:	WestFocus
Resource:	ngs.wmin.ac.uk
JobManager:	jobmanager-pbs
Kind of binary:	Sequential
Executable code of binary:	upload this [file] named *"helloyou.sh"*
Parameters:	-Iam Job0

Click on the *Job I/O tab* and specify the job input/output files and parameters used by the input/output ports.

Input ports:

Port number	Input Port's Internal File Name	Port dependent condition	Source of input directed to this port	Parametric Input details
Port 0	input	Hide	Use a text file containing your name	Hide

Output ports:

Port number	Output Port's Internal File Name	Base of Output Port's Remote File Name	Storage type	Generator
Port 1	input		Permanent	No

After specifying the job binaries and input/output files and parameters, click on the *Save button* at the bottom of the *Job I/O tab*.

Then click on the **Save on Server button** to store details of the concrete workflow.

1.1.5 Verifying the configurations of the concrete workflow

Click on the *Info button* of the concrete workflow, to inspect if there are any misconfigurations.

This is not an exhaustive verification of configuration, but does pick-up on common configuration issues.

1.1.6 Running the configured workflow

Click on the *Submit button* of the concrete workflow name to submit and execute it.
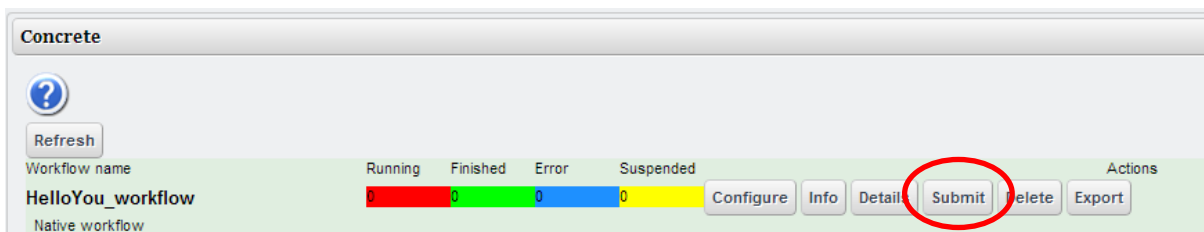
To display the workflow status during the execution, click on the *Details button*.
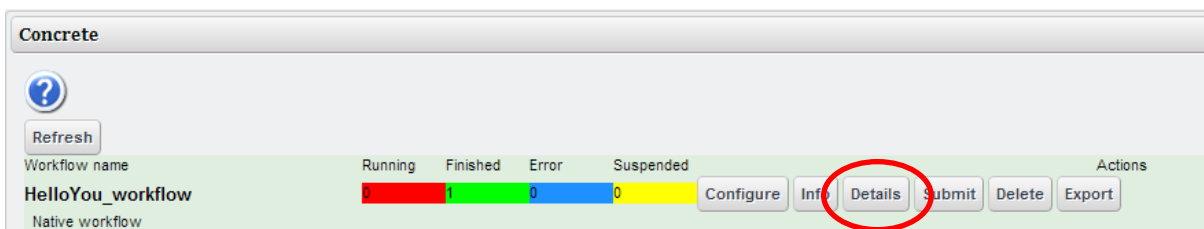
By clicking again on the *Details button*, the portal displays the execution status of the jobs.
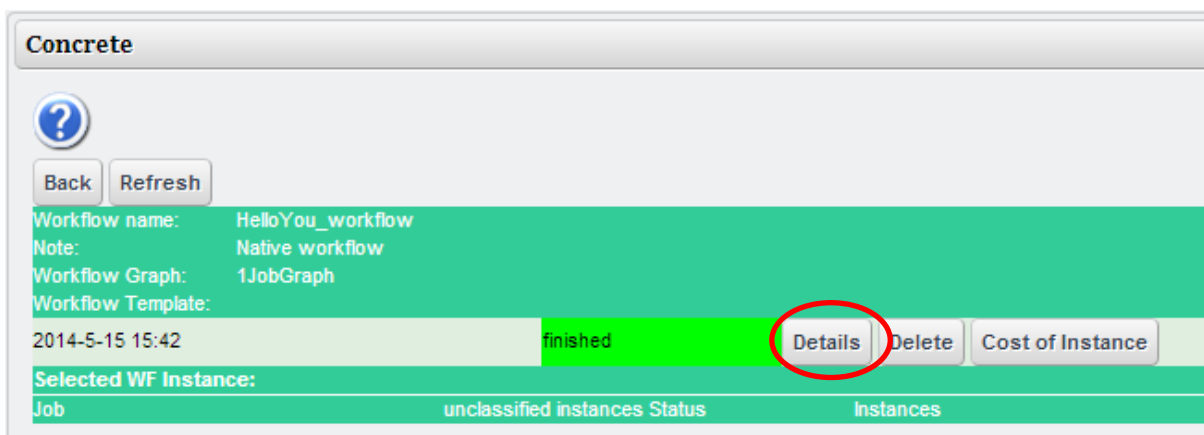
By clicking on the **View button**, a view of a specific job can be displayed.

