T001 - Basic HPC Linux

DICC

UNIVERSITI MALAYA

Session Outcomes

- Understand the difference between personal computers and HPC.
- Understand some basic components in computer system.
- Understand the concept within HPC environment.
- Understand the difference between Linux and other Operating System.
- Understand about how various stuffs in Linux work in general.
- Understand the different commands used in Linux to perform different tasks.

Software Required for This Session

Operating System	System Built-in	External Installation
Windows OS	`cmd` `powershell`	PuTTY MobaXTerm
Linux	`terminal`	
macOS	`terminal`	iTerm2

What is High Performance Computing (HPC)?

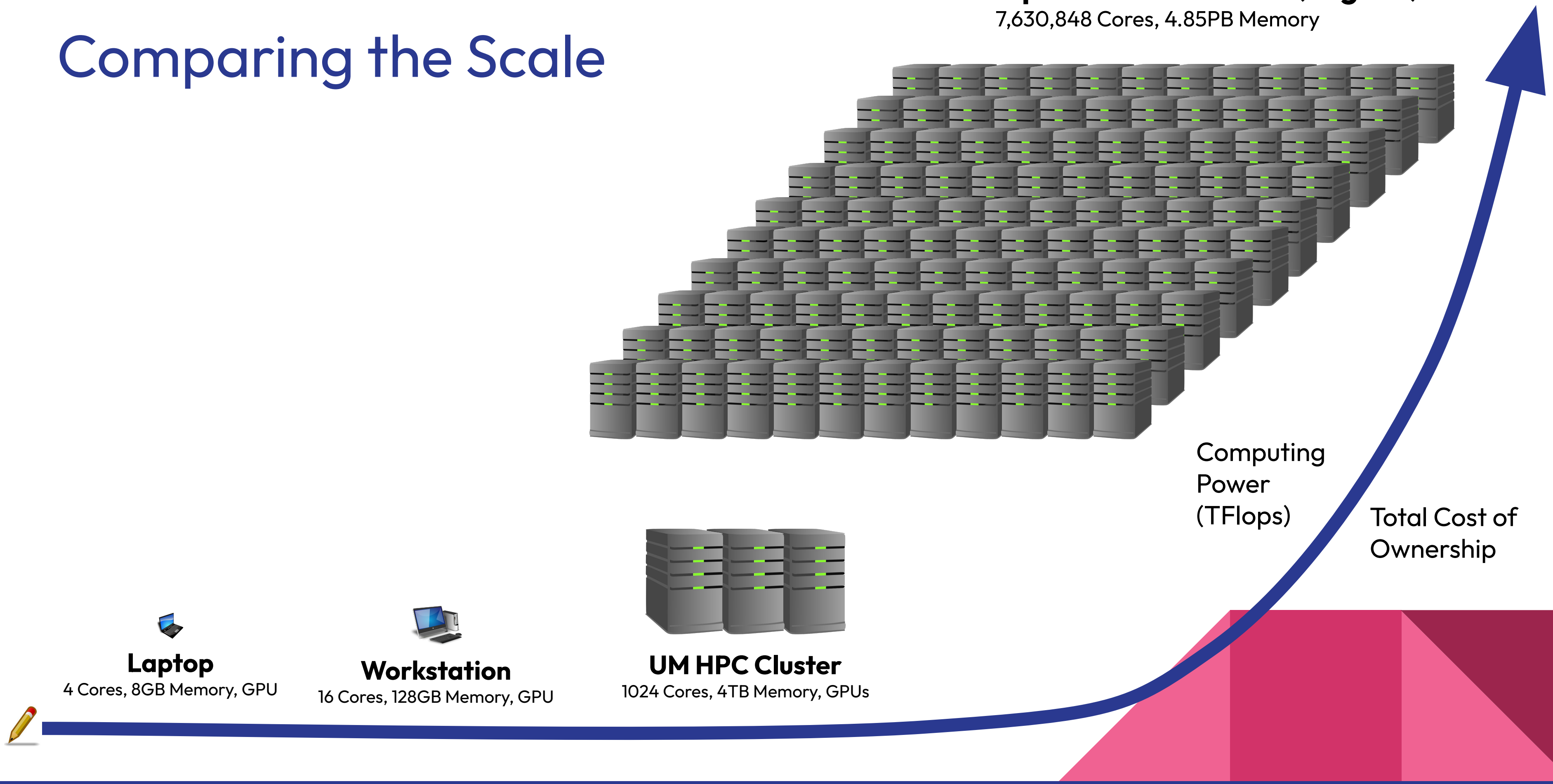
Workstation/Desktop/Laptop

Portable, affordable but limited computing power.

HPC Cluster

More investments and costs, but can be much more powerful.

