

PBS Job Submission

General Rules for PBS Job Submission

- Submit jobs using the `qsub` command.
- Monitor jobs using `qstat`, `tracejob`, and `qdel`.
- Ensure you use correct resource requests (nodes, ppn, walltime).
- Store input/output files on the Lustre filesystem, not on \$HOME.
- Use `\$TMPDIR` for temporary scratch space on compute nodes.
- Clean up after job completion using `trap` or manual commands.

PBS Limits and Errors

- Max walltime may be limited by queue (default may be 24 hrs).
- `qsub: Job exceeds queue resource limits` means you requested more than allowed.
- `qstat -f <jobid>` gives detailed job information.

ABAQUS PBS Job Script

SERIAL JOB SCRIPT

Sample job file for running Abaqus serial job for single CPU:

File Name : abaqus.cmd

#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=02:00:00

#PBS -l select=1:ncpus=1

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
abaqus job=test1 user=test.f inter >>xx
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub abaqus.cmd

SINGLE NODE JOB SCRIPT

Sample job file for running Abaqus job for 8 CPU:

File Name : abaqus.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=8
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
abaqus job=test1 user=test.f cpus=8 inter >>xx
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub abaqus.cmd

MULTI NODE JOB SCRIPT

Sample job file for running Abaqus job for 40 CPU:

File Name : abaqus.cmd

#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=48:00:00

#PBS -l select=2:ncpus=20

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

cd \$tempdir

cp -R \$PBS_O_WORKDIR/.*

abaqus job=test1 user=test.f cpus=40 inter >>xx

mv ../job\$tpdir \$PBS_O_WORKDIR/.

In the command prompt, type the command, qsub abaqus.cmd

ANSYS PBS Job Script

SERIAL JOB SCRIPT

Sample job file for running Ansys serial job for single CPU:

File Name : cfx.cmd

#!/bin/bash

```
#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=02:00:00

#PBS -l select=1:ncpus=1

tpdir=`echo $PBS_JOBID | cut -f 1 -d .`

tempdir=$HOME/scratch/job$tpdir

mkdir -p $tempdir

cd $tempdir

cp -R $PBS_O_WORKDIR/* .

cfx5solve -batch -def test.def -name test.out

mv ../job$tpdir $PBS_O_WORKDIR/.

In the command prompt, type the command, qsub cfx.cmd
```

Sample job file for running a fluent serial job :

File Name : fluent.cmd

```
#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=02:00:00

#PBS -l select=1:ncpus=1

tpdir=`echo $PBS_JOBID | cut -f 1 -d .`

tempdir=$HOME/scratch/job$tpdir

mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
fluent 3d -g -psmpi -i test.jou
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub fluent.cmd

SINGLE NODE JOB SCRIPT

Sample job file for running fluent in parallel mode within a node :

File Name : fluentpl.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=24:00:00
```

```
#PBS -l select=1:ncpus=40
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
fluent 3d -g -mpi=intel -t40 -cnf=$PBS_NODEFILE -i input.jou > fluent.out
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub fluentpl.cmd

MULTINODE JOB SCRIPT

Sample job file for running fluent in parallel mode in multiple nodes :

File Name : fluentpl.cmd

#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=48:00:00

#PBS -l select=2:ncpus=40

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

cd \$tempdir

cp -R \$PBS_O_WORKDIR/.*

fluent 3d -g -mpi=intel -t80 -cnf=\$PBS_NODEFILE -i input.jou > fluent.out

mv ../job\$tpdir \$PBS_O_WORKDIR/.

In the command prompt, type the command, qsub fluentpl.cmd

Sample job file for running Ansys in parallel mode :

File Name : cfx.cmd

#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

```

#PBS -l walltime=96:00:00

#PBS -l select=1:ncpus=8:mpiprocs=8

tpdir=`echo $PBS_JOBID | cut -f 1 -d .`

tempdir=$HOME/scratch/job$tpdir

mkdir -p $tempdir

cd $tempdir

cp -R $PBS_O_WORKDIR/* .

