Kohinoor2 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)

```
$vi serial_job.sh
#!/bin/bash
#$ -N SERIAL
#$ -cwd
#$ -S /bin/bash
#$ -q all.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
/home/$USER/matrix/matrix.x
```

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 parallel_job.sh

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

/hpcapps/mpi/openmpi/gcc/1.6.5/bin/mpirun  -np $NSLOTS  /home/$USER/matrix/matrix.x
```

Job Submission

$qsub parallel _job.sh

Queue list

1. **all.q** -- This the only default queue available.

APPLICATIONS

1. **NAMD**
   Version=2.9
   PATH=/hpcapps/NAMD_2.9_Linux-x86_64-ibverbs

   Job Script

```
#!/bin/bash
#$ -N Namd
#$ -cwd
#$ -S /bin/bash
#$ -q all.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=/hpcapps/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
```

2. **LAMMPS**
   Version=1FEB14
   PATH=/hpcapps/lammps/gcc_openmpi/1FEB14

Job scripts

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

module load openmpi-1.6.5-gcc
/hpcapps/mpi/openmpi/gcc/1.6.5/bin/mpirun  -np $NSLOTS
/hpcapps/lammps/gcc_openmpi/1FEB14/bin/lmp_openmpi_dump
```

Job Submission

```
$qsub lammps_cpu_sge.sh
```

3. **GROMACS**

CPU

Version=4.6.5
PATH=/hpcapps/gromacs/intel/4.6.5_MPI_OPENMP

Job Scripts

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

module load intel_cluster_2013
```

```
/hpcapps/gromacs/intel/4.6.5_MPI_OPENMP/bin/grompp_mpi
/hpcapps/intel/impi/4.1.1.036/intel64/bin/mpirun  -np $NSLOTS
/hpcapps/gromacs/intel/4.6.5_MPI_OPENMP/bin/mdrun_mpi
```

Job Submission

```
$qsub gromacs_cpu_sge.sh
```

4. **HOOMD**

Version=0.11.3

PATH=/hpcapps/hoomd/0.11.3

Job script

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

export OMP_NUM_THREADS=1

/hpcapps/hoomd/0.11.3/bin/hoomd lj_liquid_bmark.hoomd
```

Job submission

```
$qsub hoomd_cpu_serial_sge.sh
```

5. **CHARMM**

Version=C35B4

PATH=/hpcapps/c35b4

Job script

```
#!/bin/bash
#$ -N charmmjob
#$ -cwd
#$ -S /bin/bash
#$ -q all.q
#$ -e err.$JOB_ID
#$ -o out.$JOB_ID
#$ -pe mpi 16

module load openmpi-1.6.5-gcc
```

export CHARMM=/hpcapps/c35b4/exec/em64t/charm
export MPIRUN=/hpcapps/mpi/openmpi/gcc/1.6.5/bin/mpirun

```
$MPIRUN -v -machinefile $TMPDIR/machines -np $NSLOTS -nolocal $CHARMM < input.file
> output.file
```

COMPILERS

1. **OPENMPI – GCC**

Version = 1.6.5

PATH = /hpcapps/mpi/openmpi/gcc/1.6.5

2. **MVAPICH2**

Version = 2.0b

PATH = /hpcapps/mpi/mvapich2/gcc/2.0b

LIBRARIES

1. **ATLAS**

Path = /usr/lib64/atlas/libatlas.so

2. **LAPACK**

Path = /usr/lib64/atlas/liblapack.so

3. **BLAS**

Path = /usr/lib64/atlas/libblas.so