Comparing the Scale



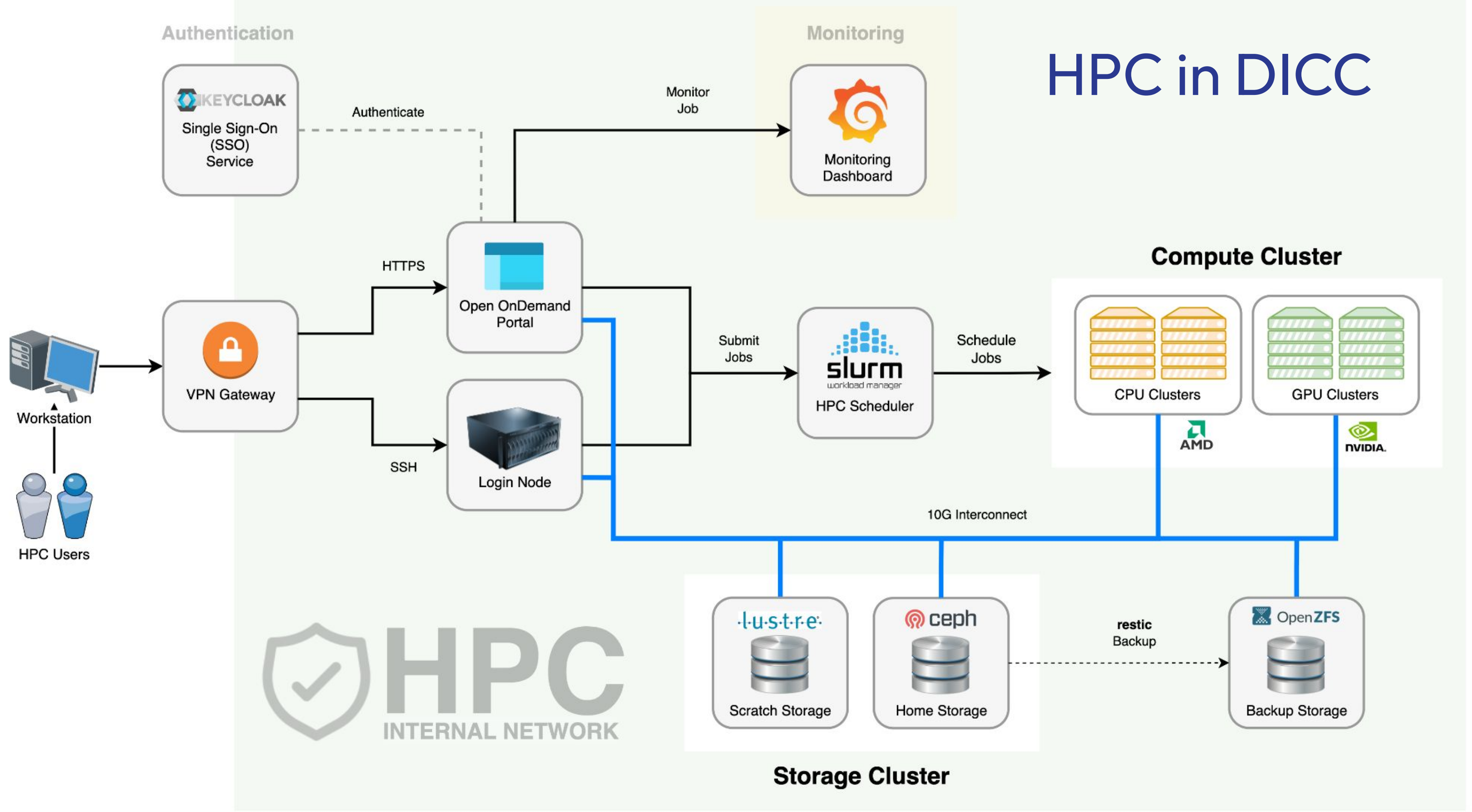
World Top HPC Data Center (Fugaku)
7,630,848 Cores, 4.85PB Memory

UM HPC Cluster
1024 Cores, 4TB Memory, GPUs

Workstation
16 Cores, 128GB Memory, GPU

Laptop
4 Cores, 8GB Memory, GPU

HPC in DICC



Authentication
KEYCLOAK
Single Sign-On (SSO) Service
Authenticate
Monitoring
Monitor Job
Monitoring Dashboard
Workstation
HPC Users
VPN Gateway
HTTPS
SSH
Open OnDemand Portal
Login Node
Submit Jobs
slurm workload manager
HPC Scheduler
Schedule Jobs
Compute Cluster
CPU Clusters
GPU Clusters
AMD
NVIDIA
10G Interconnect
lustre
Scratch Storage
ceph
Home Storage
restic Backup
OpenZFS
Backup Storage
Storage Cluster
HPC
INTERNAL NETWORK

Why HPC?

Why do people use HPC?

- **Highly parallel calculation**
  - Can be splitted into multiple small calculations and execute concurrently.
- **Large-scale tightly coupled calculation**
  - Calculation require resources that beyond what a workstation or laptop can supply.
- **Computation require use of GPU**
  - Proven to be able to utilise GPU for massive speedup.

However,

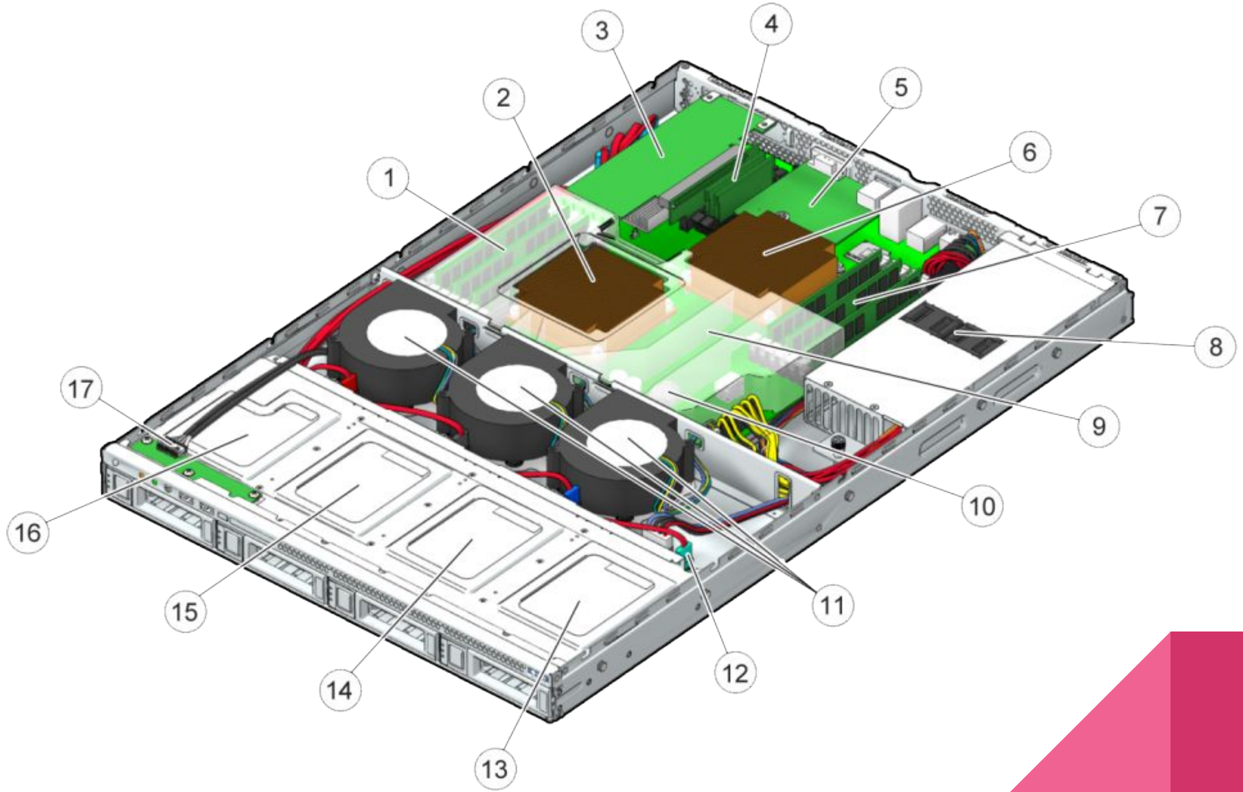
HPC is not the magic solution for everything.

