Table of Contents
1. Introduction .................................................................................................................. 3
2. Setting up the environment .......................................................................................... 3
   For regular and community cluster users on Hrothgar .................................................. 4
3. Job Submission ........................................................................................................... 6
   3.1. Script for job submission for normal queue ......................................................... 6
   3.2. Job submission ...................................................................................................... 6
   3.3. Gromacs Restart Job ............................................................................................ 7
*Community Cluster ....................................................................................................... 8
1. Introduction

GROMACS is a versatile package to perform molecular dynamics. It is primarily designed for biochemical molecules like proteins and lipids that have a lot of complicated bonded interactions, but since GROMACS is extremely fast at calculating the nonbonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems, e.g. polymers.

2. Setting up the environment

Hrothgar is equipped with SoftEnv to set up the environment with minimum work by users. The use of SoftEnv is not required but highly recommended by HPCC staff.

**Step 1: setting up user environment**

If the user environment is already set up, please skip this step.

At the first use, the user should copy two sample dot-files: dot-bashrc is the start up script which evokes SoftEnv; dot-soft contains a list of software whose specific environment variables will be set up for the user.

```bash
$ cp /lustre/work/apps/examples/dot-bashrc .bashrc
$ cp /lustre/work/apps/examples/dot-soft .soft
$ ln -s .bashrc .bash_profile
```

Log out and log in again.
Step 2: setting up Gromacs environment

For regular and community cluster users on Hrothgar

The latest version of Gromacs installed on Hrothgar is Gromacs-4.5.5 with optimization. The parallel support for Gromacs is on top of OpenMPI, so OpenMPI is the only version of MPI that can be used in order to run Gromacs in parallel. Use the following commands to add Gromacs and OpenMPI in SoftEnv:

```
$ soft add +gromacs
$ soft add +openmpi
```
If other version of MPI (e.g. MPICH) was set up, use the following command to delete it from SoftEnv:

$ soft delete +mvapich2-ib

The above procedure sets up the environment variables for the current session. It expires when the user logs out. To make path changes permanent and consisted across all nodes, execute the following commands:

$ echo +gromacs >> $HOME/.soft
$ echo +openmpi >> $HOME/.soft

CAUTION: note ">>" in the above commands, which appends to existing .soft in your home directory. If ">" is used instead of ">>", .soft file will be overwritten.
3. Job Submission

3.1. Script for job submission for normal queue

The following is a script file to submit a Gromacs job to 48 cores to the normal queue. It assumes that the input files are in the same directory with the script. The sample script and input files are available at the directory /lustre/work/apps/examples/gromacs. Use the command to copy the directory:

```
$ cp –r /lustre/work/apps/examples/gromacs gromacs
```

```bash
#!/bin/bash
#$ -cwd
#$ -S /bin/bash
#$ -V
#$ -N gromacs
#$ -j y
#$ -o $JOB_NAME.o$JOB_ID
#$ -q normal
#$ -pe fill 48
#$ -P hrothgar

unset SGE_ROOT
TOP=polymer_mon100cro50_third
MDP=mdrun_npt
GRO=mdrun
TPR=mdout
EDR=ener
grompp -f $MDP.mdp -c $GRO.gro -p $TOP.top -o $TPR.tpr
run="`which mpirun` -np $NSLOTS -machinefile $SGE_CWD_PATH/machinefile.$JOB_ID
`which mdrun` -nt 1 -s $TPR.trr -o $TPR.trr -x $TPR.xtc -c $GRO.gro -e $EDR.edr -g
md.$JOB_ID"
echo run=$run
$run
```

3.2. Job submission

$ qsub gromacs.sh - To submit your gromacs job to Hrothgar

$ qstat – To check the status of the job
3.3. Gromacs Restart Job

Since normal queue only allows a job to run for 48 hours, if your job's running for more than 48 hours, use following script to auto restart your jobs.

$ cp /lustre/work/apps/examples/gromacs/gromacs-restart.sh

Make appropriate changes in the submission script to reflect your input files.

$ qsub gromacs-restart.sh

After 48 hours status of job be changed from r to Rr.
Community Cluster
Community cluster refers to some special nodes on Hrothgar. They are purchased by some professors, and only their group can use these nodes. For example, queue kharecc is open to Dr. Khare’s group, only his group members can submit jobs to this queue. There is no time limitation for running jobs on community cluster. Consult your own research group for community cluster using.