Need to VPN to connect to our resources:

http://www.cmu.edu/computing/network/vpn/

for linux users:

http://www.cs.cmu.edu/~help/networking/vpn/vpn_linux.html

Our cluster(s):

user@ntpl-bw01.me.cmu.local

user@ntpl-bw02.me.cmu.local

user@gilgamesh.cheme.cmu.edu

or

user@172.19.10.6

user@172.19.10.14

user@128.2.52.112

If you cannot resolve the domain name explicitly. You can always check to see what the ip address is by using:

```
[jason@ntpl ~]$ /sbin/ifconfig
eth0      Link encap:Ethernet  HWaddr 00:E0:81:44:5D:B9
          inet addr:172.16.7.254  Bcast:172.16.7.255  Mask:255.255.248.0
          UP BROADCAST RUNNING MULTICAST  MTU:1500  Metric:1
          RX packets:68339299 errors:0 dropped:0 overruns:0 frame:0
          TX packets:48824629 errors:0 dropped:0 overruns:0 carrier:0
          collisions:0 txqueuelen:1000
          RX bytes:21016065686 (19.5 GiB)  TX bytes:12072127894 (11.2 GiB)
          Interrupt:25

eth1      Link encap:Ethernet  HWaddr 00:E0:81:44:5D:B8
          inet addr:172.19.10.6  Bcast:172.19.10.255  Mask:255.255.255.0
          UP BROADCAST RUNNING MULTICAST  MTU:1500  Metric:1
          RX packets:3847994 errors:0 dropped:0 overruns:0 frame:0
          TX packets:3869517 errors:0 dropped:0 overruns:0 carrier:0
          collisions:0 txqueuelen:1000
          RX bytes:338630793 (322.9 MiB)  TX bytes:4918728342 (4.5 GiB)
          Interrupt:24

lo        Link encap:Local Loopback
          inet addr:127.0.0.1  Mask:255.0.0.0
          UP LOOPBACK RUNNING  MTU:16436  Metric:1
          RX packets:38798046 errors:0 dropped:0 overruns:0 frame:0
          TX packets:38798046 errors:0 dropped:0 overruns:0 carrier:0
          collisions:0 txqueuelen:0
          RX bytes:7829260552 (7.2 GiB)  TX bytes:7829260552 (7.2 GiB)
```

ntpl-bw0x

user@ntpl-bw01.me.cmu.local

12 nodes, 4 cpu/node

user@ntpl-bw02.me.cmu.local

4 nodes, 12 cpu/node

To submit a job:

```
[jason@ntpl 6x]$ ls
1atom              log_heat_7.lammps  log_SED_16.lammps  matlab_prim.sh
in.LJAr.SED        log_heat_8.lammps  log_SED_1.lammps   matlab_toatom.sh
LJ1.in.data        log_heat_9.lammps  log_SED_2.lammps   matlab_toucell.sh
log_heat_10.lammps  log.lammps        log_SED_3.lammps   p1_lmp_perfect_SED_6x.o1654
log_heat_1.lammps   log_SED_10.lammps  log_SED_4.lammps   parallel_lmp_MD.sh
log_heat_2.lammps   log_SED_11.lammps  log_SED_5.lammps   SED_LAMMPS_DUMP.py
log_heat_3.lammps   log_SED_12.lammps  log_SED_6.lammps   SED_LAMMPS_FFT_PRIMITIVE.m
log_heat_4.lammps   log_SED_13.lammps  log_SED_7.lammps   SED_LAMMPS_FFT_toatom.m
log_heat_5.lammps   log_SED_14.lammps  log_SED_8.lammps   SED_LAMMPS_FFT_toucell.m
log_heat_6.lammps   log_SED_15.lammps  log_SED_9.lammps
[jason@ntpl 6x]$ vi parallel_lmp_MD.sh
[jason@ntpl 6x]$ qsub parallel_lmp_MD.sh
```

You need a job submission script like:

parallel_lmp_MD.sh

```
#!/bin/sh
#PBS -l nodes=1:ppn=4 :node
### Merge stderr with stdout
#PBS -j oe
### Queue name
#PBS -q default
###Job name
#PBS -N p1_lmp_perfect_SED_6x
### Declare job-non-rerunable
#PBS -r n
#PBS -V
# This job's working directory
echo Job ID: $PBS_JOBID
echo Working directory is $PBS_O_WORKDIR cd $PBS_O_WORKDIR echo Running on host `hostname` echo
Time is `date` echo Directory is `pwd` echo This job runs on the following processors:
echo `cat $PBS_NODEFILE`

RUNPATH=/home/jason/lammps/LJ/crystal/perfect/SED/6x
EXEPATH=/home/jason/lammps/lammps-30Nov10/src

cd $RUNPATH

/opt/intel/impi/3.2.2.006/bin64/mpirun -np 4 $EXEPATH/lmp_openmpi < $RUNPATH/in.LJAr.SED
```