What must you know?

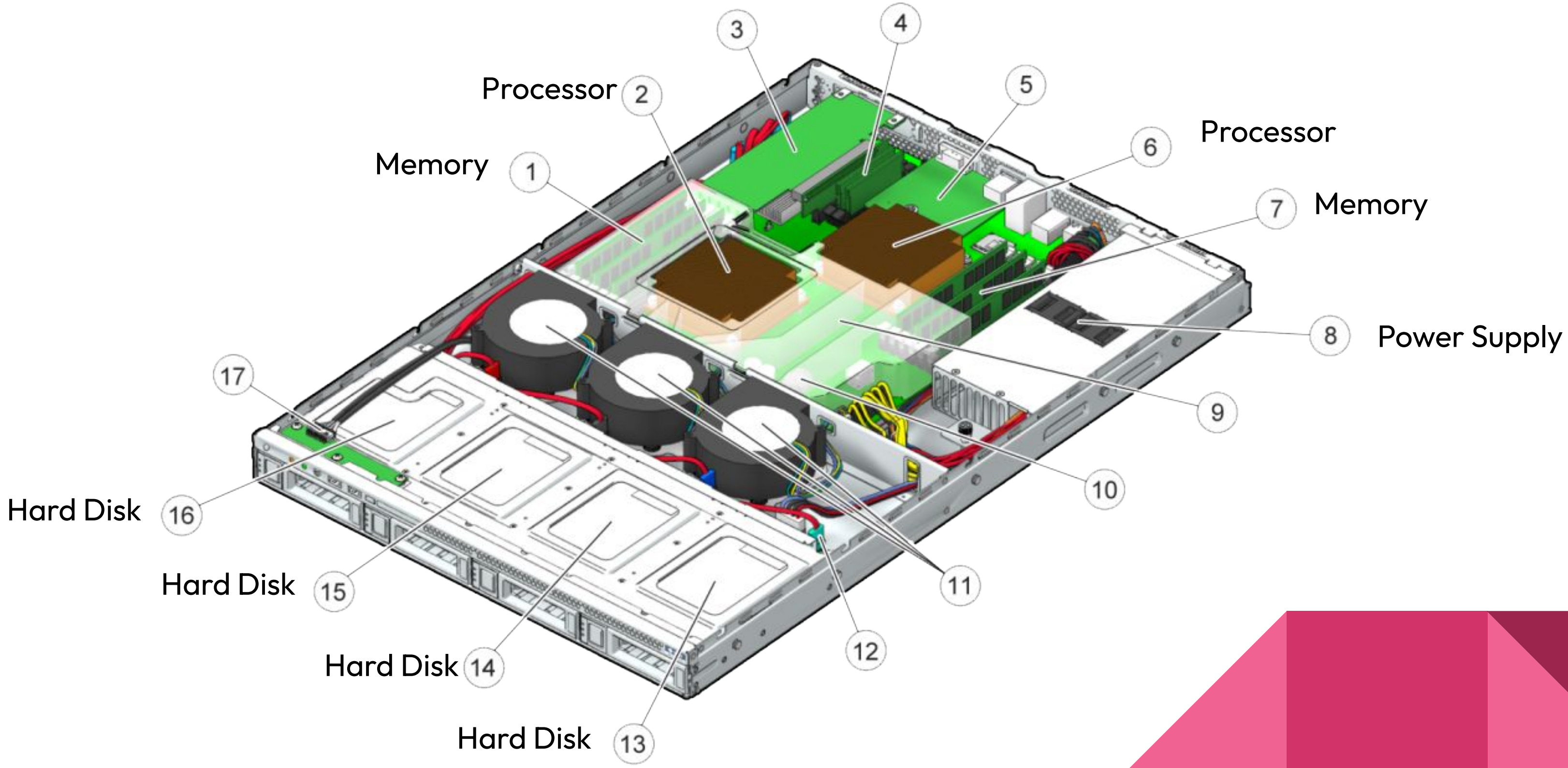
- **Basic Application Understanding**
    - To be able to run and execute your application in the HPC.
- **Basic Computer System Understanding**
    - To understand the resources type in the HPC.
- **Basic Linux Survival Skills**
    - Must have basic Linux knowledge to survive in the HPC environment.

Computer System in Layman

What is inside the Server?

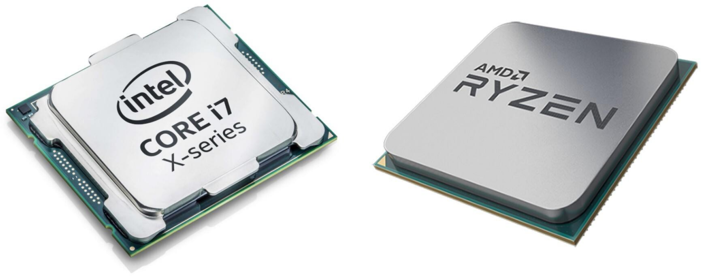


What is inside the Server?



