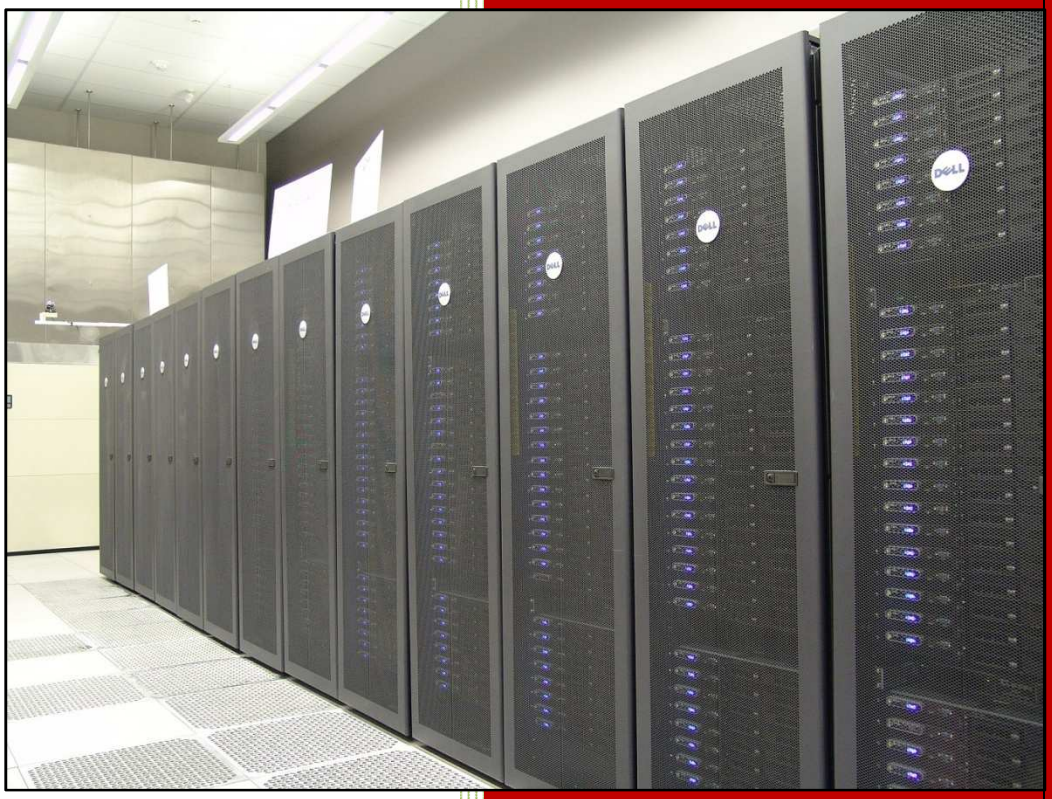
HPCC - Hrothgar

Getting Started User Guide – AMBER



High Performance Computing Center
Texas Tech University

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User Guide

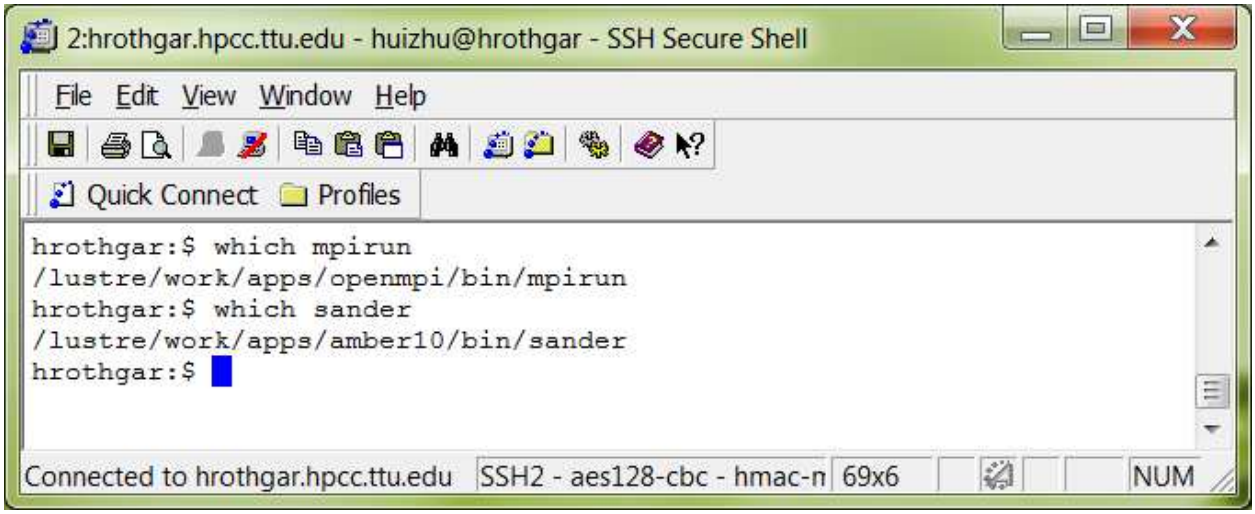
1. Introduction

AMBER is short for Assisted Model Building with Energy Refinement. It refers to two things: a set of molecular mechanical force fields for the simulation of biomolecules (which are in the public domain, and are used in a variety of simulation programs); and a package of molecular simulation programs which includes source code and demos. The latest version of AMBER installed on Hrothgar is AMBER-10. However, upon users' request, AMBER-8 is also maintained.

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. For more information about Softenv, please refer to the user guide "User's Environment" at HPCC user guides page http://www.hpcc.ttu.edu/php/NewUser.php.

