5th DEISA Training Session

CINECA, Bologna, 30th October 2007

UNICORE Exercises

1 Prerequisites

The UNICORE Client is a Java Application that requires at least **Java** Run Time Environment version **1.5** to be installed

- Check if the **SUN-Java Runtime Environment** version higher than 1.5 is installed on your computer
  - **On MS Windows** type `java -version` in a DOS box
  - **On UNIX/Linux** type `java –version` in a console
- If the execution of the command fails or if you have a java version older than 1.5 go to the **SUN web page** to download and install the latest JRE 1.5.x on your local computer, following the instructions given there.

2 Prepare and configure the Client

2.1 Install the Client

- Download `client_5.6.5_installer.jar` from **http://www.unicore.eu**-*>Download ->Core -> Client ->Download*
- Execute the installer and start the client

Linux:

- Open a console and type
  `java –jar client_5.6.5_installer.jar`
- Start client via:
  ```
  cd ~/UNICORE/bin
  ./unicore &
  ```

Windows:

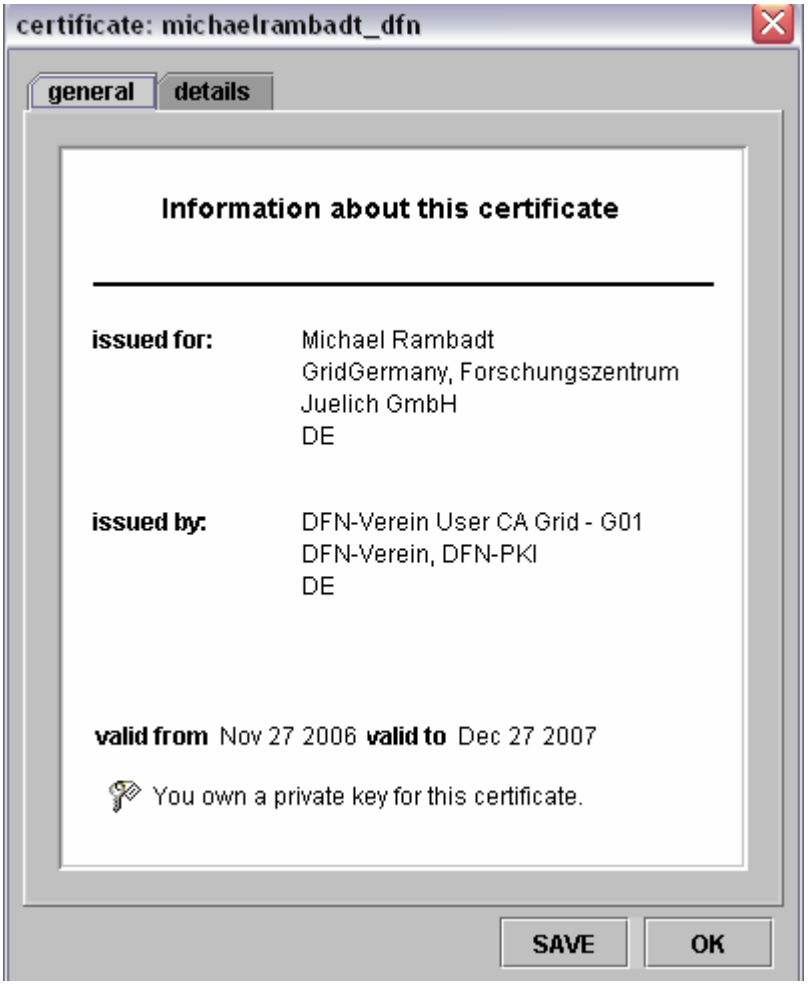
- Double-click on `client_5.6.5_installer.jar`
- by double clicking on the UNICORE desktop symbol or execute the file `UNICORE\bin\unicore.bat`

- Confirm creation of a new UNICORE keystore and choose a password.