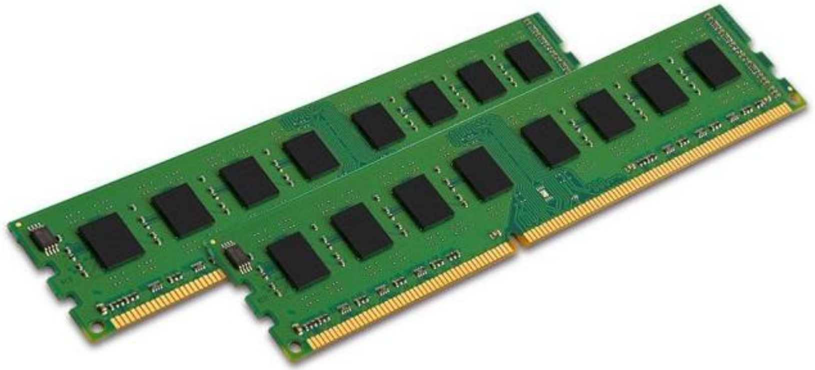
Processor in Layman

- Processor is the brain of any computer system.
  - Core - The processing core in the processor
  - Threads - Number of threads per core
  - Clock Speed - Number of CPU execution per secon
- Consumer Grade Processors:
  - Intel Core i7-1365U (10 Cores) - 5.20 GHz
  - AMD Ryzen 5 5600 (6 Cores) - 4.4 GHz
- Server Grade Processors:
  - Intel Xeon Platinum 8480+ (56 Cores) - 3.80 GHz
  - AMD EPYC 7702P (64 Cores) - 3.35 GHz



Memory in Layman

- Memory is the place where data required for CPU processing is stored.
- Common Memory Size: 1GB - 128GB per memory
- Memory Type: DDR1 - DDR5
- Newer type has lower latency, which mean faster access.
- Larger memory mean more stuff can run concurrently, and larger calculations can be supported.



GPU in Layman

- Super powerful processing unit that can dramatically accelerate additional workloads in high performance computing.
- Usually very expensive.
- Good for graphical processing, AI, accelerated mathematics calculations, and more!
- Example NVIDIA Models:
    - RTX 4090
    - Tesla A100
    - Tesla V100
    - Tesla H100

Storage in Layman

- The location where your files and directories are stored.
- Local Storage:
  - HDD
  - Hybrid-HDD
  - SSD
  - SAS
  - NL-SAS
- Network Storage:
  - NFS
  - Lustre
  - Ceph
  - GlusterFS

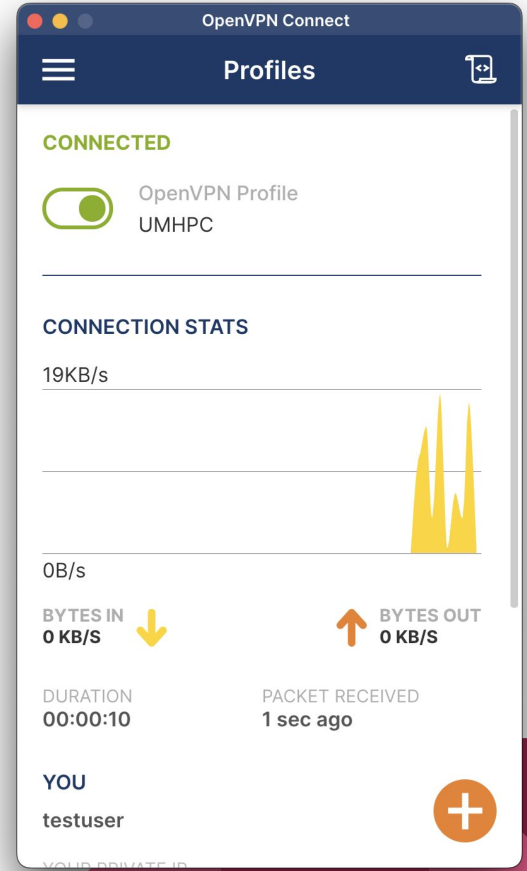
Accessing HPC Login Node

DICC Account

- DICC SSO (sso.dicc.um.edu.my)
    - Update password at DICC SSO.
    - If you forgotten your password, you can also reset your password at DICC SSO.
- Request HPC access at Service Desk.
- **DO NOT SHARE YOUR ACCOUNT !!**

VPN Connection

- Only account with HPC access can establish connection with the VPN gateway.
- Required software:
    - OpenVPN connect client
    - OpenVPN profile
- VPN Gateway:
    - `vpn01.dicc.um.edu.my`
    - `vpn02.dicc.um.edu.my`



CONNECTED

OpenVPN Profile
UMHPC

CONNECTION STATS

19KB/s

0B/s

BYTES IN
0 KB/S

BYTES OUT
0 KB/S

DURATION
00:00:10

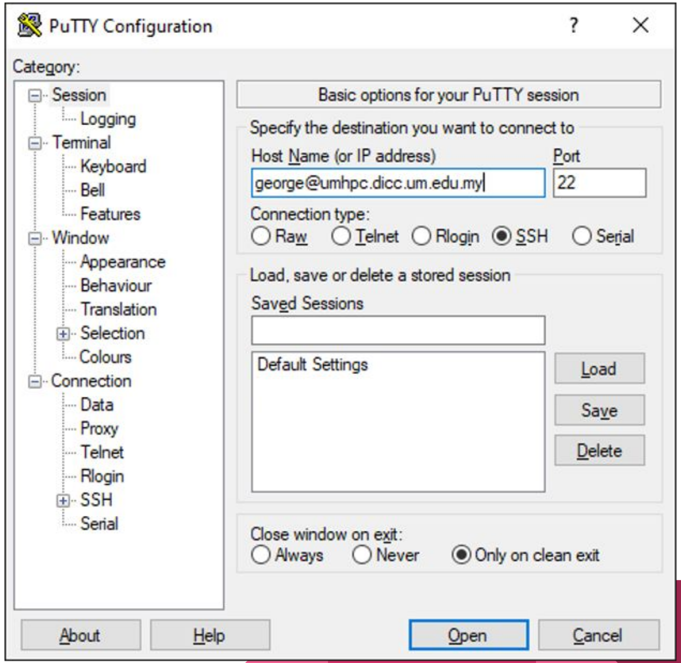
PACKET RECEIVED
1 sec ago

YOU
testuser

Connecting to HPC Login Node

- Windows users:
  - PuTTY / MobaXTerm
- Linux / Mac OS users:
  - Use **`ssh`** command
  - **`ssh username@umhpc.dicc.um.edu.my`**
- Connection details:

