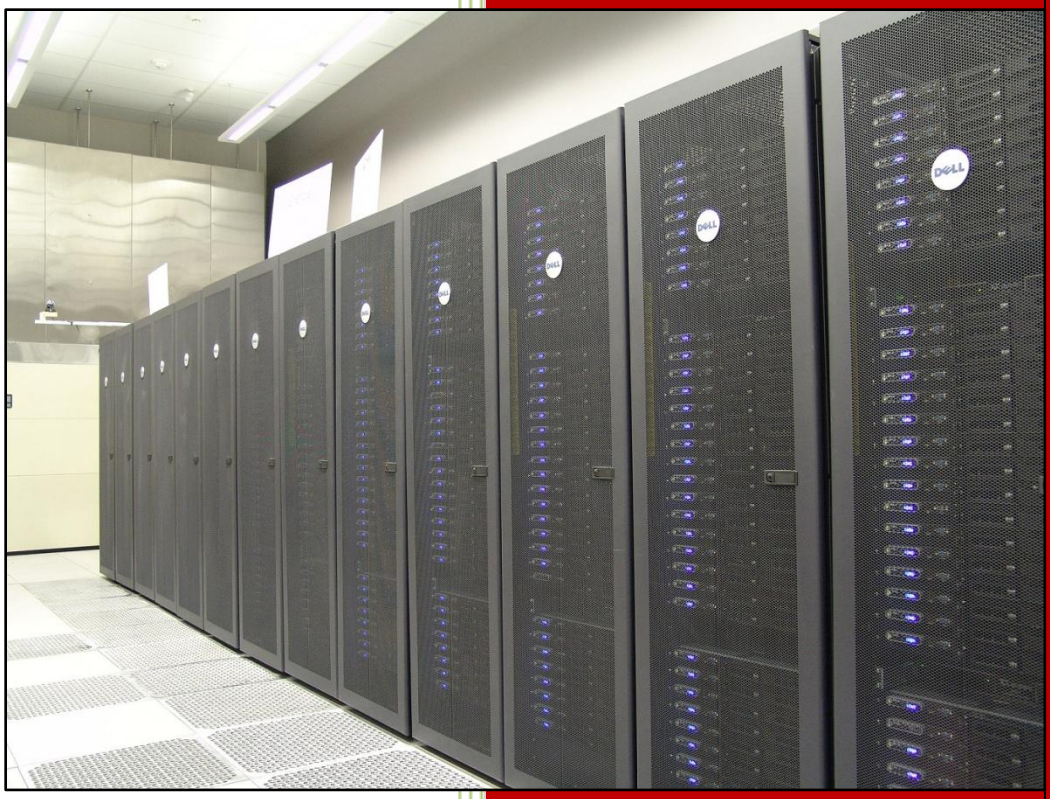
HPCC - Hrothgar

Getting Started User Guide – NAMD



High Performance Computing Center
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Table of Contents

User Guide

1. Introduction

NAMD, recipient of a 2002 Gordon Bell Award, is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects, NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters, using gigabit ethernet. NAMD uses the popular molecular graphics program VMD for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR.

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.

