Supercomputing environment

TMA4280—Introduction to Supercomputing

NTNU, IMF

February 21. 2018

Supercomputing environment

- Supercomputers use UNIX-type operating systems.
- Predominantly Linux.
- Using a shell interpreter is the only way to interact with the system.

Documentation and tutorials are usually offered on the System Administration group's website:
https://www.hpc.ntnu.no/display/hpc/User+Guide

Login

— Non-graphical interaction with the supercomputer.
— Two kinds of nodes: login/interactive nodes and compute nodes.
— Login is handled through *Secure SHell* (SSH).
— On Linux/UNIX/MacOS: pre-installed OpenSSH.
— On Windows: third-party client PuTTy.

Login

Three ingredients:

- Username: NTNU login name.
- Host: `training.hpc.ntnu.no`.
- Credential: a password or an authentication key.

```
ssh username@training.hpc.ntnu.no
```

Login

```
Last login: Wed Feb 21 16:24:19 2018 from 129.241.15.225

 /$$$$$$$$            /$$                          /$$       /$$$$$$       /$$
| $$_____/           |__/                         /$$/      |_  $$_/      | $$
| $$         /$$$$$$  /$$  /$$$$$$$            /$$/          | $$    /$$$$$$$ /$$    /$$ /$$$$$$$
| $$$$$     /$$__  $$| $$ /$$_____/           /$$/           | $$   /$$__  $$| $$   | $$| $$__  $$
| $$__/    | $$  \ $$| $$| $$                /$$/            | $$   | $$  | $$| $$   | $$| $$  \ $$
| $$       | $$  | $$| $$| $$               /$$/             | $$   | $$  | $$| $$   | $$| $$  | $$
| $$$$$$$$| $$$$$$$/| $$|  $$$$$$$       /$$/              /$$$$$$| $$$$$$$|  $$$$$$/| $$  | $$
|________/| $$____/ |__/ \_______/      |__/               |______/ \_______/ \______/ |__/  |__/
          | $$
          | $$
          |__/


To run jobs you need to generate and add public keys to authorized file:
NB!
NB! this will overwrite you existing keypair
NB!

# ssh-keygen -b 2048 -f $HOME/.ssh/id_rsa -t rsa -q -N ""
# cat $HOME/.ssh/id_rsa.pub >> $HOME/.ssh/authorized_keys

to list available modules software:
# module spider

Starting 6th of february, 2018:
Courses lectured over several afternoons will give a introduction to parallel programming.
Registration: Send an e-mail to: adm@hpc.ntnu.no
https://www.hpc.ntnu.no/display/hpc/Introduction+to+parallel+programming

To get help and support, please send email to:  help@hpc.ntnu.no
Or check our web page: http://www.hpc.ntnu.no/

Disk quota are now enabled on idun, to see your quota, command: dusage
(or quota  , see 'man quota')

Be Nice!
```

File transfer

— File transfers is performed using *Secure Copy* (`scp`).
— On Linux/UNIX/MacOS: pre-installed OpenSSH.
— On Window: third-party client *WinSCP*.

Advice: for source code and result files in text format use a revision control system like GIT.

Authentication with SSH key

- Avoid typing your password, use key authentication.
- Generate an SSH key:

```
ssh-keygen
```

- Copy the **public** key to the remote host using `scp`

```
scp ~/.ssh/id_rsa.pub username@training.hpc.ntnu.n
```

Tutorial:

https://debian-administration.org/article/530/SSH_with_authentication_key_instead_of_password

Editing files

For such small project, only a good text editor is required:

- Emacs (use locally if you can)
- Vim (handy for using remotely, a bit of a learning curve)
- Nano (simpler than Vim)
- Gedit (nice graphical editor)
- Kate (same, not installed on Lille)
- Notepad++ (good for Windows users, not installed on Lille)
- ...

In practice, non-graphical editors are preferred since working on a login node requires using the terminal: most people use Vim, Emacs, or Nano.

Graphical display (X11 forwarding)

If you want to run graphical programs on Lille you have to tunnel the display through ssh. This is called *X forwarding*.

— In Linux, it's quite easy:

```
ssh -X username@training.hpc.ntnu.no
```

Or in your `~/.ssh/config`:

```
ForwardX11 Yes
```

— In OSX, you have to start `X11.app`, then do the same.

— In Windows, you can use *X-Win32*, which is available on progdist.

This is usually not required and puts unnecessarily load on the login nodes.

Modules

As people sharing a supercomputer have different needs, the tools cannot be all installed in the default system directories. Software is offered through a *modules* system. They will not be available to you until you load the module in question.

- List all available modules:

```
module spider
```

- List available modules:

```
module avail
```

- Load a module:

```
module load gcc
```

- Load a module with a specific version:

```
module load gcc/6.3.0
module load openmpi/2.0.1
```

- List loaded modules:

```
module list
```

Modules

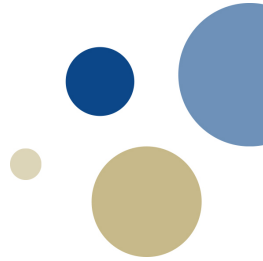
Some relevant modules for this course:

- `gcc/6.3.0`: GCC compilers (`gcc`, `g++` and `gfortran`).
- `openmpi/2.0.1`: OpenMPI implementation of MPI (*Message Passing Toolkit*).
- `openblas/0.2.19`: BLAS library.

