UBELIX submit.unibe.ch

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What is a Node?

- Individual "computers" that compose a cluster
  - Similar components
- Different type of nodes
  - Login
  - CPU compute
  - GPU compute
  - Service nodes

Login Nodes (submitXX)

Which commands are tasks for login nodes:

1. ~~python physics_sim.py~~
2. make
3. create_directories.sh
4. ~~molecular_dynamics_2~~
5. tar -xzf R-3.3.0.tar.gz

! no computation on login nodes

UBELIX software

Module environment

- multiple versions of various packages
- Preventing unintended interference
- managed via environment variables
- `$ module avail`
  - List available modules
- `$ module load <module>`
  - Load specific module
- `$ module list`
  - List loaded modules
- `$ module purge`
  - Unload all modules

BioInf Software

Vital-IT provides software for bioinformatics

- `$ module load vital-it`
- `$ module avail`

SLURM

- SLURM kills jobs, which exceed
  - memory or time limits!
  - Smaller and shorter jobs shedule faster
  - Appropriate values must be determined iteratively:

1. Make an elaborate guess for the first run
2. Check runtime and memory usage (mail, sacct)
3. Adapt values for future invocations of the same job.

- To be on the save side, add a (few hours) time and (2G) memory

Q: Where is the Output?

- Default: slurm-.out
- stderr and stdout can be split and file names be specified

Threads vs Tasks

- Threads: (***OpenMP***)
  - Single executable instance
  - Spawn and merge threads
  - **Shared memory**
  - `#SBATCH --cpus-per-task=<nr>`
- Tasks: (*MPI*)
  - Multiple executable instances
  - Communicate with each other
  - Distributed memory/multiple nodes
  - `#SBATCH --ntasks=<nr>`

Transferring Files to/from the cluster

- wget - Download files from the Internet

- Transfer files/folders from/to local desktop/laptop

```
# best practice to pack and compress first:
$ tar -zcf <tar_file> <data>
# scp [option] source destination
[user@local ~] $ scp -r myproject/ <user>@submit.unibe.ch:~/
[user@local ~] $ scp <user>@submit.unibe.ch:~/myproject/result.txt .
```

- `$ rsync -avz <source> <destination>`

- sftp client (GUI), e.g. FileZilla, MobaXterm, . . .

- Different line endings

  - UNIX: `\n` (newline)
  - Windows: `\r\n` (carriage return + newline)

- This might cause a problem!

- Convert Windows text files to UNIX format

  - `$ dos2unix <file>`

- Convert UNIX text files to Windows format

  - `$ unix2dos <file>`