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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.

![Image of terminal output showing environment variables set correctly]

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.

http://www.hpcc.ttu.edu
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.
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.

```bash
#!/bin/bash
#$ -S /bin/bash
#$ -c /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
```

```bash
#!/bin/bash
#$ -S /bin/bash
#$ -c /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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