HPCC - Hrothgar
Getting Started User Guide – NWCHEM

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User Guide

Running NWCHEM jobs on Hrothgar

1.   Setting the environment

If this is the first time you are setting up your environment on Hrothgar proceed with step 1.1, else skip to step 1.2

1.1. Setting up user environment

After you login to Hrothgar type in cd command to make sure you get back to your home directory
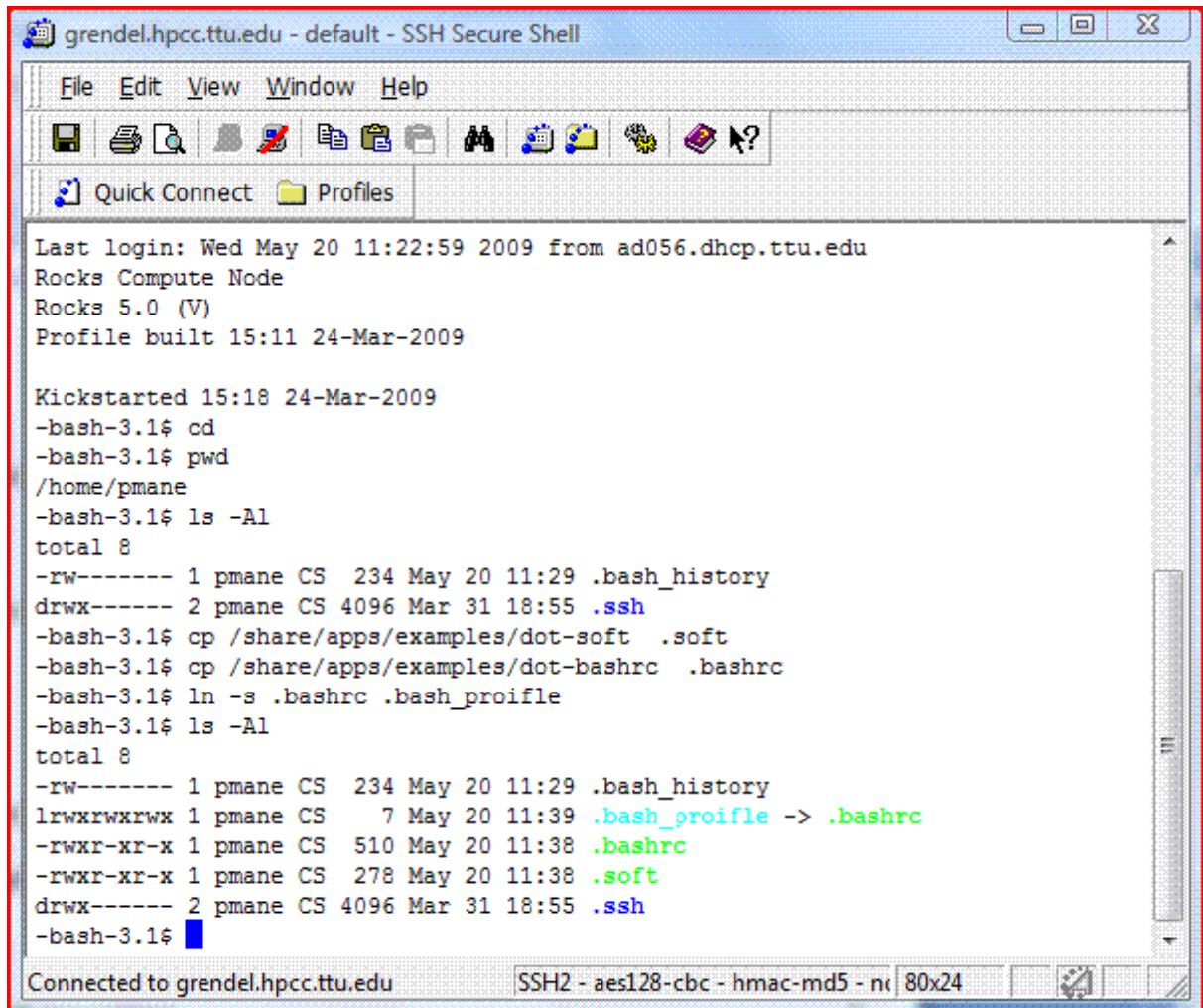
cp /share/apps/examples/dot-soft .soft

cp /share/apps/examples/dot-bashrc .bashrc

ln –s .bashrc .bash_profile

Logout and login again.

