HPC Systems Anatomy & Storage

National Supercomputer Centre (NSC), Linköping University
SNIC-PRACE training
Online @NSC 20th Apr 2021, 10:00 - ca. 15:00
When & Why to use HPC?

HPC = High Performance Computing

- **High number** of simulation or data analysis jobs
- The jobs are **too large** for a desktop/laptop
- Used in most research fields today
  - Numerical weather prediction
  - Climate simulations
  - Flow simulations
  - Materials science
  - Many disciplines within Chemistry, Physics, Biology
  - …
Desktop PC vs HPC

**Tetralith:** 1908 nodes, **Sigma:** 110 nodes

**Work node:**
- 32 cores
- 96 (384) GiB RAM
- Linux
- Omni-Path network, interconnect
- *1 - few users at a time*

**Login nodes:**
- 2 nodes
- Linux
- *Many users*

**Desktop/laptop:**
- 8 cores
- 16 GiB RAM
- Windows, MacOS (Unix), Linux
- *1 user*
Desktop PC vs HPC

Single PC/laptop
- Win, MacOS, -nix
- 1 user - not shared
- “ok” cores
- “ok” RAM
- Newest CPU?
- 1 gamer GPU?

Many nodes w/ fast interconnect
- Linux
- Many users on login nodes - shared
- More cores
- More RAM
- Cost efficient CPU
- Many high-end GPUs?

Note that HPC isn’t always the best or fastest solution… …it depends
@Login Node

- Typical access: using ssh
- For graphics, use ThinLinc
- *Many users* share login node
- Be mindful of login node usage
- Work node access via queue system (Slurm)

Login nodes:
- 2 nodes
- Linux
- *Many users*

https://www.nsc.liu.se/support/getting-started/
Some Basics

- **Linux**, see e.g. guide and forum + Simple **bash** scripting
  - Basic commands: `cd`, `pwd`, `ls`, `mkdir`, `mv`, `grep`, `less`, `cat`, `man`, ...

- **Common tools**
  - Text editors: `vi`, `gedit`, `emacs`, `nano`, ...
  - Plotting graphs: `gnuplot`, `grace`, ...
  - Analysis (basic/complex): `python`, `R`, `Matlab`, ...

- **Useful things**
  - Persistent terminal session: `screen`, `tmux`
  - Check compute usage [NSC]: `projinfo`
  - Check disk usage [NSC]: `snicquota`
Three types of storage areas available:

Personal home folder, /home/username  small 20 GiB

Project storage, owned by PI, /proj/ourstuff  large, >= 500 GiB

Work node local scratch disk (during run)

Heavy input/output  /scratch/local
Large temp. files

https://www.nsc.liu.se/support/storage/index.html
Three types of storage areas available:

- **Personal home folder**, /home/username
  - **Backup?** yes!
  - **Snapshot?** yes!

- **Project storage**, owned by PI, /proj/ourstuff
  - **Backup?** no!
  - **Snapshot?** yes!

- Work node local scratch disk (during run)
  - **Backup?** no!
  - **Snapshot?** no!

**Backup** > slow tape-drive > staff needs to check

**Snapshot** [7 days] > on disk > you can check directly

[https://www.nsc.liu.se/support/storage/snic-centrestorage/recover-deleted-files/](https://www.nsc.liu.se/support/storage/snic-centrestorage/recover-deleted-files/)
Backup your Data

- **Make your own backup** (also of work computer)!
  - Avoid learning it the hard way…
  - Use e.g. `rsync`
    - `$ man rsync`
    - `$ rsync -av username@tetralith.nsc.liu.se:datafolder`
- Your Univ. IT-dep. might help
- Data is **never 100% safe**, always some risk
Files & Folders

Permissions, who can read/write/execute a folder or file?

$ ls -l
-rw-rw-r-- 1 weiol pg_ns 0 Apr 19 20:35 testingfile

[-/d, file/dir], user [rwx], group [rwx], all [rwx]

Change permissions/group/owner using: chmod, chgrp, chown

Tip: Create a link to your project storage:

$ pwd
/home/username
$ ln -s /proj/ourproject/users/username ourproject
$ ls -l
total 1
lrwxrwxrwx 1 username group 26 Apr 18 01:06 ourproject -> /proj/ourproject/users/username
$ cd ourproject
Further Notes

- **Quota**, both file **size & numbers**!
  - Compress: tar and zip  
    ```
    $ tar cfz Results.tar.gz Results
    ```

- Odd sudden failures? Check your quota!  
  ```
  $ snicquota
  ```

- **Center storage:**
  - OK for analysis & post-processing
  - Not for long-term archiving (SNIC)

Univ. IT-dep?
Basic Security

• Unique password (non-trivial, but not overly complicated)

• Suspicion that your account is compromised -> contact NSC
  - Don’t hesitate to contact us!

• Sharing accounts is not allowed (accounts are personal)
  Share files e.g. by managing project memberships and use /proj

https://www.nsc.liu.se/support/security/