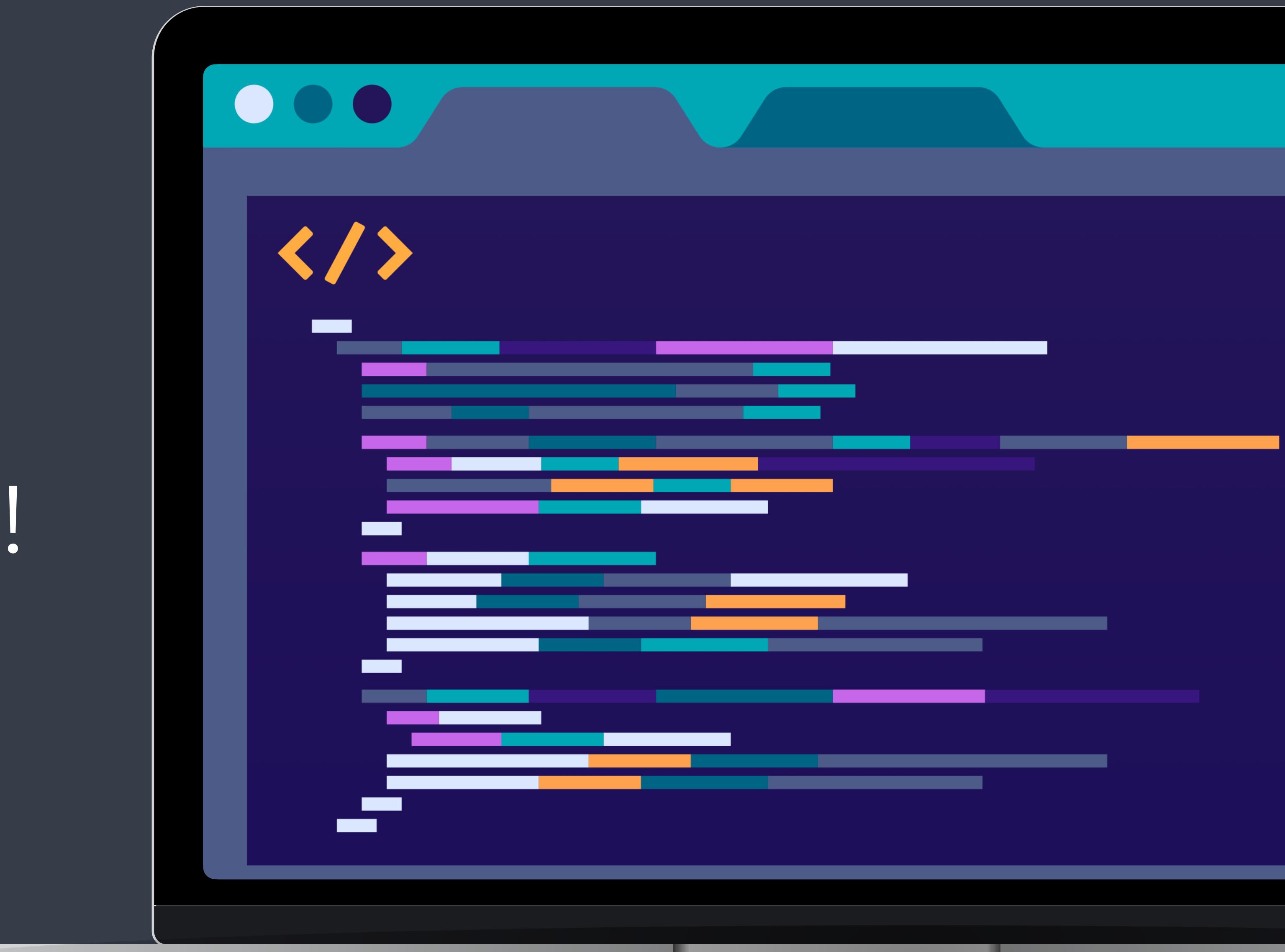
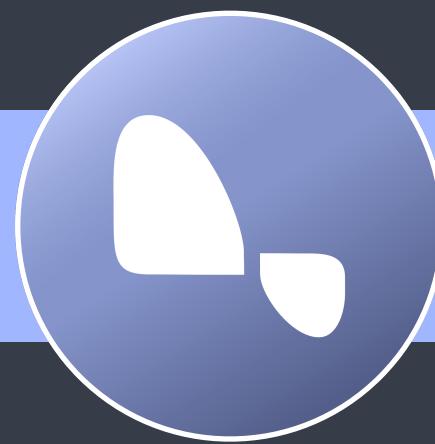


JUST BASH IT!





CENTER FOR HEALTH DATA SCIENCE (HEADS)

- Data Lab Supports Researchers at the Faculty
- Consultation, Commission & Collaboration:
 - Data science and bioinformatics analyses
- Teaching: Courses & Workshops, Seminars.