If the workflow is still running, click on the **Refresh button** to update the status.
When the execution of the workflow is successful, the status will change to *Finished* and you can click the **View finished button** to view the results of the workflow. You are able to see generated output and error messages by clicking the **std.Output** and **std.Error** buttons respectively.

The output files can be downloaded as an archive by clicking on the **Download file output button**.

1.2 Exporting the workflow to the SHIWA Repository

After a successful execution of the above workflow, you can choose to export it on the SHIWA Repository and share it with the community.
To do that, you have to click on the **Export button** of the desired workflow.

An interface is opened, from which you can choose where to export your workflow. Select the option **Remote SHIWA Repository** and click on the **Ok button**.

A new interface is presented, from which you have to select the SHIWA Repository location and enter your SHIWA Repository account credentials. Select http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/ as the repository.

For the *SHIWA Technology hackathon at EGI Community Forum 2014* event, please use user **SHIWAtraining2014**, with password **shiwa12345** .Clicking on the ***Get Groups button*** and select the only group listed.

The group used for the workshop is: "Training"

Configure the job as it is on the following screenshot and click on ***Export in WS-PGRADE/gUSE format button*** to export the workflow in the SHIWA Repository.

A message should appear confirming the successful exportation of the workflow.

The export functionality is known to work with:
- Single native workflows;
- Single non-native workflows;
- Multi-native workflows;
- Meta-workflows.

1.3 Importing and re-submitting the workflow

After the exportation, you have the possibility to import the workflow. You would have to set the Implementation in the SHIWA Repository to be publicly visible before it would be importable – this is beyond the scope of this tutorial, although has been included in the video for your information.

