

```

#!/bin/bash

#PBS -l nodes=X:ppn=XX
#PBS -q vlifesci
#PBS -A MULTIDRUG
#PBS -N XXX

#####
# compiles envs #
#####

cd $PBS_O_WORKDIR
source
/opt/intel/compilers_and_libraries_2016.2.181/linux/bin/compilervars.sh
intel64
source
/opt/intel/compilers_and_libraries_2016.2.181/linux/mkl/bin/mklvars.sh
intel64
source
/opt/intel/compilers_and_libraries_2016.2.181/linux/mpi/intel64/bin/mpiva
rs.sh release_mt

#####
# gromacs executables #
#####

GMX="/path-to-gromacs-version/gromacs/bin/gmx_mpi"
MDRUN="/path-to-gromacs-version/bin/mdrun-5.1.2"

#####
# input files #
#####

TPR=molecule_min_env

DEFFNM=molecule_min_env

##### preproc #####
$GMX grompp -f $MDP -c $CRD -p $TOP -n $NDX -o $TPR
#####

#####
# mdrun arguments #
#####
ARGS="-v -deffnm $DEFFNM -s $TPR "
#####

#####
# MPIEXEC stuff #
#####

nodefile=tmpnodefiles.$PBS_JOBID

cat $PBS_NODEFILE | sort -u > $nodefile

```

```
nodes=$(wc -l < $nodefile)
```

```
mpiexec.hydra -f $nodefile -ppn 2 -genv OMP_NUM_THREADS 8 $MDRUN $ARGS
```