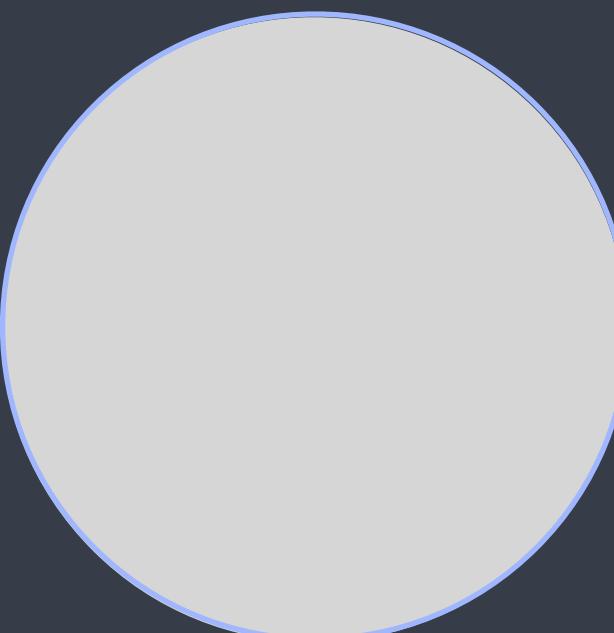
Henrike Zschach



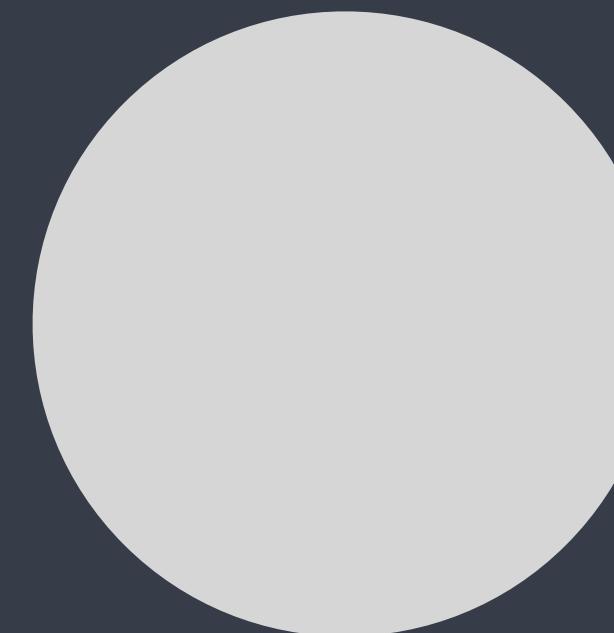
Thilde Terkelsen

COPENHAGEN UNIVERSITY LIBRARY (KUB)

- XXXXXX XXXXXX
- XXXXXX XXXXXX
- XXXXXX XXXXXX



XXXXXX XXXXXX



XXXXXX XXXXXX

JUST BASH IT!