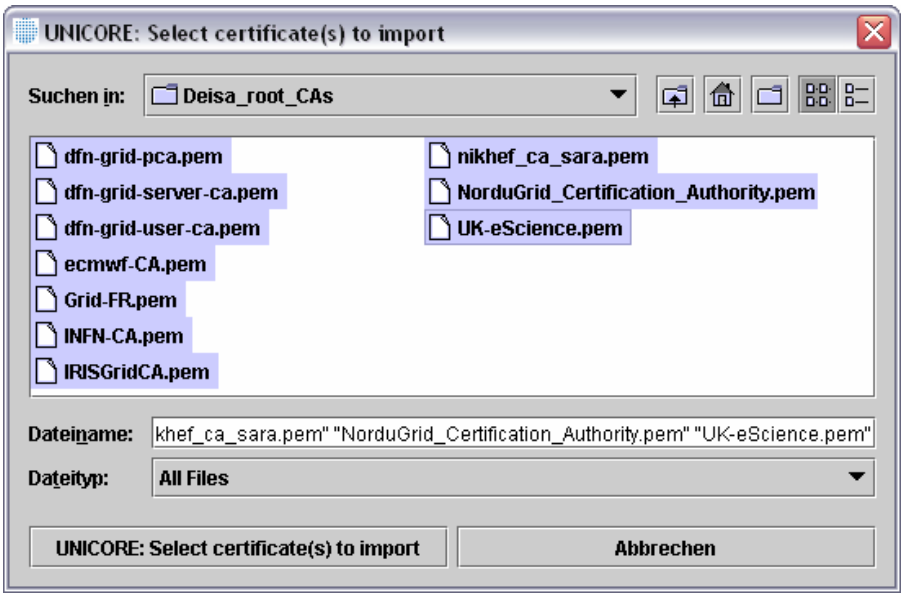
- The UNICORE password checking is quite strict so a warning might appear. Click on -> ***OK***

2.2 Import private certificate keystore (.pkcs12)

- **Prerequisites:** you have got already a signed certificate from your national CA and the corresponding .pkcs12 file on your local computer. Assuming this is called **user1.p12**
- Select ***Settings -> Keystore Editor, Action -> Import Keystore*** in the UNICORE client and select **user1.p12** within the upcoming filebrowser
- Provide your password the **user1.p12** is encrypted with
- Click ***OK.*** Your user certificate will be shown in the list of **Key entries.** If there is a problem you will be informed, otherwise you won't get any message
- Mark your certificate and click on **Details.** They should look similar to the example.



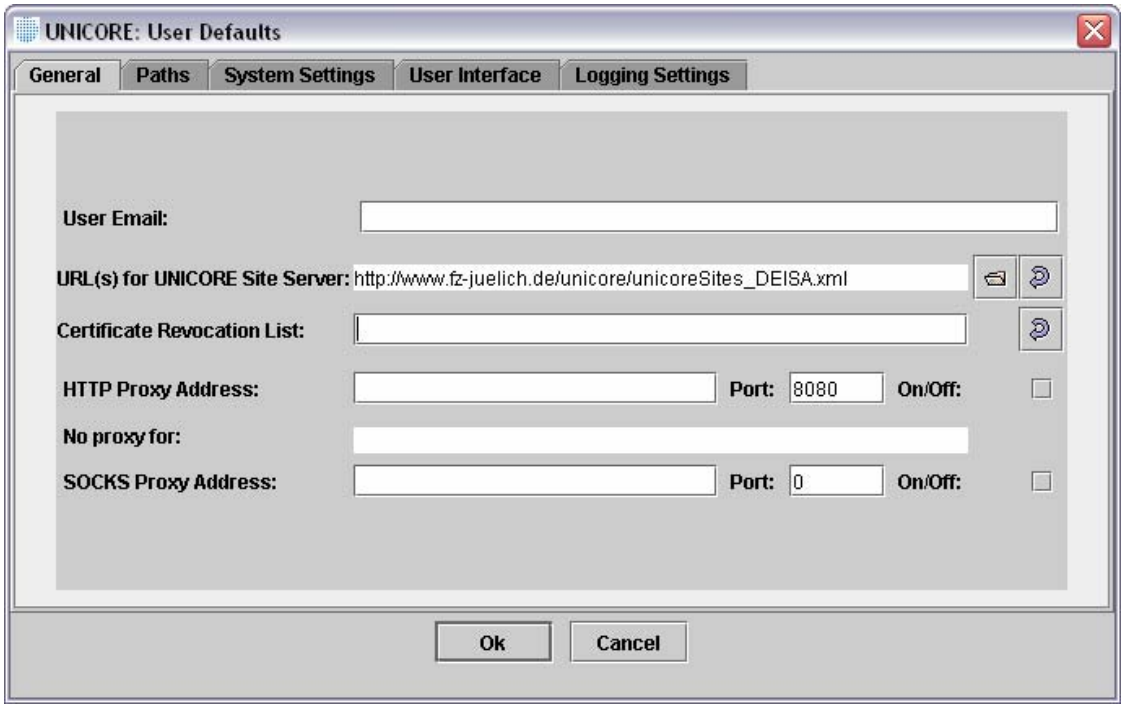
- Download the EU-GridPMA certificates from **http://winnetou.matrix.sara.nl/deisa/certs** -> Package with individual certs from CAcerts file in zip format ->unicerts.zip
- Extract the certificates to a local folder
- Import the EU-GridPMA certificates with the **UNICORE Keystore Editor**
- choose from the menu ***Action -> Import Certificate*** and select all stored certificates



- Confirm with ***OK***
- Save your keystore: ***File -> Save***.
- Exit the keystore: ***File->Exit***

