Monash eResearch Centre

MonARCH Welcomes Students from the FIT3143 Parallel Computing Course

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Learning Outcomes

1. Better understanding of HPC
    a. how to access MonARCH system
    b. what do you need installed to access a compute cluster
    c. account information, initial password, and signing into MonARCH
2. Basic Linux and Job Submission
    a. navigation, file management, directory management
    b. $HOME and Project Folders on MonARCH
    c. running the text editor
    d. managing data transfers
3. How to use a compute cluster
    a. basic concepts
    b. SLURM commands
    c. submitting your first job, checking results
4. Further reading

Introduction to High-Performance Computing

- High-performance computing is about employing the best and cost-effective technologies, from processors, storage and networks, to provide aggregated computational capabilities beyond what is typically available to the end-user
- HPC versus HTC
  - high-performance -- running a single program as quickly as possible
  - high-throughput -- running many independent programs as quickly as possible
- HPC/HTC is predominantly achieved by one or more compute clusters
- HPC/HTC are enabling technologies for larger experiments, more complex data analyses, achieving higher accuracy in computational models

Introducing MonARCH

MonARCH (Monash Advanced Research Computing Hybrid)

- university cluster for high-performance/high-throughput computing
- open for access to Monash researchers and collaborators
- hosts courses in Chemistry, Engineering and FIT that require access to advanced tools or hardware, like lots of CPU cores, or GPU devices
- made up of over 83 servers connected via a fast network
- runs on top of the Monash internal cloud
- over 233 active users in the past 90 days
- 40-50 active users who together run 400-500 calculations at once

What you need to access MonARCH

On Windows you will need two applications:

- an **`ssh`** client
  - `putty`
    - https://the.earth.li/~sgtatham/putty/latest/w64/putty.exe
  - MobaXterm
    - https://download.mobatek.net/2032020060430358/MobaXterm_Portable_v20.3.zip
- a secure copy client (for data file transfers)
  - `WinSCP`
    - https://winscp.net/download/WinSCP-5.17.7-Portable.zip
  - `FileZilla` (choose the appropriate OS)
    - https://filezilla-project.org/download.php?show_all=1

On Linux and Mac OS systems, the commands **`ssh`** and **`scp`** are pre-installed
FileZilla is available on these platforms

Where to get info about my MonARCH Account

FIT3143 staff and students are assigned individual user accounts on MonARCH; and your user account is distinct from your Monash username.

Your Monash username is the word before the @ in your email address, e.g.:

```
abcd0001@student.monash.edu
```

Use **+** on MobaXterm => new connection => enter this as the address:

```
118.138.234.199
```

When prompted for a username, enter your Monash username; then enter you **MyMonash** password.   Read the message displayed.

Logging into the MonARCH cluster

Keep your password secure, do not share this with anyone.

By now, you should know your assigned MonARCH (HPC) username:

it is prefixed by “`fit`” followed by three decimal digits, e.g., `fit015`

On MobaXterm, create a new connection using this address:

`monarch.erc.monash.edu`

with your assigned HPC username (e.g., `fit015`) and then enter your given password.

On successful SSH access into MonARCH

You will see a “`Welcome to MonARCH`” MOTD (message-of-the-day)

If there are any updates on cluster availability, we will be posting the information on the MOTD.

Below the MOTD, you should see a command prompt, e.g.,

```
[fit015@monarch-login1 ~]$
```

awaiting your textual commands.

```
************************************************************
* Welcome to MonARCH                                       *
*                                                          *
* For assistance, please contact: mcc-help@monash.edu      *
* Documentation: https://docs.monarch.erc.monash.edu       *
************************************************************

  - Useful SLURM Commands:
     squeue
     SQ                       for extended info on jobs
     sbatch <slurm_script_file>
     scontrol show job <JOBID>
     scancel <JOBID>

  - M3/MonARCH User Scripts:
     show_job
     show_job <JOBID>
     show_cluster

************************************************************
Please limit CPU-intensive processes on this login node
to a maximum of 20 minutes. Please use the sbatch command
to submit longer processes to the queue. There is a short
partition for jobs that take a maximum of 24 hours.
************************************************************

NOTE: Your respective $HOME folders are currently backed-up.
The Lustre project & scratch folders are NOT backed-up.
Please ensure that you keep a copy of IMPORTANT data
outside of MonARCH. We will soon support Lustre backups.

************************************************************
```

First Commands on MonARCH

You are now within your "home folder", we call `$HOME`, also called `~`

First commands:

