

TIFR Hyderabad

Kohinoor3 CLUSTER QUEUE DETAILS

QUEUE_NAME	TIMELIMIT	CORES	QUEUE_TYPE
compute	48.00.00	260	CPU
gpu	120.00.00	40	GPU/CUDA

SAMPLE SCRIPT

Sample script for compute queue

```
#!/bin/bash
#PBS -l nodes=1:ppn=20
#PBS -N <job name>
#PBS -q compute
module /required/modules
cd $PBS_O_WORKDIR
Command to be executed (gmx mdrun -s new.tpr -g md.log -nb gpu -v >& log)
```

Sample script for gpu queue

```
#!/bin/bash
#PBS -l nodes=1:ppn=20
#PBS -N <job name>
#PBS -q gpu
module load /required/modules
cd $PBS_O_WORKDIR
Command to be executed (gmx mdrun -s new.tpr -g md.log -nb gpu -v >& log)
```

Note: Please use the following syntax for generating nodes while running MPI jobs

```
mpirun -machinefile $PBS_NODEFILE -np <no of procs> <executable>
```
