

QCG Client - Cheat Sheet



QosCosGrid

www.qoscogrid.org
docs.plgrid.pl/qcg



Client Documentation

EN	www.qoscogrid.org/trac/qcg-broker/wiki/client_user_guide
PL	docs.plgrid.pl/qcg-client

UI (Submit host)

PCSS	<code>ssh plguser@qcg.man.poznan.pl</code>
WCSS	<code>ssh plguser@ui.plgrid.wcss.wroc.pl</code>
CYFRONET	<code>ssh plguser@zeus.cyfronet.pl</code>
ICM	<code>ssh plguser@ui.grid.icm.edu.pl</code>

Basic Commands

<code>qcg-sub <i>script.qcg</i></code>	Submit a job
<code>qcg-list</code>	List active jobs
<code>qcg-info <i>JOB_ID</i></code>	Get job information
<code>qcg-peek <i>JOB_ID</i></code>	Peek job output
<code>qcg-cancel <i>JOB_ID</i></code>	Delete job
<code>qcg-connect <i>JOB_ID</i></code>	Connect Interactively
<code>qcg-resub <i>JOB_ID</i></code>	Resubmit job

Basic script directives

<code>#QCG queue=plgrid</code>	Queue name
<code>#QCG host=Cluster</code>	Target resource name
<code>#QCG nodes=N:P</code>	Parallel topology (N -nodes, P - cores per node)
<code>#QCG procs=P</code>	Number of cores without particular topology
<code>#QCG walltime=PT8H</code>	Max job walltime
<code>#QCG memory=1024</code>	Total memory requirement (in megabytes)
<code>#QCG grant=MyGrant</code>	Grant/Allocation Id
<code>#QCG note=Info</code>	Short description of the job
<code>#QCG application=g09</code>	Request application
<code>#QCG argument=et.gjf</code>	Application argument
<code>#QCG module=namd</code>	Request module
<code>#QCG module = nwchem/6.0</code>	Request particular version of module

Clusters (#QCG host)

Reef (PSNC)	<code>reef.man.poznan.pl</code>
Inula (PSNC)	<code>inula.man.poznan.pl</code>
Nova (WCSS)	<code>nova.wcss.wroc.pl</code>
Zeus (Cyfronet)	<code>zeus.cyfronet.pl</code>
Galera+ (TASK)	<code>galera.task.gda.pl</code>
Hydra (ICM)	<code>hydra.icm.edu.pl</code>

Staging directives

<code>#QCG input=input.txt</code>	Standard input file name
<code>#QCG output=out.txt</code>	Standard output file name
<code>#QCG error=err.txt</code>	Standard error file name
<code>#QCG stage-in-file = input_file.txt</code>	Name of the file to be staged in
<code>#QCG stage-in-dir = inputs</code>	Name of the directory to be staged in
<code>#QCG stage-out-file = results.dat</code>	Name of the file to be staged out
<code>#QCG stage-out-dir = outputs</code>	Name of the directory to be staged out
<code>#QCG stage-out-dir = ./ -> results</code>	Stage out complete job working directory

Advance script directives

<code>#QCG monitor = monitor.sh</code>	Monitor script
<code>#QCG preprocess = mkdir</code>	Job prolog command
<code>#QCG postprocess = tar cvf results.tar *</code>	Job epilog command
<code>#QCG native=-r n</code>	Arguments passed directly to the batch system
<code>#QCG reservation=r</code>	Local Reservation Identifier

Example Job Script (I)

```
#!/bin/bash
#QCG queue=plgrid-testing
#QCG host=reef.man.poznan.pl
#QCG output=output
#QCG error=error
#QCG stage-in-dir=inputs -> inputs
#QCG stage-out-file=output.tgz -> output.tgz

/bin/tar -czf output.tgz inputs/*
```

Example Job Script (II)

```
#QCG queue=plgrid-long
#QCG name=etanal
#QCG note=etanal Gaussian
#QCG output=${JOB_ID}.output
#QCG error=${JOB_ID}.error
#QCG stage-in-file=etanal.gjf -> etanal.gjf
#QCG stage-out-file=results.tar -> ${JOB_ID}.tar
#QCG nodes=1:12
#QCG host=galera.task.gda.pl
#QCG walltime=P7D
#QCG notify=mailto:jon@example.com
#QCG memory=15360
#QCG application=g09
#QCG argument=etanal.gjf
#QCG postprocess=tar cvf results.tar *
```