2.3 Make DEISA Gateways known to the client

- Select ***Settings -> User Defaults General->URL(s) for UNICORE Site Server***
- Remove the existing URL (if any)
- Type **http://www.fz-juelich.de/unicore/unicoreSites_DEISA.xml** in this field

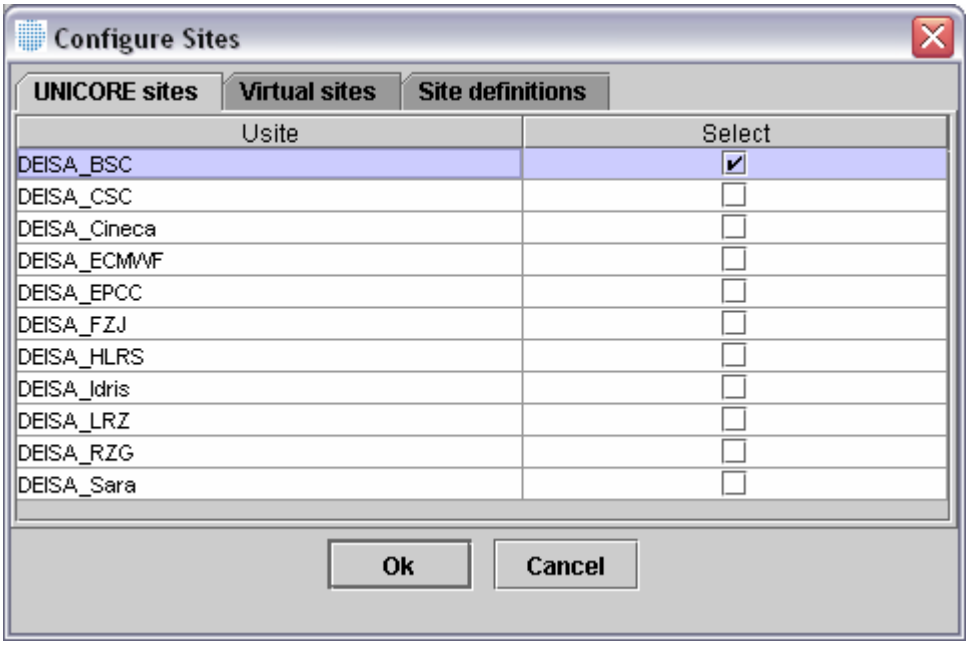


- confirm with ***OK***

2.4 Configure your Home site as UNICORE Site

All DEISA users are expected to use their Home site as UNICORE Site (e.g. DEISA_BSC) for job submission. Only if the Home Site is not available other UNICORE Sites might be used instead. Each UNICORE Site contains the same Virtual Sites or target supercomputer resources.
Therefore configure the UNICORE client just to show your Home site as UNICORE Site as follows:

- Select from the menu of the UNICORE client ***Settings->Configure sites***
- In the "Configure Sites editor" deselect all UNICORE Sites **expect from your Home site and DEISA_FZJ, and DEISA_CINECA** for backup
- For a user with Home site BSC the UNICORE sites configuration should look as follows:



- Confirm with ***OK***

2.5 Refresh the actual settings

To refresh the actual settings of the UNICORE client with the actual configuration, select ***Settings -> Clear Cache***

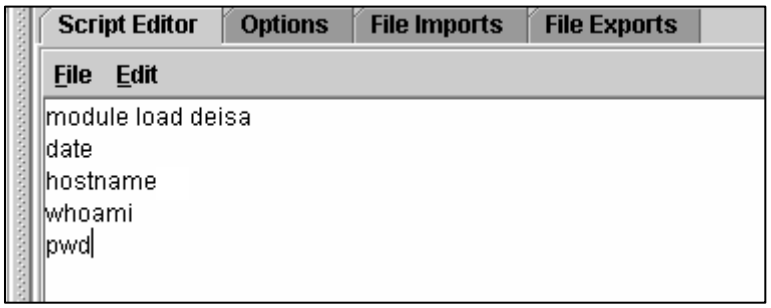
3 Use the Client

3.1 Run a simple script

- Select from the menu of the UNICORE client ***File -> New Job***.
- Select your DEISA Home Site (**UNICORE Site e.g. DEISA_CINECA**) and a **Virtual Site** (**e.g. FZJ JUMP**)

