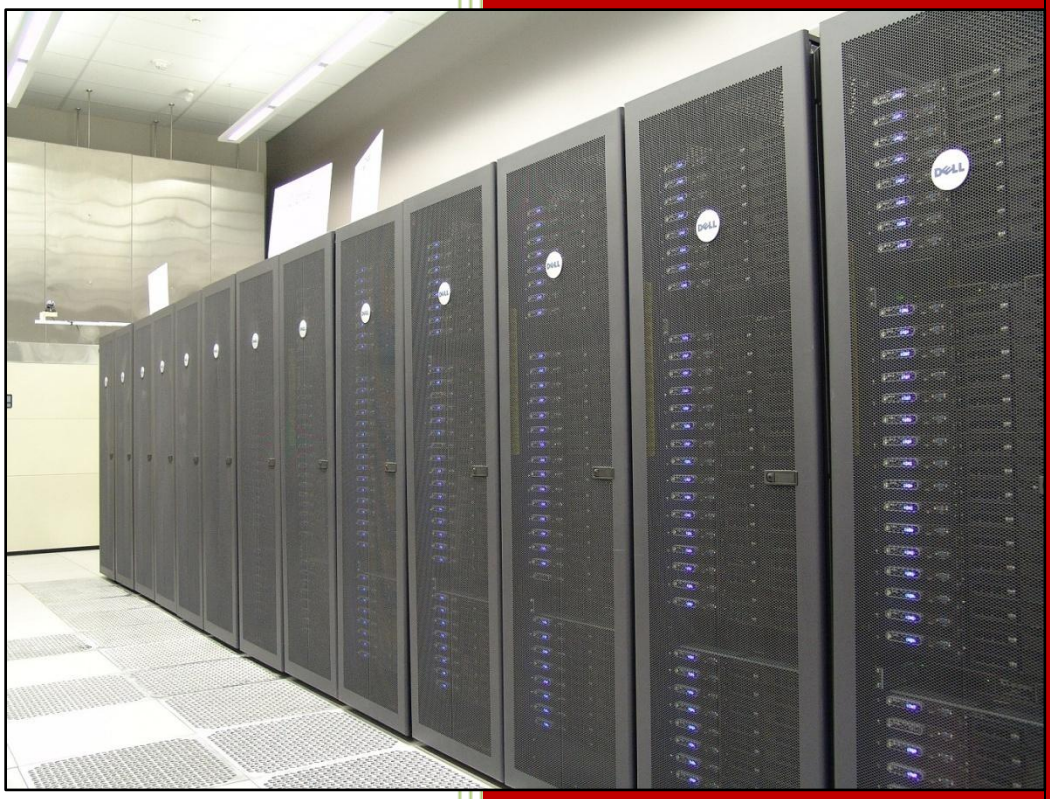
HPCC - Hrothgar

Getting Started User Guide – LAMMPS



High Performance Computing Center
Texas Tech University

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User Guide

1. Introduction

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is a classical molecular dynamics simulation code designed to run efficiently on parallel computers. It was developed at Sandia National Laboratories, a US Department of Energy facility, with funding from the DOE. It is an open-source code, distributed freely under the terms of the GNU Public License (GPL). The current version of LAMMPS is 15 Jan 2010.

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.