PROGRAM

XX:XX-XX:XX - INTRODUCTION TO COMMANDLINE

XX:XX-XX:XX - NAVIGATING FILES AND DIRECTORIES

XX:XX-XX:XX - PROJECT ORGANIZATION & BACKUP

XX:XX-XX:XX - WORKING WITH FILES

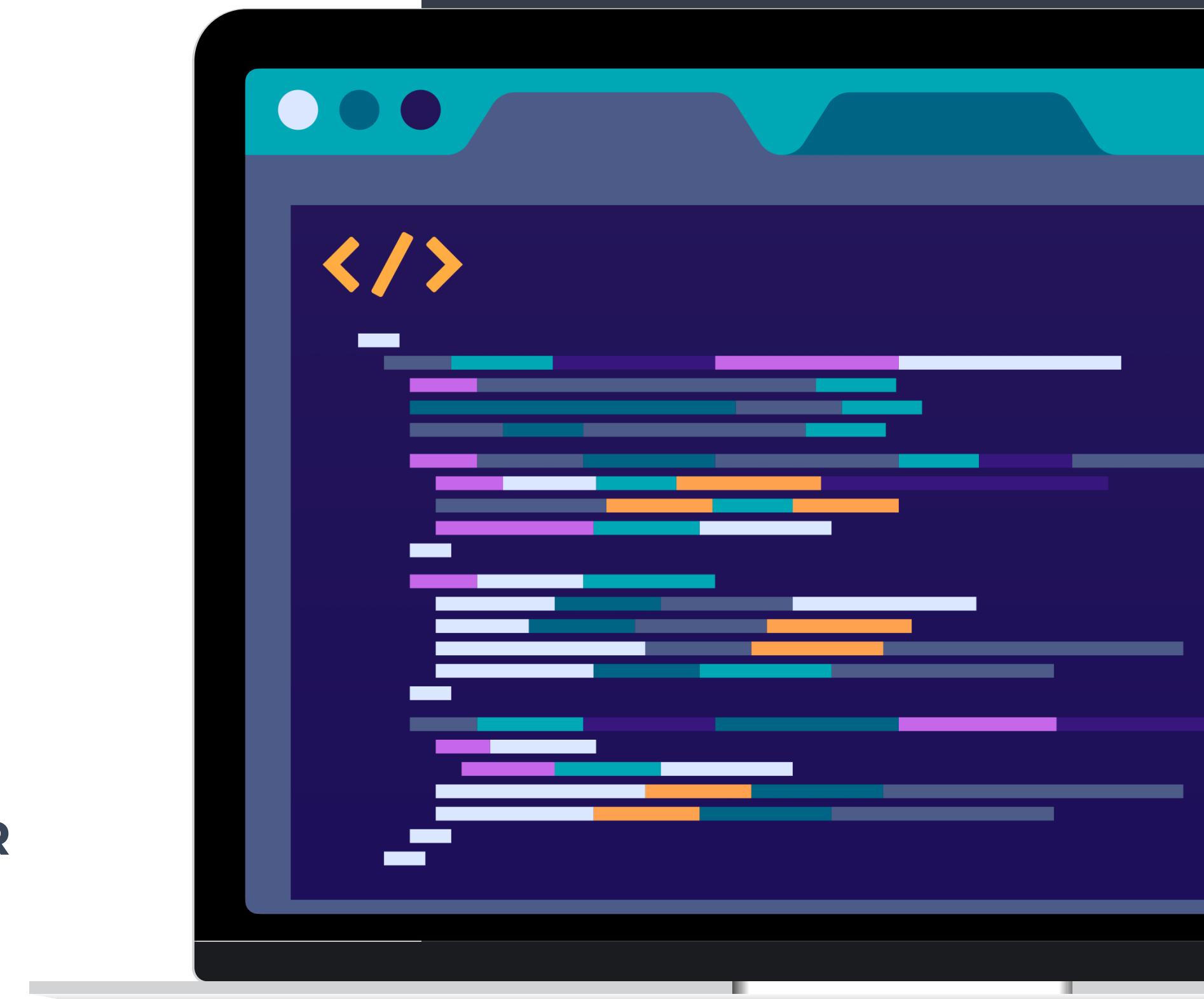
XX:XX-XX:XX - MORE BASH COMMANDS

XX:XX-XX:XX - REDIRECTION & PIPES

XX:XX-XX:XX - SHELL SCRIPTS & LOOPS

XX:XX-XX:XX - SOFTWARE INSTALLATION UPKEEP & MORE

XX:XX-XX:XX - WORKFLOW LANGUAGE & COMPUTE POWER



COURSE MATERIALS:

<https://github.com/Center-for-Health-Data-Science/Just-Bash-It>



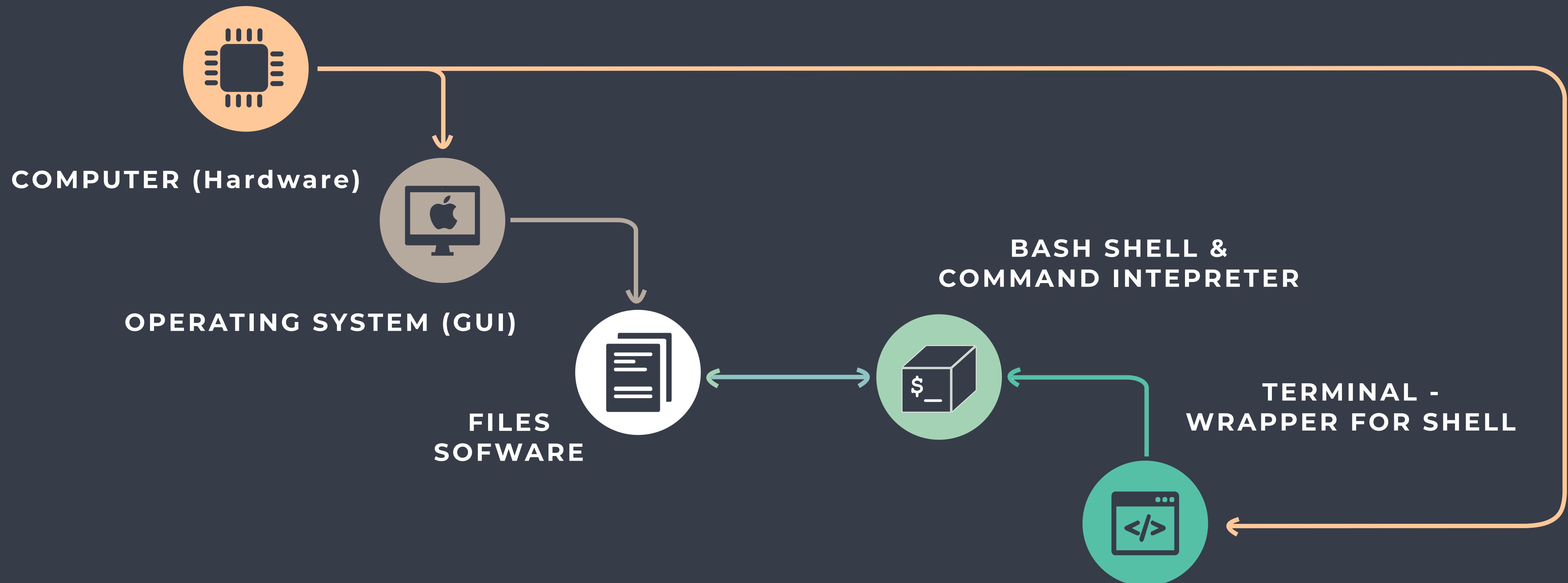
```
Last login: Fri Jun 24 15:05:34 on ttys000  
[kgx936@SUN1007442 ~ % echo "Just Bash It"  
Just Bash It  
kgx936@SUN1007442 ~ % █
```