Above process will ensure that your user shell has the required setting to use various applications. If the user does not know how to log on to the appropriate cluster please refer user guides at http://www.hpcc.ttu.edu/newuser.php - connect to server (Windows/Linux)

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```
grendel.hpcc.ttu.edu - default - SSH Secure Shell

File   Edit   View   Window   Help

Quick Connect    Profiles

Last login: Wed May 20 11:22:59 2009 from ad056.dhcp.ttu.edu
Rocks Compute Node
Rocks 5.0 (V)
Profile built 15:11 24-Mar-2009

Kickstarted 15:18 24-Mar-2009
-bash-3.1$ cd
-bash-3.1$ pwd
/home/pmane
-bash-3.1$ ls -Al
total 8
-rw------- 1 pmane CS  234 May 20 11:29 .bash_history
drwx------ 2 pmane CS 4096 Mar 31 18:55 .ssh
-bash-3.1$ cp /share/apps/examples/dot-soft  .soft
-bash-3.1$ cp /share/apps/examples/dot-bashrc  .bashrc
-bash-3.1$ ln -s .bashrc .bash_proifle
-bash-3.1$ ls -Al
total 8
-rw------- 1 pmane CS  234 May 20 11:29 .bash_history
lrwxrwxrwx 1 pmane CS    7 May 20 11:39 .bash_proifle -> .bashrc
-rwxr-xr-x 1 pmane CS  510 May 20 11:38 .bashrc
-rwxr-xr-x 1 pmane CS  278 May 20 11:38 .soft
drwx------ 2 pmane CS 4096 Mar 31 18:55 .ssh
-bash-3.1$