To check job status:

```
[jason@ntpl ~]$ qstat
Job id                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - -----
2492.ntpl                 ...0.2_r310x16LH jason          255:05:3 R default
2493.ntpl                 ....2_r310x16_re jason          260:22:0 R default
[jason@ntpl ~]$ qstat -n

ntpl.bw01.me.cmu.local: Torque Server @ ntpl.bw01.me.cmu.local
                                                            Req'd  Req'd   Elap
Job ID                  Username Queue    Jobname          SessID NDS   TSK Memory Time  S Time
----------------------- -------- -------- ---------------- ------ ----- --- ------ ----- - -----
2492.ntpl.bw01.m        jason    default  owl_3DLsc59WLJ0.  26864     1  --    --    --  R 42:59
   n016/7+n016/6+n016/5+n016/4+n016/3+n016/2+n016/1+n016/0
2493.ntpl.bw01.m        jason    default  owl_3DLsc59WLJ0.  26999     1  --    --    --  R 42:58
   n016/11+n016/10+n016/9+n016/8
```

To delete a job:

```
[jason@ntpl ~]$ qdel 2492
```

To check job status/timings:

```
/home/jason/.pbs_spool/2492.ntpl.bw01.me.cmu.local.OU

  995000  0.085111238 -0.0017991423 -0.0010303413 -0.0010038524    -3.91734    -4.044088   0.12674804    153736.84
 1000000  0.085225177 -0.0010769173 0.00020226436 -0.00014742846   -3.9173497   -4.0442674   0.12691772
153736.84
Loop time of 5598.58 on 8 procs for 1000000 steps with 2640 atoms
```

To check node status:

```
[root@ntpl ~]# ssh n016
[root@ntpl ~]# top

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+   P COMMAND
10319 jason     25   0  108m  10m 8116 R 100.0  0.0   2:30.35  3 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
10321 jason     25   0  114m  10m 7388 R 100.0  0.0   2:28.05  7 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
10322 jason     25   0  108m 7728 5600 R 100.0  0.0   3:43.76  2 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
10324 jason     25   0  114m 9292 5556 R 100.0  0.0   3:40.60  5 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
27124 jason     25   0  114m  10m 6832 R 100.0  0.0   2529:50 10 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
27125 jason     25   0  114m   9m 6456 R 100.0  0.0   2606:44 11 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
27121 jason     25   0  115m  12m 8808 R 99.7  0.1   2665:28  8 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
27122 jason     25   0  108m 9676 7460 R 99.7  0.0   2736:48  1 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
10325 jason     25   0  114m 9.8m 6248 R 52.2  0.0   3:07.87  6 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
10326 jason     25   0  108m 7676 5420 R 50.2  0.0   3:06.57  4 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
27126 jason     25   0  108m 9056 6776 R 50.2  0.0   2607:03  0 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
10323 jason     25   0  108m 8984 6852 R 49.8  0.0   1:53.20  0 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
27120 jason     25   0  115m  13m 9596 R 49.8  0.1   2600:07  4 /home/jason/lammps/lammps-30Nov10/src/lmp_openmpi
```

File Permissions

Sometimes you need to change permissions on folders if current files in folder do not have rwx:

[root@n016 16x]# ls -l
total 86M
-rw-rw-r-- 1 jason jason 629 Feb 10 14:36 2_replaceXYZ.py
-rw-rw-r-- 1 jason jason 103K Feb 10 14:40 final8.txt
-rw-rw-r-- 1 jason jason 9.4K Feb 15 16:44 F_NEMD.in
-rw-rw-r-- 1 jason jason 9.4K Feb 17 23:10 F_restart.in
drwxrwxrwx 2 jason jason 4.0K Feb 20 10:58 LH
-rw-rw-r-- 1 jason jason 784 Feb 16 12:31 lmp_restart.sh
-rw-rw-r-- 1 jason jason 775 Feb 14 21:52 lmp_run.sh

To change permissions, use chmod:

[root@n016 1D_3Ligands]# ls
16x final8.txt r4.5 r5.5
[root@n016 1D_3Ligands]# chmod -R 777 ./16x

Now the permissions read:

[root@n016 16x]# ls -l
total 86M
-rwxrwxrwx 1 jason jason 629 Feb 10 14:36 2_replaceXYZ.py
-rwxrwxrwx 1 jason jason 103K Feb 10 14:40 final8.txt
-rwxrwxrwx 1 jason jason 9.4K Feb 15 16:44 F_NEMD.in
-rwxrwxrwx 1 jason jason 9.4K Feb 17 23:10 F_restart.in
drwxrwxrwx 2 jason jason 4.0K Feb 20 10:58 LH
-rwxrwxrwx 1 jason jason 784 Feb 16 12:31 lmp_restart.sh
-rwxrwxrwx 1 jason jason 775 Feb 14 21:52 lmp_run.sh

Gilgamesh

user@gilgamesh.cheme.cmu.edu

http://gilgamesh.cheme.cmu.edu/doc/gilgamesh.html

gilgamesh.cheme.cmu.edu is a computing cluster housed in the Department of Chemical Engineering at CMU.

The cluster consists of 640 cores distributed on 20 nodes:

2 nodes with 32 cores 256 GB RAM/node (nodes n00-n01)
6 nodes with 32 cores 128 GB RAM/node (nodes n02-n07)
12 nodes with 32 cores 64GB RAM/node   (nodes n08-n19)