For your convenience, there is already a publicly visible Implementation of this workflow on the Repository. The workflow is named ***HelloYou_workflow***. Click on the ***Workflow -> Import tab*** to open the ***Import page***.
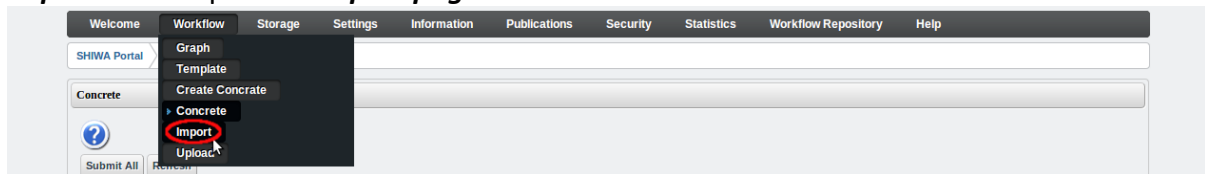
Click on the ***Remote SHIWA Repository button*** to open the interface for importing your workflow.
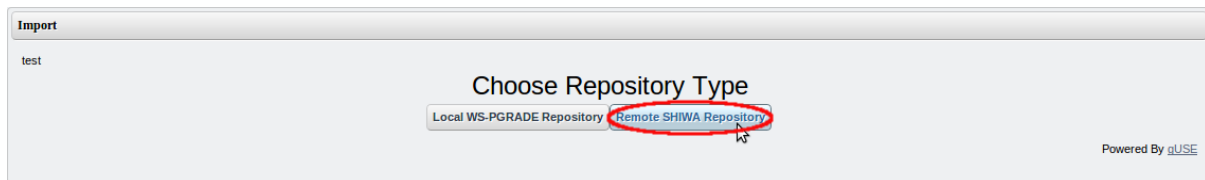
The menu open, select the SHIWA Repository location (http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/) and click on the ***Get Public Bundles button***.
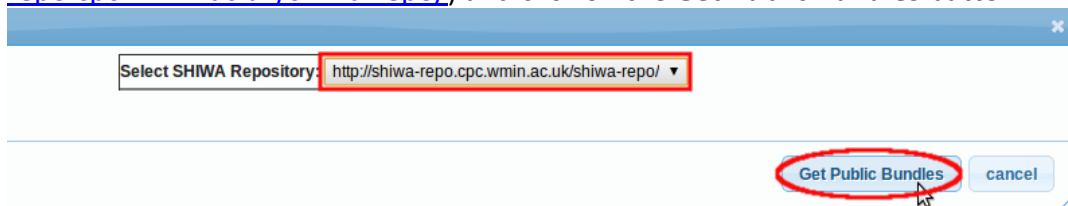
You can see the list of all exported workflows within then SHIWA Repository. Search for the workflow you just exported in the previous subsection, select it and click on the ***Import Selected button***.
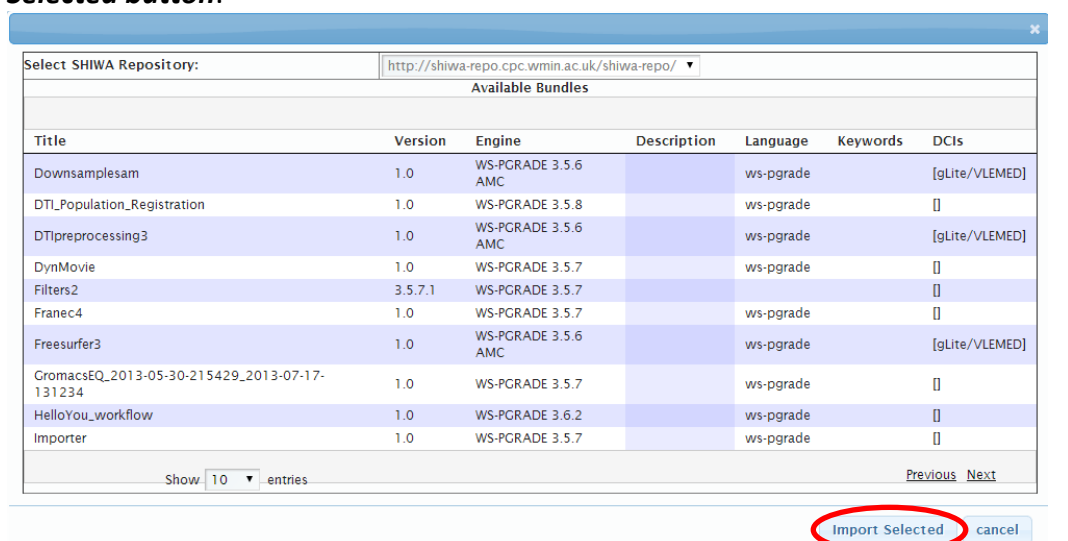
A confirmation message should appear to announce the successful importation.
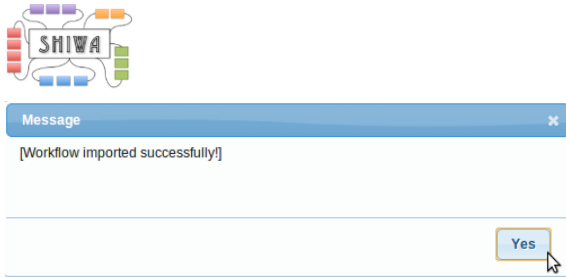
You can now go back the **Concrete page** by clicking on the **Workflow -> Concrete tab**. You should see the new imported workflow – this will be denoted by a time stamp after the name. To check if everything went well, click on the **Submit button** on the newly imported workflow, wait until the end of the execution and check if you get a finished result and not an error.

Tutorial 2: Extension of workflow from Tutorial 1 to a meta-workflow including both native and non-native workflows

In this section, you will see how to extend WS-PGRADE workflows and use the selection functionality within the SHIWA Portal and Repository to simplify the configuration of an associated workflow. The workflow in question will be a *"concatenation of strings"* job corresponding to the "*concatTwoStrings*" workflow available in the SHIWA Repository and deployed as Submittable through the Submission Service. Then, once this workflow selected, the creation, configuration and execution of the workflow will be discussed.

2.1 Extend graph of workflow

The portal allows developers to extend workflows. As long as the graph is only extended – with the existing jobs neither being removed nor changed - the configurations of existing jobs will persist.

Click on the *Edit* button from the workflow configuration interface, to edit the Graph.

2.2 Use the Graph Editor to extend the workflow

Add two jobs to the Graph:
- Job1 should be structure the same as Job0:
    - 1 input port, change the name of the port to : input
    - 1 output port, change the name of the port to : output
- Job2 should be structured with two input ports and one output port:
    - 2 input ports, without touching the name: PORT0, PORT1
   - 1 output port, without touching the name: PORT2

Now connect each of the output (grey) ports of jobs Job0 and Job1 to each of the two input ports of Job2. Then save the extended graph, as a different name.
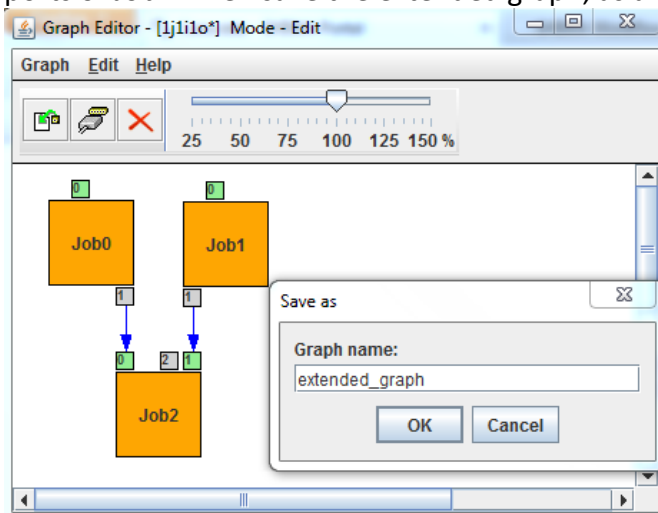
2.3 Copy the workflow and fit to the extended Graph

The portal will allow users copy the workflow and attempt to fit the copied workflow to a new Graph.