Connected to grendel.hpcc.ttu.edu        SSH2 - aes128-cbc - hmac-md5 - n  80x24
```

One can verify if the required files are copied correctly by using 'ls –Al' command as shown in the snapshot above.

1.2. Setting up nwchem information to user shell
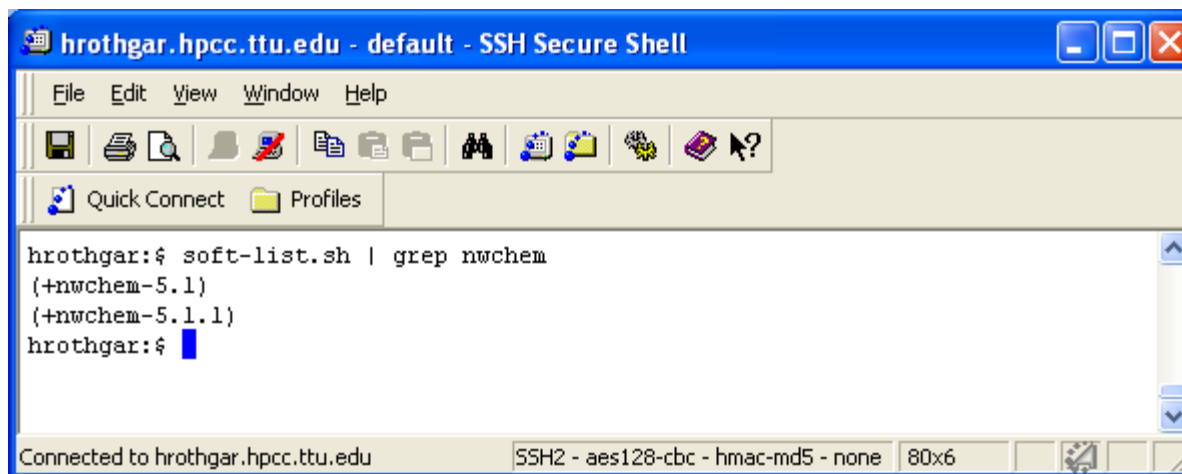
Type in:

> *$ bash*

> *$ soft-list.sh | grep nwchem*

Above command will list available nwchem soft-env setting.

(+nwchem-5.1)
(+nwchem-5.1.1)

The two options are equivalent. If there are multiple installations of NWChem, +nwchem-5.1 points to the latest version. Currently, the latest installation of NWChem is the version 5.1.1, and it is compiled by OpenMPI.
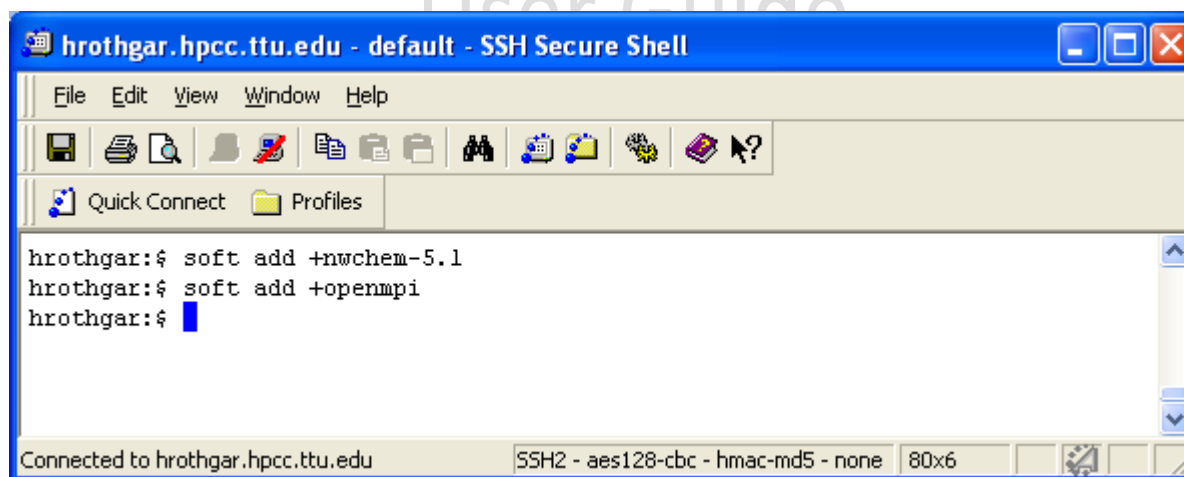

To set up the environment for regular NWChem use:

$ soft add +nwchem-5.1

$ soft add +openmpi

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 +nwchem-5.1 >> $HOME/.soft

$ echo +openmpi >> $HOME/.soft