“

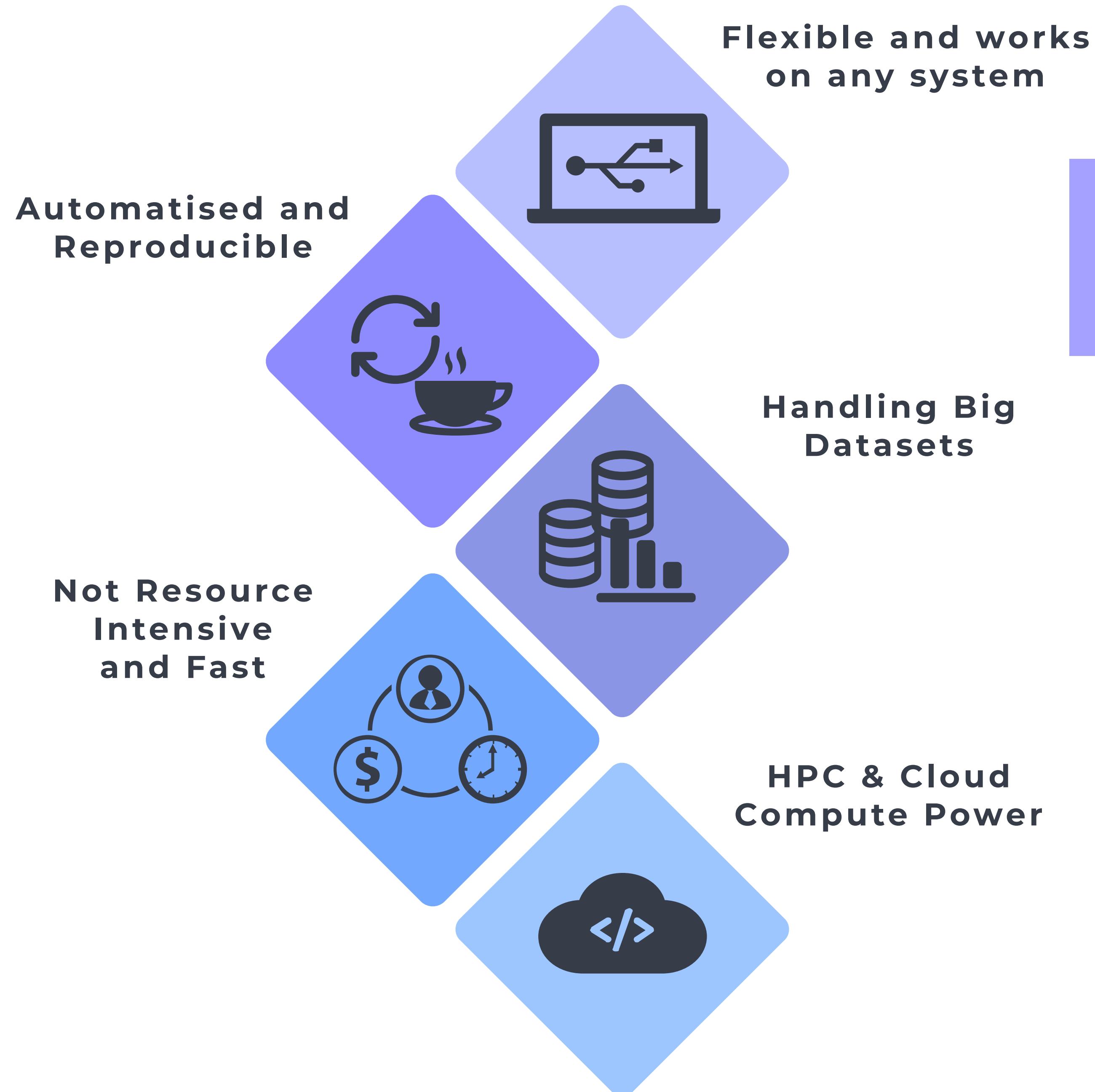
“What is a shell, a terminal, a command-line, and what is bash?”

“How do these concepts connected to my computer?”

TERMINOLOGY



- You open the terminal on your computer
- You type bash commands
- Commands are interpreted and fed to the OS



SELL IT TO ME!

Benefits of bash & command line:

- Do a lot with minimum effort on any system.
- Your analysis will be reproducible, automated and parallelized.
- Fast processes, less computationally intensive.
- Power to handle big data and heavy computations.

A COUPLE OF EXAMPLES



REGISTRY DATA

Drug adverse effects and mortality:

Person sensitive
Huge files, many columns
Different formats



SEQUENCING DATA

Single Cell RNA from Cystic Fibrosis:

Paired-end sequencing
300 patients
Two fastq files per patient



DATABASES

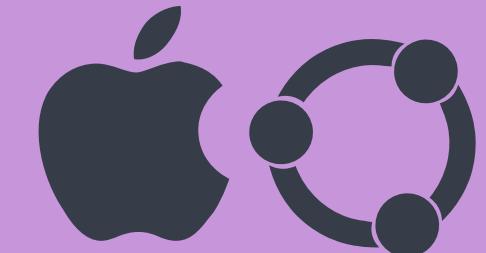
Drug Databases - molecular structure & interaction:

Multiple large databases
Different formats
Maybe not downloadable

HOW DO I GET A BASH SHELL?

YEAH!
YOU HAVE A BASH SHELL &
TERMINAL ALREADY.

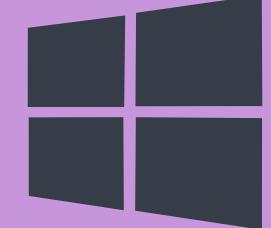
Search for terminal on your
laptop and open it.



OS X or UBUNTU

YOU NEED TO INSTALL A BASH SHELL/TERMINAL:

- **MobaXterm:** <https://mobaxterm.mobatek.net/download.html>
- **Cygwin:** <https://www.cygwin.com/index.html>
- **Cmder:** <https://cmder.net/>
- **PuTTY:** <https://www.putty.org/>



WINDOWS

In this course Windows users will be working on **MobaXterm**.

