Kohinoor queuing document

List of SGE Commands:

qsub : Submit a job to SGE

qstat : Determine the status of a job

qdel : Delete a job

qhost : Display Node information

Some useful commands

$qstat –f	--	**Specifies a "full" format display of information**
$qstat –j <JOBID>	--	**get the information about a specific job.**
$qstat –g c	--	**displays a cluster queue summary**
$qstat –u <Username>	--	**displays the jobs and queues being associated with the users**
$qstat –u “*”	--	**displays a running jobs of all users**
$qsub <script.sh>	--	**submit a job**
$qdel –f <JOBID>	--	**delete a specific job**
$qhost –j	--	**displays all the jobs running on the hosts along with queues**

Sample Model script explanation

#!/bin/bash	--	**Run the script under the bash shell**
#$ -N CPMD	--	**The name of the job**
#$ -cwd	--	**Execute the job from the current working directory**
#$ -S /bin/bash	--	**Specifying the shell for the job**
#$ -q short.q	--	**The name of cluster queues**
#$ -e err.$JOB_ID	--	**The Standard error of the Job**
#$ -o out.$JOB_ID	--	**The Standard output of the Job**
#$ -pe orte <core>	--	**The name of Parallel Environment with no of cores**

Sample script for Serial Jobs (Single core jobs)

```
$vi abinit_cpu_sge.sh
#!/bin/bash
#$ -N ABINIT
#$ -cwd
#$ -S /bin/bash
#$ -q serial.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
/export/data/apps/abinit/6.12.3/intel-ompi/bin/abinit
```

Job Submission

$qsub abinit_cpu_sge.sh

Note: For serial, the "#$ -pe" option is not required. If used job gets rejected by SGE.

Sample script for Parallel (MPI) Jobs (Multi cores jobs)

$vi abinit_cpu_sge.sh

```
#!/bin/bash
#$ -N ABINIT
#$ -cwd
#$ -S /bin/bash
#$ -q long.q/short.q/gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16

/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS
/export/data/apps/abinit/6.12.3/intel-ompi/bin/abinit
```

Job Submission

$qsub abinit_cpu_sge.sh

Queue list

1. **gpu.q** -- This queue is for gpu/cuda jobs, with no time limit.
2. **long.q** -- This queue is for long parallel jobs, with 15 days time limit.
3. **short.q** -- This queue is for short parallel jobs, with 5 days time limit.
4. **serial.q** -- This queue is for serial jobs (single core), with no time limit.

1. **ABINIT**
   Version=6.12.3
   PATH=/export/data/apps/abinit/6.12.3

   Job Script

   The following job script is adequate for running of ABINIT application

   $vi abinit_cpu_sge.sh

```
#!/bin/bash
#$ -N ABINIT
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
```

```
#$ -pe orte 16


/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS
/export/data/apps/abinit/6.12.3/intel-ompi/bin/abinit
```

Job Submission

```
$qsub abinit_cpu_sge.sh
```

2. **CPMD**
   Version=3.15.3
   PATH=/export/data/apps/cpmd/3.15.3

   Job Script

```
#!/bin/bash
#$ -N CPMD
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16


/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS
/export/data/apps/cpmd/3.15.3/intel-ompi/cpmd.x
```

   Job Submission

```
$qsub cpmd_cpu_sge.sh
```

3. **GROMACS**

   CPU

   Version=4.5.5
   PATH=/export/data/apps/gromacs/4.5.5

   Job Scripts

```
#!/bin/bash
#$ -N Gromacs
#$ -cwd
#$ -S /bin/bash
#$ -q serial.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID


/export/data/apps/gromacs/4.5.5/intel/bin/grompp_mpi
```

/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun -np $NSLOTS
/export/data/apps/gromacs/4.5.5/intel/bin/mdrun_mpi

Job Submission

$qsub gromacs_cpu_sge.sh

GPU

Version=
PATH=/export/data/apps/gromacs-gpu

Job scripts

#!/bin/bash
#$ -N GMX-GPU
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -l gpu=1

/export/data/apps/gromacs/4.5.5/intel-ompi/bin/grompp_mpi

#$ -v LD_LIBRARY_PATH=/export/data/apps/gromacs-gpu:/export/data/apps/gromacs-gpu/cuda23/lib64

