

HPC School - Beginner

\$1-2 - Don't fear the command line

High Performance Computing & Big Data Services













Before we start

Objectives:

- get acquainted to the linux command line interface (CLI)
- be able to manipulate the file system
- be able to decrypt complicated commands

Prerequisite: you should be able to connect to the HPC cluster



A little bit of history

- Computers before the early 80s'
 - o room sized, expensive
 - o as powerful as a modern scientific calculator
 - multi user
 - o central computer / terminal model
- Philosophy
 - use resources as efficiently as possible
 - textual human/machine interface (shell)
 - small specialized programs

Similarities with the modern HPC and Cloud ethos







Connect to the HPC cluster





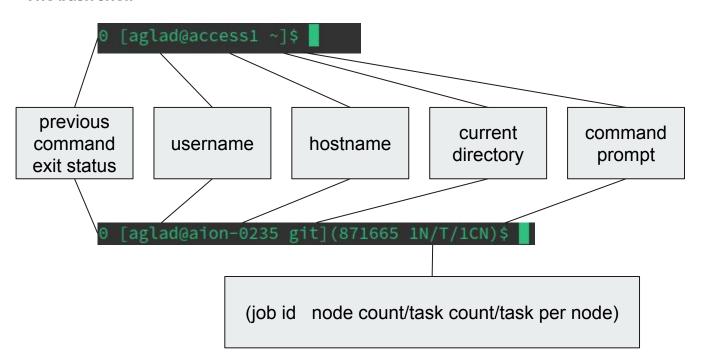






The command prompt









The linux file system

- Tree structure starting at /
 - No drives as in windows (c:, ...)
- Strong conventions
 - System directories
 - /etc configuration files
 - /bin built-in programs
 - /usr 'user system resource' other installed programs, libraries, ...
 - /home users personal directories
 - Program installation follows conventions
 - difficult to know what is installed
 - the system able to provide **completion**
- Files and directories
 - o ~ shorthand for /home/users/<user_name>
 - current directory
 - .. parent directory
 - .filename hidden file/directory

```
drwxr-xr-x 5 root root 4096 Sep 7 15:25 .

drwxr-xr-x 5 root root 4096 Jul 21 09:41 .

-rw------ 1 hpcuser hpcuser 59 Jul 21 19:26 .bash_history
-rw-r--r-- 1 hpcuser hpcuser 57 Jan 9 2022 .bash_profile
-rw-r--r-- 1 hpcuser hpcuser 3824 Jan 14 2022 .bashrc
drwxr-xr-x 13 hpcuser hpcuser 4096 Aug 7 09:55 .cache
drwxr-xr-x 14 hpcuser hpcuser 4096 Aug 7 09:54 .config
-rw-r--r-- 1 hpcuser hpcuser 4096 Aug 7 09:51 Desktop
-rw-r--r-- 1 hpcuser hpcuser 4096 Aug 7 09:51 Documents
drwxr-xr-x 2 hpcuser hpcuser 4096 Aug 7 09:51 Documents
drwxr-xr-x 2 hpcuser hpcuser 4096 Aug 7 09:51 Documents
```

Access rights

- o user group
- o d[rwx][rwx][rwx]
 - directory [user][group][other]
 - read write execute/navigate





Anatomy of a command

program [flags]... [arguments]...

- flags = options that change the behavior of the program
 - not sensitive to order
 - long flags more readable, annoying to type
 - start with -- e.g. --all
 - can have parameters e.g. --format=long --ignore foo
 - o short flags condensed, difficult to parse
 - start with e.g. -1 -a
 - can be combined e.g. -la. The order of the tags is not relevant -la = -al
 - can also have parameters e.g. -I foo
- arguments = parameters of the program
 - positional
 - o number of arguments depends on the program
- example all these commands are equivalent
 - \$1s -la
 - \$1s -a -1
 - \$1s --format=long -a





A little bit of help

- Manual page ← more comprehensive
 - o man <command>
 - e.g. \$ man ls
- Help flag ← when a man page does not exist
 - < <command> --help
 - e.g. \$ 1s --help

```
SYNOPSIS
ESCRIPTION
      Sort entries alphabetically if none of -cftuvSUX nor --sort is speci-
      -A, --almost-all
      --author
Manual page ls(1) line 1 (press h for help or q to quit)
```





A little bit of help



- What does the **echo** command do?
- What does the which command do?





