Introduction to the UNIX Command Line

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Where to find this presentation

Find the presentation at https://tinyurl.com/ytt3kdm3.

Goals of presentation

- ► How to access UCL UNIX systems
- ► How to use the UNIX command line

Information on the Web

Astrophysics Wiki

https:

//liveuclac.sharepoint.com/sites/PhysAstAstPhysGrp This Wiki is freely viewable and editable by all members of the department. Please use it to record information that you think will be useful to others (including your future self). Be bold!

UCL Research Computing Platforms

https://www.rc.ucl.ac.uk/

Stack Overflow

http://stackoverflow.com/ (But will it survive ChatGPT?)

Computing Environment for Astrophysics

- Large datasets requiring substantial processing followed by sophisticated statistical analysis
- Calculations often done on specialised high-performance computing (HPC) machines having large filesystems and large RAM; calculations are often broken into pieces that can be run simultaneously ('in parallel') across many processors.
- Much useful software is made freely available within the community. Software quality is usually high; documentation quality is more variable.
- Many users write their own software.

Local Computing Environment

You will have your own local machine, which might be:

- ► PC (Windows)
- Mac
- ► Linux

Also there are shared Linux machines:

- General purpose Astrophysics servers available from outside UCL: zuserver1 and zuserver2
- UCL Cosmology HPC clusters: splinter and hypatia
- ► Other UCL clusters: Myriad and Kathleen
- ► National clusters: DiRAC (UK) and NERSC (US)

Work patterns

Several work patterns are possible:

- Write and test a program on your local machine; use the local machine to remotely connect to a server; upload the program to the server and run it there;
- Or do all your work locally (requires small data sets);
- Or use the local machine to remotely connect to a server and do all your work there.

Accessing remote machines

Credentials

- ➤ You will need a *username* and *password* for any machine that you want to access.
- Contact Edd Edmondson (e.edmondson@ucl.ac.uk) or John Deacon (j.deacon@ucl.ac.uk) to get these credentials.

The full names of the Astro servers are:

- zuserver1.star.ucl.ac.uk
- zuserver2.star.ucl.ac.uk
- splinter-login.star.ucl.ac.uk
- hypatia-login.hpc.phys.ucl.ac.uk

Software for connecting

How to connect to a shared machine

- Windows PC: use PuTTY (or MobaXterm, which uses PuTTY);
- ► Mac: go to the Terminal window and use ssh;
- Linux machine: go to the Terminal window and use ssh.

Visibility

- zuserver* (≡ zuserver1 or zuserver2) can be seen from anywhere.
- ▶ If you are on the UCL network then you can see any Astro or UCL HPC server.
- ▶ If you are not on the UCL network then to connect to Astro or UCL HPC servers (except zuserver*) you must set up a Virtual Private Environment. For details see https://www.ucl.ac.uk/isd/services/get-connected/ucl-virtual-private-network-vpn. An alternative is to logon to zuserver* and from there logon to the server.

Using PuTTY for remote connections from Windows

- If you don't have PuTTY you can download it from http://www.putty.org/.
- ➤ On the 'Connection/SSH/X11' tab, click on 'enable X11 forwarding' and set 'X display location' to 'localhost:0' this is necessary for handling graphical output.
- On the Session tab, set the Host Name as appropriate e.g. zuserver1.star.ucl.ac.uk.

Using ssh for remote connections from Mac and Linux

- ► Syntax: ssh -YC username@servername
- ► The 'Y' option is necessary for handling graphical output.

X-Windows client

- ▶ If the remote program that you are running produces graphical output, then you must have a program (an 'X-Windows client') running on your local machine to display this graphical output.
- On Windows you can use XMing (https://sourceforge.net/projects/xming/) or Exceed (available on the UCL Desktop).
- On Mac you can use XQuartz.
- On Linux you don't need to do anything special the graphical interface is already an X-server.

Unix

- Unix and Unix-like computer operating systems have become the industry standard for scientific research.
- Unix was started in 1969 by Ken Thompson, Dennis Ritchie, and others.
- Unix is multi-tasking and multi-user, with a modular design: the operating system provides various single-purpose tools that may be linked together for more complicated tasks.
- ▶ Unix has a reputation for efficiency, robustness, and security.

Linux

- Linux is a popular 'Unix-like' operating system.
- ► Linux was created by Linus Torvalds, and was first released in 1991. His motivation was to avoid restrictive software licenses.
- splinter and hypatia use a version of Linux called 'CentOS'.
- Free and open source.