First, users can check whether the environment variables for Amber and OpenMPI are set by commands ***which mpirun*** and ***which sander***. If they are set correctly, ***which mpirun*** should return "/lustre/work/apps/openmpi/bin/mpirun", and ***which sander*** should return either "/lustre/work/apps/amber10/bin/sander", or "/lustre/work/apps/amber8/bin/sander", like the screen shot below.

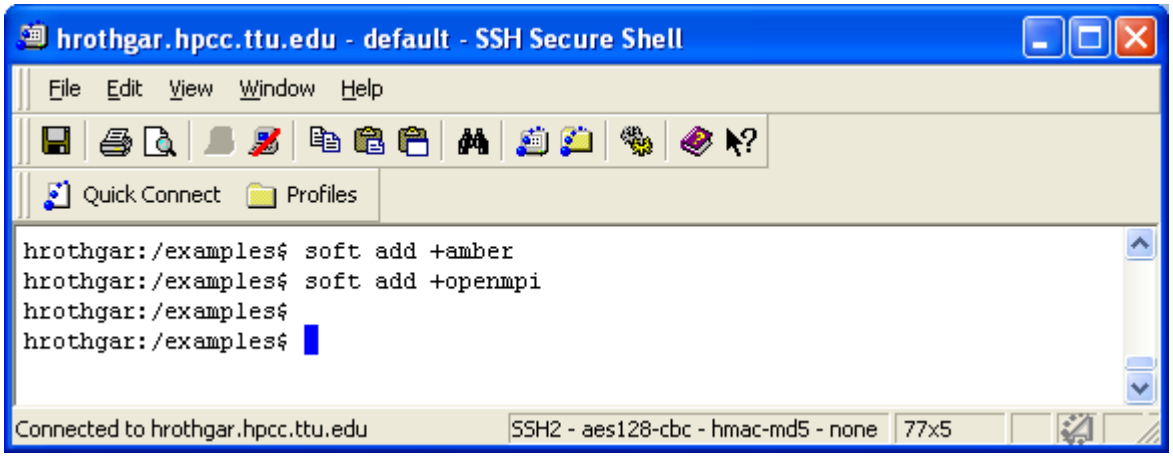


If it returns "/lustre/work/apps/amber8/bin/sander", the user's account has set up the environment for AMBER-8. If it is the version that the user needs to use, skip this section and go to Section 3 Job Submission.

If it returns message like "no sander found", or the user wants to use another version of Amber, follow the below steps to set up the environment variables.

