PBS/Torque --Beowulf-- user manual

NU-Grid Beowulf is a cluster of 5 work station, dual core single processor and 4 GB of memory running OpenSuse 11.1, Torque PBS 2.3.6, native schedule running for now, and also have Maui 2.3.6 patch 21 installed.

Workstation :-

Each workstation acting as an exec machine and a node, so you can submit your job from any machine inside the beowulf to any other machine, using a single username called "nu", with UID 1000, and connection is via SSH using RSA keys.

The machines are :-

mahmoud 192.168.10.248 running pbs_mom "client"
fadi 192.168.10.249 running pbs_mom "client"
masterhead 192.168.10.250 running pbs_server, pbs_sched and pbs_mom "client"
hamish 192.168.10.251 running pbs_mom "client"
ahmed 192.168.10.252 running pbs_mom "client"

Please not we are not using DNS to resolve the IP address, but we have them static in /etc/hosts of each node.

PBS client commands :-

To check the current status for Queue/jobs :-
qstat -Q "summary for the queues."
qstat -q "summary for all the running jobs."
qstat -f "very detailed summary about the running jobs."

To check the current status for nodes
qnodes "summary for all nodes."
qnodes "mahmoud summary for the node mahmoud."

To submit a job and let torque manage which node will run your job just do :-
qsub my_job_or_mpi.sh

To submit a job to a node or some nodes " in case of MPI "
qsub -l nodes=mahmoud,masterhead,fadi my_job_or_mpi.sh

To request number of nodes :-
qsub -l nodes=3 my_job_or_mpi.sh
Submitting a serial job :-

Serial job is a job / task that depends on other jobs / tasks to be completed, for example :- we have job A ,B and C should be completed before job D starts, in this case we can add options to job D qsub command to check on A, B ,C jobs before it starts :-

```
qsub -W depend=afterok:A_JOBID,afterok:B_JOBID,afterok:C_JOBID JOB_D_.sh
```

in this case job D will not run before jobs A ,B and C return OK and completed.

**PBS important Variables to include in your job bash script :-**

Please not to add a PBS directive it should look like #PBS -N job_name , the "#" is not a comment in this case

```
#PBS -N job_name "To add job name"
#PBS -j oe "Mix the standard output and the error together"
#PBS -q batch "Specify the queue"
#PBS -m abe "Send email when job begins and when job terminated"
#PBS -M nu@masterhead "Email address to send the report, in this case it can be also nu@mahmoud"
```

**PBS standard variables you can use :-**

```
$PBS_O_HOST "Host that did run the qsub."
$PBS_O_QUEUE "The queue where the job running.
$PBS_JOBID "Job ID should be something like 234.masterhead"
$PBS_JOBNAME "Job name"
$PBS_O_WORKDIR "Working directory where the job got submitted usually it is /home/nu on the compute node where the PBS will write all the output of your job in case you didn't specify a place to write the output"
```

**How to run :-**

You will need to copy all your data to the compute node “where the job is getting executed“ including your program , data and any special files needed to get your task done, this can be done in stagein stage in the run_serial script or you can copy the files manual if you want to. Also note that the output is always in the compute node in /home/nu or in your specified output directory in your job, and you also can get the data back by stageout stage in the run_serial script of manual using scp / rsync method, no passwords required when you are using nu user.

**References:-**

http://www.nersc.gov/nusers/systems/franklin/running_jobs/
http://qcd.phys.cmu.edu/QCDcluster/pbs/run_serial "script"
http://masterhead/run_serial "my script for Mahmoud's task script – please note it need modifications"