Hostname	: **`umhpc.dicc.um.edu.my`**
Port	: **22**
Connection Type	: **SSH**


PuTTY Configuration

Basic options for your PuTTY session

Specify the destination you want to connect to

Host Name (or IP address): george@umhpc.dicc.um.edu.my

Port: 22

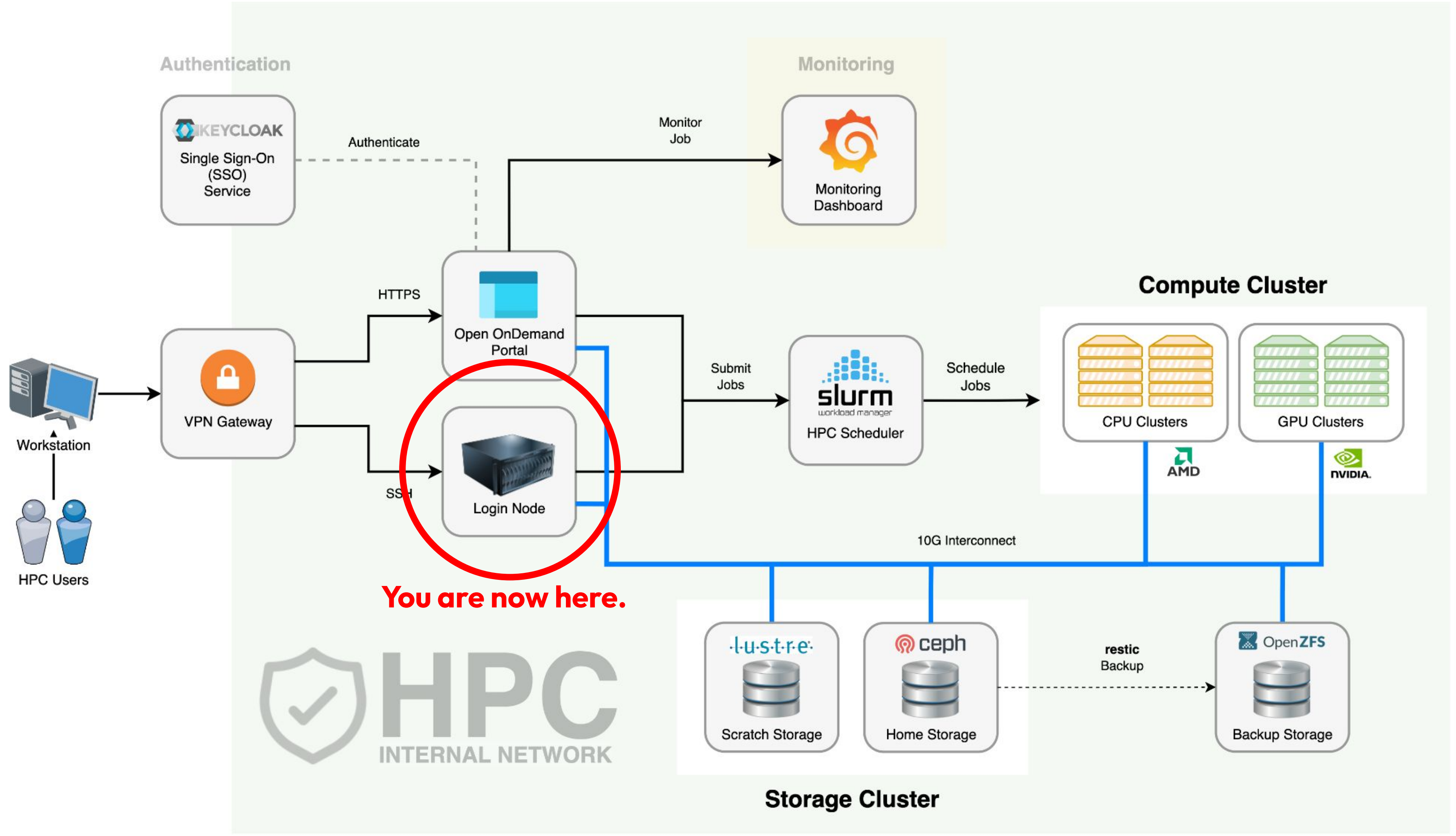
Connection type: Raw Telnet Rlogin [✓ SSH] Serial

Load, save or delete a stored session

Saved Sessions

Default Settings

Close window on exit: Always Never [✓ Only on clean exit]


Authentication
KEYCLOAK
Single Sign-On (SSO) Service
Authenticate
Monitor Job
Monitoring
Monitoring Dashboard
HTTPS
Open OnDemand Portal
Compute Cluster
Workstation
VPN Gateway
Submit Jobs
slurm workload manager
HPC Scheduler
Schedule Jobs
CPU Clusters
GPU Clusters
AMD
NVIDIA
SSH
Login Node
HPC Users
10G Interconnect
You are now here.
lustre
Scratch Storage
ceph
Home Storage
restic Backup
OpenZFS
Backup Storage
HPC
INTERNAL NETWORK
Storage Cluster

Basic Introduction to Linux

CRAY®

a Hewlett Packard Enterprise company

Windows OS

Ubuntu

openSUSE

Linux OS

Rocky Linux

Mac OS

CentOS

CRAY®

a Hewlett Packard Enterprise company

HPE Cray OS

Redhat

Scientific Linux

Kubuntu

What is Linux OS?

- Open source UNIX-like operating system.
- Many distributions and flavours:
  - Fedora
    - RedHat, CentOS, Rocky Linux
  - Debian
    - Ubuntu, Kubuntu
  - SUSE
    - SLES, OpenSUSE
- Widely used in server environments where performance matter.