`pwd`	-	displays the working directory (where you are)
`echo $HOME`	-	try this command and compare its output with above
`date`	-	display the system date and time
`cal 2019`	-	show the calendar for 2019
`fortune`	-	try this
`clear`	-	clears the terminal window
`passwd`	-	change your MonARCH password (do this soon)

Introducing MonARCH

- “CPU-only” nodes (three configurations)
- “GPU” nodes (two configurations)
- 1,476 physical CPU cores
- over 400 TB of Lustre storage
- compute nodes are virtual machines on the Monash Research Cloud

Login node: `monarch.erc.monash.edu`

`monarch-login1.erc.monash.edu`

`monarch-login2.erc.monash.edu`

Data Transfer: `monarch-dtn.erc.monash.edu`

Docs: `https://docs.monarch.erc.monash.edu`

```
show_cluster
```

```
gf01          K80      gpu    18   206   3   Running
gp01          P100     gpu     0   153   0      Busy
gp02          P100     gpu     0   142   0      Busy
gp03          P100     gpu     0   166   0      Busy
hs03          CPU    short     0     1   0      Busy
hs04          CPU    short     0    34   0      Busy
hs05          CPU    short     0    34   0      Busy
hs06          CPU     comp     0    54   0      Busy
hs12          CPU     comp     6    63   0   Running
hs13          CPU     comp     0    59   0      Busy
hs14          CPU     comp     0    65   0      Busy
hs16          CPU     comp     0    62   0      Busy
hs17          CPU     comp     0    49   0      Busy
mi00          CPU     comp     4    43   0   Running
mi01          CPU     comp     3    28   0   Running
mi02          CPU     comp     7    10   0   Running
mi05          CPU     comp     4    27   0   Running
mi06          CPU     comp     1    68   0   Running
mi07          CPU     comp     0    11   0      Busy
mi08          CPU     comp     0    26   0      Busy
mi09          CPU     comp     0    21   0      Busy
mi11          CPU     comp     2     7   0   Running
mi12          CPU     comp     6    68   0   Running
mi14          CPU     comp     0    12   0      Busy
mi15          CPU     comp     4    30   0   Running

                         Summary:
+------------+------------+------------+------------+------------+
|            | CPUS       | Nodes      | K80 GPUs   | P100 GPUs  |
|------------+------------+------------+------------+------------|
| Available  | 89   ( 6%) | 0    ( 0%) | 6    (25%) | 0    ( 0%) |
| In Use     | 1255 (85%) | 53   (91%) | 2    ( 8%) | 6    (50%) |
| Down       | 132  ( 9%) | 5    ( 9%) | 16   (67%) | 6    (50%) |
| Reserved   | 0    ( 0%) | 0    ( 0%) | 0    ( 0%) | 0    ( 0%) |
| ---------- | ---------- | ---------- | ---------- | ---------- |
| Total      | 1476       | 58         | 24         | 12         |
+------------+------------+------------+------------+------------+
```

Files, Directories and Paths

In Unix/Linux, everything is a file; even a directory is just a special file.

Each file on the system is identifiable by its absolute path.

A path is a string that specifies the name & location of a file (or directory); it consists of characters separated by zero or more / ("forward slash" character)

Examples of absolute paths:

are there relative paths?

```
/home/fit014
/usr/local/dos2unix/7.4.0/bin/dos2unix
/mnt/lustre/projects/fs19/tutorial/rawimages
```

Further reading: https://en.wikipedia.org/wiki/Path_(computing)

Files, Directories and Paths (relative paths)

A relative path is one that does not have a leading / ("forward slash" character)

Each file on the system is identifiable by its absolute path. Any absolute path can also be specified as a relative path.

Examples of relative paths:

```
python           ?≡?  ./python
bin/dos2unix      ≡   ./bin/dos2unix
./fs19/tutorial/demo.zip
```

two special relative paths:

.	-	this directory
..	-	the parent directory

Use of relative paths in your program **can break your access to data** if the program is run from another folder on the system.

