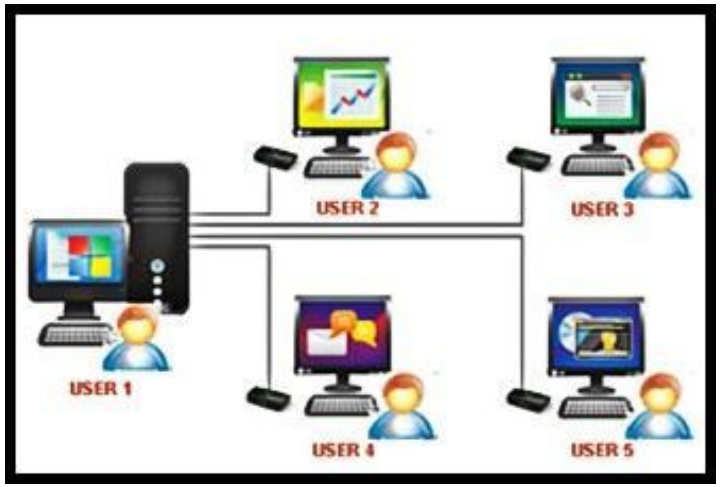
Lab1: Getting started

Objective

- Basic UNIX/Linux commands
- How to use ParamShakti Supercomputer
- Chemistry Software

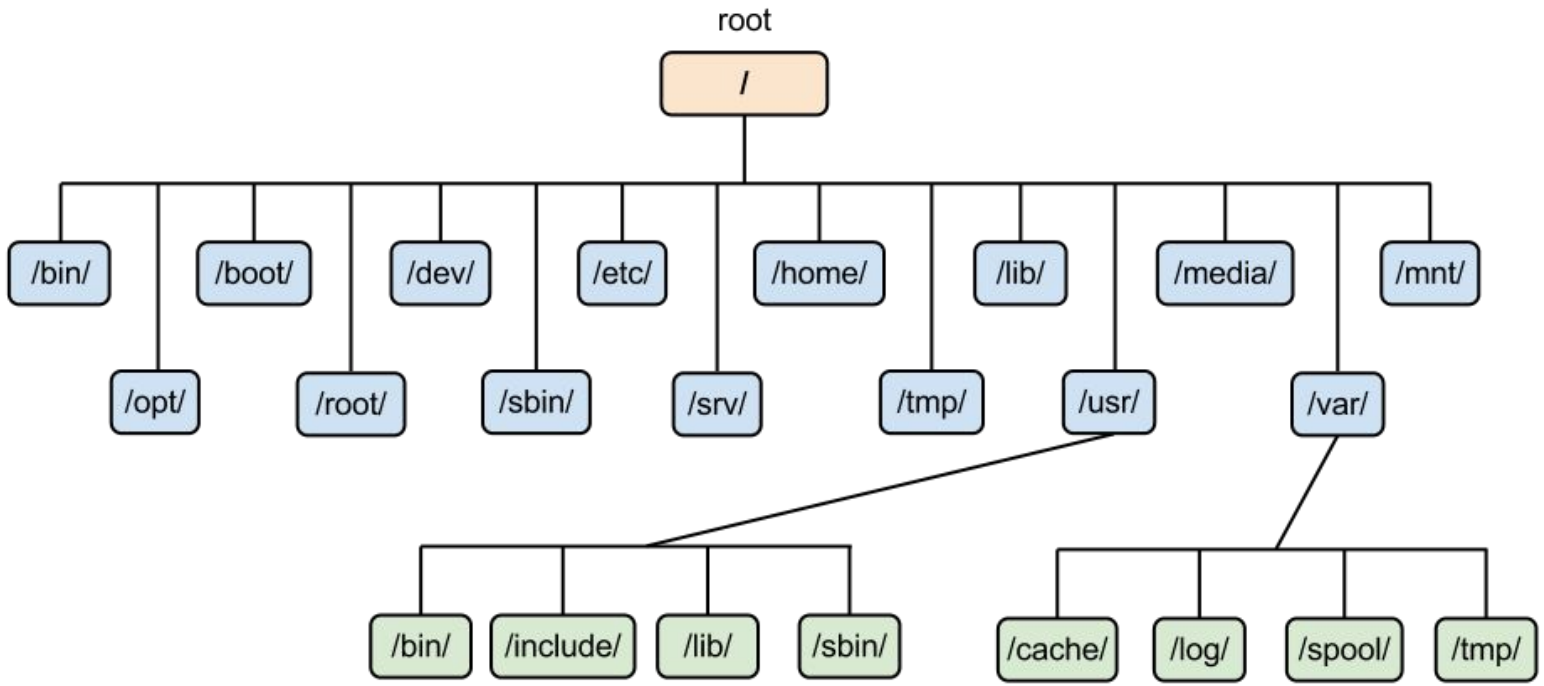
Why Linux

- A Multi-user system
- A multitasking system
- A Repository of applications
- Pattern matching
- Programming facility
- Documentation



https://www.itrelease.com/2014/08/advantages-disadvantages-multi-user-operating-system/