Fedora Linux in DICC

- Free, open source
- Reliable
- Lightweight
- Allow multiple concurrent connections

CentOS

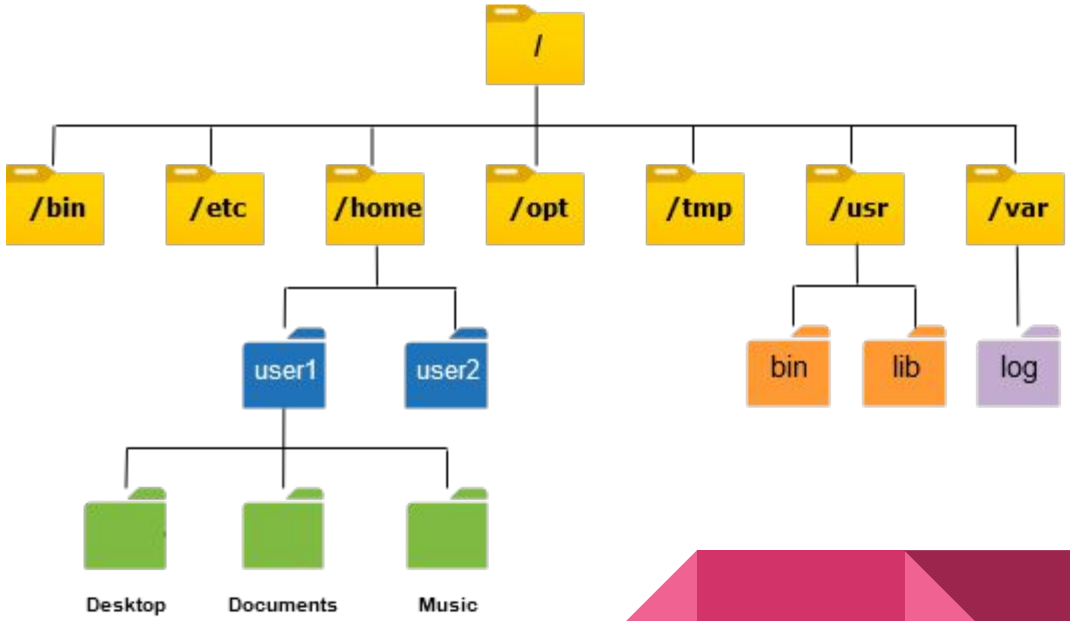
Rocky Linux™

User Roles in Linux

- Super Users
  - System Administrator that can access everything on the system.
- Regular Users
  - Can only access files and directories owned by themselves.
  - All HPC users belongs to this group.
- Service Users
  - System users that are used to run system services.

Directories in Linux

- Tree-like directory structure.
- Everything start with root directory "/":
  - `/home/user/`
  - `/opt/app/exe/`
  - `/tmp/scratch/`
  - `/dev/usb1/`
- No Windows C/D/E drives in Linux OS



Linux Commands

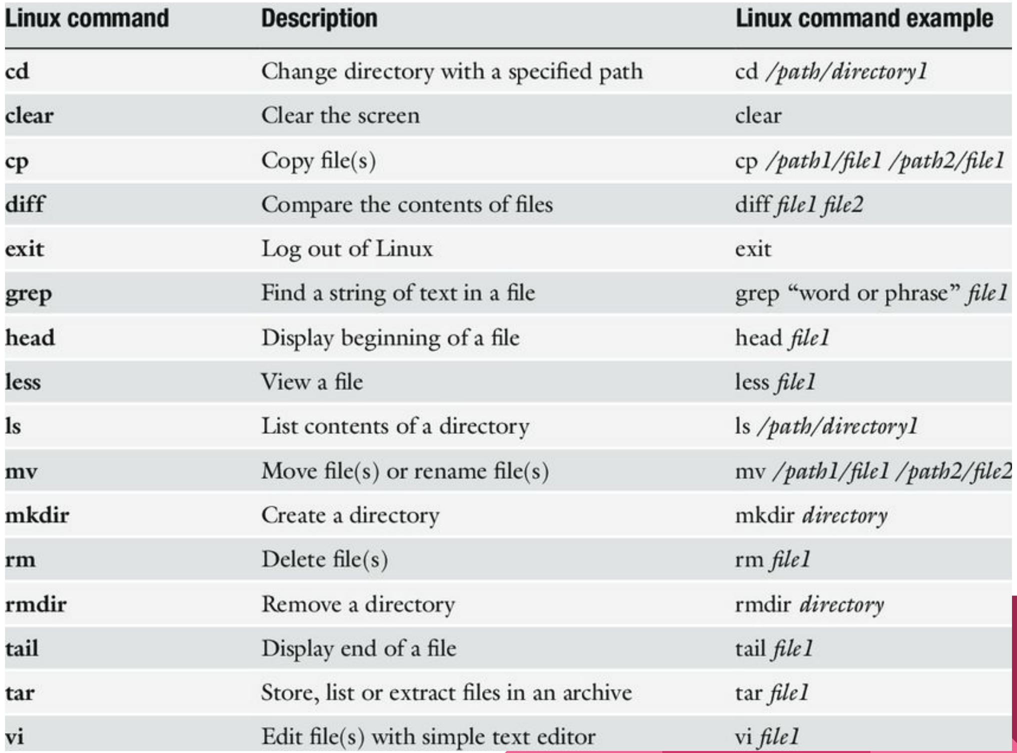
Linux Command Structure

$$\underbrace{\texttt{\$}}_{\texttt{prompt}} \quad \underbrace{\texttt{ls}}_{\texttt{command}} \quad \underbrace{\texttt{[-a] [-b] [-c]}}_{\texttt{option}} \quad \underbrace{\texttt{[arg1] [arg2] [arg3]}}_{\texttt{arguments}}$$

- `ls -lah /home/user/george`
- `cd /tmp`
- `df`

Basic Linux Commands

- Instructions to perform basic actions in Linux.
  - Copy file
  - Move file
  - List directory
  - Navigate to another directory
  - Remove file or directory
  - Create new directory
  - Search for file or directory
- `Ctrl + C` to cancel instruction.



