High Performance Computing & Big Data Services

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LUXEMBOURG
LET'S MAKE IT HAPPEN

# HPC School - Beginner

S1-2 - Don't fear the command line

UNIVERSITÉ DU LUXEMBOURG

# 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

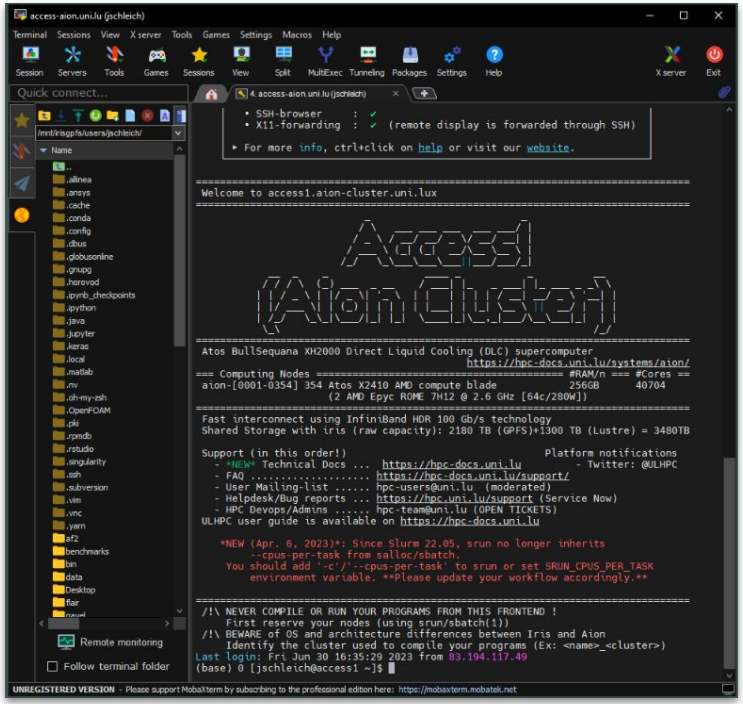
# A little bit of history

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

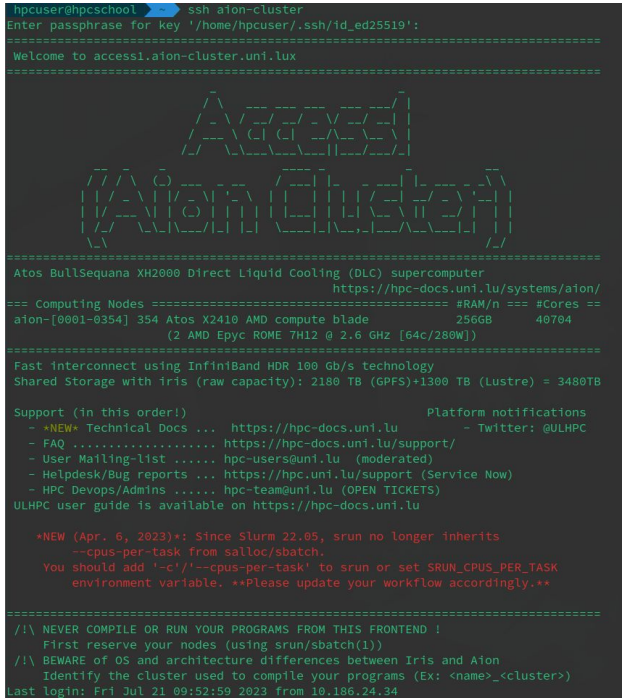
Similarities with the modern HPC and Cloud ethos