Linux file system



- Directory in Linux is similar to a “Folder” in Windows OS
- Files are organized into directories and sub-directories
- Directories are separated by forward slash (/)

Source: https://freedompenguin.com/articles/how-to/learning-the-linux-file-system/

Getting started

- Log in with your username and passwd
- Normal user vs Super user
- Locate terminal
- Applications → System Tools → Terminal
- Program & Process – Process: Executes the program/command or performs the work
- All Linux commands are CASE SENSITIVE
- Type one or two characters of a command and HIT TAB (twice) for knowing the list of all commands starting with these characters

Getting started

- “*” character means match everything
- “?” character means match any one character
- [0-4] or [m-s] matches a range of characters
- **Piping**
  - ls -l | grep "file"
  - cat text.txt | wc -w
  - sort file.txt | uniq
  - ps aux | grep "chrome" | awk '{print $2}'

Getting started

- ctrl+c halts the current command
- ctrl+z stops the current command and resume it with fg in the foreground or bg in the background
- Login to remote system: ssh
  - ssh -X remote_username@remote_hostname OR

    Eg: ssh -X sandeep@10.3.55.120
- Copying files: scp
  - scp -r remote_username@remote_hostname:~/file1 . OR
  - scp -r file1 remote_username@remote_hostname:~

Basic Linux commands

Sl. No.	Command	Description
1	mkdir dir	create directory
2	cd dir	change directory
3	pwd	present working directory
4	ls	list files and directories
5	ls -ltr	sorting the listing by time modification
6	touch file	creates an empty file
7	cp file1 file2	copy files
8	cp -r dir1 dir2	copy directory dir1 to directory dir2
9	mv file1 file2	rename file1 to file2
10	rm -i file	remove file1 (interactive mode)

Basic Linux commands

Sl. No.	Command	Description
11	rmdir dir1	remove directory
12	history	prints all recent commands to stdout
13	cat file	prints contents of the file
14	head file	outputs first 10 lines
15	tail file	outputs last 10 lines
16	top	display all running processes
17	kill -9 PID	kill the process with process id
18	bg	list all stopped jobs or resume the stopped job in the background
19	fg	Brings the most recent job to the foreground
20	date	displays today date and time

Basic Linux commands

Sl. No.	Command	Description
21	grep -i [pattern] file	search for a pattern in file and print it to stdout
22	find -iname “file”	search for a file in current directory recursively
23	./file	executes a file in current directory
24	../../file	executes a file two levels above the current directory
25	zip file.zip file1 file2 or unzip file.zip	compress/uncompress the files

How to use ParamShakti

Login details

username:

password:

ssh -X username@paramshakti.iitkgp.ac.in

You need to enter Captcha followed by the password.

Login details

testuser6	Test!@3
testuser7	Test!@3
testuser8	Test!@3
testuser9	Test!@3
testuser10	Test!@3

How to navigate

There are two partitions

/home/username

/scratch/username

Work in the /scratch/username directory always

Chemistry Software

List of software packages

- For molecules,
  - Gaussian 16 (https://gaussian.com/gaussian16/)

- For periodic systems,
  - Quantum Espresso (https://www.quantum-espresso.org/)

- For Visualization
  - Avogadro (https://avogadro.cc/)

Gaussian script

```
#!/bin/bash

#SBATCH -J gaussian # name of the job
#SBATCH -p shared # name of the partition: available options "shared medium large gpu"
#SBATCH -N 1 # no of nodes
#SBATCH -n 1 # no of processes
#SBATCH -t 2:00:00 # walltime in HH:MM:SS, Max value 72:00:00
#SBATCH -c 4 # no of threads per rank

#list of modules you want to use, for example
module load apps/gaussian/16/gnu

g16 -m=5gb - p=${SLURM_CPUS_PER_TASK} input.com
```

References

1. Your Unix :The Ultimate Guide, Das, Sumitabha
2. https://gaussian.com/gaussian16/
3. https://www.quantum-espresso.org/
4. https://avogadro.cc/