You should have **installed this shell** via. instructions in the introduction email.

WHAT WILL I LEARN TODAY?



The BASICS OF BASH

- The terminal
- Navigation w. bash
- Read, Edit, Copy

1

ORGANIZATION & STRUCTURE

- Directory Structure
- Paths & Permission
- Reproducibility

2

MORE BASH COMMANDS

- Manipulate files
- Subset, Count
- Print, Sort, Match
- Cut, Paste, Split

3

SCRIPTS & AUTOMATIZATION

- Stdin & Stdout
- Piping
- Loops & Scripts
- Pipelines

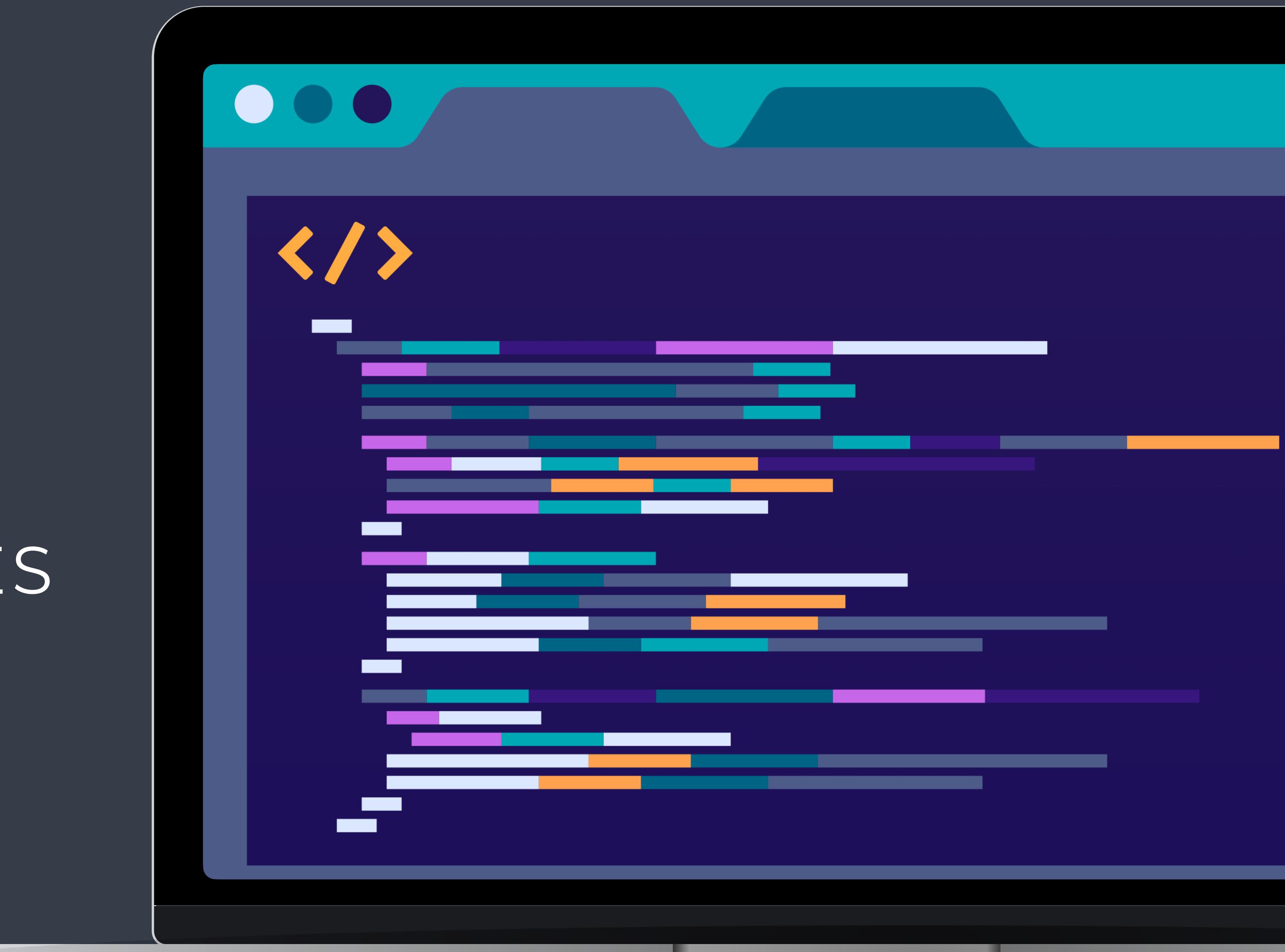
4

STORAGE, BACKUP & MORE...