# Connect to the HPC cluster

Mobaxterm

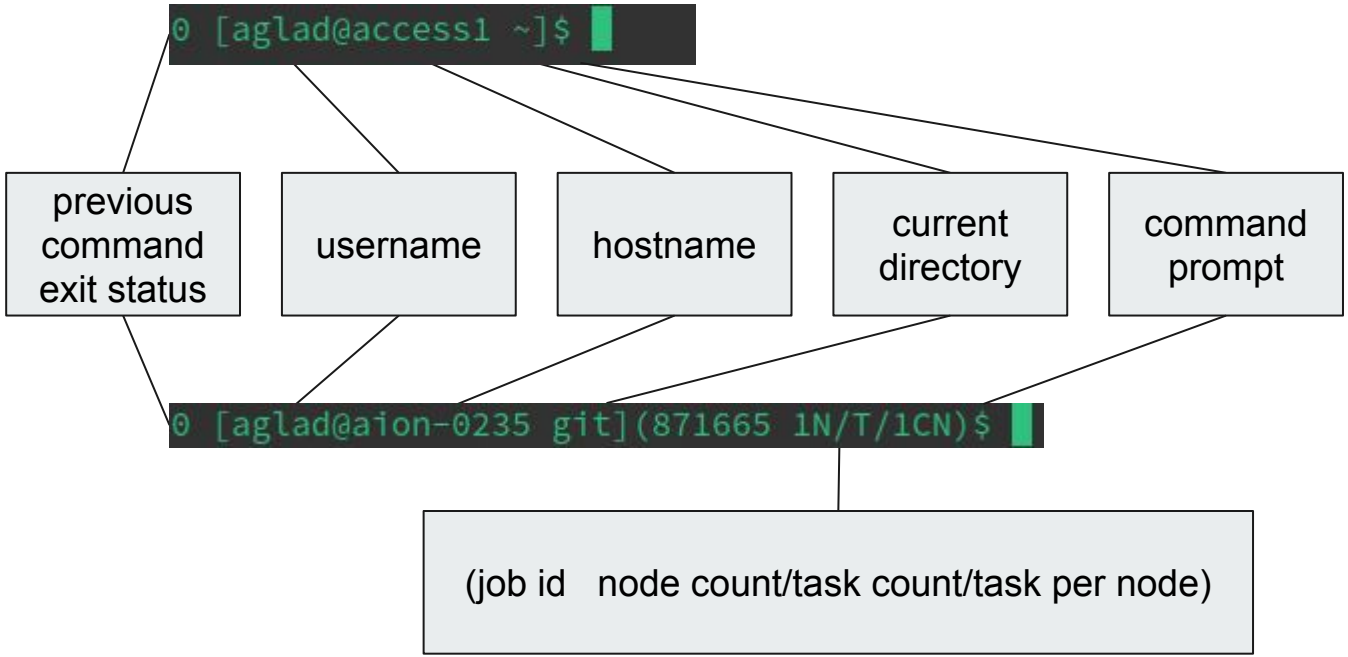



CLI



# The command prompt

## The bash shell



# 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
  - **~** - shorthand for **/home/users/<user_name>**
  - **.** - current directory
  - **..** - parent directory
  - **.filename** - hidden file/directory

```
total 512
drwx------ 18 hpcuser hpcuser   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     21 Jan  9  2022 .bash_logout
-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      0 Jul 21 11:12 data.dat
drwxr-xr-x  2 hpcuser hpcuser   4096 Aug  7 09:51 Desktop
-rw-r--r--  1 hpcuser hpcuser   4855 Oct 30  2017 .dir_colors
drwxr-xr-x  2 hpcuser hpcuser   4096 Aug  7 09:51 Documents
drwxr-xr-x  2 hpcuser hpcuser   4096 Aug  7 09:51 Downloads
```

- Access rights
  - user - group
  - **d[rwx][rwx][rwx]**
    - directory [user][group][other]
    - read - write - execute/navigate

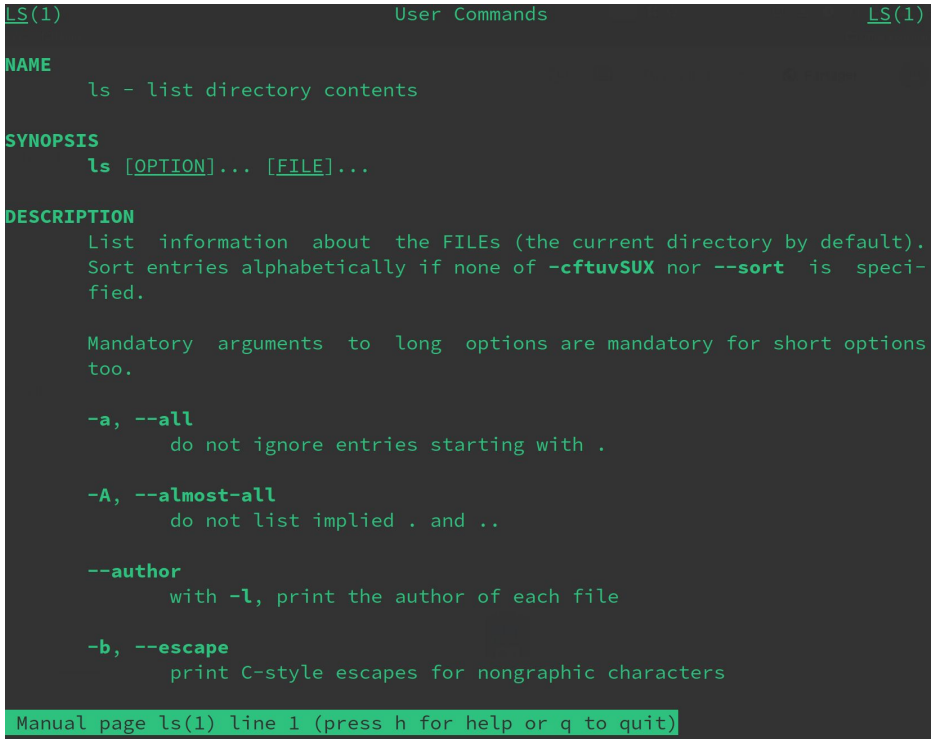
# Anatomy of a command

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`
  - short flags - condensed, difficult to parse
    - start with - e.g. `-l -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
  - number of arguments depends on the program
- example - all these commands are equivalent
  - `$ls -la`
  - `$ls -a -l`
  - `$ls --format=long -a`