A little bit of help

Now, you do it!



- What does the echo command do?
- What does the which command do?

```
NAME

echo - display a line of text

SYNOPSIS

echo [SHORT-OPTION]... [STRING]...
echo LONG-OPTION

DESCRIPTION

Echo the STRING(s) to standard output.
```

```
WHICH(1) General Commands Manual WHICH(1)

NAME
     which - shows the full path of (shell) com-
     mands.

SYNOPSIS
```

which [options] [--] programname [...]

DESCRIPTION

Which takes one or more arguments. For each of its arguments it prints to stdout the full path of the executables that would have been executed when this argument had been entered at the shell prompt. It does this by searching for an executable or script in the directories listed in the environment variable PATH using the same algorithm as bash(1).



Lëtz build ourselves a little playground

```
Go to the home directory
$ cd
Pull the repository containing the files
$ git clone https://github.com/ULHPC/hpc-school-for-beginners.git
Check the content
You should see a couple of files and directories. Check that the CLI directory is present.
$ 1s ~/hpc-school-for-beginners
Go to the directory containing the files for the tutorial
$ cd hpc-school-for-beginners/CLI
```





Navigating through the file system

Tab autocompletes paths and your commands

- pwd print working directory
 - show the full path of the current directory
 - useful to know where you are
- 1s list
 - list the files and directories in the current directory
 - add a path in argument to show the content of another directory
 - o -a flag shows hidden files and directories
 - -1 formats the output and shows access right
- **cd c**hange **directory**
 - o cd with no argument returns you to your home dir
 - o cd /<path> go the the indicated absolute path
 - e.g.\$ cd /home/users/hpcuser/foo/
 - o cd ./<path> or cd <path> go to the relative path
 - e.g. \$ cd ./foo then \$ cd nestedFoo
 - o cd .. go to the parent directory
 - e.g. from ~/foo/nestedFoo & cd ../../dir

[hpcuser@hpcschool git]\$ pwd
/home/hpcuser/git



```
[hpcuser@hpcschool CLI]$ ls -la
total 24
drwxr-xr-x 6 root root 4096 Sep 8 14:27 .
drwxr-xr-x 4 root root 4096 Sep 8 14:27 ..
drwxr-xr-x 2 root root 4096 Sep 8 14:27 docs
```

```
[hpcuser@hpcschool CLI]$ cd docs [hpcuser@hpcschool docs]$
```





Navigating through the file system



- go to your home directory
- from there, go to the tutorial directory hpc-school-for-beginners/CLI/playground
- go back a level then to the docs directory

```
[hpcuser@hpcschool CLI]$ tree -d

docs
final_boss
playground
backup
files
experiments
data
scripts
temp
```





Navigating through the file system



- go to your home directory
- from there, go to the tutorial directory
 hpc-school-for-beginners/CLI/playground
- go back a level then to the docs directory

```
[hpcuser@hpcschool CLI]$ tree -d

docs
final_boss
playground
backup
files
experiments
data
scripts
temp
```

```
[hpcuser@hpcschool git]$ cd
[hpcuser@hpcschool ~]$ 
[hpcuser@hpcschool ~]$ cd hpc-school-for-beginners/CLI/
playground/
[hpcuser@hpcschool playground]$ 
[hpcuser@hpcschool playground]$ cd ../docs/
[hpcuser@hpcschool docs]$
```





Executing programs and scripts

- Built-in and installed software
 - Built-in commands come with the shell
 - Installed software
 - via package manager or install scripts
 - copies files according to conventions
 - The OS is aware of their existence/location
 - just type their name (e.g. 1s, cd)
 - the tab key proposes completion
 (e.g. 1 + tab -> all executables starting with 'l')
- Scripts and non installed software
 - Launcher scripts (.sh), precompiled software from archives
 - The OS is usually **not** aware of their existence
 - must be executable
 - called using its path/name (either absolute (starts with /) or relative (starts with ./)





Executing programs and scripts

Now, you do it!