Your personal and project spaces on MonARCH

`${HOME}`	-	your personal $HOME directory
		good for source codes, configuration files, etc.
		not good for HPC with lots of data
`${HOME}/fs19`	-	shortcut to the project folder for FIT3143
	-	a symbolic link to absolute path `/mnt/lustre/fs19`
`${HOME}/fs19/${USER}`	-	your personal project space
	-	prepare and submit your jobs within this folder
	-	accessible only to you & your lecturer/tutors
	-	Note: `/mnt/lustre` sits on the fast parallel FS

Basic Navigation and Directory Management

`ls`	-	list the file names in current directory
`mkdir` *path*	-	create an empty directory
`rmdir` *path*	-	removes an empty directory
`cd` *path*	-	change into the given path/directory
`cd ..`	-	change into the enclosing directory
`cd`	-	change into your `$HOME` directory
`tree`	-	visualise the directory structure

Or try this sequence:

```
cd; mkdir A; cd A; mkdir a b c; cd; tree
```

Something to try:

```
cd
mkdir 2019
ls
cd 2019
mkdir jan feb mar
ls
cd jan
mkdir wk1
cd ../mar
mkdir wk1
cd ../feb
mkdir wk1 wk2
cd
tree
```

Navigating your way within MonARCH

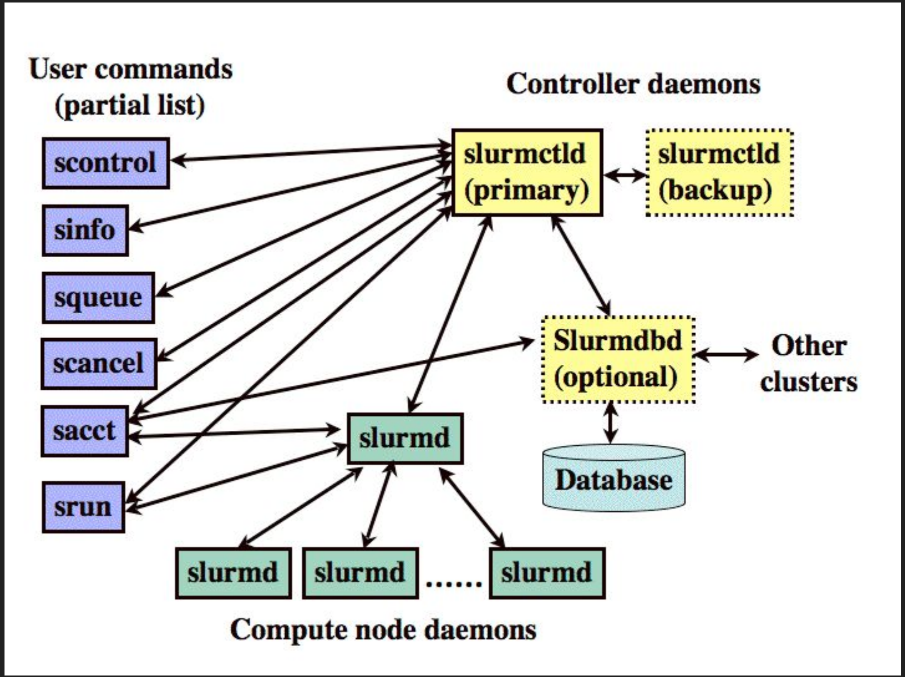
Key commands:

`cat` *path*	-	displays the contents of *path* (try this on a folder?)
		be careful running this on a binary file
`cp` *src dest*	-	makes a copy of *src* into *dest* (both are paths)
`mv` *src dest*	-	moves or renames files (or folders)
`rm` *path*	-	permanently deletes the given file
`ls -l`	-	long directory listing (equivalent shortcut `ll`)
`cd`	-	go back `$HOME`
`cd` *path*	-	change into the given path / folder

SLURM Scheduler

MonARCH uses SLURM as its resource manager and job scheduler:

- fair share scheduling policy
- no fixed CPU allocation, jobs are prioritised based on history of usage



Source: https://slurm.schedmd.com/overview.html

Interacting with the SLURM Job Scheduler

`sbatch jobscript.sh`	- to submit a job for batch execution; returns the unique JobID if successful
`squeue -u ${USER}`	- to display the status of my jobs on the queue
`scontrol show job` *{jobid}*	- to check the status of a job and other details
`sacct -j` *{jobid}*	- to check the accounting information of a given job
`scancel` *{jobid}*	- to delete a job that you own given its unique JobID
`scancel -u ${USER}`	- to delete all your jobs on the cluster

Commands unique to MonARCH:

`sq`	- this is a convenient shortcut to “**`squeue -u ${USER}`**”
`SQ`	- detailed listing of all user jobs (useful to determine job position in the queue)
`show_cluster`	- to see the status of all nodes on the cluster

