



## Running a computational application on the Grid

How To

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1







# Computational aspects of the code Very basic Porting and submission





Each run independent from the other

- Can be executed several times for different sets of input parameters (parameter study job)
- Executed via the classical command line interface
- Execute via a so called "Scientific Gateway"





## Compile

- -Right libraries (Blas, Lapack, libg2c)
- -Right compiler (ifort, g95)
- -Right option for compiler (-static, -Bstatic, -static-libcxa)

\$ Idd exec\_name

not a dynamic executable

### Executable: KB or MB





alex@ui:~\$ cat test.jdl

Type = "Job"; JobType = "Normal"; Executable = "code.sh"; StdOutput = "std.out"; StdError = "std.err"; InputSandbox = {"code.sh","code","input1.in","input2.in","input3.in"}; OutputSandbox = {"std.out","std.err","output1.out","output2.out"};



## **Prepare script file**



alex@ui:~\$ cat code.sh #!/bin/bash EXE=code date echo echo "Executing \$EXE" chmod 755 \$EXE ls -1 time ./\$EXE echo echo "List directory after Executing" ls -1 date exit 0







Create a valid VOMS proxy:

\$ glite-voms-proxy-init -voms compchem

Your identity: /C=IT/O=INFN/OU=Personal Certificate/L=University of Perugia Dept

Maths and CompSci/CN=Alessandro Costantini

Cannot find file or dir: /home/alex/.glite/vomses

Creating temporary proxy ...... Done

Contacting voms.cnaf.infn.it:15003 [/C=IT/O=INFN/OU=Host/L=CNAF/

CN=voms.cnaf.infn.it]

"compchem" Done

Creating proxy ...... Done Your proxy is valid until Tue Oct 9 00:56:49 2007





#### List-match of the resources:

\$ glite-wms-job-list-match -a test.jdl

Connecting to the service https://gliterb00.cnaf.infn.it:7443/glite\_wms\_wmproxy\_server

COMPUTING ELEMENT IDs LIST

\*CEId\*

- ce0.bordeaux.inra.fr:8443/cream-pbs-compchem
- ce0.m3pec.u-bordeaux1.fr:8443/cream-pbs-compchem
- ...







Submit a job to the WMProxy:

\$ glite-wms-job-submit -a -o idjob test.jdl

Connecting to the service https://gliterb00.cnaf.infn.it:7443/glite\_wms\_wmproxy\_server

==== glite-wms-job-submit Success ====

The job has been successfully submitted to the WMProxy

Your job identifier is:

https://gliterb00.cnaf.infn.it:9000/wJbzJtuHdkLXNbIxmLV0Uw

The job identifier has been saved in the following file:

/home/alex/idjob







#### Monitor the status of the job:

\$ glite-wms-job-status -i idjob

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**BOOKKEEPING INFORMATION:** 

Status info for the Job : https://gliterb00.cnaf.infn.it:9000/wJbzJtuHdkLXNbIxmLV0Uw

Current Status: Running

Status Reason: Job successfully submitted to Globus

Destination: ce.grid.unipg.it:2119/jobmanagerlcgpbsshort

Submitted: Mon Oct 8 13:03:57 2007 CEST

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Retrieve the output:

\$ glite-wms-job-output --dir \$HOME\_PATH/test -i idjob

JOB GET OUTPUT OUTCOME

Output sandbox files for the job:

https://gliterb00.cnaf.infn.it:9000/wJbzJtuHdkLXNbIxmLV0Uw

have been successfully retrieved and stored in the directory:

/home/alex/test





#### Submit multiple jobs:

\$ cd JDL-collection/
\$ ls -l
test1.jdl test2.jdl test3.jdl

\$ glite-wms-job-submit -a -o idjob\_multi --collection jdl

Connecting to the service https://gliterb00.cnaf.infn.it:7443/glite\_wms\_wmproxy\_server

The job has been successfully submitted to the WMProxy

Your job identifier is:

https://gliterb00.cnaf.infn.it:9000/wFvdNrgSewDGNcjktOZ1Yw

The job identifier has been saved in the following file:

/home/alex/idjob\_multi





## Hands on







#### Host: ui2.grid.unipg.it Username: studentxx (xx=01..20) Passwd: TCCM12

ssh <Username>@ui2.grid.unipg.it







#ls grid-example.tar

Untar #tar -xf <file>.tar





Type = "Job"; JobType = "Normal"; Executable = "test.sh"; StdOutput = "std.out"; StdError = "std.err"; InputSandbox = {"test.sh"}; OutputSandbox = {"std.out"};





Prepare bash script (test)

exit 0