H3ABioNet

Pan African Bioinformatics Network for H3Africa

16SrRNA Intermediate Bioinformatics Online Course: Int_BT_2019

Introduction to the command line and R

Introduction to the command line

Learning Objectives

- To give a background on Unix and the fundamentals of the OS
- To introduce the shell
- To give a breakdown of command usage and some of the most important commands
- To give an intro to command line editors
- To give an intro to a compute cluster and resources manager
- To give an intro to workflow tools
- To give an intro to software containerisation

Learning Outcomes

- To understand the background of the Unix environment
- To understand the need for using the command line for scientific computing
- To be comfortable with navigating the environment, doing file and directory manipulations, and working with pipes and filters
- To understand a cluster environment basics and be able to submit an interactive job
- To be familiar with workflow tools
- To be familiar with software containerisation

What is Unix

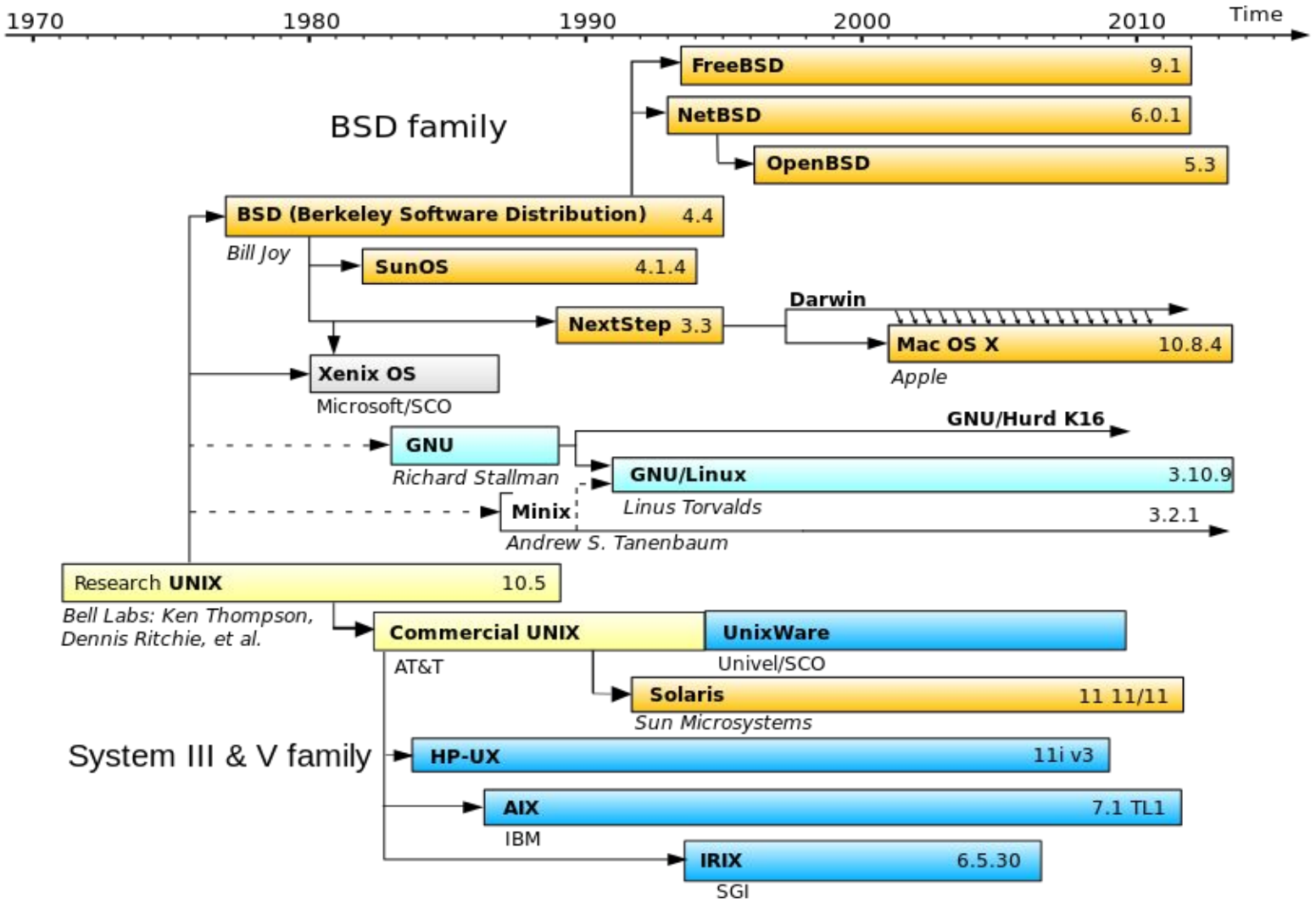
- A stable, multi-user, multitasking operating system for servers, desktops and laptops that exists in many variants