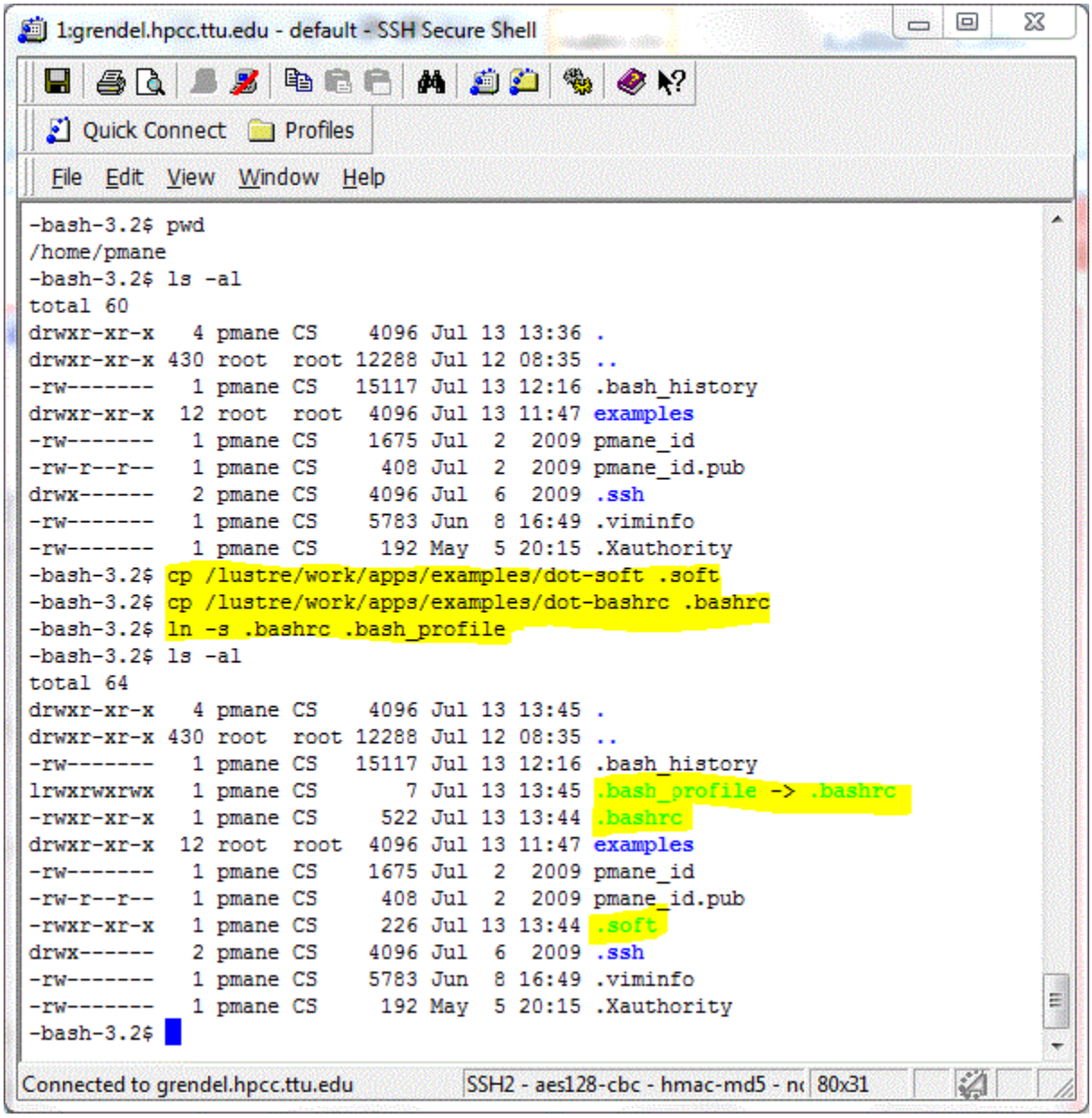
2.1 Setting up user environment

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.

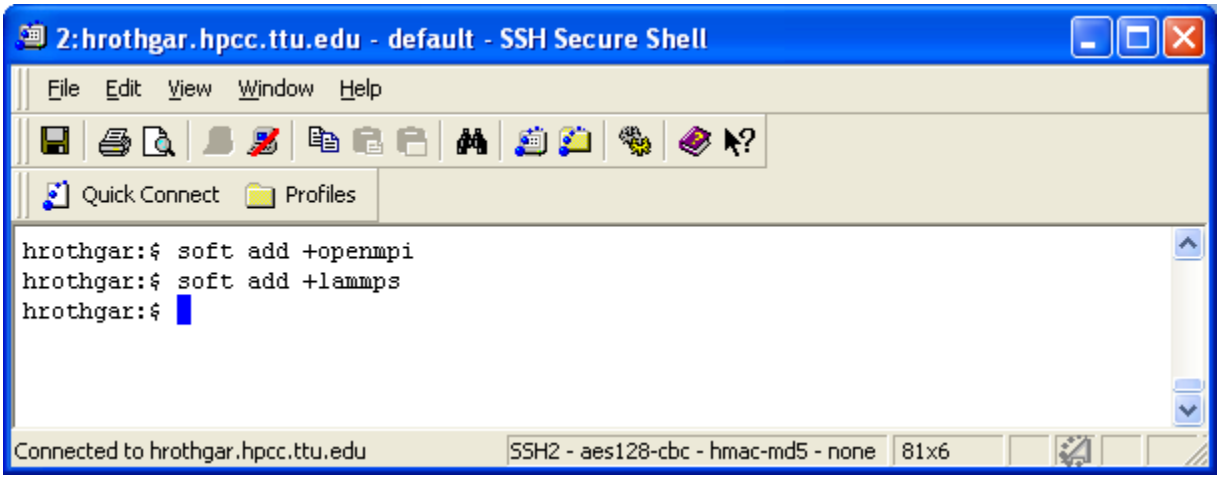


2.2 Setting up LAMMPS environment for submitting the jobs

The latest version of LAMMPS is installed on Hrothgar. The parallel support for LAMMPS is on top of OpenMPI, so OpenMPI is the only version of MPI that can be used in order to run LAMMPS in parallel. Use the following commands to add LAMMPS and OpenMPI in SoftEnv for submitting the jobs to the normal and community queue:

$ soft add +openmpi

$ soft add +lammps

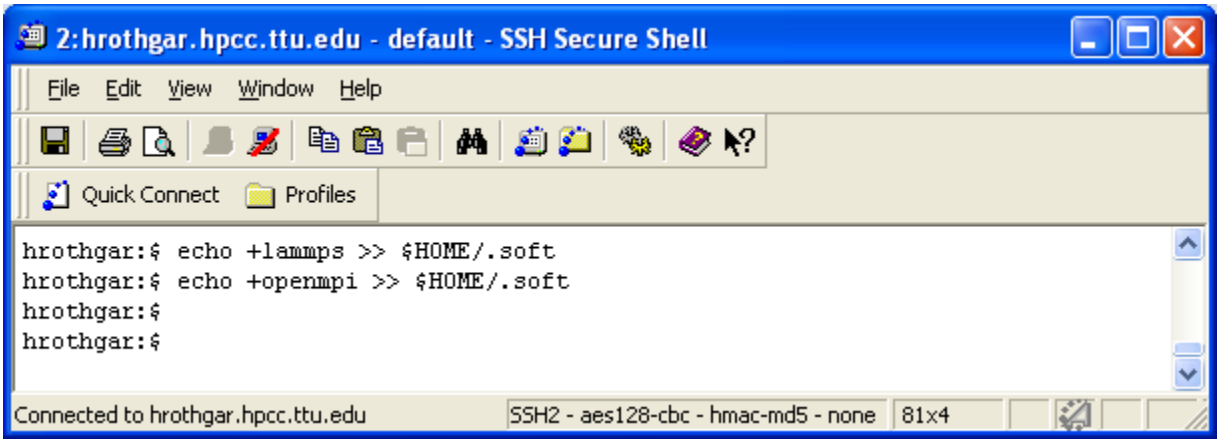


If other version of MPI (e. g. MPICH) was set up, use the following command to delete it from SoftEnv:

$ soft delete +mvapich-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 commands:

$ echo +lammps >> $HOME/.soft
$ echo +openmpi >> $HOME/.soft



3. Job Submission

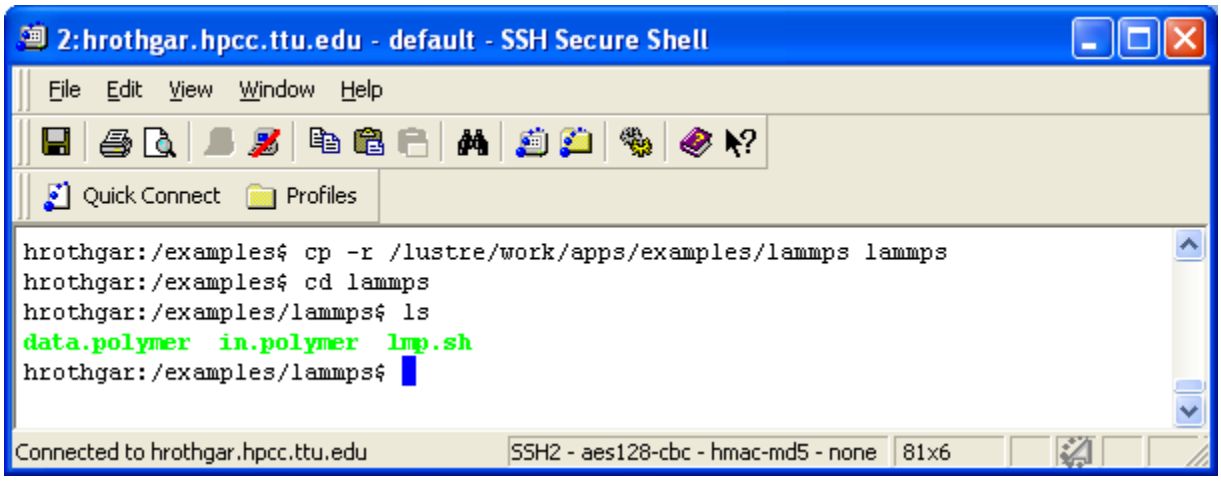
3.1. Script for job submission to the normal queue

The following is a script file to submit a LAMMPS job to 24 cores for a 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/lammps. Use the command to copy the directory:

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

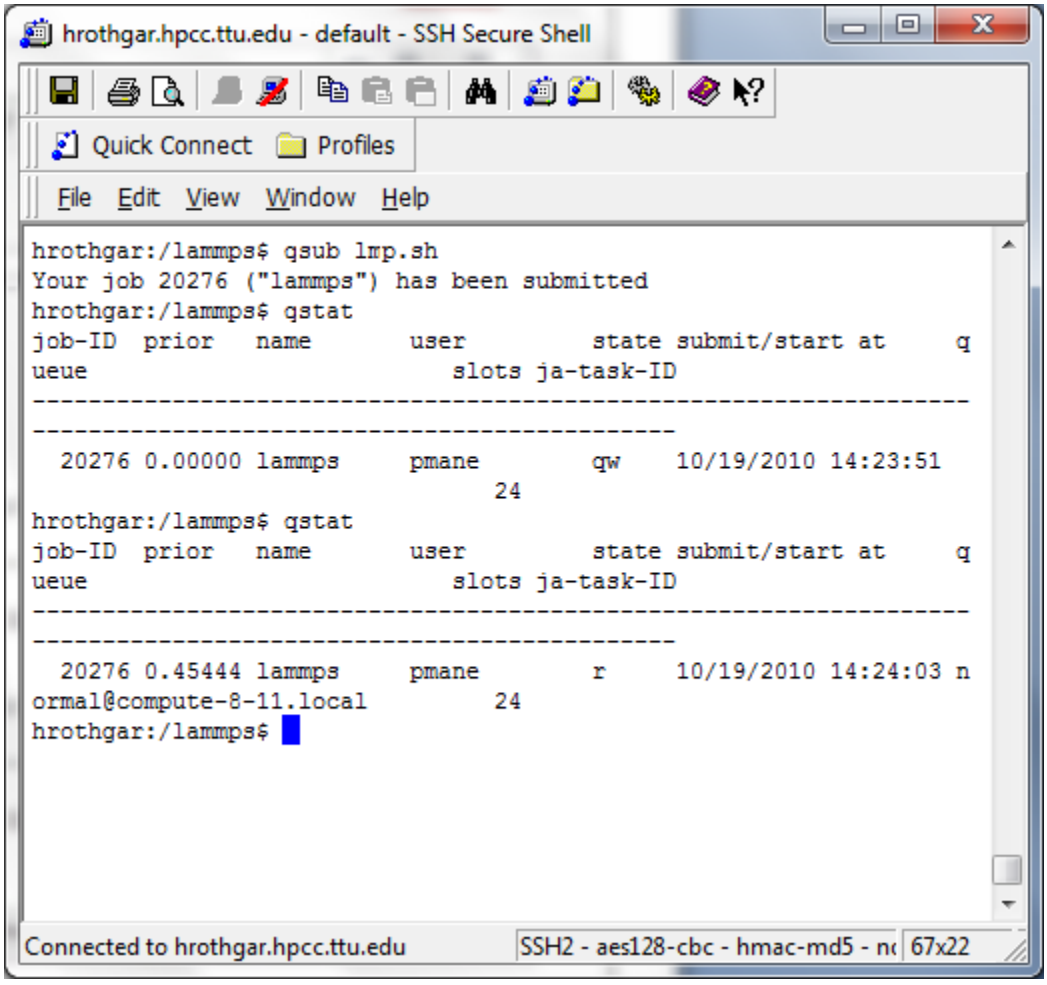
```
#!/bin/bash
#$ -V
#$ -cwd
#$ -j y
#$ -S /bin/bash
#$ -N lammps
#$ -o $JOB_NAME.o$JOB_ID
#$ -e $JOB_NAME.e$JOB_ID
#$ -q normal
#$ -pe fill 24
#$ -P hrothgar

unset SGE_ROOT

/usr/mpi/intel/openmpi/bin/mpirun  -np $NSLOTS -machinefile machinefile.$JOB_ID
/lustre/work/apps/lammps-4Jul10/src/lmp_linux < in.polymer
```



3.2. Job submission

$ qsub lmp.sh - To submit your LAMMPS job to Hrothgar

$ qstat – To check the status of the job


hrothgar.hpcc.ttu.edu - default - SSH Secure Shell
Quick Connect
Profiles
File Edit View Window Help
hrothgar:/lammps$ qsub lmp.sh
Your job 20276 ("lammps") has been submitted
hrothgar:/lammps$ qstat
job-ID prior name user state submit/start at q
ueue slots ja-task-ID
20276 0.00000 lammps pmane qw 10/19/2010 14:23:51
24
hrothgar:/lammps$ qstat
job-ID prior name user state submit/start at q
ueue slots ja-task-ID
20276 0.45444 lammps pmane r 10/19/2010 14:24:03 n
ormal@compute-8-11.local 24
hrothgar:/lammps$
Connected to hrothgar.hpcc.ttu.edu
SSH2 - aes128-cbc - hmac-md5 - n
67x22

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For Additional Assistance Contact: hpccsupport@ttu.edu

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

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