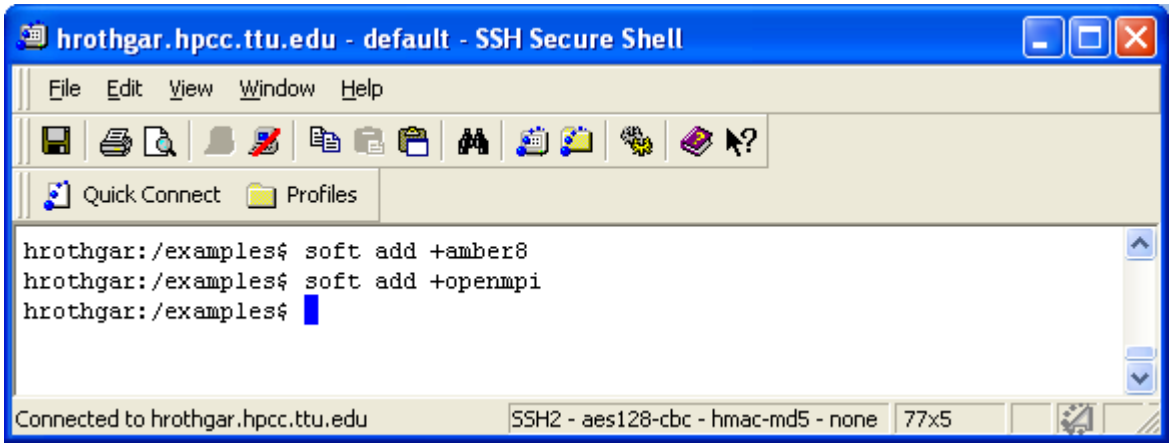
To set up Amber environment variables in current session:

$ soft add +amber
$ soft add +openmpi



The option +amber tracks the latest version of AMBER installed on Hrothgar. Currently it points to AMBER-10. If a user wants to use AMBER-8, run the following commands instead:

$ soft add +amber8
$ soft add +openmpi



Type “which sander” to verify that one of AMBER commands can be. In this way the environment variables is valid only in the current session. It expires when the user logs out.

To set up abaqus environment variables permanently:

To make path changes permanent and consisted across all nodes, execute the following commands:

$ echo +amber >> $HOME/.soft

$ echo +openmpi >> $HOME/.soft

$ resoft

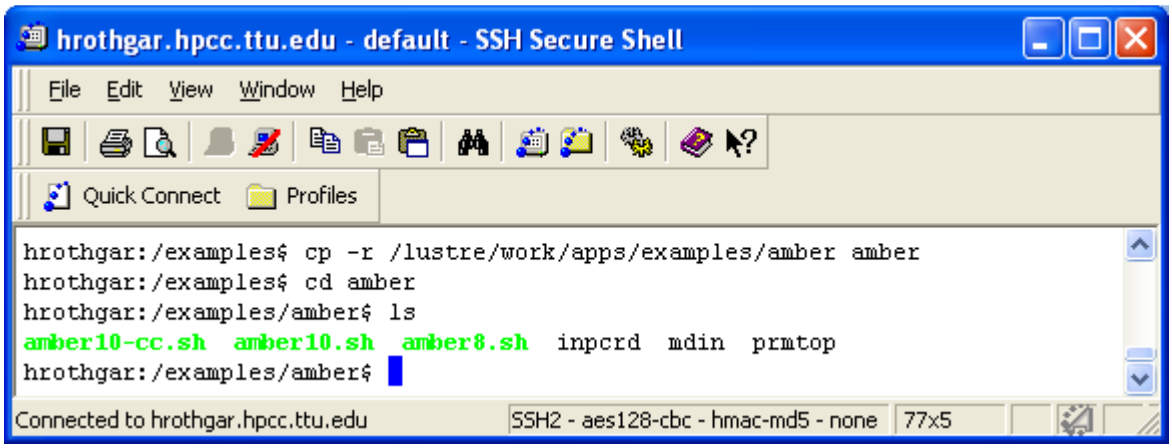
Similarly, if the user needs to use AMBER-8, replace +amber with +amber8 in the command.

3. Job Submission

3.1. Script for job submission

Sample scripts for AMBER jobs submission are available at /lustre/work/apps/examples/amber. They assume that the input files are in the same directory with the script. Use the command to copy the directory:

$ cp –r /lustre/work/apps/examples/amber amber



The following is is the content of the file *amber10.sh*, which is a script file to submit an AMBER10 job.

```
#!/bin/bash
#$ -cwd
#$ -S /bin/bash
#$ -V
#$ -N amber10
#$ -j y
#$ -o $JOB_NAME.o$JOB_ID
#$ -e $JOB_NAME.e$JOB_ID
#$ -q normal
#$ -P hrothgar
#$ -pe mpi 24

unset SGE_ROOT

mpirun -np $NSLOTS -machinefile machinefile.$JOB_ID /lustre/work/apps/amber10/bin/sander.MPI
-O -i mdin -o md.out.$JOB_ID -inf md.mdinfo.$JOB_ID
```