- Unix systems are characterised by a modular design:
  - a set of simple tools that each perform a limited, well-defined function
  - with a unified filesystem as the main means of communication and
  - a shell scripting and command language to combine the tools to perform complex workflows.

- Unix flavours
  - Sun Solaris, Mac OS X, GNU/Linux, UnixWare, FreeBSD, OpenBSD, IBM IAX, HP UX

- GNU/Linux distributions
  - Difference is in package managers, directory structure, file naming, suitability (servers vs desktops)
  - Debian, Ubuntu, Fedora, openSUSE, SUSE Linux Enterprise, Scientific Linux, Redhat, CentOS

Timeline



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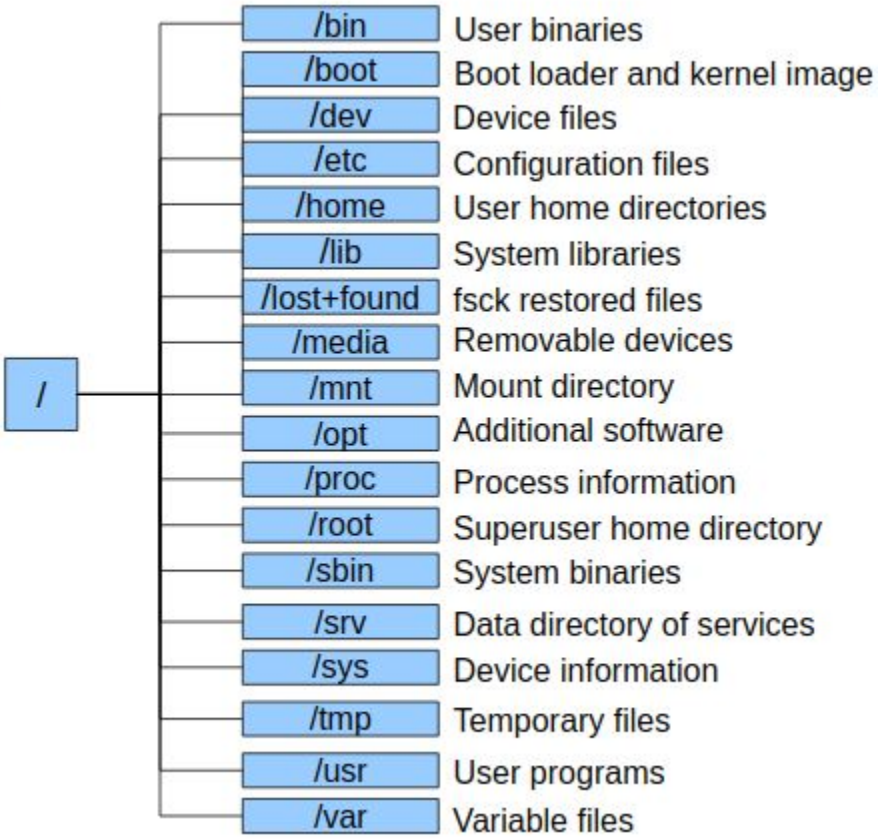
Fundamentals

- Different Unix flavours but fundamentally the same
  - Kernel
    - Allocates time and memory to programs, handles storage and communication
  - Shell
    - Interface between user and kernel. Command line interpreter (CLI)
  - Terminal / Console
    - Interface to the shell
- Comply to POSIX standards
- Username, password, home directory, group, permissions, default shell
- Processes (PID)
- Directory structure and files