Linux command	Description	Linux command example
cd	Change directory with a specified path	cd */path/directory1*
clear	Clear the screen	clear
cp	Copy file(s)	cp */path1/file1 /path2/file1*
diff	Compare the contents of files	diff *file1 file2*
exit	Log out of Linux	exit
grep	Find a string of text in a file	grep "word or phrase" *file1*
head	Display beginning of a file	head *file1*
less	View a file	less *file1*
ls	List contents of a directory	ls */path/directory1*
mv	Move file(s) or rename file(s)	mv */path1/file1 /path2/file2*
mkdir	Create a directory	mkdir *directory*
rm	Delete file(s)	rm *file1*
rmdir	Remove a directory	rmdir *directory*
tail	Display end of a file	tail *file1*
tar	Store, list or extract files in an archive	tar *file1*
vi	Edit file(s) with simple text editor	vi *file1*

→ clear

Clear Screen

Usage : `clear`

Clear the entire terminal screen output.

Examples :

- `clear`

Command Manual

Usage : `man <command>`

Display the manual for the command, if any.

Examples :

- `man ls`
- `man cd`
- `man touch`
- `man clear`

List Directory Contents

Usage : `ls <destination>`

List information about the files (the current directory by default)

Options :

• `-a`	list all files including hidden files
• `-l`	use long listing format
• `-h`	print sizes in human-readable format
• `-i`	print index number of each file

Examples :

- `ls -lah /tmp`
- `ls -l /opt`
- `ls /home`

Alias for ls command

Usage	:	**`ll <destination>`**
		Alias for `ls -l`.
Options	:	

● `-a`	list all files including hidden files
● `-h`	print sizes in human-readable format
● `-i`	print index number of each file

Examples :

- `ll -ah /tmp`
- `ll /home`
- `ll -h /lustre/user/george`

Navigate to Another Directory

Usage : **`cd <destination>`**

Navigate or move to another directory in the system.

Examples :

- `cd /home/user/george`
- `cd /lustre/user/george`
- `cd /tmp`
- `cd`
- `cd -`
- `cd ~`

Print Working Directory

Usage	:	**`pwd`**
		Print the full path to current directory.
Examples	:	

- `pwd`

Create Directory

Usage	:	**`mkdir <destination>`**
		Create the directory if it does not already exist.
Options	:	
● `-p`		Make parent directories if necessary
Examples	:	

- `mkdir -p /home/user/george/sampledir`

- → clear
- → man
- → ls
- → ll
- → cd
- → pwd
- → mkdir
- → touch

Update File Timestamps

Usage : `touch <filename>`

Update the access and modification times of file to current time.

Will automatically create file if absent.

Options :

`-c`	Do not create file if absent

Examples :

- `touch /home/user/george/empty`

Programmers Text Editor

Usage : `vi <filename>`

Use vi editor to edit the specified file.

Examples :

- `vi /home/user/george/file01`
- `vi /lustre/user/george/file02`

- → clear
- → man
- → ls
- → ll
- → cd
- → pwd
- → mkdir
- → touch
- → vi

Mode Switching in vi Editor

$$\begin{tikzcd} \text{Command Mode (Default)} \arrow[r, shift left, "i"] & \text{Insert Mode} \arrow[l, shift left, "esc"] \end{tikzcd}$$

Command Mode (Default)

`arrow keys`	to navigate
`u`	to undo action
`dw`	to cut word
`yy`	to copy the current line
`dd`	to cut whole line
`P`	to paste before your cursor
`p`	to paste after your cursor
`:w`	to save the file
`:wq`	to save the file and quit
`:q!`	to quit without saving

Insert Mode

- Can only type in Insert Mode

WYSIWYG Text Editor

Usage : `nano <filename>`

Use nano editor to edit the specified file.

Examples :

- `nano /home/user/george/file01`
- `nano /lustre/user/george/file02`

Commands in nano Editor

- WYSIWYG - What you see is what you get
- Useful shortcuts:

`Ctrl + x`	exit
`Ctrl + o`	save
`Ctrl + w`	search
`Ctrl + k`	cut
`Ctrl + u`	paste
`Ctrl + g`	help menu

Print File Content

Usage : `cat <filename>`

Print the contents of the file on the terminal.

Examples :

- `cat /home/user/george/file01`
- `cat /lustre/user/george/file02`

Print Last Part of File

Usage : `tail [-n K] <filename>`

Print the last K lines of the file contents on the terminal.

Print a last 10 lines by default.

Examples :

- `tail /home/user/george/file01`
- `tail -n 25 /lustre/user/george/file02`

Inspect File in Scrollable Mode

Usage : `less <filename>`

Inspect the file in a scrollable mode.

Options :

`-S`	Do not wrap lines

Examples :

- `less /home/user/george/file01`
- `less -S /lustre/user/george/file02`

Simple Exercise (Part 01)

Let’s Practise

- Create new directory **`training01`** in your home directory.
- Navigate to the created directory.
- Create a file named **`data.txt`** with following content using your desired text editor:

```
I have some sample data.
I have more sample data.
I have even more sample data.
```

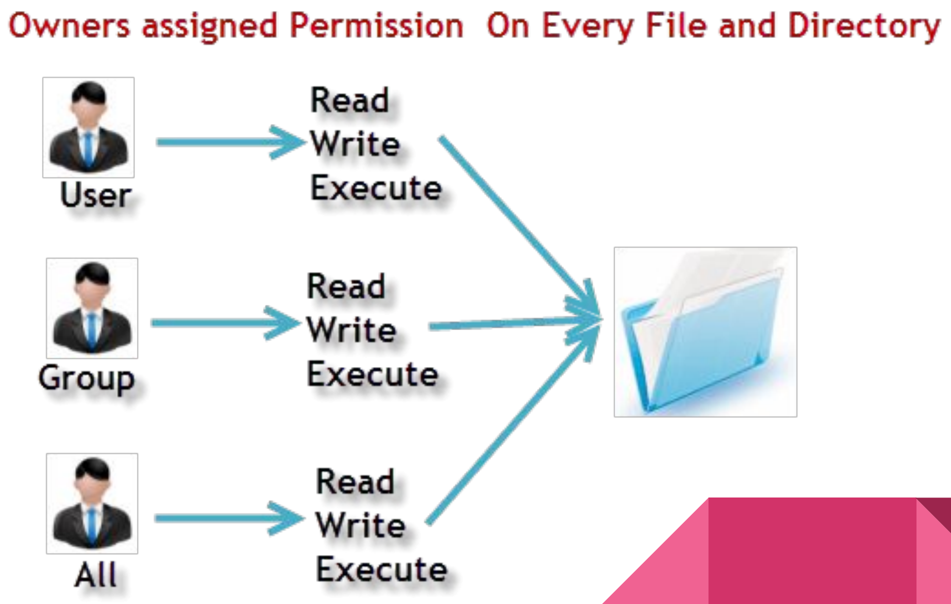
- Check the content of current directory and ensure **`data.txt`** present.
- Print out the content of the **`data.txt`** and verify.