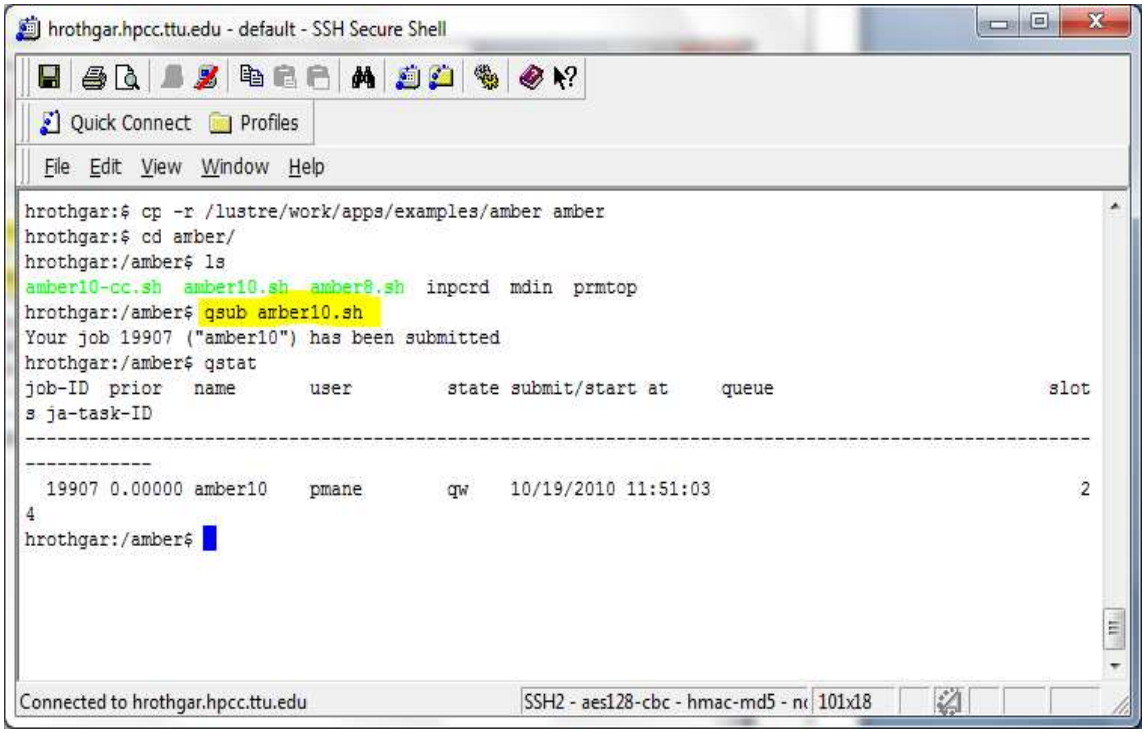
The following is a script file (*amber8.sh*) to submit an AMBER8 job to 12 cores, but run the program *sander* over 8 cores. Note that besides the installation directory, the name of the executable is different in AMBER10 and AMBER8. In AMBER10, the executable's name is *sander.MPI*, but in AMBER8, the name is *sander*. AMBER8 also requires the number of cores used for running *sander* in parallel to be power of 2, but AMBER10 does not have this restriction. For this reason, the number after "-np" option is 8 instead of $NSLOTS. The differences are highlighted in yellow in the scripts.


```
#!/bin/bash
#$ -cwd
#$ -S /bin/bash
#$ -V
#$ -N amber8
#$ -j y
#$ -o $JOB_NAME.o$JOB_ID
#$ -e $JOB_NAME.e$JOB_ID
#$ -q normal
#$ -pe mpi 12

unset SGE_ROOT

mpirun -np 8 -machinefile machinefile.$JOB_ID /lustre/work/apps/amber8/bin/sander -O -i mdin -o
md.out.$JOB_ID -inf md.mdinfo
```

3.2 Job submission

$ qsub amber10.sh - To submit your AMBER10 job to normal queue.

$ qstat – To check the status of the job



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