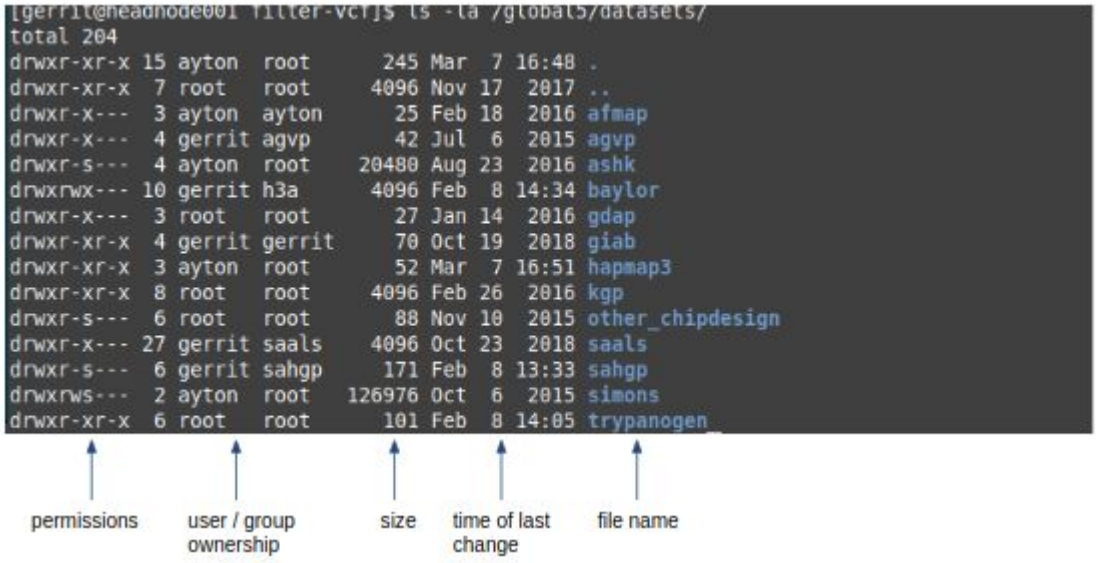
Ubuntu files structure

```
trainee@mgwvm: ~
trainee@mgwvm:~$ ls -1d /*/ | sort
/bin/
/boot/
/cdrom/
/dev/
/etc/
/home/
/lib/
/lib32/
/lib64/
/lost+found/
/media/
/mnt/
/opt/
/proc/
/root/
/run/
/sbin/
/selinux/
/srv/
/sys/
/tmp/
/usr/
/var/
```



Permissions

- In multi-user systems, access and access restrictions are key
- Typically, you are the owner of every file/directory you create or bring into a system
- What other files and directories you can read, write or execute will depend on how the system is set up



Shell

- Command line interface to the operating system (browsing file system and issuing commands)
- All in all a programming language
- Shell scripts provide a way to automate repetitive tasks
- Different shells with different features

Command anatomy

command -options/flags [**input**] [**output**]

- Depending on the command the **input** can be read from the *stdin* stream, the output from a previous command or from a file
- Depending on command the **output** can be send to the *stdout* stream, to the **input** of the next command or to a file
- Error messages are normally send to the *stderr* stream
- Do get more detail information about command flags and usage make use of the man pages. e.g. `man ls`

List of important commands

File management	
`ls`	List files
`cd`	Change directory
`pwd`	Print working directory
`mkdir`	Make a new, empty directory
`rmdir`	Remove an empty directory
`cp`	Copy files
`scp / ssh`	Do a secure copy from or to a remote machine / login to remote machine
`rm`	Remove files
`mv`	Move files or directories (rename)
`find`	Find files or folders based on name, date, size, ownership or other parameters
`tar`	Build an archive of files
`gzip / bzip2`	Compression tools
Permissions	
`chown`	Change ownership of files/directories
`chgrp`	Change group ownership of files/directories
`chmod`	Change permissions (mode) of files/directories
`groups`	Report the group(s) you belong to
`id`	Report your username, userid, group(s) and group id(s)
`newgrp`	Set you default group for the current shell

