LINUX WORKSHOP

05 RSB Computer Cluster

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Learning Objectives

- Learn the configuration of RSB computer cluster
- Learn the data storage policy of RSB cluster
- Learn the job scheduling system

- Write and run the variant calling pipeline

RSB Computer Cluster

The RSB computer cluster consists of 4 servers, including 2 CPU servers and 2 GPU servers. The servers work together and are controlled and scheduled by SLURM.

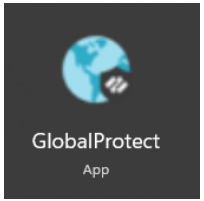
The specs of 4 servers:

1. `dayhoff.rsb.anu.edu.au`
   - 1TB of RAM
   - 196 Cores
   - 100TB of data storage
   - Ubuntu 20.04 Linux
   - GPU, 2 Nvidia A30's
   - DELL PowerEdge R750 + MD1400
2. `fisher.rsb.anu.edu.au`
   - 1TB of RAM
   - 56 Cores
   - 50TB of data storage
   - Ubuntu 20.04 Linux
3. `wright.rsb.anu.edu.au`
   - 1TB of RAM
   - 64 Cores
   - 70TB of data storage
   - Ubuntu 20.04 Linux
4. `thor.rsb.anu.edu.au`
   - 170GB of RAM
   - 80 Cores
   - 9 NVIDIA GeForce RTX 2080
   - Rocky Linux 8.9 (compat with RHEL8)

Assessing RSB servers

To access the RSB server, we need to:

1. Connect to GlobalProtect
2. Connect to server using `ssh` command
3. Using your UID as account name and ANU password



- `ssh (u number)@dayhoff.rsb.anu.edu.au`
- for example ssh u2474733@dayhoff.rsb.anu.edu.au

Welcome message

And you can also see the current usage of the server.

```
  System information as of Tue 25 Feb 2025 04:38:50 PM AEDT

  System load:    28.98              Processes:              2289
  Usage of /home: 83.5% of 106.49TB  Users logged in:        25
  Memory usage:   48%                IPv4 address for eno8303: 150.203.73.37
  Swap usage:     47%

  => /boot is using 97.6% of 973MB
  => There are 6 zombie processes.
New release '22.04.5 LTS' available.
Run 'do-release-upgrade' to upgrade to it.


##############################################################################################

WELCOME TO
 ____                  __              ___    ___
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The Research School of Biology Bioinformatics server.

If you have not received access approval from your supervisor please logout.
For instructions on usage please see the Core user guide here:
https://infrawiki.rsb.anu.edu.au/doku.php?id=rsb_it:infrastructure:userdoco:studentservers

##############################################################################################
Last login: Tue Feb 25 16:32:27 2025 from 10.28.44.187
```

Data storage locations on RSB server

- Home directory: /mnt/data/(server)/home/UID, 100GB per user
- Groups directory: /mnt/data/(server)/home/groups, 500GB per group
- Projects directory: /mnt/data/(server)/home/projects, 250GB per project

Scratch Space: /mnt/data/(server)/home/scratch/…

- No limitation
- Data not backed up
- Files will be deleted after 130 days
- You can store temporary files here

Job Scheduling System - SLURM

A **job scheduling system**, also called **Workload Management System** or **Cluster Management** System, is a software designed to efficiently allocate and manage computing resources in a distributed computing environment.

These systems are commonly used by **high-performance computing clusters**, **data centres**, and other **large-scale computing infrastructures**.

Their primary purpose is to optimise the utilisation of available resources while ensuring **fair access** to those resources for multiple users.

slurm workload manager

PBS Professional®

Job Scheduling System - SLURM

The RSB cluster uses SLURM, which is an open-source project.

The NCI's supercomputer **Gadi** uses PBS Professional. It has a similar syntax to SLURM, and you can quickly learn PBS Pro after you learn SLURM.

slurm workload manager

PBS Professional®

SBATCH script

To submit a job to SLURM, you need to write a SBARCH script which includes a SBATCH header with several settings.

```
#!/bin/bash
#SBATCH --job-name=job_00
#SBATCH --output=/path/to/output/job_00.out
#SBATCH --error=/path/to/output/job_00.err
#SBATCH --partition=Standard
#SBATCH --time=1:00:00                          # [hh:mm:ss]
#SBATCH --mem=5G
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --mail-user=u_id@anu.edu.au
#SBATCH --mail-type=ALL
```

- `job-name` : the name of your job. You can name it anything.
- `output` : path and filename to store the output log file of this job. It contains information that should be printed on the screen.
- `error` : path and filea to store the error log file of this job. It contains all the error messages has in this job.
- `partition` : is the queue you want to submit your job to. It is used to separating jobs to different queues. We only have one partition on the cluster which is called `Standard`, so all the jobs will be submitted to the same queue.
- `time` : time limit for this job. Format in `days-hh:mm:ss`.
- `mem` : RAM size you want to allocate.
- `nodes` : each node is an independent computer. On our cluster, we have 3 nodes which is dayhoff, wright, and fisher. If you are using parallel processing, you may want to separate your sub-jobs to different nodes to spread the workload.
- `ntasks` : the number of tasks included in this job. It is used when doing parallel processing with `srun` command. If there is no `srun` command, your entire script would be 1 task.
- `cpus-per-taks` : number of CPUs you want to allocate for each task.
- `mail-user` : the email address to receive messages.
- `mail-type` : types of messages you want to receive. `ALL` for everything. `BEGIN` for job begins execution. `END` for job finishes. `FAIL` for job fails.

SBATCH script

On the cluster, you have to specify every directory and file from root /.

To use conda environment, write this in your SBATCH script:

```
source /opt/conda/bin/activate /mnt/data/wright/home/[u_id]/.conda/envs/[env-name]
```

The second path is where conda install packages in our environment.

You can use `cd ~/.conda/envs` to see what's inside.

Avoid using `cd` command in the SBATCH script, it sometimes doesn't work.

Submit a job

Let’s save our SBATCH script to “job.sh”. The SBATCH script is also a shell script.

To submit a job, we run `sbatch job.sh`.

Practise

Modify your previous shell script and submit it as a SLURM job.

THANK YOU

Contact Us

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