- Manage Software
- Workflows
- Backups
- Computing Power

5

1. NAVIGATING FILES & DIRECTORIES



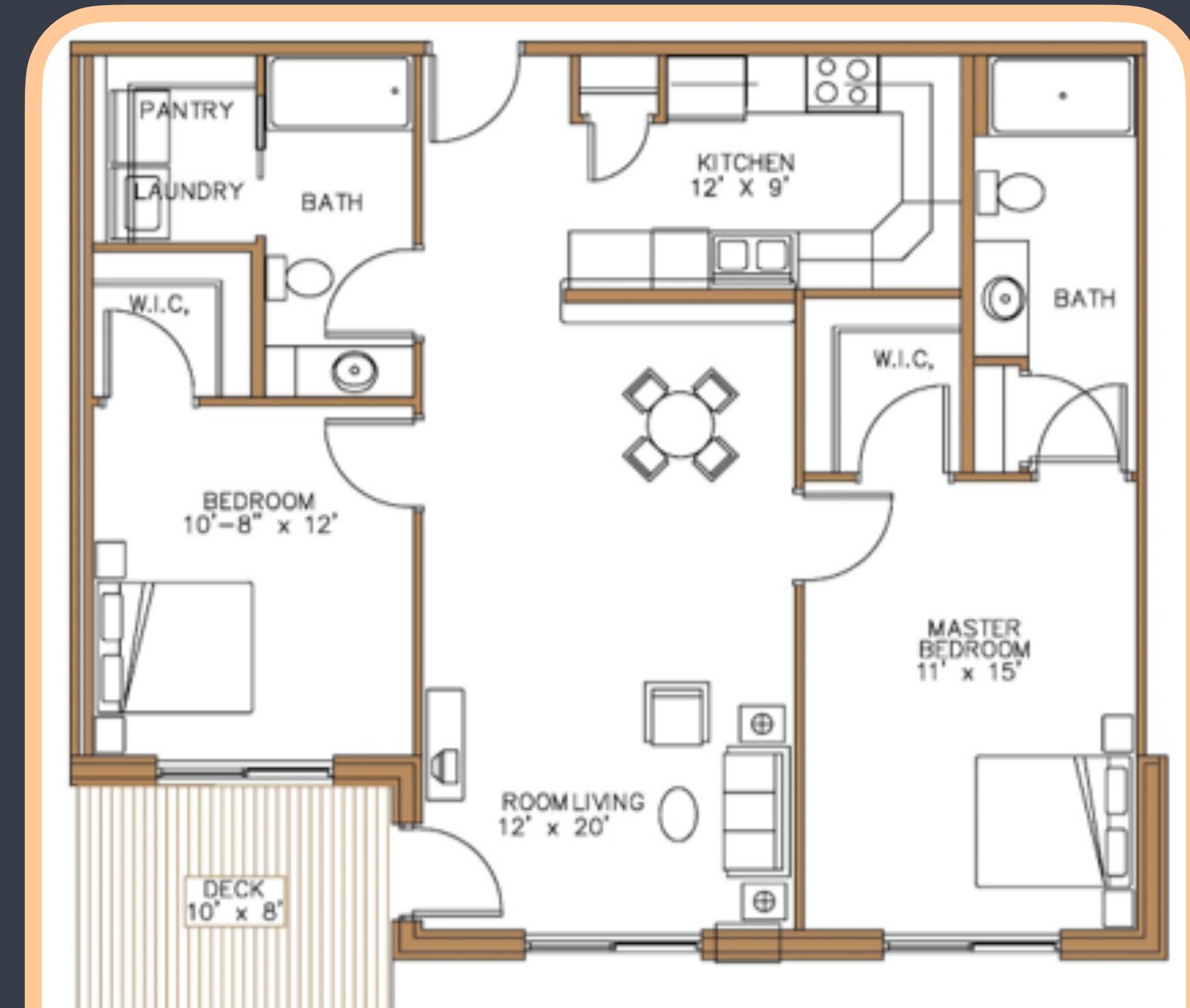
NAVIGATING FILES AND DIRECTORIES

- **Where am I on my computer? (And what does that mean?)**
- **How can I move around on my computer?**
- **What are files and directories?**
- **How can I see what files and directories I have?**
- **How can I specify the location of a file or directory on my computer?**