List of important commands

Resource monitoring	
`top`	See the top resource-hungry processes
`df`	See how much disk space is free
`du`	Report numbers and sizes of files on disk
`free`	Show available and cached memory
Job control	
`which`	Display full path of command
`ps`	View active processes
`<cntrl>-c`	Kill current job
`<cntrl>-z`	Suspend current job
`bg`	Put suspended job in background
`fg`	Bring a suspended job into the foreground
Filtering/Reporting	
`grep`	Search for substrings in a file or pipeline
`awk / sed`	Pattern scanning and text processing / stream editor for transforming text
`sort`	Sort lines alphabetically or numerically
`wc`	Count lines, words, characters
`cat`	Print file or files to standard output
`more / less`	Text viewing programs
`head / tail`	View start or end of a file or pipeline

Redirection and piping

Piping and redirection summary	
> file	Output redirection, overwrite
>> file	Output redirection, append
< file	Input redirection
commandA | commandB	Pipe output from commandA to commandB

Things to be aware of

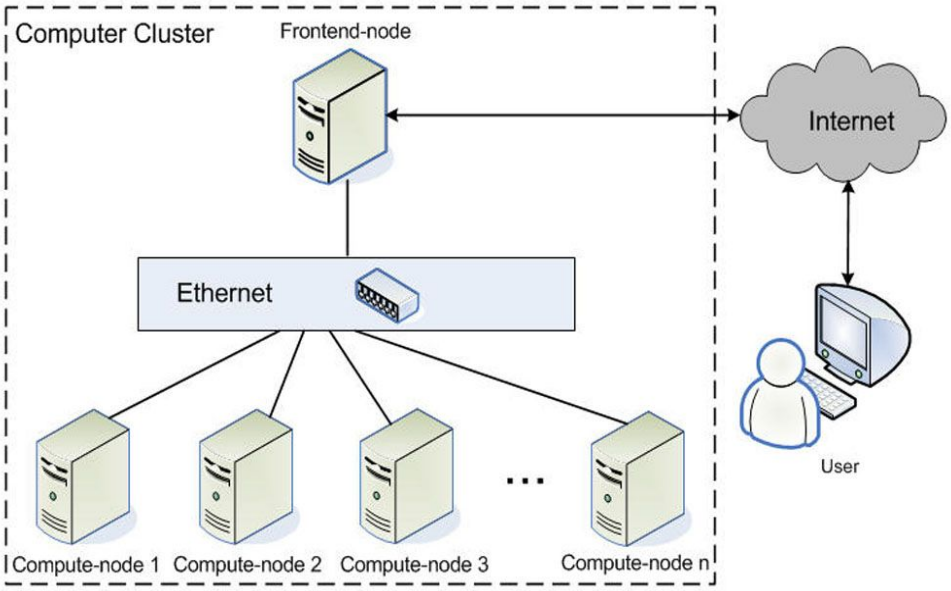
- File and directory naming is case sensitive.
- Keep away from using strange characters in file names otherwise it needs to be escaped.
- Bash shell features
  - Command and filename completion with **tab** key
  - Browse through history with up and **down** keys
  - Search for previous commands with **cntrl-r**
- Many ways to accomplish the same thing using various combinations of piping together commands.
- In the shell deleting files is forever.

Editors

- Learn to use a shell editor and the shortcut keys
- Command line options for editors: `vi, emacs, nano, pico`
- `nano` is a easy editor to start with

Compute cluster

- A compute cluster consist of single machines that work together so that in many respects they can be viewed as a single system.
- A resource and scheduler monitors job resources and assigns jobs to nodes.
- A job scheduler operates efficiently if resources are fairly distributed across users of the system.
- A job scheduler uses certain criteria to decide if jobs should run e.g.
  - Job priority
  - Compute resource availability (memory/cpu)
  - Execution time allocated to user
  - Number of simultaneous jobs allowed for a user
  - Estimated execution time
  - Elapsed execution time
  - Job dependency