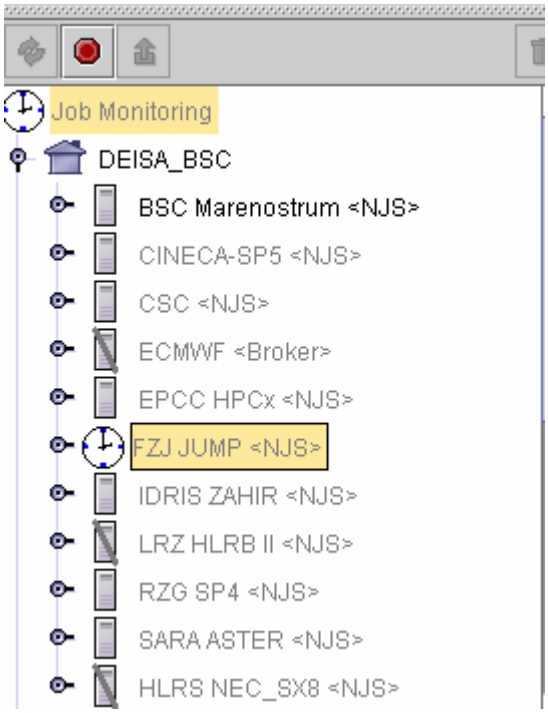
- **Important note:** BSC Marenostrum, ECMWF and HLRS_NEC_SX8 are **not** available for the training session use!

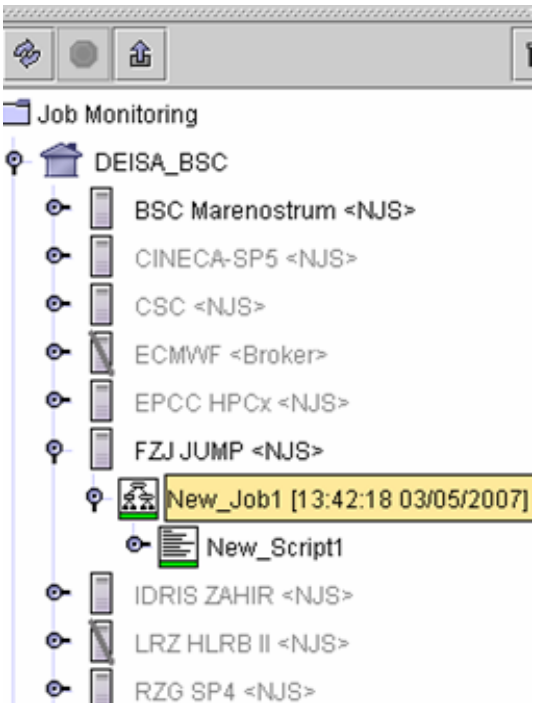
- Select ***Job Preparation -> Add Script***
- Type a simple bash script in the UNICORE script editor



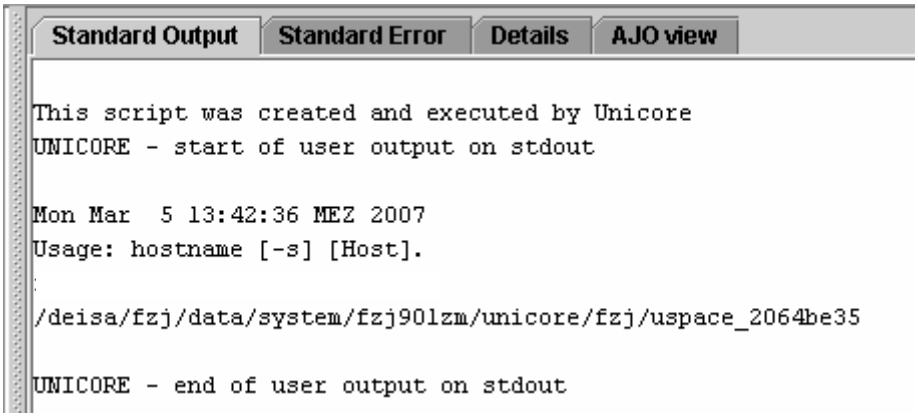
- Right-click on the job and choose ***Submit*** or click on
  The job will be submitted to the supercomputer of your Home site.

- Right-click on the target system the job has been submitted to in the lower left ***Job Monitoring*** window and choose ***Refresh*** or click on You should see your job now coloured in yellow (indicating that the job is queued), red (indicating that the job has been failed) or green (indicating that the job has run successfully).





- Right-click on the job in the lower left window and choose ***Fetch output*** or click on .
  In the right part of the screen you should now see the output of your script.

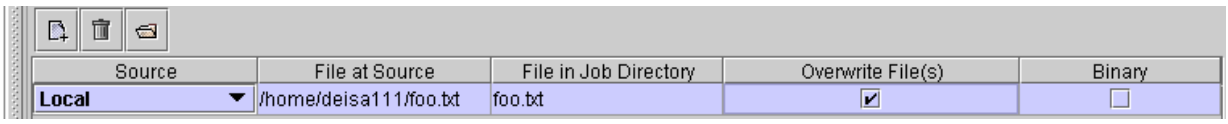


3.2 Hold, resume, and abort a job

- To create a job that runs a little longer, add to the script `sleep 20` and submit the job as before. Right-click on the target system in the **Job Monitoring** Window and choose ***Refresh***. You should see your second job coloured in yellow and blue, indicating that the job is being executed/run. Right-click on the job and choose ***Hold Job***. Then right-click on the job and choose ***Resume Job***. You can try ***Abort Job*** (after job is hold) as well.