- Go to ~/hpc-school-for-beginners/CLI
- Run the backup script located in playground/scripts/backup.sh with the file playground/files/important.txt as an argument
- Check the content of the playground/backup directory

backup.sh is a custom script and does not have a man page or --help flag.
Usage is \$./backup.sh <file_to_backup>







Executing programs and scripts

Now, you do it!



- Go to ~/hpc-school-for-beginners/CLI
- Run the backup script located in playground/scripts/backup.sh with the file playground/files/important.txt as an argument
- Check the content of the playground/backup directory

backup.sh is a custom script and does not have a man page or --help flag.
Usage is \$./backup.sh <file_to_backup>

```
[hpcuser@hpcschool ~]$ cd hpc-school-for-beginners/CLI
[hpcuser@hpcschool CLI]$ ls -l playground/backup/
total 0
[hpcuser@hpcschool CLI]$ ./playground/scripts/backup.sh
  playground/files/important.txt
[hpcuser@hpcschool CLI]$ ls -l playground/backup/
total 4
-rw-r--r- 1 hpcuser hpcuser 20 Sep 11 16:32 important.
txt-230911-16:32.bak
[hpcuser@hpcschool CLI]$
```







Manipulating files (1/2)

- mkdir make directory
 - o create a directory at the designated path
 - \$ mkdir test
 - **mkdir** i_dont_exist/test -> The command fails because the i_dont_exist directory does not exist.
 - **s** mkdir -p i_dont_exist/test -> Recursively creates the directories if they do not exist.



- cp copy
 - copy a file cp <source> <destination>
 - \$ cp ./dir/file.txt file(copy).txt
 - \$ 1s -> you should see test.txt
 - copy a directory use the -r flag
 - \$ cp -r ./dir ./foo/nestedFoo
 - \$ cp -r ./dir ./foobar
 The command fails. The foobar directory doesn't exist.
 - copy files using a pattern
 - \$ cp dir/* foo copies all files in dir to foo
 - \$ cp dir/*.txt foo copies all files ending in .txt in dir to foo





Manipulating files (1/2)



- Create a 'manual_backup' directory in the CLI directory
- Make a backup of
 ~/hpc-school-for-beginner/CLI
 /playground/temp/experiment.out in the
 'manual_backup' directory





Manipulating files (1/2)



- Create a 'manual_backup' directory in the CLI directory
- Make a backup of
 ~/hpc-school-for-beginner/CLI
 /playground/temp/experiment.out in the
 'manual_backup' directory

```
[hpcuser@hpcschool CLI]$ mkdir manual_backup
[hpcuser@hpcschool CLI]$ ls
docs final_boss manual_backup playground
[hpcuser@hpcschool CLI]$ cp playground/temp/experiment.
out ./manual_backup/experiment_backup.out
[hpcuser@hpcschool CLI]$ ls manual_backup/
experiment_backup.out
```





Manipulating files (2/2)

- rm remove file
 - There is no bin. Deleted files cannot be recovered.
 - delete a file
 - \$ rm ~/hpcschool/foo/data.dat
 - delete a directory
 - \$ rm -r ~/hpcschool/foo/nestedFoo
 - force deletion
 - \$ rm -f -r ~/hpcschool/foo
- mv move file
 - move a file/directory (cut and paste)
 - \$ mv test.txt foo/test.txt
 - rename a file/directory = moving a file to the same directory
 - \$ mv foo/test.txt foo/temp.txt
 - o move and rename a file
 - \$ mv foo/temp.txt ./test.txt



up and down arrows navigate through recent commands







Manipulating files (2/2)