Click on the *Fit copied workflow to a new graph* to attempt to fit the configured concrete to a new Graph.
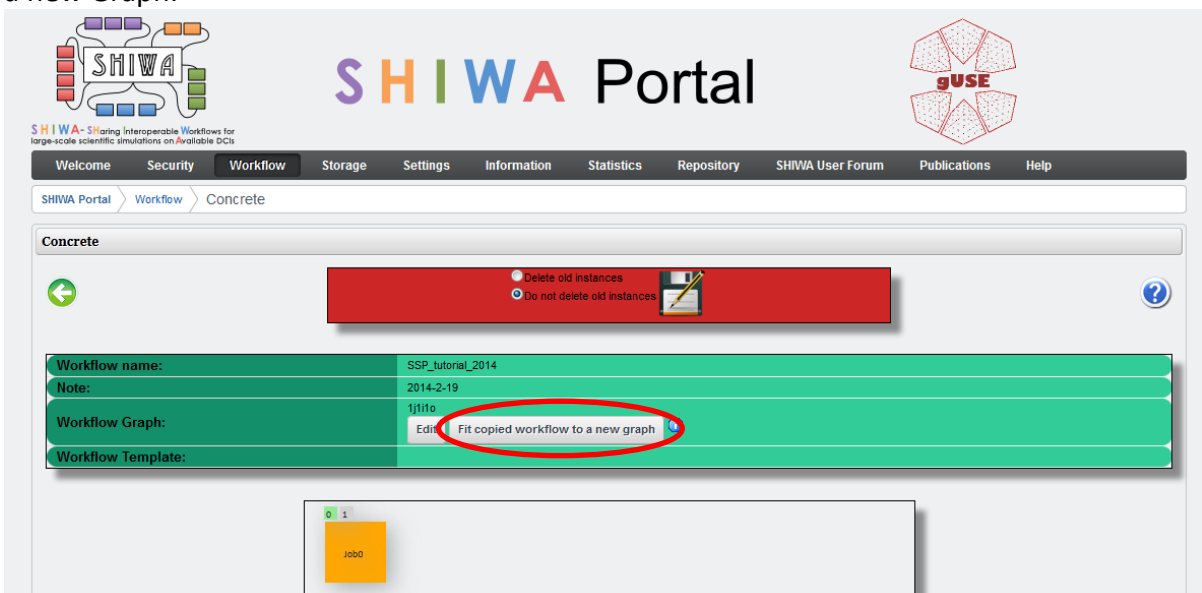
Now select the new graph. Make sure you specify a name for the new workflow – failure to this will overwrite the existing workflow, which may destroy job configurations.
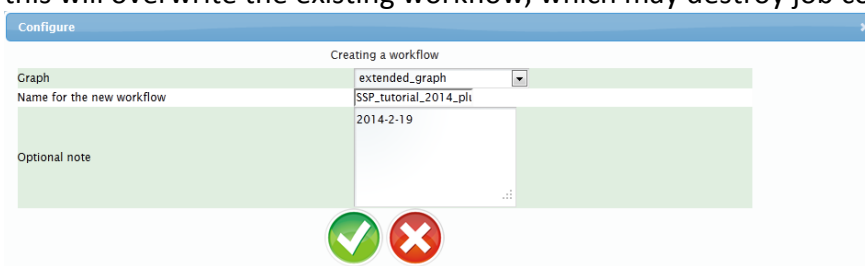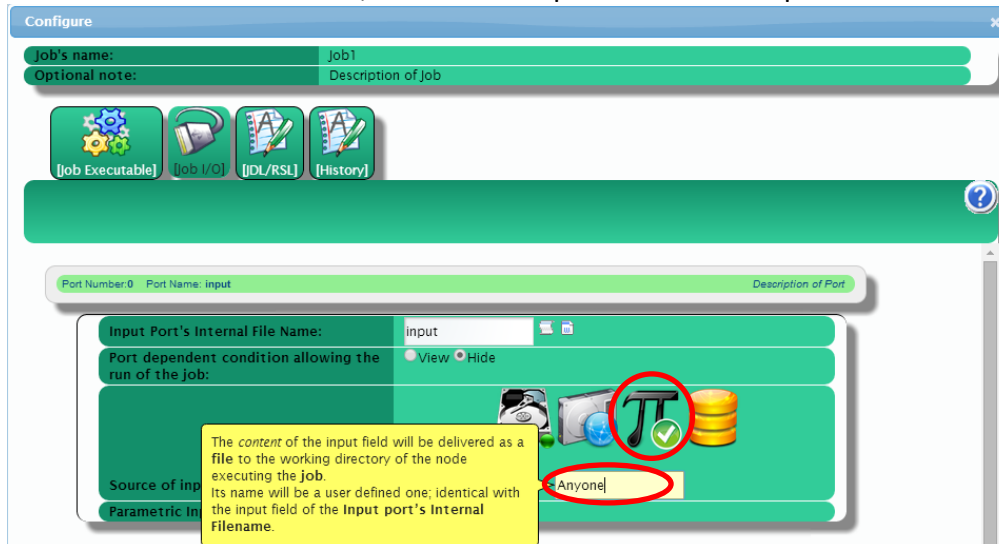
2.4 Configuration of second native job