nodes=`cat ${PBS_NODEFILE}`

nodes=`echo $nodes | sed -e 's/ /,/g'`

cfx5solve -double -def "FC0.25.def" -par-dist $nodes -start-method "Intel MPI
Local Parallel"

mv ../job$tpdir $PBS_O_WORKDIR/.

```

In the command prompt, type the command, qsub cfx.cmd

NOTE : ncpus and mpiprocs should be same

COMSOL PBS Job Script

Note to create inputfile to Running COMSOL on Clusters COMSOL cluster jobs can be launched from the COMSOL Desktop and the command line. To run COMSOL on a cluster, the feature must be enabled by clicking the Show button and selecting Advanced Study Options. Then in the Model Builder, right-click a Study node and select Cluster Computing to create cluster jobs. In Job configuration use default settings

SERIAL JOB SCRIPT

Sample job file for running Comsol serial job for single CPU:

File Name : comsol.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
comsol batch -inputfile infile.mph -outputfile out.mph -batchlog out.log
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub comsol.cmd

SINGLE JOB SCRIPT

Sample job file for running comsol in parallel mode within a node :

File Name : comsolpl.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```


#PBS -e errorfile.err

#PBS -l walltime=24:00:00

#PBS -l select=1:ncpus=40

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

cd \$tempdir

cp -R \$PBS_O_WORKDIR/.*

comsol batch -inputfile infile.mph -outputfile out.mph -batchlog out.log

mv ../job\$tpdir \$PBS_O_WORKDIR/.

In the command prompt, type the command, qsub comsolpl.cmd

MULTINODE JOB SCRIPT

Sample job file for running comsol in parallel mode in multiple nodes :

File Name : comsolpl.cmd

#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=48:00:00

#PBS -l select=2:ncpus=20

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
comsol batch -inputfile infile.mph -outputfile out.mph -batchlog out.log
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, *qsub comsolpl.cmd*

Gaussian09 PBS Job Script

SERIAL JOB SCRIPT(For running in local scratch folder)

Sample job file for running Gaussian09 for single CPU in local scratch folder:

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=/lscratch/$PBS_O_LOGNAME/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
module load gaussian09
```

```
g09 inputfile
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

SERIAL JOB SCRIPT(For running in local scratch folder)

Sample job file for running Gaussian09 Linda within single node in local scratch folder:

The Gaussian input file must have below lines to run Linda job,

```
%nproclinda=1  Note: must match select in the job submission script
```

```
%nprocshared=4  Note: must match ncpus in the job submission script
```

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=4
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=/lscratch/$PBS_O_LOGNAME/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
module load gaussian09
```

```
g09 inputfile
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

SERIAL JOB SCRIPT(For running in LFS scratch folder)

Sample job file for running a Gaussian09 Linda within single node with LFS scratch:

```
#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=02:00:00

#PBS -l select=1:ncpus=4

tpdir=`echo $PBS_JOBID | cut -f 1 -d .`

tempdir=$HOME/scratch/job$tpdir

mkdir -p $tempdir

cd $tempdir

cp -R $PBS_O_WORKDIR/*.

module load gaussian09

g09 inputfile

mv ../job$tpdir $PBS_O_WORKDIR/.
```

GROMACS PBS Job Script

SERIAL JOB SCRIPT

Sample job file for running Gromacs serial job for single CPU:

File Name : gromacs.cmd

```
#!/bin/bash

#PBS -l walltime=02:00:00

#PBS -e errorfile.err
```

```
#PBS -o logfile.log

#PBS -l select=1:ncpus=1

tpdir=`echo $PBS_JOBID | cut -f 1 -d .`

tempdir=$HOME/scratch/job$tpdir

mkdir -p $tempdir

cd $tempdir

cp -R $PBS_O_WORKDIR/*.

mdrun -s test.tpr >> output

mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub gromacs.cmd

SINGLE NODE JOB SCRIPT

Sample job file for running gromacs in parallel mode within a node:

File Name : gromacs.cmd

```
#!/bin/bash

#PBS -l walltime=24:00:00

#PBS -e errorfile.err

#PBS -o logfile.log

#PBS -l select=1:ncpus=40

tpdir=`echo $PBS_JOBID | cut -f 1 -d .`

tempdir=$HOME/scratch/job$tpdir

mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
mpirun -np 40 -hostfile `which mdrun_mpi` -s -v -deffnm test.tpr
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub gromacs.cmd

MULTINODE JOB SCRIPT

Sample job file for running gromacs in parallel mode in multiple nodes :

Sample job file for running a gromacs parallel job multiple nodes :

File Name : gromacs.cmd