3.3 File import

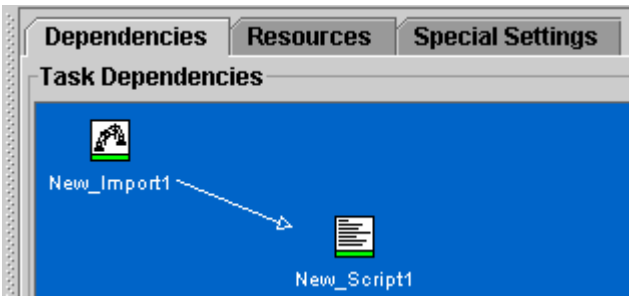
- Create an arbitrary text file **`foo.txt`**. Create a new job (***File -> New Job***) and select a site where it should run.
- Select ***Job Preparation-> Add Import***. In the right part of the screen, click on the leftmost icon to create a new file entry
  - In the first column, choose e.g. **Local**
  - Choose the file to import from the UNICORE file browser Or enter the complete path to your text file (e.g. /home/deisa111/foo.txt) into the second column.
  - In the third column enter the new name of the text file, use the same name **foo.txt**.

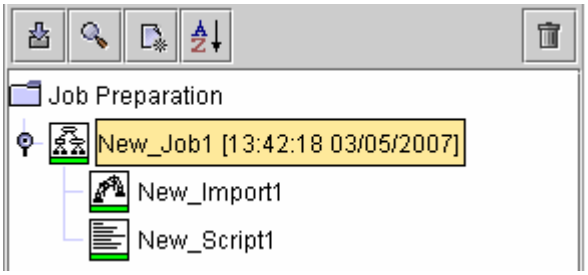


- To display the content of the imported file add a UNICORE script (***Job Preparation-> Add Script)*** to the job with the following content:

```
cat foo.txt
```

- As it is, the **script task** and the **import task** would run independent of each other in arbitrary order. But the script should be executed after the import has finished, so we have to create a **workflow**:
- Click on the job and look at the blue window on the right hand side.
- Click on the file import with the right mouse button (don't release the button yet) and drag an arrow to the script.





- Now submit the job and fetch the output as above.

3.4 If-then-else job

- Create a new file (foo2.txt) which is different from foo.txt
- Create a new job and select the Site where it should run. Add an ***import*** task as before (***Job Preparation-> Add File Import)***, but then create a task for both foo.txt and foo2.txt.

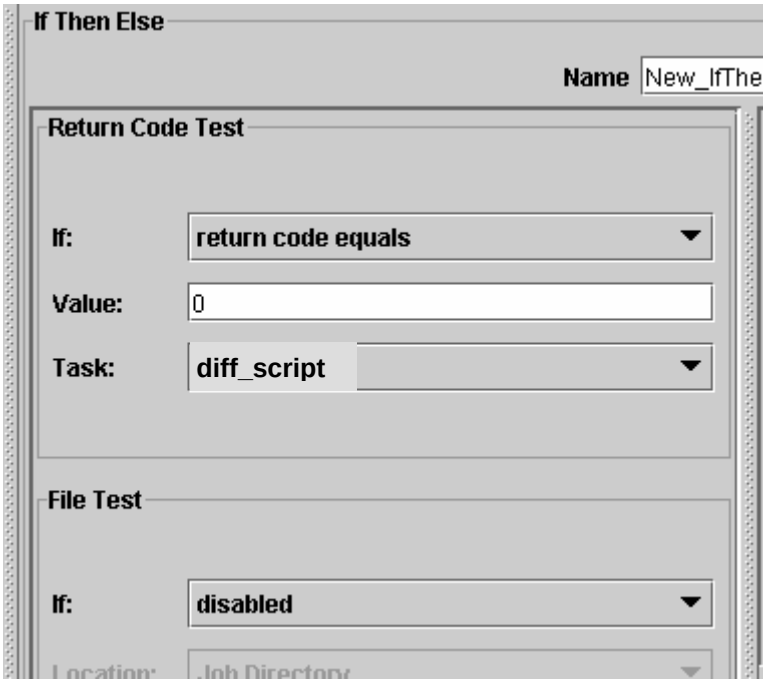
Source	File at Source	File in Job Directory	Overwrite File(s)	Binary
Local	/home/deisa111/foo.txt	foo.txt	☑	☐
Local	/home/deisa111/foo2.txt	foo2.txt	☑	☐