- Delete the ~/hpc-school-for-beginner/CLI
 /playground/temp directory and its content
- Move the backup of experiment.out to the hpc-school-for-beginners/CLI/playground/ files/experiment/data directory and rename it test001.com





Manipulating files (2/2)



- Delete the ~/hpc-school-for-beginner/CLI /playground/temp directory and its content
- Move the backup of experiment.out to the hpc-school-for-beginners/CLI/playground/ files/experiment/data directory and rename it test001.com

```
[hpcuser@hpcschool CLI]$ ls playground/
backup files scripts temp
[hpcuser@hpcschool CLI]$ rm -r playground/temp
[hpcuser@hpcschool CLI]$ ls playground/
backup files scripts
[hpcuser@hpcschool CLI]$
```

```
[hpcuser@hpcschool CLI]$ ls playground/files/experiments/data
test003.com test034.com test072.com test156.com
test013.com test057.com test077.com
test014.com test061.com test101.com
test021.com test065.com test121.com
[hpcuser@hpcschool CLI]$ ls manual_backup/
experiment_backup.out
[hpcuser@hpcschool CLI]$ mv manual_backup/experiment_backup.out playground/files/experiments/data/test001.com
[hpcuser@hpcschool CLI]$ ls playground/files/experiments/data
test001.com test021.com test065.com test121.com
test003.com test034.com test072.com test156.com
test013.com test057.com test077.com
test014.com test061.com test101.com
[hpcuser@hpcschool CLI]$ ls manual_backup/
[hpcuser@hpcschool CLI]$ ls manual_backup/
[hpcuser@hpcschool CLI]$
```



Reading and writing files (1/2)

- cat concatenates files and write to the standard output
 - 0 \$ cat <filename>
 - e.g. \$ cat dir/data.csv
- less reading longer files
 - 0 \$ less <filename>
 - e.g. \$ less dir/data.csv
 - o scroll with arrows/page up/page down
 - quit with q
- tail show the last lines of a text file
 - 0 \$ tail <filename>
 - \$ tail -n 25 <filename> specify the number of displayed lines
 - \$ tail -f <filename> follow new lines
- chaining commands the | operator
 - o allow to pass the output of a command to the next one
 - \$ ls -la /usr/bin | less
- grep filtering utility
 - \$ 1s /usr/bin | grep update
 - 9 \$ grep pattern filename

ctrl-r allows to search your command history







Reading and writing files (1/2)

Now, you do it!



- Launch playground/scripts/tailMe.sh & and follow the output file (tailMe.out)
- In playground/files/experiments/data, find all files that contain data about Methylene (with a capitalized M)

The tailMe.sh script writes data to the tailMe.out file every second for a minute.



Adding an '&' at the end of a command will make it run in the background. You will not see any output but it will not block the terminal while it is running.

Hit ctrl + c to interrupt any running program





Reading and writing files (1/2)

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Hit ctrl + c to interrupt any running program

```
[hpcuser@hpcschool CLI]$ ./playground/scripts/tailMe.sh &
[1] 13509
[hpcuser@hpcschool CLI]$ ls
docs final_boss manual_backup playground tailMe.out
[hpcuser@hpcschool CLI]$ tail -f tailMe.out
processing 9/60
processing 10/60
processing 11/60
processing 12/60
[hpcuser@hpcschool data]$ cat test001.com | grep Methylene
Methylene uhf forces
```

```
[hpcuser@hpcschool data]$ cat test001.com | grep Methylen Methylene uhf forces
[hpcuser@hpcschool data]$ grep Methylene test*.com
test001.com:Methylene uhf forces
test034.com:Methylene cisd/3-21g
test065.com:Methylene mp2 density, fully in-core
test065.com:Methylene mp2 density
test065.com:Methylene mp2 density, quartic out of core
test065.com:Methylene mp2 density, quintic out of core
test065.com:Methylene mp2 using l802/l901
test065.com:Methylene mp2 use=l903
test077.com:Methylene ump2 scan
```



Reading and writing files (2/2)