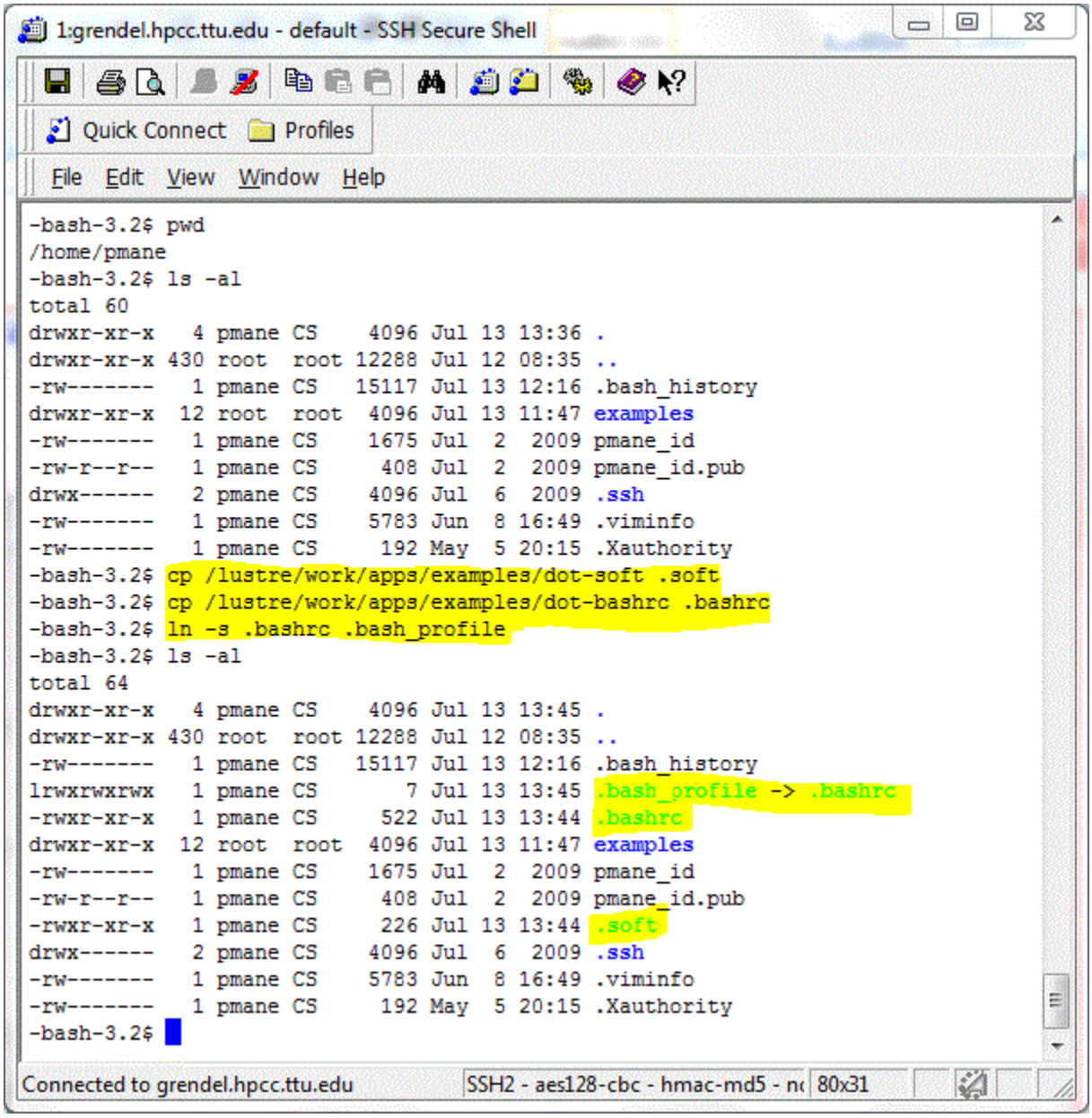
Step 1: setting up user environment

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.


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

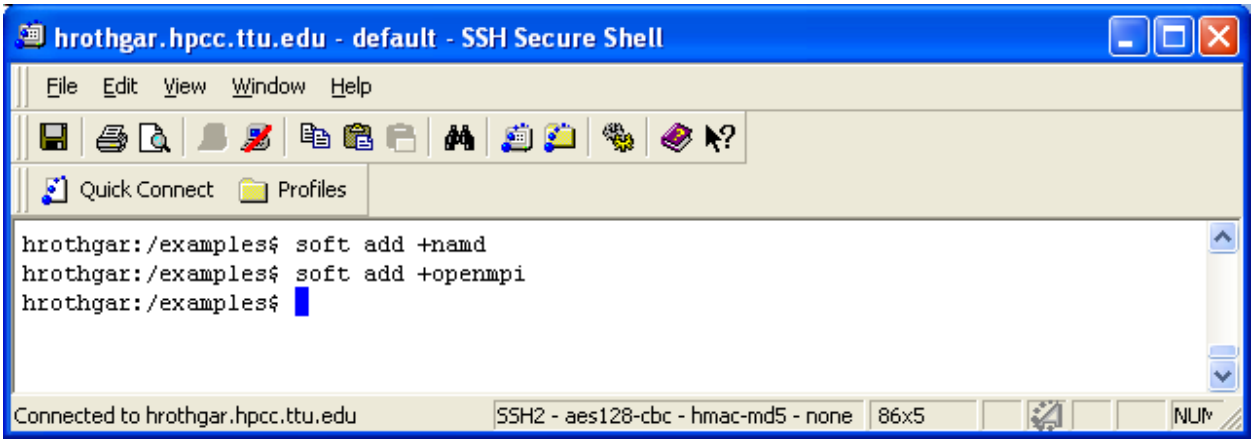
Log out and log in again.