Job1 should be configured in the same was as Job0 was configured in the previous tutorial. The only differences should be:

- The string entered in the Parameter box should read "-Iam Job1".

- In the Job I/O tab, for PORT 0, click the π symbol – this will enable you enter in a value in the text box, which will be passed into the input file.


Save the concrete at this stage.

2.5 Browsing the SHIWA Repository and selecting a non-native workflow

A new feature of the portal allows the selection of non-native workflow deployed as Submittable through the Submission Service through the SHIWA Repository tab. If an implementation exists within the SHIWA Repository and is deployed as Submittable through the Submission Service, you can select it and easily access to it during the configuration of the workflow as it will be explained in the next part of this tutorial.

Click on the *Repository tab* to access to the SHIWA Repository embedded website.
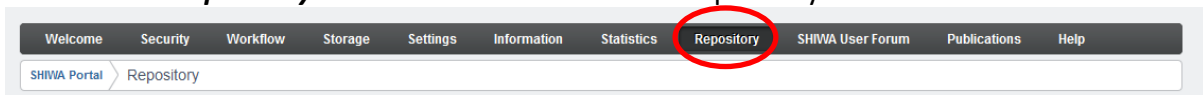
Then, in the *Find Workflows field*, enter "*concat*" and click on the *Search button* to launch the research of the "*concatTwoStrings*" existing workflow.
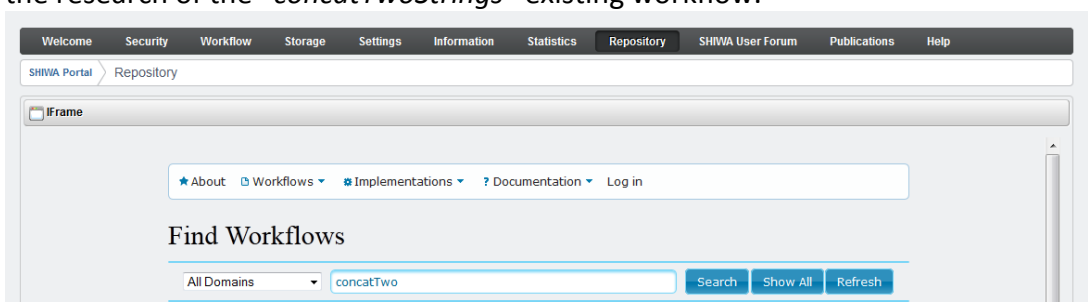
A short description of the workflow and its implementation appear. This workflow is composed of two inputs and one output. This information has to be known when you want to include this workflow within a WS-PGRADE workflow, to create a graph with a corresponding job, with the correct number of input and output ports.

To make the selection of the workflow, you have to click on the *blue arrow button*.
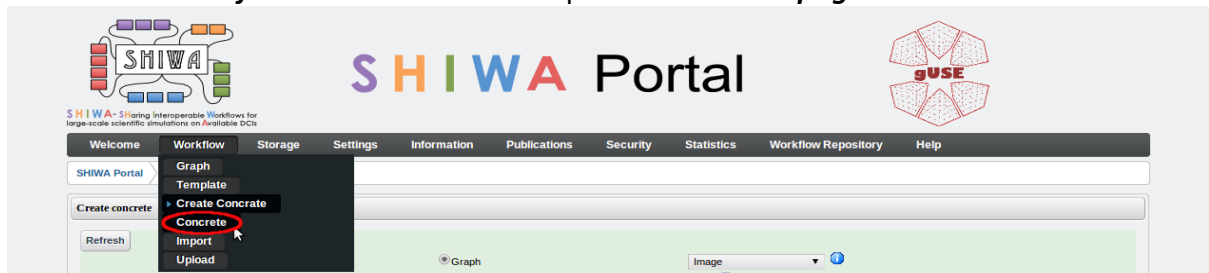

A message is displayed confirming the selection and the button is crossed. The portal and the repository offer the possibility to select as much as implementations as you want.