Submitting your first sample job

1. Change to your project folder:

```
cd ~/fs19/${USER}
pwd
```

2. Make a copy of the demo.zip:

```
cp ../tutorial/demo.zip .
ll
```

3. Unzip the file and cd into `demo`:

```
unzip demo.zip
ll
cd demo
```

4. Submit the “demo.job”:

```
sbatch demo.job
sq
```

5. Check for output:

```
ll
tree
cat slurm*.out
```

6. View any one of the output JPEGs:

```
cd blackwhite
display filename
cd ../sharpened
```

MPI job script template *(when running all 8 mpi processes on one node)*

```
#!/bin/bash
#SBATCH --job-name=np_8_job       ### name your job
#SBATCH --time=00:30:00           ### hh:mm:ss or dd-hh:mm:ss
#SBATCH --mem=32G                 ### set this to 8 ntasks x 4 GB
#SBATCH --ntasks=8                ### launch one python process
#SBATCH --cpus-per-task=1         ### single-threaded processes
#SBATCH --ntasks-per-node=8       ### set this to ntasks if ntasks <= 16
#SBATCH --account=fit3143         ### SLURM setting
#SBATCH --reservation=fit3143     ### reserved nodes

module load openmpi/1.10.7-mlx
srun path-to-mpi-executable
```

1/2 hours max per job

1 cpu max per task

Active as of 27/08/2020

one running max per user

MPI job script template *(same 8 processes but on two nodes)*

```
#!/bin/bash
#SBATCH --job-name=np_32_job      ### name your job
#SBATCH --time=00:30:00           ### hh:mm:ss or dd-hh:mm:ss
#SBATCH --mem=32G                 ### memory setting is max @ 4 GB per core
#SBATCH --ntasks=8                ### launch one python process
#SBATCH --cpus-per-task=1         ### single-threaded processes
#SBATCH --ntasks-per-node=4       ### four per node
#SBATCH --account=fit3143         ### SLURM setting
#SBATCH --reservation=fit3143     ### reserved nodes

module load openmpi/1.10.7-mlx
srun path-to-mpi-executable
```

32 tasks is the current max per job

1/2 hours max per job

8 tasks for this job

1 cpu max per task

4 tasks per node, two nodes

Active as of 27/08/2020

one running max per user

MPI job script template *(beyond 16 cores, you need two nodes)*

32 tasks is the current max per job

```
#!/bin/bash
#SBATCH --job-name=np_32_job      ### name your job
#SBATCH --time=00:30:00           ### hh:mm:ss or dd-hh:mm:ss
#SBATCH --mem=32G                 ### memory setting is max @ 4 GB per core
#SBATCH --ntasks=32               ### launch one python process
#SBATCH --cpus-per-task=1         ### single-threaded processes
#SBATCH --ntasks-per-node=16      ### this is the max as each node has 16 cores only
#SBATCH --account=fit3143         ### SLURM setting
#SBATCH --reservation=fit3143     ### reserved nodes

module load openmpi/1.10.7-mlx
srun path-to-mpi-executable
```

1/2 hours max per job

32 tasks max per job

1 cpu max per task

Active as of 27/08/2020

one running max per user

MPI + OpenMP job script template *(4 MPI processes on two nodes)*

16 cpu cores allocated to this job, 8 cores per node

```
#!/bin/bash
#SBATCH --job-name=mpi_omp_4x4_job    ### name your job
#SBATCH --time=00:30:00               ### hh:mm:ss or dd-hh:mm:ss
#SBATCH --mem=32G                     ### memory setting is max @ 4 GB per core
#SBATCH --ntasks=4                    ### launch one python process
#SBATCH --cpus-per-task=4             ### multi-threaded processes
#SBATCH --ntasks-per-node=2           ### two processes per node
#SBATCH --account=fit3143             ### SLURM setting
#SBATCH --reservation=fit3143         ### reserved nodes

module load openmpi/1.10.7-mlx
srun path-to-mpi-executable
```

1/2 hours max per job

4 tasks for this job

4 cpu per mt process

2 tasks per node, two nodes

Active as of 27/08/2020

one running max per user

MPI Demo Hello World Job

Self study and further reading

Install WinSCP or FileZilla and download/upload files into MonARCH

Running a text editor (nedit or nano). Alternatively, you may edit a file from Windows, upload to MonARCH, but will need to run: `dos2unix` to clean up the file.

Please read through the Getting-Started document:

https://docs.google.com/document/d/1Ewa49D00zYk1GK3Lg__ZxR-w0tUepW69U536w-owDZs

How to pick a secure but easy-to-remember password:

https://xkcd.com/936/

Further help with Unix/Linux:

http://www.ee.surrey.ac.uk/Teaching/Unix/

Thank you for your time.

Your questions welcome.

First point of contact ⇒ your tutor/lecturer

For help with cluster-related issues, email:

`mcc-help@monash.edu`

On the subject, please include this tag: `[FIT3143]`