Step 2: setting up Gromacs environment

The latest version of NAMD installed on Hrothgar is NAMD 2.7 Parallel support for NAMD 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 +namd
$ 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 command:

```
$ echo +namd >> $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

The sample script and input files are available at the directory */lustre/work/apps/examples/namd*. Use the command to copy the directory:

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

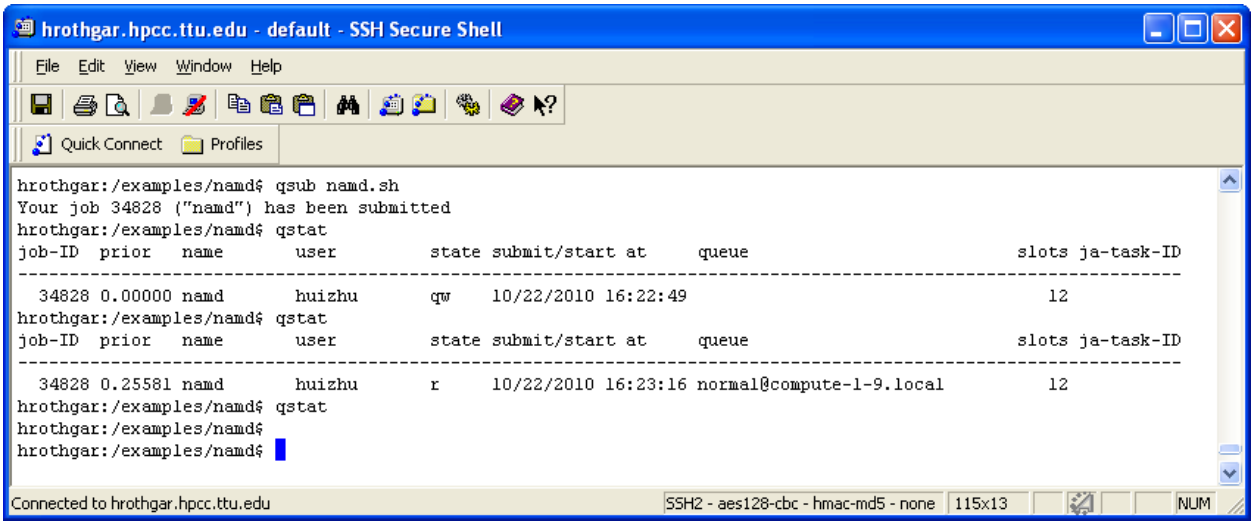
In the directory, namd.sh is the script for submitting a NAMD job to 12 cores. It's content is shown as below. It assumes that the input files are in the same directory with the script.

```
#!/bin/bash
#$ -cwd
#$ -S /bin/bash
#$ -V
#$ -N namd
#$ -j y
#$ -o $JOB_NAME.o$JOB_ID
#$ -q normal
#$ -pe mpi 12
#$ -P hrothgar

unset SGE_ROOT

INPUT_CONF=bpti.namd
OUTPUT_LOG=OUTPUT.log
mpirun -np $NSLOTS -machinefile machinefile.$JOB_ID namd2 $INPUT_CONF >
$OUTPUT_LOG
```

3.2. Job submission

$ qsub namd.sh - To submit your NAMD job to Hrothgar

$ qstat – To check the status of the job



In the above screen shot, the output of the first *qstat* command indicate that the job is in "qw" state, which means it is waiting in the queue. The second *qstat* command indicates that the job is in "r" state, which means it is running. The third *qstat* command returns nothing, which means the job finished.

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For Additional Assistance Contact: hpccsupport@ttu.edu

For Comments/Suggestions on user guide hpcc@ttu.edu

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