#$ -v OPENMM_PLUGIN_DIR=/export/data/apps/gromacs-gpu

#$ -v OPENMM_PLATFORM=Cuda,CudaDevice=1

export LD_LIBRARY_PATH=/export/data/apps/gromacs-gpu:/export/data/apps/gromacs-gpu/cuda23/lib64

export OPENMM_PLUGIN_DIR=/export/data/apps/gromacs-gpu

export OPENMM_PLATFORM=Cuda,CudaDevice=0

/export/data/apps/gromacs-gpu/mdrun-openmm

Job Submission

$qsub gromacs_gpu_sge.sh

4. **HOOMD**

CPU

Version=0.11.0

PATH=

Job script

#!/bin/bash

```
#$ -N hoomd-cpu
#$ -cwd
#$ -S /bin/bash
#$ -q serial.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -v OMP_NUM_THREADS=1

export OMP_NUM_THREADS=1

/usr/bin/hoomd lj_liquid_bmark.hoomd
```

Job submission

```
$qsub hoomd_cpu_serial_sge.sh
```

GPU

Version=0.11.0

PATH=

Job script

```
#!/bin/bash
#$ -N hoomdgpu
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 1
#$ -l gpu=1
#$ -v OMP_NUM_THREADS=1

export OMP_NUM_THREADS=1

/usr/bin/hoomd lj_liquid_bmark.hoomd
```

Job submission

```
$qsub hoomd_gpu_sge.sh
```

5. **LAMMPS**

CPU

Version=
PATH= /export/data/apps/lammps-cpu

Job scripts

```
#!/bin/bash
#$ -N LAMMPS-CPU
#$ -cwd
```

```
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16


/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS /export/data/apps/lammps-cpu/30Aug12/bin/lmp_openmpi
```

Job Submission

```
$qsub lammps_cpu_sge.sh
```

GPU

Version=
PATH= /export/data/apps/lammps-cuda

Job scripts

```
#!/bin/bash
#$ -N Lammps-cuda
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -l gpu=1


#$ -v LD_LIBRARY_PATH=/export/data/apps/gromacs-gpu:/export/data/apps/gromacs-gpu/cuda23/lib64

export LD_LIBRARY_PATH=/export/data/apps/gromacs-gpu:/export/data/apps/gromacs-gpu/cuda23/lib64

/export/data/mpi/openmpi/1.6.1/intel/bin/mpirun -np 1  /export/data/apps/lammps-cuda/bin/lmp_cuda  -sf cuda -v g 1 -v x 16 -v y 16 -v z 16 -v t 100 < in.lj.cuda
```

Job Submission

```
$qsub lammps_gpu_sge.sh
```

6. NAMD

CPU

Version=2.9
PATH= /export/data/apps/NAMD_2.9_Linux-x86_64-ibverbs

Job script

```
#!/bin/bash
#$ -N Namd
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe mpi 32


nodefile=$TMPDIR/namd2.nodelist
echo group main > $nodefile
awk '{ for (i=0;i<$2;++i) {print "host",$1} }' $PE_HOSTFILE >> $nodefile


cat $nodefile
dir=/export/data/apps/NAMD_2.9_Linux-x86_64-ibverbs
$dir/charmrun ++remote-shell ssh ++nodelist $nodefile +p$NSLOTS $dir/namd2 apoa1.namd
```

Job Submission

```
$qsub namd_cpu_sge.sh
```

GPU

Version=2.9
PATH=/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA

Job scripts

```
#!/bin/bash
#$ -N Namd-CUDA
#$ -cwd
#$ -S /bin/bash
#$ -q gpu.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -l gpu=1
#$ -v LD_LIBRARY_PATH=/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA:
$LD_LIBRARY_PATH


export  LD_LIBRARY_PATH=/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA:
$LD_LIBRARY_PATH

/export/data/apps/NAMD_2.9_Linux-x86_64-multicore-CUDA/namd2 +idlepoll  apoa1.namd
```

Job Submission

```
$qsub namd_gpu_sge.sh
```

7. QUANTUM ESPRESSO

Version=5.0
PATH= /export/data/apps/q-espresso/5.0

Job scripts

```
#!/bin/bash
#$ -N QEspresso
#$ -cwd
#$ -S /bin/bash
#$ -q long.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16


/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS /export/data/apps/q-espresso/5.0/intel-ompi/bin/pw.x –in input file > file.out
```

Job Submission

```
$qsub qespresso_cpu_sge.sh
```

8. SIESTA

Version=3.1
PATH= /export/data/apps/siesta/3.1

Job script

```
#!/bin/bash
#$ -N SIESTA
#$ -cwd
#$ -S /bin/bash
#$ -q short.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe orte 16


/export/data/mpi/openmpi/1.4.5/intel/bin/mpirun  -np $NSLOTS  /export/data/apps/siesta/3.1/intel-ompi/bin/siesta
```

Job submission

```
$qsub siesta_cpu_sge.sh
```