Add a UNICORE script (***Job Preparation-> Add Script)*** and name it `diff_script`

The script contains

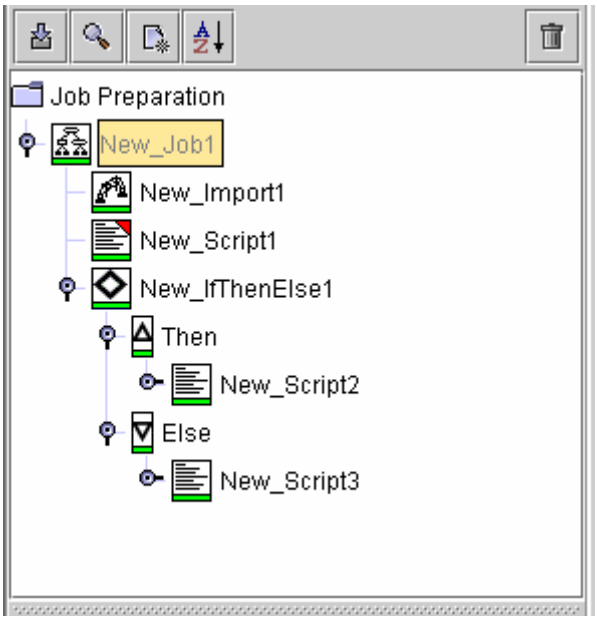
```
diff foo.txt foo2.txt > diff_output
```

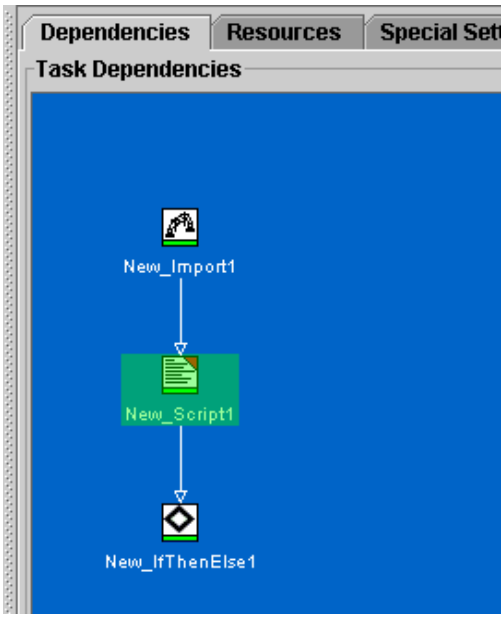
- To add an if-then-else task, select ***Job Preparation-> Add If Then Else***.
- In the right part of the screen you can now configure the **if-then-else task**.
- In the uppermost part labelled "**Return Code Test**" choose from the first drop down menu ***return code equals*** and leave the according value at zero.
- From the second drop down menu choose `diff_script`.



- The if-then-else task has two subjobs: Then and Else.
  - Select the Then-part and add a script ***Job Preparation-> Add Script***.
  - Enter: `echo "Files are equal!"` in the UNICORE script editor
  - Add a script to the Else-part as well with the following content:

    `echo "Files differ!"`
- Now go to the workflow edit window and drag an arrow from the Import Task to the diff script and from the diff script to the If-Then-Else-Task. Submit your job.
- If the files are different UNICORE's `diff_script task` will be red. That is because in this case the diff command returns "1" and UNICORE interprets the return values with different colours. It doesn't mean that there is a UNICORE error.





3.5 File export

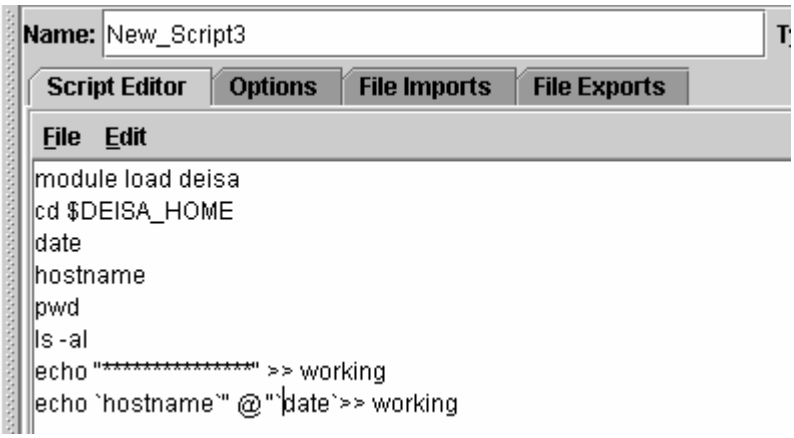
- Add an export task to the above job (***Job Preparation-> Add Export)***
- Create a new entry and enter `diff_output` in the first column. Choose **Local** from the drop down menu, browse the file system with and enter something like `diff_output as file name` in the third column. If you want to run the job multiple times, select "***Overwrite File(s)***" as well.
- In the workflow editor, drag an arrow from the **`if-then-else`** task to the **`file export`** task.
- Submit your job. You should now have a copy of `diff_output` with the output of your diff-script on your local workstation

3.6 DEISA GPFS and UNICORE

This example is to show the functionality and strength of DEISA GPFS within UNICORE.