Note that if you use CMake to build your programs, you may need to pass the compiler you want to use:

```
mkdir build
cd build
CXX=g++ CC=gcc FC=gfortran cmake ..
```

Modules



```
[aurelila@lille-login2 ~]$ module avail

------------------------------- /share/apps/modules/all/Core --------------------------------
   EasyBuild/3.3.0        Go/1.8.1             foss/2017a                      (D)
   FLUENT/18.0            Java/1.8.0_92        icc/2017.1.132-GCC-6.3.0-2.27
   FLUENT/18.2     (D)    MATLAB/2016b         ifort/2017.1.132-GCC-6.3.0-2.27
   GCC/4.9.3-2.25         MATLAB/2017a  (D)    intel/2017a
   GCC/5.4.0-2.26         foss/2016a
   GCC/6.3.0-2.27  (D)    foss/2016b

------------------------------ /share/apps/modulefiles/Core ---------------------------------
   easybuild/2.9.0    gcc/6.2.0        matlab/R2016b
   gcc/4.9.4          gcc/6.3.0 (D)    python/2.7.3

  Where:
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the
"keys".
```

Modules

Modules have dependencies: for example openmpi cannot be loaded unless a compiler has been loaded already:

```
[aurelila@lille-login2 ~]$ module load openmpi
Lmod has detected the following error:  These module(s) exist but cannot be
loaded as requested: "openmpi"

   Try: "module spider openmpi" to see how to load the module(s).
```

Load gcc first:

```
[aurelila@lille-login2 ~]$ module load gcc openmpi
```

You can add this line in your shell profile or write a script to do it.

Batch scheduler/Queuing system

To schedule jobs run by users, a queueing system is installed on supercomputers:

- each job submitted is appended to the queue with a given priority,
- then launched when reaching the top of the queue (`training` on Lille),
- status (success/failure) is reported accordingly,
- computational time n core.hour is charged to the project (maximum resource is 20 processes on 2 nodes).

A simple job:

```
echo "sleep 30;echo hello world"|qsub -q training \
  -W group_list=itea_lille-tma4280 \
 -lselect=2:ncpus=20:mpiprocs=20
```

Batch scheduler/Queuing system

The status of the training queue can be inspected:

```
[aurelila@lille-login2 ~]$ qstat -Q training
Queue              Max   Tot Ena Str   Que   Run   Hld   Wat   Trn   Ext Type
---------------- ----- ----- --- --- ----- ----- ----- ----- ----- ----- ----
training             0     0 yes yes     0     0     0     0     0     0 Exec
```

The status of jobs for a given username can be displayed:

```
[aurelila@lille-login2 ~]$ qstat -u username
```

Running jobs on Lille

After compiling your program, you have to write a *job script*. Example (the *pi* program):

```
#!/bin/bash

#PBS -N pi
#PBS -A itea_lille-tma4280
#PBS -W group_list=itea_lille-tma4280
#PBS -l walltime=00:01:00
#PBS -l select=2:ncpus=20:mpiprocs=16

cd $PBS_O_WORKDIR
module load openmpi
mpiexec ./pi 1000000
```

Running jobs on Lille

```
#PBS -N pi
```

My job is called “pi”.

```
#PBS -A itea_lille-tma4280
```

The time spent executing this job should be charged to `itea_lille-tma4280`.

```
#PBS -l walltime=00:01:00
```

The walltime limit for this job is one minute.

```
#PBS -l select=2:ncpus=20:mpiprocs=16
```

I want two units of 20 CPUs each (two nodes, that is) and I want 16 processes on each of them (32 in total). On Lille, `ncpus` should *always* be equal to 20.

Running jobs on Lille

```
cd $PBS_O_WORKDIR
```

Ensure that we are in the correct directory. This should always be in your job script.

```
module load openmpi
```

Make sure the `openmpi` module is loaded so that the `mpiexec` command is available to run MPI programs.

```
mpiexec ./pi 1000000
```

Run the program.

Running jobs on Lille

Submit a job using `qsub`:

```
qsub job.sh
5723717.service2
```

`qsub` will reply with a job ID number. You can ask for the status of your job with

```
qstat -f 5723717.service2
```

or see a list of all jobs running and queued

```
qstat
```

Running jobs on Lille

When the program has completed, the accumulated output will be written to files in the same folder you launched it from.

```
ls
job.sh   pi   pi.c   pi.e5723717   pi.o5723717
```

The e-file contains stderr (empty?) and the o-file contains output from stdout (the most interesting one).

```
cat pi.o5723717
Agent pid 21651
pi=3.141593e+00, error=8.437695e-14, duration=2.177000e-03
Start Epilogue v3.0.1 Wed Jan 27 14:18:27 CET 2016
clean up
End Epilogue v3.0.1 Wed Jan 27 14:18:28 CET 2016
```

Other PBS options

```
#PBS -o stdout
#PBS -e stderr
```

I want my output files to have more sensible names.

```
#PBS -m abe
```

I want an e-mail notification when the job starts (`b`), ends (`e`) or if it aborts (`a`).

```
#PBS -M some@where.com
```

. . . and this is where that e-mail should be sent to.

```
#PBS -l ...:ompthreads=16
```

for 16 OpenMP threads per process.

See https://www.hpc.ntnu.no/display/hpc/PBS+Professional

More information

The NTNU HPC Wiki has a very good user guide.

https://www.hpc.ntnu.no/display/hpc/User+Guide