Command shell

- ▶ In Linux you will use a 'command shell', a text environment in which you type commands and receive text output.
- ▶ Not GUI! Reflects the hardware limitations current when Unix was created. Low-tech and reliable e.g. for remote access.
- Various command shell programs are used: bash, csh, tcsh, zsh, etc. Use echo \$0 to see which one is in use.
- ▶ This presentation assumes bash. Other shells may use different names for some of the commands discussed.
- ▶ New accounts on UCL Astro servers get given tcsh as a shell. But if you don't use Starlink software, it's safe to ask to be switched to bash.

Directory structure

- ► Everything is organised around files (which may be data files or program files i.e. instructions to be executed).
- ► Files live in directories. There is a hierarchical tree structure of directories.
- ► The *root* directory (the base of the directory tree) is called /.
- ► Sample file name: /home/ucapwhi/foo.txt
- ▶ Note use of slash '/', not backslash '\' as in Windows.
- ► Case sensitivity: 'Foo' and 'foo' are different strings.

Working directory

- ► The shell is always pointed at one particular directory, known as the *working directory*.
- Use pwd ('print working directory') to see the current working directory.
- ▶ Refer to files in the working directory simply via the file name (example foo.txt) and refer to files in other directories by directory name plus file name (example /home/ucapwhi/foo.txt).

Abbreviations for directories

- ▶ Full stop . is an abbreviation for the working directory.
- ► Two full stops ... is an abbreviation for the parent of the working directory.
- Hyphen is an abbreviation for the most-recent previous working directory – useful if you need to flip back and forth between directories!
- ► Tilde ~ is an abbreviation of the user's home directory e.g. /home/ucapwhi/. Many configuration files are located here by default.

Navigating the directory tree

- Use cd to change working directory. Example: cd ../data/des/.
- Use 1s to list the files in the current working directory; use 1s <dir> to list the files in another directory.

Keyboard speedups

- Linux has several speedups that make it efficient to use the keyboard to type commands.
- Keyboard interfaces predate more modern graphical interfaces; they are less friendly for new users, but are low-tech, robust, and very efficient for experienced users.

Keyboard shortcuts: tab

- Use the tab key to autocomplete commands, directory names and filenames.
- If what you have typed so far doesn't have a unique autocompletion, then it will complete up to the first ambiguous character.
- This will influence your naming conventions for directories and files!

Keyboard shortcuts: up and down arrows

- Use up arrow to scroll backwards through previous commands, and then down arrow to scroll forwards again.
- ► Follow with Enter to execute an old command that you have scrolled back to, or ctrl+c to cancel.

Keyboard shortcuts: ctrl+r

- Use ctrl+r to search backwards through previous commands (reverse-i-search).
- Type a substring (not necessarily initial) of the sought-for command.
- ► Example: ctrl+r push will bring up the most recent command that included the substring push.
- ► Follow with Enter to execute, ctrl+c to cancel, or ctrl+r to search further back.

Keyboard shortcuts: alias

- Use alias to create your own abbreviations for long commands.
- Example: alias s='cd /share/ucapwhi/almanac_project/'
- ▶ It's boring to retype all your aliases at the start of your session.
 So instead put them in a batch file that autoexecutes at login
 this will be named ~/.bashrc or something similar.

Environment variables (1)

- ► The operating system maintains a global namespace of 'environment variables' to store configuration information.
- ► The following commands are specific to bash other shells use different commands.
- Use set to see all environment variables;
- Use echo \$<variable_name> to see the value of one environment variable (e.g. echo \$PATH);
- ► Use export \$F00='my_string' to set an environment variable F00.

Environment variables (2)

- Variables PATH and PYTHONPATH are used frequently (to maintain lists of directories in which to search for executable programs and Python modules, respectively).
- Linux has no equivalent of the Windows Registry; configuration is done via the directory structure and the environment variables.

Structure of commands

Structure

```
[command] -[option(s)] [argument]
```

Examples

```
ls -la
mkdir my_experiments
cp hello.cpp new_hello.cpp
```

Command reference

- For help with <command> (in increasing order of verbosity):
 <command> -h or <command> --help
 man <command>
 info <command>
- http://www.computerhope.com/unix.htm is a useful reference for Linux commands.

File management

- ▶ Use mkdir <dir> to make a new directory
- ▶ Use rm -rf <dir> to delete a directory and its contents (including subdirectories). This is irreversible!
- Use cp <source> <destination> to copy a file and mv <source> <destination> to move a file.

File contents

- ▶ Use cat <file> to show the contents of a file as text and xxd <file> to show the contents of a file as bytes.
- ▶ Use head <file> or tail <file> to show the first or last few lines in a file helpful if the file is large!
- Use grep to search for text with a file or files.