THE DIRECTORY TREE

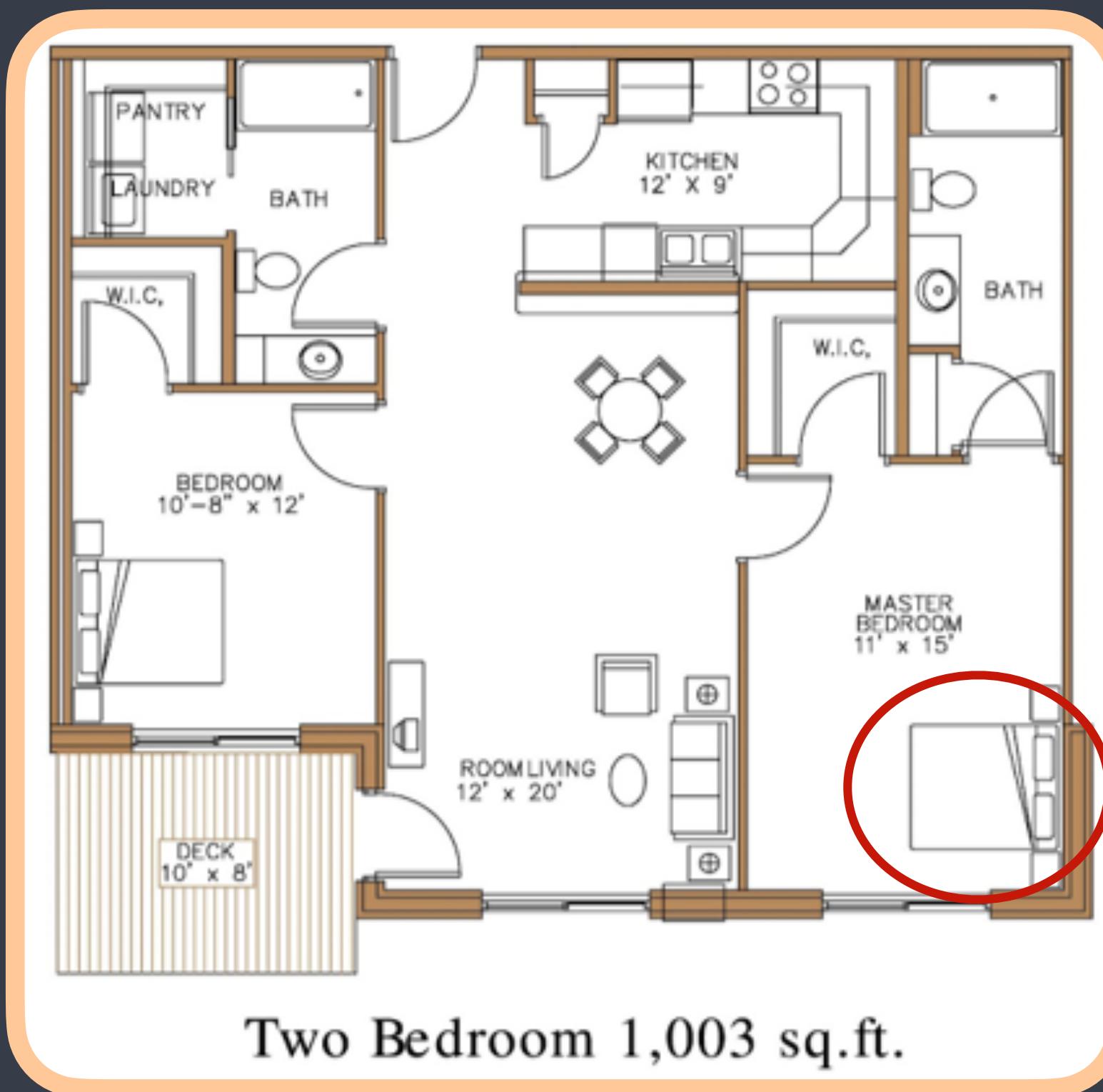
Your computer is **like a house**:

- It has different rooms, i.e. **directories** which contain items, i.e. **files**.
- You cannot be in two different rooms at the same time.
- Your files are items in the house and they are in specific places. Your bed is in your bedroom.
- In order to interact with your item **you need to know where it is**.
- You can move items from one room to another.

