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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

   ```bash
   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](http://www.hpcc.ttu.edu/newuser.php) - connect to server (Windows/Linux)
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
```
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
# -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`
edo 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