- > and >> redirect the standard output (i.e. output of a command in the terminal) to a file
 - % ls /usr/bin > all_bins.txt
 - creates or opens in overwrite mode the all_bins.txt file and write the output of ls /usr/bin in it
 - % ls -la /usr/bin >> all_bins.txt
 - creates or opens in append mode the all_bins.txt file and write the output of Is -Ia /usr/bin in it
- the nano text editor
 - o \$ nano [filename]
 - basic usage
 - write with your keyboard
 - move the cursor with the arrow keys
 - shortcuts
 - at the bottom of the screen
 - accessible via ctrl + <key>
 - e.g. save: ctrl + o; quit: ctrl + x







Changing permissions

chmod - **ch**ange file **mod**e bits allows you to change access rights on your files and directories

```
8 14:27 .
drwxr-xr-x
            4 root
                      root
                               4096 Sep
drwx----- 19 hpcuser
                      hpcuser 4096 Sep
                                         8 14:30 ...
drwxr-xr-x
            6 root
                      root
                               4096 Sep
                                         8 14:27 CLI
drwxr-xr-x
            8 root
                               4096 Sep
                                         8 14:27 .git
                      root
                               6213 Sep
                                         8 14:27 README.mc
            1 root
                      root
-rw-r--r--
```

Why?

- give/restrict access to other people
- make some files executable

\$ chmod 744 <filename>

- first number for the owner, second for the owner's group, third for everyone else
- octal mode
 - 0 1 = execute
 - \circ 2 = write
 - 0 4 = read

- sum the numbers to adjust the rights
 - 7 = 1+2+4 = x + w + r
 - 4 = read only

- for directories
 - execute allows to cd into
 - write allows to create/delete files
 - read allows to see the content of the directory





Changing permissions



- make CLI/playground/files/secret.txt readable only to you
- make CLI/playground/scripts/helloWorld.sh executable and run it





Changing permissions



- make CLI/playground/files/secret.txt readable only to you
- make CLI/playground/scripts/helloWorld.sh executable and run it

```
[hpcuser@hpcschool files]$ ls -la secret.txt
-rw-r--r-- 1 hpcuser hpcuser 10 Sep 11 16:03 secret.txt
[hpcuser@hpcschool files]$ chmod 700 secret.txt
[hpcuser@hpcschool files]$ ls -la secret.txt
-rwx----- 1 hpcuser hpcuser 10 Sep 11 16:03 secret.txt
[hpcuser@hpcschool files]$
```

```
[hpcuser@hpcschool scripts]$ ls -l helloWorld.sh
-rw-r--r- 1 hpcuser hpcuser 32 Sep 11 16:03 helloWorld.sh
[hpcuser@hpcschool scripts]$ ./helloWorld.sh
bash: ./helloWorld.sh: Permission denied
[hpcuser@hpcschool scripts]$ chmod 744 helloWorld.sh
[hpcuser@hpcschool scripts]$ ls -l helloWorld.sh
-rwxr--r-- 1 hpcuser hpcuser 32 Sep 11 16:03 helloWorld.sh
[hpcuser@hpcschool scripts]$ ./helloWorld.sh
hello world!
```





Moving data

- Rsync is a utility that allows to synchronize data between machines
 - upload/download files
 - synchronize files between servers
 - resume interrupted transfers
- Push data
 - \$ rsync -azvu <source> [user@]<host>:<destination>
 - \$ rsync -azvu data_directory aion-cluster:my_data
- Pull data
- Flags
 - o a archive mode (recursive, copies files, rights, links, ...)
 - o z compress data during transfer (speeds up transmission)
 - o v verbose (display what is going on)
 - o u update (skip files that are newer on the receiver)
 - P progress bar (monitor big transfers)





Moving data

Now, you do it!



 copy the content of the CLI/docs directory to your machine to get this presentation and a command line interface cheat sheet pdf Run rsync from your laptop, not from the HPC. Finding the HPC cluster from your laptop is easier than finding your laptop from the cluster.