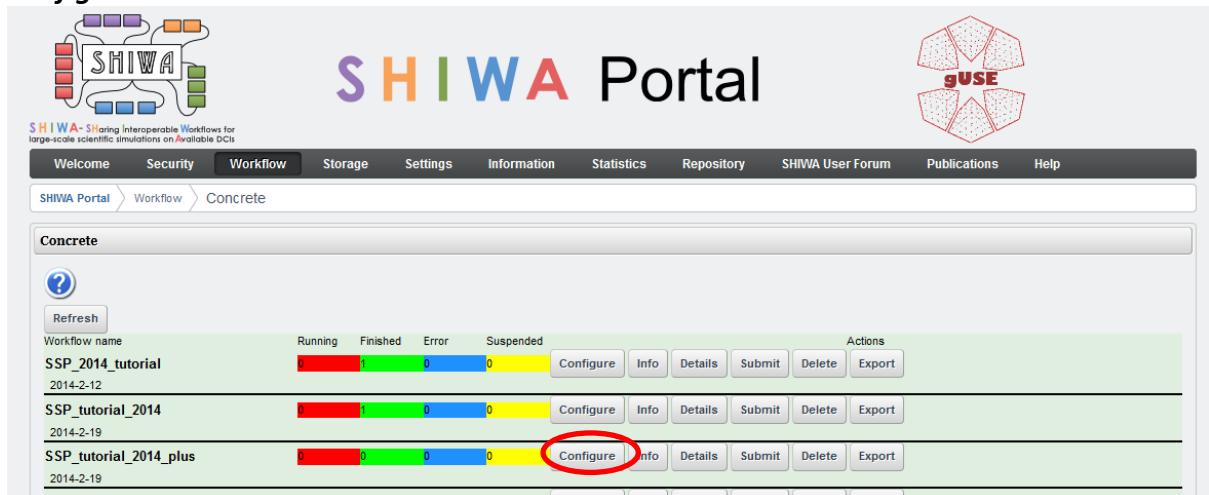### 2.5.1 Configuring the non-native job within the concrete workflow
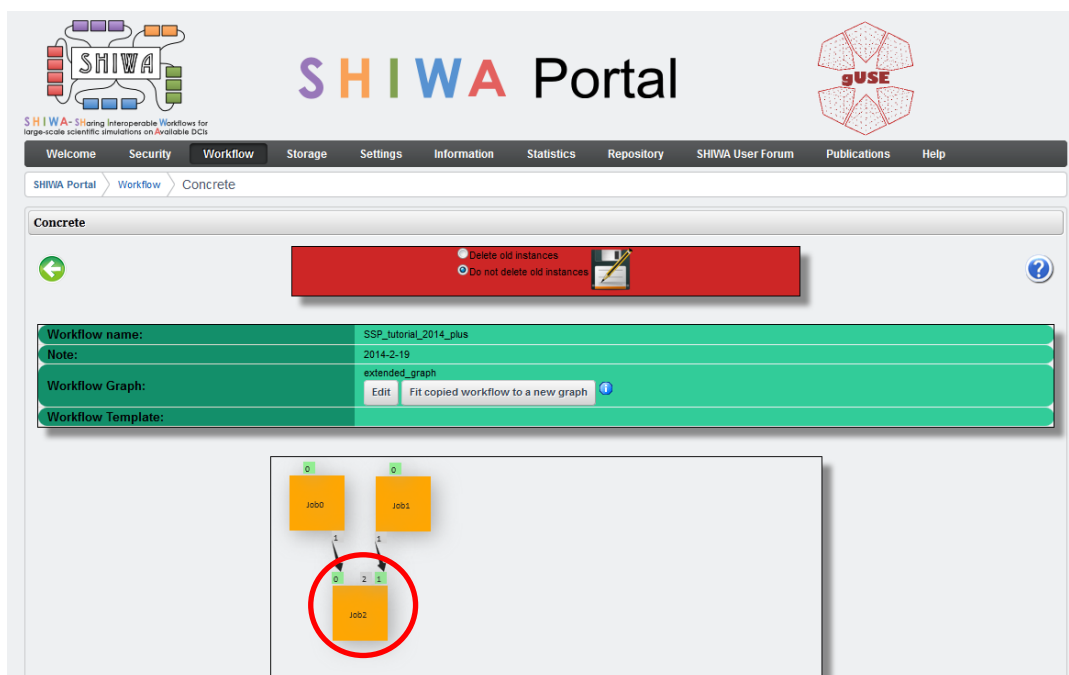
Click on the *Workflow tab -> Concrete* to open the *Concrete page*.