Controlling processes

- Use top to see all the processes running on a server (not just your own); type q to exit top. Helpful if someone seems to be hogging the processor!
- Use kill to stop one of your own processes.
- Use watch to run a command repeatedly.
- Use nohup or screen to let a command continue to run even after you exit your session.
- ▶ Use & at the end of a command to have it run in the background; control is then immediately returned to you. Use jobs to see what is running in the background, and fg to move a job from background to foreground.

Long command lines

- ► Concatenate several commands onto one long command using semicolon e.g. cd ~; cat .bashrc; cd -.
- ► Conversely use \ to split one long command over two lines.

Wildcards

- Some commands take *sets* of filenames as an argument. For example rm <set of filenames> will remove multiple files.
- Such sets can be given as a space-separated list (example rm foo1.txt foo2.txt), or else using wildcards (example rm foo*.txt).
- ► The wildcards are
 - * (matches zero or more characters) and
 - ? (matches preceisely one character).

vim

- vim (an improved version of vi) is a text editor that is found on almost every UNIX machine.
- Some familiarity with vim is therefore useful, as it's often the fastest way to make small edits to text files.
- ▶ Bad news: the key commands for vim are very different from those that have become standard on personal computers. Good news: vim can be useful even if you know only a few commands.
- The minimum you need to know is how to exit vim if you get into it by accident: esc: q! enter.

Redirection

- ► Use > to redirect the text output from a program to go to a file instead of the screen. Example: ls > listing.txt.
- ► Conversely use < to allow text input to a program to be taken from a file rather than the keyboard.
- Use the pipe symbol | to allow output from one program to be used an input for another. Example: ifconfig | grep UP.

bash scripts

- ▶ bash comes with a Turing-complete scripting language in which you can write programs.
- ► Such scripts are usually used for control of processing (rather than for e.g. actual processing of data).
- ► The language has some idiosyncrasies (e.g. fi instead of end_if).
- ► Every programs return an integer return code (0 = success) that can be used in conditional statements.
- ▶ It is common to use the extension .sh for such files.

Example bash script

```
#!/usr/bin/env bash
source /mnt/lustre/tursafs1/home/dp327/dp327/share
cd /mnt/lustre/tursafs1/home/dp327/dp327/shared/lf
rm -f /mnt/lustre/tursafsl/home/dp327/dp327/sharec
/mnt/lustre/tursafs1/home/dp327/dp327/shared/lfi r
/mnt/lustre/tursafsl/home/dp327/dp327/shared/lfi r
/mnt/lustre/tursafs1/home/dp327/dp327/shared/lfi r
echo stop > /mnt/lustre/tursafs1/home/dp327/dp327/
pvthon3 /mnt/lustre/tursafs1/home/dp327/dp327/shar
mkdir -v ./fof/
mv -v *.fofstats* ./fof/
chmod g+w -vR ./fof/
cd /mnt/lustre/tursafs1/home/dp327/dp327/shared/lf
tar -czvf run017.fof.tar.gz ./run017/fof/
test -f ./run017.fof.tar.gz && rm -rfv ./run017/fc
tar -czvf run017.tar.gz ./run017/
test -f ./run017.tar.gz && rm -v ./run017/run*
```

How to run a bash script

bash myscript.sh

Alternatively make the script executable:

- ► Add #!/usr/bin/env bash at the top of the file
- ► Then chmod +x myscript.sh

Then just need to call ./myscript.sh

Scripts and environment variables

- lt's natural to write a script that sets environment variables.
- ▶ But this doesn't work! The script gets a *copy* of the environment; this copy gets amended by the script, but is then discarded when the script stops.
- So instead use source e.g. source my_set_environ_vars.sh

Modules

- ▶ Both splinter and hypatia use the module package to give access to software packages (typically by setting appropriate environment variables).
- Example: on splinter, module load dev_tools/oct2021/hdf5-1.12.1 makes version 1.12.1 of the hdf5 package available.
- Use module avail to see what you can load and module list to see what you have loaded.
- ► If desired, you can extend this system to include your own software.

HPC environments

- splinter and hypatia are high-performance computing (HPC) clusters.
- ► Each has many linked computers (called nodes). Most nodes are compute nodes; these are available for processing. The login node (which you login to) is special. Use it for control, for editing and for compiling, but not for heavy processing!
- srun --pty bash will give you a session on one of the compute nodes.
- Alternatively you can use sbatch to launch an unattended job on one or several compute nodes.