We need to add the **-e 'ssh -p 8022'** flag to access the custom ssh port of the cluster.





Moving data

Now, you do it!



 copy the content of the CLI/docs directory to your machine to get this presentation and a command line interface cheat sheet pdf Run rsync from your laptop, not from the HPC. Finding the HPC cluster from your laptop is easier than finding your laptop from the cluster.



We need to add the **-e** 'ssh **-p** 8022' flag to access the custom ssh port of the cluster.

```
aglad@hpcschool ~/tmp rsync -azvu -e 'ssh -p 8022' aglad@access-aion.uni.lu:~/hpc-school-for-b eginners/CLI/docs/CLI_Cheat_Sheet.pdf ~/tmp receiving incremental file list CLI_Cheat_Sheet.pdf

sent 43 bytes received 134,552 bytes 89,730.00 bytes/sec total size is 175,255 speedup is 1.30 aglad@hpcschool ~/tmp ls ~/tmp CLI_Cheat_Sheet.pdf aglad@hpcschool ~/tmp
```

Do the same for the other file or copy the whole directory at once.





Final Boss

```
$ man bash > tmp.dat
$ cat tmp.dat | grep -i bash | wc -l
```

Find out what these commands are doing. Don't run them yet!





Final Boss

```
$ man bash > tmp.dat
$ cat tmp.dat | grep -i bash | wc -l
```

Find out what these commands are doing. Don't run them yet!

- first command
 - o redirect the content of the man page command for the bash program to the tmp.dat file
- second command
 - o display the content of the tmp.dat file (cat) and
 - o pipe the result to grep. Only keep the lines that contain 'bash' while ignoring the case and
 - o pipe the output to wc which will count the number of lines (-I flag)
- summary: count the number of lines containing 'bash' (case insensitive) in the man page of the bash program





Final Boss - Phase 2

- \$ export HPL_VERSION=2.3
- \$ wget --continue http://www.netlib.org/benchmark/hpl/hpl-\${HPL_VERSION}.tar.gz
- \$ tar xvzf hpl-\${HPL_VERSION}.tar.gz

Find out what these commands are doing? Don't run them yet! You might need the help of google on this one!



Is your friend





Final Boss - Phase 2

```
$ export HPL_VERSION=2.3
$ wget --continue http://www.netlib.org/benchmark/hpl/hpl-${HPL_VERSION}.tar.gz
$ tar xvzf hpl-${HPL_VERSION}.tar.gz
```

Find out what these commands are doing? Don't run them yet! You might need the help of google on this one!

- set an environment variable
- download a file from netlib.org. The name of the file depends on the value of the environment variable that has been set previously. If the file was partially downloaded, continue instead of redownloading everything.
- extract the files (x) from a gzip archive (z) in the hpl-2.3.tar.gz file (f) and show the logs (v)





Final Boss - Final form

Make ~/hpc-school-for-beginners/CLI/final_boss/runme.sh executable and run it.

What did it do? How can you get rid of it? The script might contain clues and you have all the keys...





Final Boss - Final form

Make ~/hpcschool/data/runme.sh executable and run it.

What did it do? How can you get rid of it? The script might contain clues and you have all the keys...

- Too many files to be deleted one by one. Maybe they all have a pattern in common?
- It seems that you don't have the rights to remove files in this directory





Final Boss - Final form

Make ~/hpc-school-for-beginners/CLI/final_boss/runme.sh executable and run it.

What did it do? How can you get rid of it? The script might contain clues and you have all the keys...

- Too many files to be deleted one by one. Maybe they all have a pattern in common?
- It seems that you don't have the rights to remove files in this directory
- Regain write rights on the directory \$ chmod 700 ~/hpc-school-for-beginners/CLI
- All files finish with a 1. Delete them using a pattern. \$ rm -f ~/hpc-school-for-beginners/CLI/*1

Never trust random scripts and commands found on the internet. Try to understand them first!

Your rights are limited and you cannot really hurt the HPC cluster.

You could easily lose you data however.





Useful resources - explainshell.com