Select the concrete workflow corresponding to the extended workflow by clicking on the *Configure tab*.

The portal displays the graph of the selected concrete workflow. To configure the workflow job, click on the Job2 on the workflow graph.

Specify both the job binary and input/output files and parameters. To specify job binaries, click on the **Job Executable tab**. The job executable configuration is done in two steps.

The first step is to select the corresponding workflow implementation from the SHIWA Repository for the job. Select "*shiwa*" as **Type** of the Job Executable tab. Select the **SHIWA Submission Service** "*to complete*". Select the **SHIWA Repository** is "*http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo*". Then select the **Submittable Execution None (SEN)** "*to complete*". You can see that the list is divided into two parts, the first part being workflows selected within the SHIWA Repository. The "*concatTwoStrings*" workflow should appear in this first part of the list.

Select **WestFocus** from the list of Resources available.

Click the green tick at the bottom of the interface, to save the configurations at this stage. Then you should see this screen.
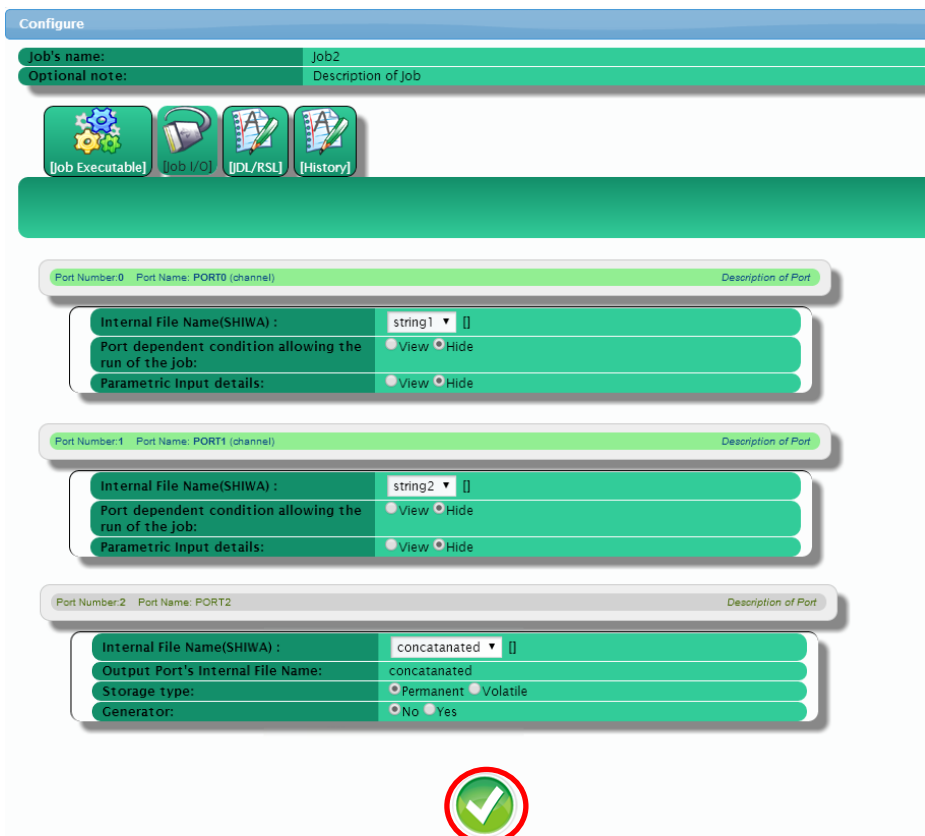
Click on the *Job I/O tab* and specify the job input/output files and parameters used by the input/output ports.

Input ports:

Port number	Internal File Name(SHIWA)	Port dependent condition allowing the job to run:	Parametric Input details:
0	string1	Hide	Hide
1	string2	Hide	Hide

Output ports:

Port number	Internal File Name(SHIWA)	Storage type:	Generator:
2	concatenated	Permanent	No

Do not forget to click the greet tick to save the configurations.

After specifying the job binaries and input/output files and parameters, click on the *Save button* at the bottom of the *Job I/O tab*.
Then click on the *Save on Server button* to store details of the concrete workflow.