```
#!/bin/bash
```

```
#PBS -e errorfile.err
```

```
#PBS -o logfile.log
```

```
#PBS -l walltime=24:00:00
```

```
#PBS -l select=2:ncpus=40
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
echo $PBS_NODEFILE
```

```
module load intel2020 gromacs2019.6
```

```
mpiexec.hydra -np 80 -genv OMP_NUM_THREADS=1 -genv I_MPI_PIN=1 -genv  
I_MPI_FABRICS=shm:ofi -machinefile ${PBS_NODEFILE} --ppn 40  
/lfs/sware/gromacs2019.6/bin/gmx mdrun -s test.tpr -deffnm test -rdd 1.4 -v  
  
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub gromacs.cmd

Mathematica PBS Job Script

File Name : math.cmd

SERIAL JOB SCRIPT

Sample job file for running Mathematica serial job for single CPU:

File Name : cfx.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
/lfs/sware/mathematica11.2/Executables/math -noprompt -script test.m >  
output.txt
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub math.cmd

MATLAB PBS Job Script

SERIAL JOB SCRIPT

Sample job file for running Matlab serial job for single CPU:

File Name : matlab.cmd

```
#!/bin/bash
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -e errorfile.err
```

```
#PBS -o logfile.log
```

```
#PBS -l select=1:ncpus=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
matlab < mathsample.m
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub matlab.cmd

SINGLE NODE JOB SCRIPT

Sample job file for running Matlab job in single node:

File Name : matlab.cmd

#!/bin/bash

#PBS -l walltime=24:00:00

#PBS -e errorfile.err

#PBS -o logfile.log

#PBS -l select=1:ncpus=40

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

cd \$tempdir

cp -R \$PBS_O_WORKDIR/.*

matlab < mathsample.m

mv ../job\$tpdir \$PBS_O_WORKDIR/.

In the command prompt, type the command, qsub matlab.cmd

NAMD PBS Job Script

SERIAL JOB SCRIPT

Sample job file for running NAMD serial job for single CPU:

File Name : namd.cmd

#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=24:00:00

#PBS -l select=1:ncpus=1

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

cd \$tempdir

cp -R \$PBS_O_WORKDIR/.*

export

LD_LIBRARY_PATH=/lfs/sware/namd/tcl8.5.5/unix/lib:\$LD_LIBRARY_PATH

*charmrun /lfs/sware/namd/NAMD_2.6_Linux-amd64/namd2 inputfile >
outfile*

mv ../job\$tpdir \$PBS_O_WORKDIR/.

In the command prompt, type the command, qsub namd.cmd

SINGLE NODE JOB SCRIPT

Sample job file for running NAMD job for single node:

File Name : namd.cmd

#!/bin/bash

#PBS -l walltime=24:00:00

#PBS -e errorfile.err

#PBS -o logfile.log

#PBS -l select=1:ncpus=40

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
NODELIST=/tmp/charmrn-nodelist.$PBS_JOBID
```

```
cat $PBS_NODEFILE | sed -e 's/^/host /' > $NODELIST
```

```
export CONV_RSH=ssh
```

```
charmrn +p40 ++remote-shell ssh ++nodelist $NODELIST  
/lfs/sware/namd/NAMD_2.9b1_Linux-x86_64-ibverbs/namd2 inputfile >  
output file
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub namd.cmd

MULTI NODE JOB SCRIPT

Sample job file for running NAMD job for multiple nodes:

File Name : namd.cmd

```
#!/bin/bash
```

```
#PBS -l walltime=48:00:00
```

```
#PBS -e errorfile.err
```

```
#PBS -o logfile.log
```

```
#PBS -l select=2:ncpus=40
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
NODELIST=/tmp/charmrun-nodelist.$PBS_JOBID
```

