MedCMU HPC Cheat Sheet

Guide to general Linux and SLURM commands

Accessing raptor MedCMU HPC

Logging in from a terminal

hostname for raptor cluster is 10.128.1.10

```
ssh username@hostname
```

Add -X parameter to display graphical windows

GUI Clients

MobaXterm	SSH/FTP client for windows
SSH FS in VS Code	SSH/FTP client for Windows, MacOS, Linux
FileZilla	FTP client for Windows, MacOS, Linux

File Transfer Commands

Copying an entire directory to a remote server

```
rsync -rvz dir username@hostname:/dir
```

Copying an entire directory from a remote server to local

```
rsync -rvz username@hostname:/dir dir
```

MedCMU HPC Directory

`/home/username`	User's personal home directory (100 GB quota)
`/project/project`	Project directory (1 TB quota)
`/scratch/project`	Temporary space for project use. Files will be automatically deleted 30 days after created (1 TB quota)
`/common`	Shared resources such as databases (read-only access)

Basic Linux File Management

`ls`	Lists files and directories
`pwd`	Print current working directory
`man command`	Displays the manual page for a specific command
`cd dir`	Changes the working directory to dir
`cd ..`	Changes the working directory to parent directory
`cd ../..`	Changes the working directory to the parent directory two levels up
`touch file`	Creates an empty file named file
`cp f1 f2`	Copies file f1 as file f2
`mkdir dir`	Creates a directory named dir
`rm file`	Removes a file named file
`rm -r dir`	Removes a directory named dir and its contents recursively
`mv f1 f2`	Renames file f1 to f2
`mv f1 dir`	Moves file f1 to a directory named dir
`ln -s f1 link`	Creates a symbolic (shortcut) named link that point to f1
`wget url`	Downloads a file from the url
`gzip file`	Compresses file suing GZip
`gunzip file.gz`	Decompress the file file.gz

`tar xzvf \`
`file.tar.gz`
	Extracts the file file.tar.gz

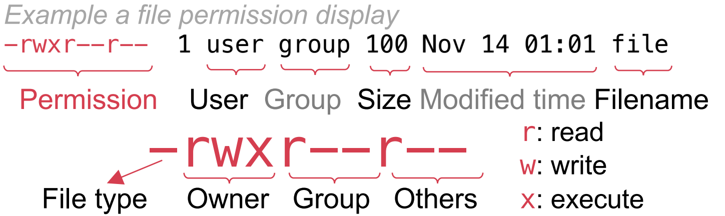
Viewing and Editing Text Files

`cat file`	Prints the entire content of file
`head file`	Displays the first 10 lines of file by default
`tail file`	Displays the last 10 lines of file by default
`grep pattern file`	Searches for lines containing pattern in file and displays

File Permission Commands

`ls -l`	Displays a detailed list of files, including file permissions, ownership, size, and modification date

Example a file permission display



```
-rwxr--r--  1 user group 100 Nov 14 01:01 file
```

Permission User Group Size Modified time Filename

-rwxr--r--

File type Owner Group Others

r: read

w: write

x: execute

`chmod g+rw file`	Grants read and write permissions to the group for the specified file
`chmod -R g+rw dir`	Recursively grants read and write permissions to the group for all files and directories inside the specified dir directory

Environment Modules

`module avail`	Lists all available modules
`module load module`	Loads a specified module in to environment

`module unload \`
`module`
	Unloads a specified module from the environment

`module list`	Lists all currently loaded modules in the environment
`module purge`	Unloads all loaded modules
`ml spider keyword`	Search for modules that matched to specified keyword
`Which cmd`	Displays the location of the executable for the specified cmd
`cmd --help`	Displays information on how to use the specified cmd tool

Mamba Environment

`module load mamba`	Loads the Mamba environment module
`micromamba env list`	Lists all available environments in Mamba

`micromamba activate \`
`env_name`
	Activates the specified environment (env_name)

`micromamba deactivate`	Deactivates active environment
`micromamba info`	Displays current environment and config

`micromamba create \`
`-n env_name \`
`-c conda-forge \`
`package_name`
	Creates environment named env_name by download package_name from conda-forge

`micromamba list`	Lists all installed packages in the active environment

Apptainer (Singularity) container

`apptainer pull \`
`  img.sif \`
`  docker://img:tag`
	Pulls an image from Docker Hub and save it as img.sif

`apptainer shell \`
`  img.sif`
	Starts a shell inside the container img.sif

`apptainer exec \`
`  img.sif cmd`
	Executes command cmd in a container img.sif

`apptainer exec \`
`  --nv img.sif cmd`
	Executes command cmd inside the container img.sif with GPU support

Submit Jobs on the HPC Cluster

RAPTOR Cluster Partitions

Partition	Cores	GPUs	RAM (GB)	Time limit	Workload
short	1	-	8	8 h	Development job for generic application
compute	96	-	1,289	-	Generic application
gpu	96	2	385	-	GPU application

SLURM Job Management

`sinfo`	Displays the status of the cluster and its partitions
`squeue`	Displays the job queue, including waiting and running jobs
`sacct`	Displays job accounting information, such as completed jobs and resource usage

`sbatch \`
`  script.sh`
	Submits a batch script (script.sh) for job execution

`srun cmd \`
`  parameter`
	Runs an interactive job with the specified command (cmd) and its parameters

`scancel job_id`	Cancels the job with the specified job_id

srun and sbatch common options

Option	Short	Description
`--job-name`	`-J`	Assign a memorable name to the job
`--account`	`-A`	Account to charge the job's usage to
`--partition`	`-p`	Partition to run the job on
`--cpus-per-task`	`-c`	Number of cores each task will use
`--mem`		Memory required per node
`--mem-per-cpu`		Memory required per core
`--ntasks`	`-n`	Number of tasks to start (Each task uses at least one core)
`--nodes`	`-N`	Minimum number of nodes Each node needs to run at least one task.
`--time`	`-t`	Time limit (wall time) in `dd-hh:mm:ss` format
`--gpus`	`-G`	GPU card that you want
`--x11`		Allow applications to use graphics
`--pty`		Run an interactive application
`--output`	`-o`	File name for job output
`--error`	`-e`	File name for job errors
`--mail-user`		Send email alerts to the specified user for job state changes
`--mail-type`		Send an email for events: BEGIN: Job stars END: Jobs finishes normally FAIL: Job encounters a problem ALL: All of the above

Example sbatch Script

File: SeqQuanlity.sbatch

```
#!/bin/bash

#SBATCH --job-name=DemoSeqQuality
#SBATCH --partition=short
#SBATCH --time=1:00:00
#SBATCH --cpus-per-task=1
#SBATCH --mem=8G
#SBATCH --mail-user=email@cmu.ac.th
#SBATCH --mail-type=END
#SBATCH --output=DemoSeqQuality_%j.out
#SBATCH --error=DemoSeqQuality_%j.err

module load fastqc
mkdir qc
fastqc -o qc /common/demo/*.fastq.gz
```

Example of interactive job

Run bash interactive mode

```
srun --pty bash
```

Run python with interactive mode

```
module load python

srun -p short -t 1:00 --mem=1G \
  -c 1 -n 1 --pty python
```

Run apptainer with interactive mode with 1 GPU

```
module load apptainer

srun -p gpu -G 1 \
  apptainer exec --nv img.sif cmd params
```

Check allocated and usage resource

`myquota`	Displays data storage quota
`sbalance`	Displays computing quota

MedCMU HPC Documentation and Support

Website	https://cmu.to/medcmu-hpc
Email	nattawet.sri@cmu.ac.th
Booking consult	https://cal.com/nattawet-sri/30min