- ❏ `mkdir ~/training01`
- ❏ `cd ~/training01`
- ❏ `nano data.txt` or `vi data.txt`
- ❏ `ls -l` or `ll`
- ❏ `cat data.txt` or `less data.txt`

File Permissions and Ownership

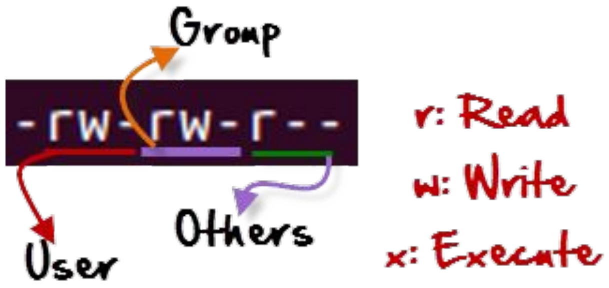
File Permissions and Ownership in Linux

- **File Ownership**
  - User
  - Group
  - All
- **File Permissions**
  - Read
  - Write
  - Execute



Example Permissions & Ownership

- User **`john`** is a member of **`alpha`**.
- Can user **`john`** read the content of the files with following permissions?
  - `rwx --- ---    john     john    1.sh`
  - `rw- r-- r--    george   alpha   2.sh`
  - `rwx rwx rwx    william  beta    3.sh`
  - `rwx --- r--    george   alpha   4.sh`



Important !!

DO NOT

set your home directory or scratch directory to permission 777 !!

→ chmod

Changing Permission

Usage : `chmod <permission> <filename>`

Change the permission bits of the file or directory.

Examples :

```
● chmod +x /home/user/george/file01
● chmod 700 /home/user/george/file02
● chmod u=rwx,g=-,o=- /home/user/george/dir01
● chmod 644 /home/user/george/dir02
```

→ chmod

→ chown

Changing Ownership

Usage : `chown [-R] <owner>:<group> <filename>`

Change the owner of the file or directory to another owner and group.

Options :

- `-R` Also include changing the owner for children within the directory.

Examples :

- `chown george:george file.txt`
- `chown george:alpha file.txt`
- `chown george:george dir`
- `chown -R george:george dir_with_files`

Script Execution

Usage : `source <filename>`

Execute script without execution permission bit.

Examples :

- `source example.sh`
- `source dir/example.sh`
- `example.sh`
- `dir/example.sh`

→ chmod
→ chown
→ source

Direct Script Execution

Usage : `./<filename> or <path/to/file>`

Execute script with execution permission bit.

Examples :

- `./example.sh`
- `dir/example.sh`

Copy File

Usage : `cp [-R] <source> <destination>`

Copy file or directory from source to destination.

Options :

• `-R`	Recursively copy directories and files.

Examples :

- `cp file.txt copy_of_file.txt`
- `cp -R dir copy_of_dir`
- `cp dir/* dir2/`
- `cp dir/file.txt dir2/copy_of_file.txt`

Move / Rename File

Usage : `mv <source> <destination>`

Move file or directory from source to destination.

Can also be used to rename file.

Examples :

- `mv file.txt file2.txt`
- `mv dir dir2`
- `mv dir/* dir2/`
- `mv file.txt dir2/`

Remove File / Directory

Usage : `rm <file>`

Remove the specified file or directory

Options :

`-r`	remove directories and their contents recursively
`-f`	ignore nonexistent files and arguments, never prompt
`-i`	prompt before every removal

Examples :

```
rm /home/user/george/test.txt
rm -r /home/user/george/test
```

Linux Shell Variables

- A variable is a character string to which we can assign any value.
- Can contain the following characters:
  - letters (a to z or A to Z)
  - numbers (0 to 9)
  - underscore character (_)
- Example valid variables:
  - `_ALI`
  - `TOKEN_A`
  - `VAR_1`
- Example invalid variables:
  - `2_VAR`
  - `-VARIABLE`
  - `VAR1-VAR2`
  - `VAR_A!`

Linux Shell Variables

- The following are examples to define a variable:
  - `NAME=“George”`
  - `VAR1=“input.txt”`
  - `VAR2=100`
- Readonly variable is a variable that cannot be changed, once defined:
  - `NAME=“George”; readonly NAME`
  - executing `NAME=“John”` again will give an error message:
    - `/bin/sh: NAME: This variable is read only.`
- Unsetting variables:
  - `unset NAME`

Linux Shell Variables

- Accessing the variables:
  - `echo $NAME`
  - `echo “Hello $NAME - hope you're well.”`
  - `echo “Your file can be located as ${NAME}.txt”`
  - `touch ${NAME}.txt`

Bash Profile

- Users can define what they wish to do automatically on login in the user **bash profile**.
- Every single lines defined in **bash profile** will be executed on user login.
- General use case:
  - Export variables
  - Run command
  - Activate custom environment
  - Load application module
  - Customise bash prompt
- Location of the file:
  - **`~/.bash_profile`**

Simple Exercise (Part 02)

Let’s Practise

- Navigate to the **`training01`** directory created earlier.
- Create a script named **`script.sh`** with the following content.

```
#!/bin/sh

echo Hello HPC!!
echo I am now in $(pwd) directory.
echo These are the contents from $1.
cat $1
```

- Add executable permission to the **`script.sh`**.
- Execute **`script.sh`** with **`data.txt`** as argument.
- Remove the directory **`training01`**.

❏ `cd ~/training01`

❏ `nano script.sh` or `vi script.sh`

❏ `chmod +x script.sh`

❏ `./script.sh data.txt`

❏ `cd ~`

❏ `rm -r training01` or `rm -rf training01`

Any Questions?