

Lecture 1: The high-performance computing environment

1 Course introduction

"lab course" lab is Amarel cluster
a) general intro to scientific computing
b) electronic structures c) MD simulation

2 A brief history of operating systems

a) Unix 70's Bell Labs → Linux
b) Microsoft MS-DOS → Windows 10, 11 → WSL
c) Apple MacOSX derived from Unix, called Darwin
iOS app "ish"

3 The command line and file system

GUI vs CLI: terminal-based
jupyter-based
\$, >
good for documenting, repeat
" remote access

folder aka directory

/home/<netid>/

/usr

/projects

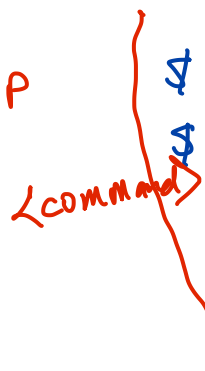
/tmp

shared space on Amarel

4 The "shell"

OS ↔ "shell" ↔ user interaction
/usr/bin/bash

- ① --help
- h
- ② man



```
$ ls
$ gl6
```

→ list of files in the current folder
→ shell look for a program called 'gl6'

echo \$PATH

```
/usr/bin:/usr/local/bin:/bin:
/home/dacase/bin
```

which gl6

ls -l

5 stdin/stdout/stderr and pipes

default stdin is keyboard; stdout, stderr screen

```
$ ls > directory.txt
< redirect stdin
2> redirect stderr
```

create a new file with a list of file names

```
$ ls | wc ⇒ 6 17 256
#lines #words #characters
```

on the screen

```
$ ls | wc | awk '{print $1}' <ret> FIFO
```

6 ~~Shell variables and programming~~

a) the various commands operate in parallel

wc command ~~wait~~ keeps reading its input until <EOF> is found

b) each program does one thing well
" " uses stdin, stdout, stderr

↳ combine individual programs with pipes

echo "ls | wc | awk '{ }'" > count-files

```
$ bash count-files ⇒ $ countfiles
cf ↓
```

7 Introduction to AWK

...more AWK