# A little bit of help

- Manual page ← *more comprehensive*
  - `man <command>`
    - e.g. `$ man ls`
- Help flag ← *when a man page does not exist*
  - `<command> --help`
    - e.g. `$ ls --help`



# A little bit of help

*Now, you do it!*

- 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?

```
ECHO(1)


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://gitlab.uni.lu/hlst/hpc-school-for-beginners.git
```

*Check the content*

*You should see a couple of files and directories. Check that the CLI directory is present.*

```
$ ls ~/hpc-school-for-beginners
```

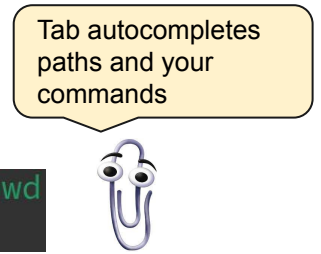
*Go to the directory containing the files for the tutorial*

```
$ cd hpc-school-for-beginners/CLI
```

# Navigating through the file system

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

*Now, you do it!*

- 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

*Now, you do it!*

- 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. **`ls`**, **`cd`**)
    - the tab key proposes completion
      (e.g. **`l + 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

```
[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]$
```

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

# Manipulating files (1/2)

- `mkdir` - make directory
  - 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.
    - `$ 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`
    - `$ ls` -> 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)

*Now, you do it!*

- 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)

*Now, you do it!*

- 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)

up and down arrows navigate through recent commands

- `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`
  - move and rename a file
    - `$ mv foo/temp.txt ./test.txt`

# Manipulating files (2/2)

*Now, you do it!*

- 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)

*Now, you do it!*

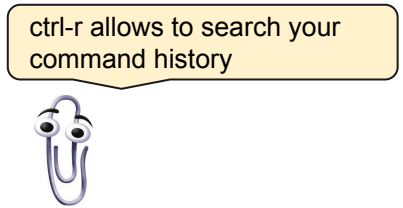
- Delete the `~/hpc-school-for-beginner/CLI/playground/temp` directory and its content
- Move the backup of experiment.out to the `hpc-school-for-beginners/CLI/playground/files/experiment/data` directory and rename it `test001.com`

```
[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]$
```

# Reading and writing files (1/2)

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



# 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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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.

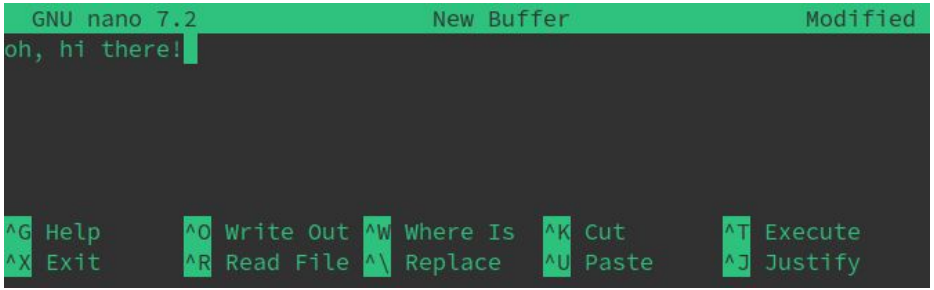
Hit ctrl + c to interrupt any running program

```
[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]$ 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 **ls -la /usr/bin** in it
- the nano text editor
  - `$ 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

```
drwxr-xr-x  4 root    root    4096 Sep  8 14:27 .
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    root    4096 Sep  8 14:27 .git
-rw-r--r--  1 root    root    6213 Sep  8 14:27 README.md
```

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
  - 1 = execute
  - 2 = write
  - 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

*Now, you do it!*

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

# Changing permissions

*Now, you do it!*

- 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
  - `$ rsync -azvu [user@]<host>:<source> <destination>`
  - `$ rsync -azvu aion-cluster:my_data data_directory`
- Flags
  - a - archive mode (recursive, copies files, rights, links, ...)
  - z - compress data during transfer (speeds up transmission)
  - v - verbose (display what is going on)
  - 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
  - redirect the content of the man page command for the bash program to the tmp.dat file
- second command
  - display the content of the tmp.dat file (cat) and
  - pipe the result to grep. Only keep the lines that contain ‘bash’ while ignoring the case and
  - pipe the output to wc which will count the number of lines (-l flag)
- summary: count the number of lines containing ‘bash’ (case insensitive) in the man page of the bash program

# Final Boss - Phase 2

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$ 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!

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Find out what these commands are doing? Don't run them yet!
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- 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 `~/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…

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- 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.