## 2.6 Verifying the configurations of the concrete workflow

Click on the *Info button* of the concrete workflow, to inspect if there are any misconfigurations which the portal has pick-up.
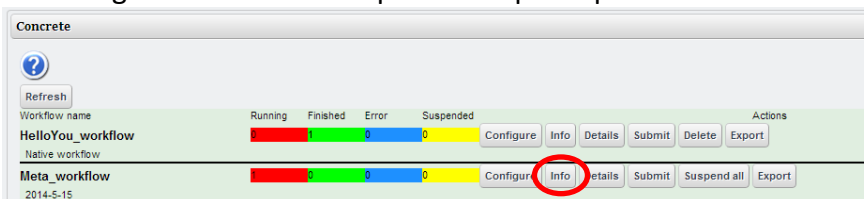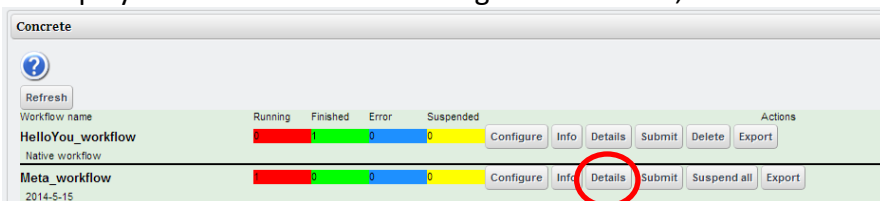

This is not an exhaustive verification of configuration, but does pick-up on common configuration issues.
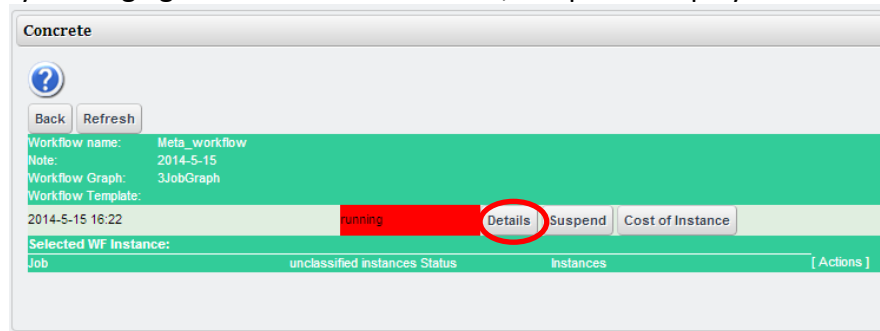
2.7 Running the configured workflow

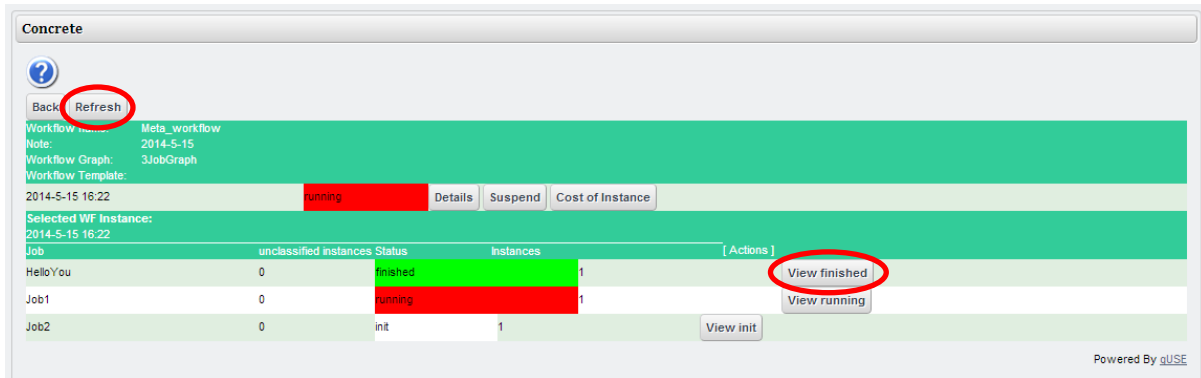Click on the *Submit button* of the concrete workflow name to submit and execute it.
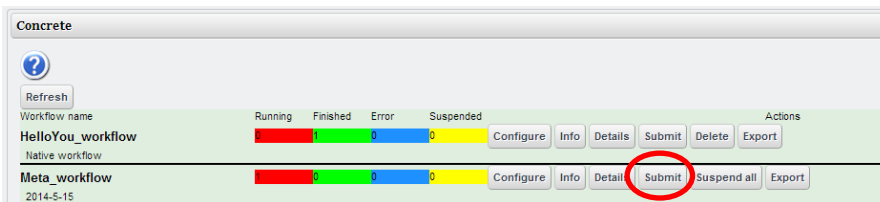
To display the workflow status during the execution, click on the *Details button*.

By clicking again on the *Details button*, the portal displays the execution status of the jobs.

By clicking on the respective *View button*, a view of a specific job can be displayed.

Click on the **Refresh button** to update the status.

2.8 Retrieving results of the workflow

When the execution of the workflow is successful, the status should be changed to *Finished* and you should be able to see generated output and error messages. Output files can be downloaded as an archive by clicking on the **Download file output button**.