

HPCC - Hrothgar

Getting Started User Guide – LAMMPS



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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.

```

1:grendel.hpcc.ttu.edu - default - SSH Secure Shell
Quick Connect Profiles
File Edit View Window Help

-bash-3.2$ pwd
/home/pmane
-bash-3.2$ ls -al
total 60
drwxr-xr-x  4 pmane CS   4096 Jul 13 13:36 .
drwxr-xr-x 430 root  root 12288 Jul 12 08:35 ..
-rw-----  1 pmane CS  15117 Jul 13 12:16 .bash_history
drwxr-xr-x 12 root  root  4096 Jul 13 11:47 examples
-rw-----  1 pmane CS  1675 Jul  2 2009 pmane_id
-rw-r--r--  1 pmane CS   408 Jul  2 2009 pmane_id.pub
drwx-----  2 pmane CS  4096 Jul  6 2009 .ssh
-rw-----  1 pmane CS  5783 Jun  8 16:49 .viminfo
-rw-----  1 pmane CS   192 May  5 20:15 .Xauthority
-bash-3.2$ cp /lustre/work/apps/examples/dot-soft .soft
-bash-3.2$ cp /lustre/work/apps/examples/dot-bashrc .bashrc
-bash-3.2$ ln -s .bashrc .bash_profile
-bash-3.2$ ls -al
total 64
drwxr-xr-x  4 pmane CS   4096 Jul 13 13:45 .
drwxr-xr-x 430 root  root 12288 Jul 12 08:35 ..
-rw-----  1 pmane CS  15117 Jul 13 12:16 .bash_history
lrwxrwxrwx  1 pmane CS      7 Jul 13 13:45 .bash_profile -> .bashrc
-rwxr-xr-x  1 pmane CS   522 Jul 13 13:44 .bashrc
drwxr-xr-x 12 root  root  4096 Jul 13 11:47 examples
-rw-----  1 pmane CS  1675 Jul  2 2009 pmane_id
-rw-r--r--  1 pmane CS   408 Jul  2 2009 pmane_id.pub
-rwxr-xr-x  1 pmane CS   226 Jul 13 13:44 .soft
drwx-----  2 pmane CS  4096 Jul  6 2009 .ssh
-rw-----  1 pmane CS  5783 Jun  8 16:49 .viminfo
-rw-----  1 pmane CS   192 May  5 20:15 .Xauthority
-bash-3.2$

```

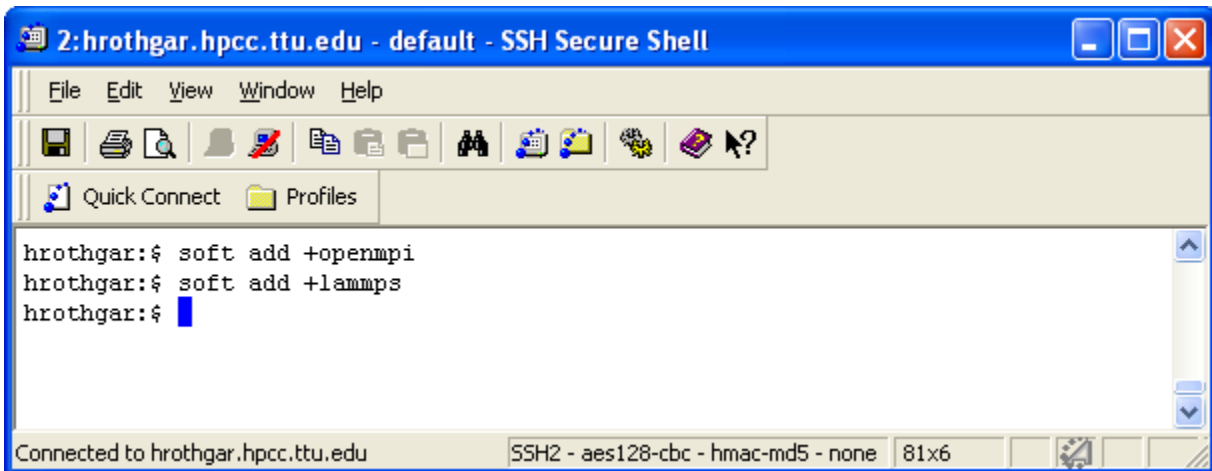
Connected to grendel.hpcc.ttu.edu SSH2 - aes128-cbc - hmac-md5 - n 80x31