```
cat $PBS_NODEFILE | sed -e 's/^/host /' > $NODELIST
```

```
export CONV_RSH=ssh
```

```
charmrun +p80 ++remote-shell ssh ++nodelist $NODELIST  
/lfs/sware/namd/NAMD_2.9b1_Linux-x86_64-ibverbs/namd2 inputfile >  
output file
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub namd.cmd

OPENMP Job Script

SINGLE NODE JOB SCRIPT

Sample job file for running openmp job :

File Name : openmp.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=24:00:00
```

```
#PBS -l select=1:ncpus=20
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
export OMP_NUM_THREADS=20
```

```
./a.out
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub openmp.cmd

OPENFOAM

SERIAL JOB SCRIPT

Sample job file for openfoam for running in serial :

File Name : openfoam.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=24:00:00
```

```
#PBS -l select=1:ncpus=1:mpiprocs=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
simpleFoam
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub openfoam.cmd

C and FORTRAN PBS Job Script

SERIAL JOB SCRIPT

Sample job file for running C Code in serial job in single CPU:

File Name : csample.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
gcc inputfile.c
```

```
./a.out >output.txt
```

```
rm a.out
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub csample.cmd

Sample job file for running Fortran Code in serial job in single CPU:

File Name : fsample.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.f
```

```
gfortran inputfile.f
```

```
./a.out >output.txt
```

```
rm a.out
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub fsample.cmd

PARALLEL JOB SCRIPT

Sample job file for running C Code in multiple nodes:

File Name : csample1.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=24:00:00
```

```
#PBS -l select=2:ncpus=20
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/* .
```

```
mpicc inputfile.c
```

```
mpiexec.hydra -np 40 -genv OMP_NUM_THREADS=1 -genv I_MPI_PIN=1 -genv  
I_MPI_FABRICS=shm:ofi -hostfile $PBS_NODEFILE ./a.out >output.txt
```

```
rm a.out
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub csample1.cmd

Sample job file for running Fortran Code in multiple nodes:

File Name : fsample1.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=24:00:00
```

```
#PBS -l select=2:ncpus=20
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d `
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/* .
```

```
mpif90 inputfile.f
```

```
mpiexec.hydra -np 40 -genv OMP_NUM_THREADS=1 -genv I_MPI_PIN=1 -genv  
I_MPI_FABRICS=shm:ofi -hostfile $PBS_NODEFILE ./a.out >output.txt
```

```
rm a.out
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub fsample1.cmd

Open Source Software Job Scripts

SERIAL JOB SCRIPT

Sample job file for running any open source software in serial job in single CPU:

File Name : sample.cmd

```
#!/bin/bash
```

```
#PBS -o logfile.log
```

```
#PBS -e errorfile.err
```

```
#PBS -l walltime=02:00:00
```

```
#PBS -l select=1:ncpus=1
```

```
tpdir=`echo $PBS_JOBID | cut -f 1 -d .`
```

```
tempdir=$HOME/scratch/job$tpdir
```

```
mkdir -p $tempdir
```

```
cd $tempdir
```

```
cp -R $PBS_O_WORKDIR/*.
```

```
absolute_path_of_executable inputfile
```

```
mv ../job$tpdir $PBS_O_WORKDIR/.
```

In the command prompt, type the command, qsub sample.cmd

PARALLEL JOB SCRIPT

Sample job file for running any opensource software in multiple nodes:

File Name : sample1.cmd

#!/bin/bash

#PBS -o logfile.log

#PBS -e errorfile.err

#PBS -l walltime=24:00:00

#PBS -l select=2:ncpus=20

tpdir=`echo \$PBS\_JOBID | cut -f 1 -d .`

tempdir=\$HOME/scratch/job\$tpdir

mkdir -p \$tempdir

cd \$tempdir

cp -R \$PBS_O_WORKDIR/* .

**mpiexec.hydra -np 40 -genv OMP_NUM_THREADS=1 -genv I_MPI_PIN=1 -genv
I_MPI_FABRICS=shm:ofi -hostfile \$PBS_NODEFILE
absolute_path_of_executable inputfile**

mv ../job\$tpdir \$PBS_O_WORKDIR/.

In the command prompt, type the command, qsub sample1.cmd