Step 1:

- Create a new UNICORE workflow with ***File->New Job***
- Rename the job to "**DEISA_job**"
- Select your Home site as **UNICORE Site** (e.g. **DEISA_CINECA** for the CINECA users) and the **Virtual Site FZJ JUMP**
- Click on "**DEISA_job**"
- Add a sub job to the job (***Job Preparation->Add Sub Job***)
- Rename the first sub job from "**New_Sub_Job1**" to "**CINECA-Job**"
- Click on "IDRIS" and select the **UNICORE Site DEISA_CIINECA** and the **Virtual Site CINECA-SP5**. This means that this sub job will be executed on the CINECA supercomputer
- Click on "CINECA-Jobt" and select ***Job Preparation->Add Script***
- Rename the script from "**New_Sctript1**" to "**start_at_CINECA**"
- Enter the following script:



<u>Step 2:</u>

- Click on "DEISA_job"
- Add a 2nd subjob to "DEISA_job" (***Job Preparation->Add Sub Job***)
- Rename the 2nd subjob from "**New_Sub_Job2**" to "**FZJ**"
- Click on "FZJ" and select your Home site as **UNICORE Site** and the **Virtual Site FZJ JUMP**. This means that this 2nd subjob will be executed on the FZJ supercomputer
- Click on "FZJ" and select ***Job Preparation->Add Script***
- Rename the script to "**continue_at_FZJ**"
- Enter the above script

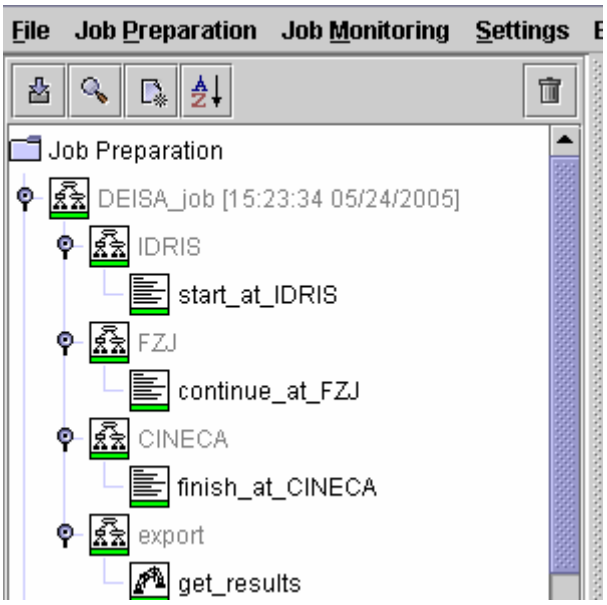
<u>Step 3:</u>

- Click on "DEISA_job"
- Add a third subjob to "DEISA_job" (***Job Preparation->Add Sub Job***)
- Rename the third subjob from "**New_Sub_Job3**" to "**CINECA**"
- Click on "CINECA" and select your Home site as **UNICORE Site** and the **Virtual Site CINECA-SP5**. This means that this third subjob will be executed on the CINECA supercomputer
- Click on "CINECA" and select Job ***Preparation->Add Script***
- Rename the script to "**finish_at_CINECA**"
- Enter the above script

Step 4:

- Click on “DEISA_job”
- Add a fourth subjob to “DEISA_job” (***Job Preparation->Add Sub Job***)
- Rename the forth subjob from “**New_Sub_Job4**” to “**export**”
- Click on “export” and select your Home site as **UNICORE Site** and the **Virtual Site RZG SP4**. This means that this fourth subjob will be executed on the RZG supercomputer
- Click on “export” and select ***Job Preparation->Add Export***
- Rename the new export task to “**get_results**”
    - Create a new export task by clicking on
    - Type in File in Job Directory: $DEISA_HOME/working
    - Choose as Destination: Local
    - Choose as File at Destination your local desktop directory

- Click on “DEISA_job” It should look as follows:



- Now submit the job and fetch the output as above.
- Have a look in the local copy of “working”. The data from all sites the job has been submitted to should be available.