PBS and SLURM

- PBS and SLURM are popular job scheduling systems
- Both have different ways in defining submissions scripts. See https://github.com/grbot/batch-system-comp

PBS

```
#!/bin/bash
#PBS -l nodes=1:ppn=1
#PBS -l walltime=01:00:00
#PBS -N ech_count
#PBS -d .
#PBS -M gerrit.botha@uct.ac.za
#PBS -m abe
#PBS -q UCTlong

##### Running commands
echo "Date is ";date
echo "hostname is ";hostname
exe="echo_count.sh count.txt 100"
$exe
```

SLURM

```
#!/bin/bash
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH -t 01:00:00
#SBATCH -J echo_count
#SBATCH -o echo_count.o%j
#SBATCH -e echo_count.e%j
#SBATCH --mail-user=gerrit.botha@uct.ac.za
#SBATCH --mail-type=begin
#SBATCH --mail-type=end
##SBATCH -p Main

##### Running commands
echo "Date is ";date
echo "hostname is ";hostname
exe="./echo_count.sh count.txt 100"
$exe
```

PBS and SLURM interactive sessions

- PBS doing an interactive submission (getting onto a compute node, requesting 1 node and 1 core and reserve for 2 hours)

  - `$ qsub -I -l nodes=1:ppn=1 -l walltime=02:00:00`

- SLURM doing an interactive submission (getting onto a compute node, requesting 1 node and 1 core and reserve for 2 hours)

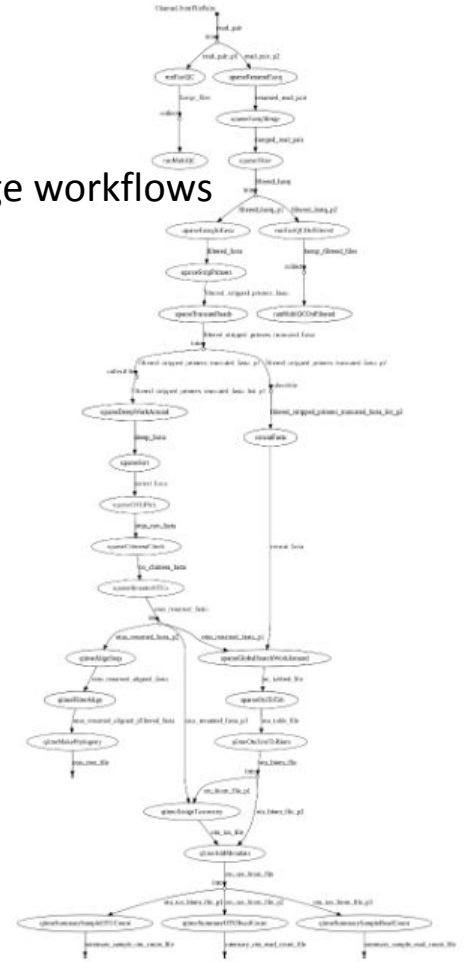
  - `$ srun --nodes=1 --ntasks=1 --time=120 --pty bash`

Workflow tools

- Nextflow
  - Provides a language and engine
  - Language are based on Groovy
  - Relative easy to learn and can easily be applied to simple and large workflows
  - Not modular at moment but will be in DSL 2.0
  - Nextflow example code on Ilifu are here with demo here

- CWL (Common Workflow Language)
  - Language only, tools such as cwltool an Toil provides the engine
  - Modular and very structured
  - Large community support similar to what is found for Nextflow.

- WDL (Workflow Descriptive Language)
  - Language only, Cromwell provides the engine
  - Used by Broad Institute and supported in GA4GH workflows.



Software containers

- A container is a standard unit of software that packages up code and all its dependencies so the application runs quickly and reliably from one computing environment to another.
- Use operating-system-level virtualization to deliver software in packages called containers
- Most popular technologies are Docker and Singularity
- Depending on what is available at you facility it is sometimes a less administrative hassle to package your software or software suite in a container.
- Before building a container have a look at https://quay.io/organization/biocontainers to see if an image of the tool does not exist already.
- SIngularity images can be build from Docker images
- Due to Docker security issues it is most likely that only Singularity is supported on your cluster environment.