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
```



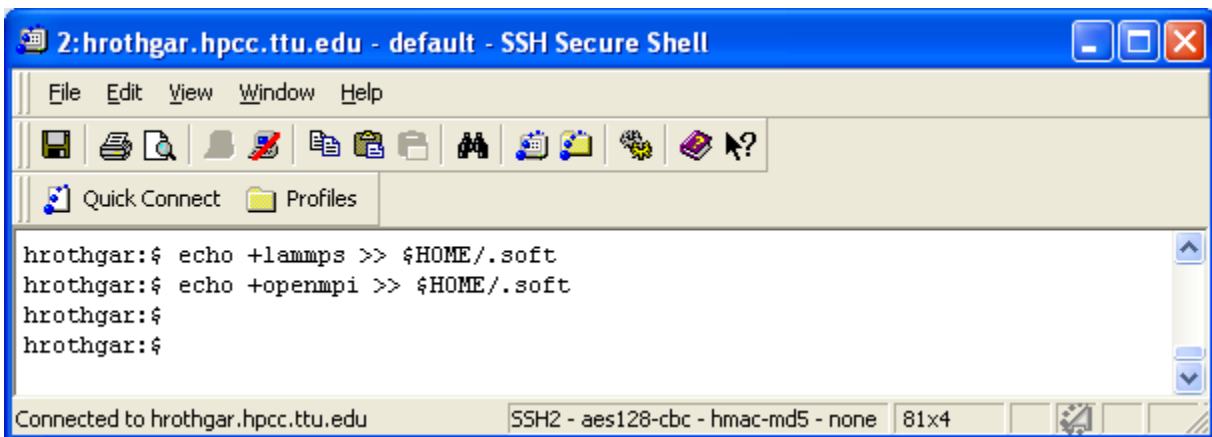
```
2:hrothgar.hpcc.ttu.edu - default - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
hrothgar:$ soft add +openmpi
hrothgar:$ soft add +lammps
hrothgar:$
Connected to hrothgar.hpcc.ttu.edu  SSH2 - aes128-cbc - hmac-md5 - none  81x6
```

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



```
2:hrothgar.hpcc.ttu.edu - default - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
hrothgar:$ echo +lammps >> $HOME/.soft
hrothgar:$ echo +openmpi >> $HOME/.soft
hrothgar:$
hrothgar:$
Connected to hrothgar.hpcc.ttu.edu  SSH2 - aes128-cbc - hmac-md5 - none  81x4
```

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

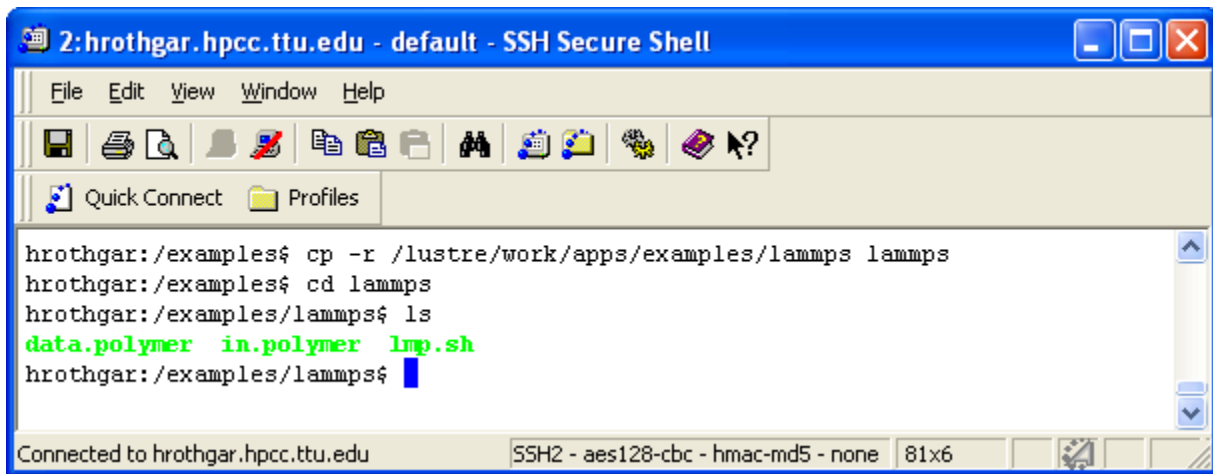
are available at the directory /lustre/work/apps/examples/lammps. Use the command to copy the directory:

```
$ 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/imp_linux < in.polymer
```

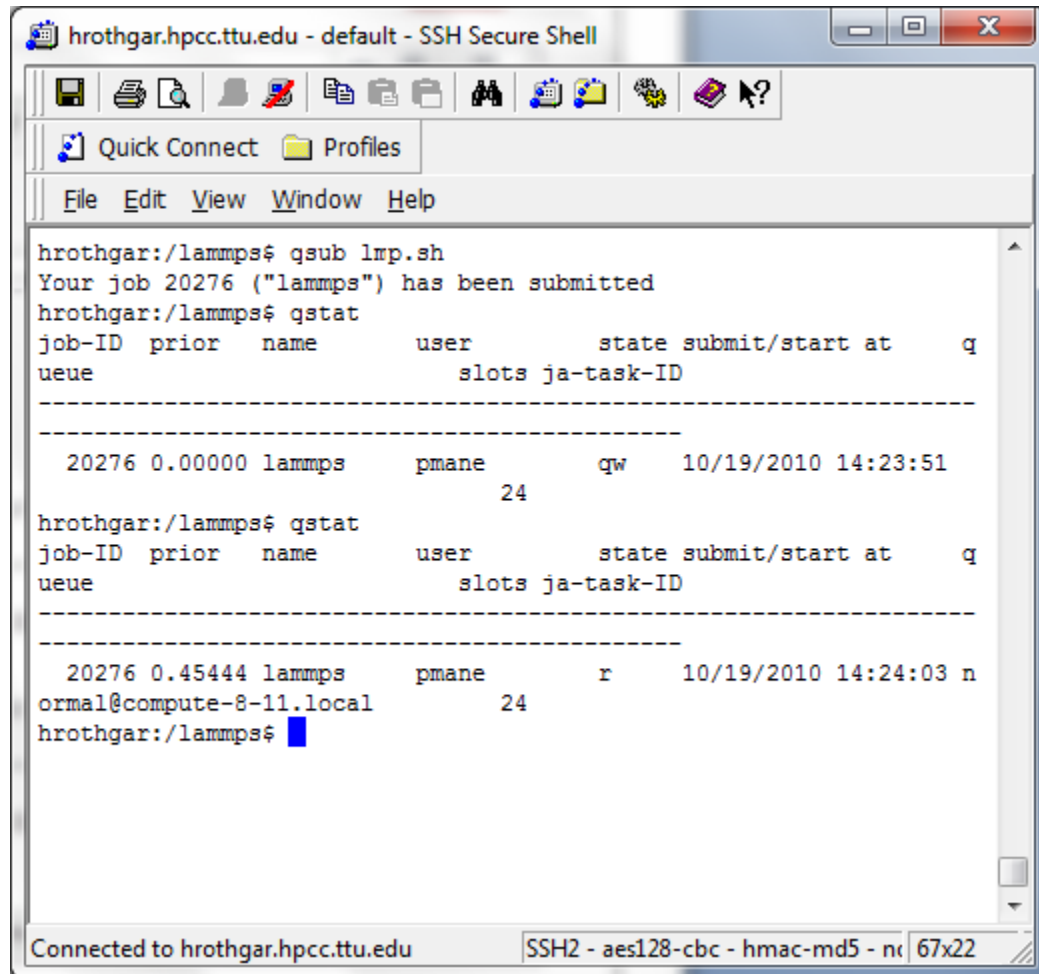


```
2:hrothgar.hpcc.ttu.edu - default - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
hrothgar:/examples$ cp -r /lustre/work/apps/examples/lammps lammps
hrothgar:/examples$ cd lammps
hrothgar:/examples/lammps$ ls
data.polymer in.polymer imp.sh
hrothgar:/examples/lammps$
```

3.2. Job submission

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

\$ qstat - To check the status of the job



```
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 - nc 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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