4 Access the DCPE with UNICORE

- Create a new job with following script

```
module load deisa
cd $DEISA_HOME
pwd
ls
module list
module avail
```

- Create a new job with the following script:

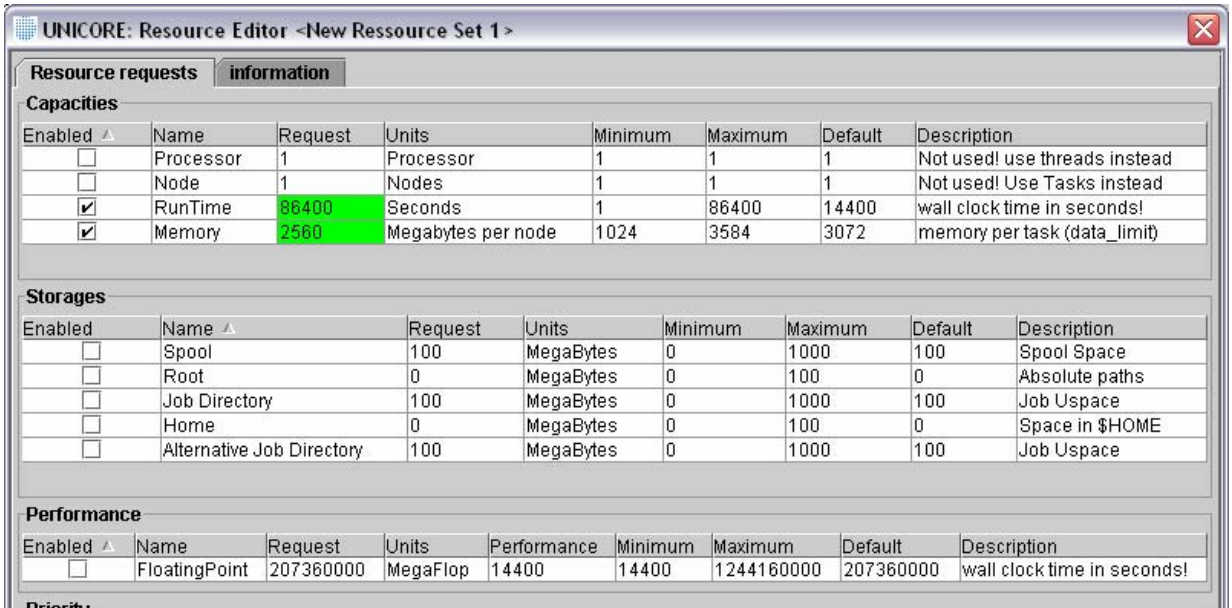
```
module load cpmd
module list
echo “CPMD-PATH:” $PATH
module unload cpmd
module list
echo “CPMD-PATH:” $PATH


module load nag
module list
module load fftw
module list
echo $DEISA_FFLAGS
echo $DEISA_LDFLAGS
module switch fftw fftw/3
module list
echo $DEISA_FFLAGS
echo $DEISA_LDFLAGS


module whatis fortran
module help fortran
module display fortran
```

5 Defining resources with UNICORE

- Mark the job and click on ***Resources*** in the upper right window
- Add a new resource set by clicking on
- Edit the resource set by clicking on
  - The ***Resource Editor*** appears - enable the values you want to change by clicking in the corresponding squares of the first row
  - you can change the values by double clicking the ***Request*** row
  - Your values have to be between the given ***Minimum*** and ***Maximum***
  - when you have finished editing the resource set click ***OK***
  - for each task in your job you can create an own resource set
  - to merge the resource set with the corresponding task select the lower right ***Tasks*** window and click on the task



Enabled	Name	Request	Units	Minimum	Maximum	Default	Description
☐	Processor	1	Processor	1	1	1	Not used! use threads instead
☐	Node	1	Nodes	1	1	1	Not used! Use Tasks instead
☑	RunTime	86400	Seconds	1	86400	14400	wall clock time in seconds!
☑	Memory	2560	Megabytes per node	1024	3584	3072	memory per task (data_limit)

Enabled	Name	Request	Units	Minimum	Maximum	Default	Description
☐	Spool	100	MegaBytes	0	1000	100	Spool Space
☐	Root	0	MegaBytes	0	100	0	Absolute paths
☐	Job Directory	100	MegaBytes	0	1000	100	Job Uspace
☐	Home	0	MegaBytes	0	100	0	Space in $HOME
☐	Alternative Job Directory	100	MegaBytes	0	1000	100	Job Uspace

Enabled	Name	Request	Units	Performance	Minimum	Maximum	Default	Description
☐	FloatingPoint	207360000	MegaFlop	14400	14400	1244160000	207360000	wall clock time in seconds!

6 Hints for further usage

6.1 What site resources are available?

You can have a look at the resources of a site by clicking on the magnifying glass next to the Vsites List. Next to the tab of the workflow editor you can find a tab called ”Resources” where you can specify the requirements of your job.