```
hrothgar:/examples$ echo +nwchem-5.1 >> $HOME/.soft
hrothgar:/examples$ echo +openmpi >> $HOME/.soft
hrothgar:/examples$ 
```

To remove nwchem from your user environment

soft delete +nwchem-5.1

2. Job Submission

2.1. Script for job submission for normal queue

The following is a script file named nwchem.sh to submit a NWChem job to 24 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/nwchem. Use the command to copy the directory:
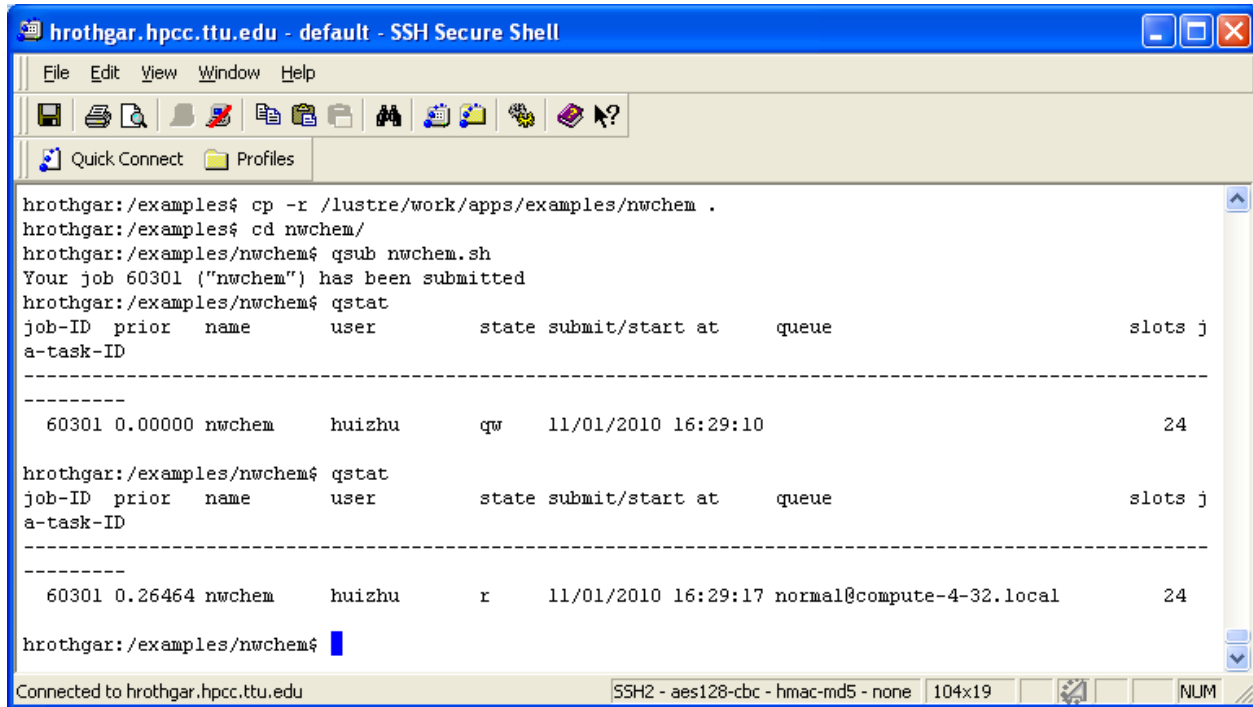
$ cp –r /lustre/work/apps/examples/nwchem nwchem

```
#$ -V
#$ -cwd
#$ -j y
#$ -q normal
#$ -S /bin/bash
#$ -N nwchem
#$ -pe fill 24
#$ -P hrothgar
unset SGE_ROOT
for i in `more machinefile.$JOB_ID | grep compute | uniq` ;do for j in `seq 1 11`;do echo $i >>
newmachinefile; done; done
NCORES=`more newmachinefile | grep compute |  wc -l`
echo $NCORES
ldd `which nwchem`
ldd `which mpirun`
/usr/mpi/intel/openmpi/bin/mpirun  -machinefile $SGE_O_WORKDIR/newmachinefile -np $NCORES
/lustre/work/apps/nwchem-5.1.1/bin/LINUX64/nwchem  siosi3.nw
```

2.2. Job submission

$ qsub nwchem.sh - To submit a NWChem job to Hrothgar

$ qstat – To check the status of the job

```
hrothgar:/examples$ cp -r /lustre/work/apps/examples/nwchem .
hrothgar:/examples$ cd nwchem/
hrothgar:/examples/nwchem$ qsub nwchem.sh
Your job 60301 ("nwchem") has been submitted
hrothgar:/examples/nwchem$ qstat
job-ID prior   name       user        state submit/start at    queue                        slots j
a-task-ID
-------------------------------------------------------------------------------------------------
---------
  60301 0.00000 nwchem     huizhu       qw    11/01/2010 16:29:10                              24

hrothgar:/examples/nwchem$ qstat
job-ID prior   name       user        state submit/start at    queue                        slots j
a-task-ID
-------------------------------------------------------------------------------------------------
---------
  60301 0.26464 nwchem     huizhu       r     11/01/2010 16:29:17 normal@compute-4-32.local    24

hrothgar:/examples/nwchem$ 
```

 Last updated: 11/01/2010
For Additional Assistance Contact: **hpccsupport@ttu.edu**

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

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