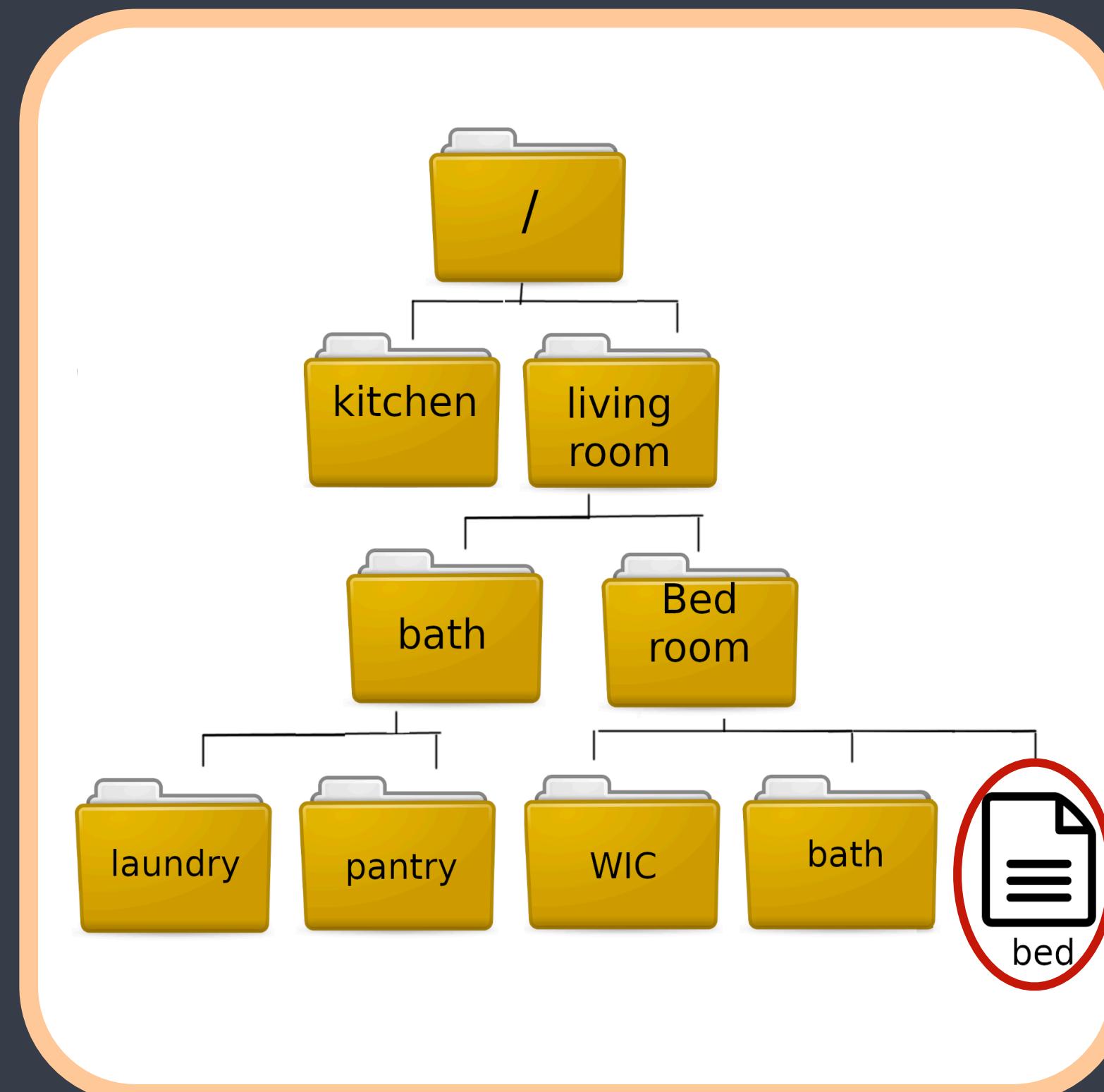


THE DIRECTORY TREE

A loose translation of the floor plan into a directory tree:



The **directory tree** is hierarchical and starts at the 'root' = '/'

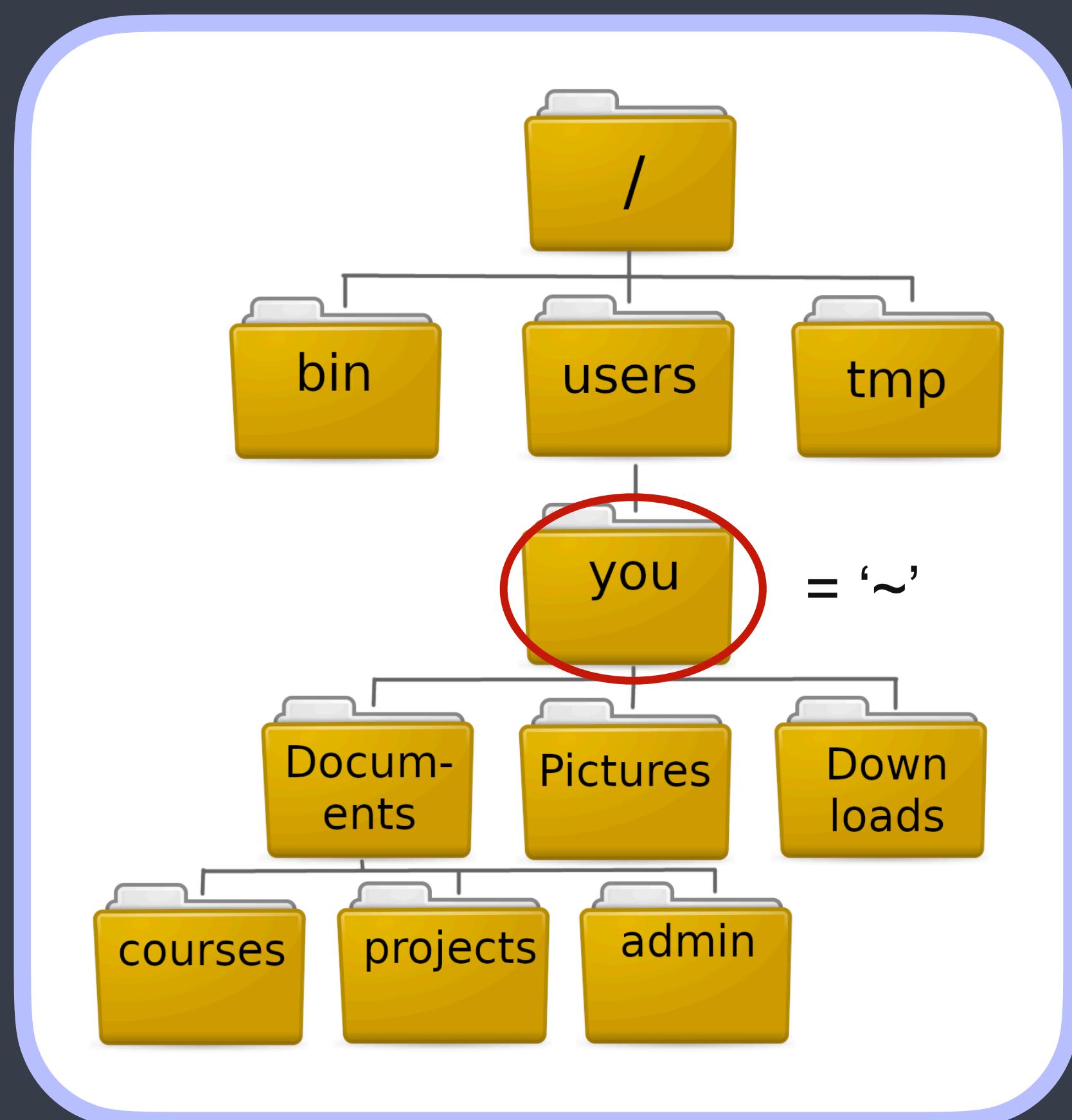


THE HOME DIRECTORY

- When you open your terminal you are in your home directory.
- The directory you are currently in is called your **working directory (wd)** - you can **check it**:

```
$ pwd
```

- **Open your terminal and check where you are!**
- Your home directory is also represented by the symbol ‘~’ (**tilde**).
- You may notice this symbol later when looking at your current directory or changing to another directory.



LISTING CONTENT

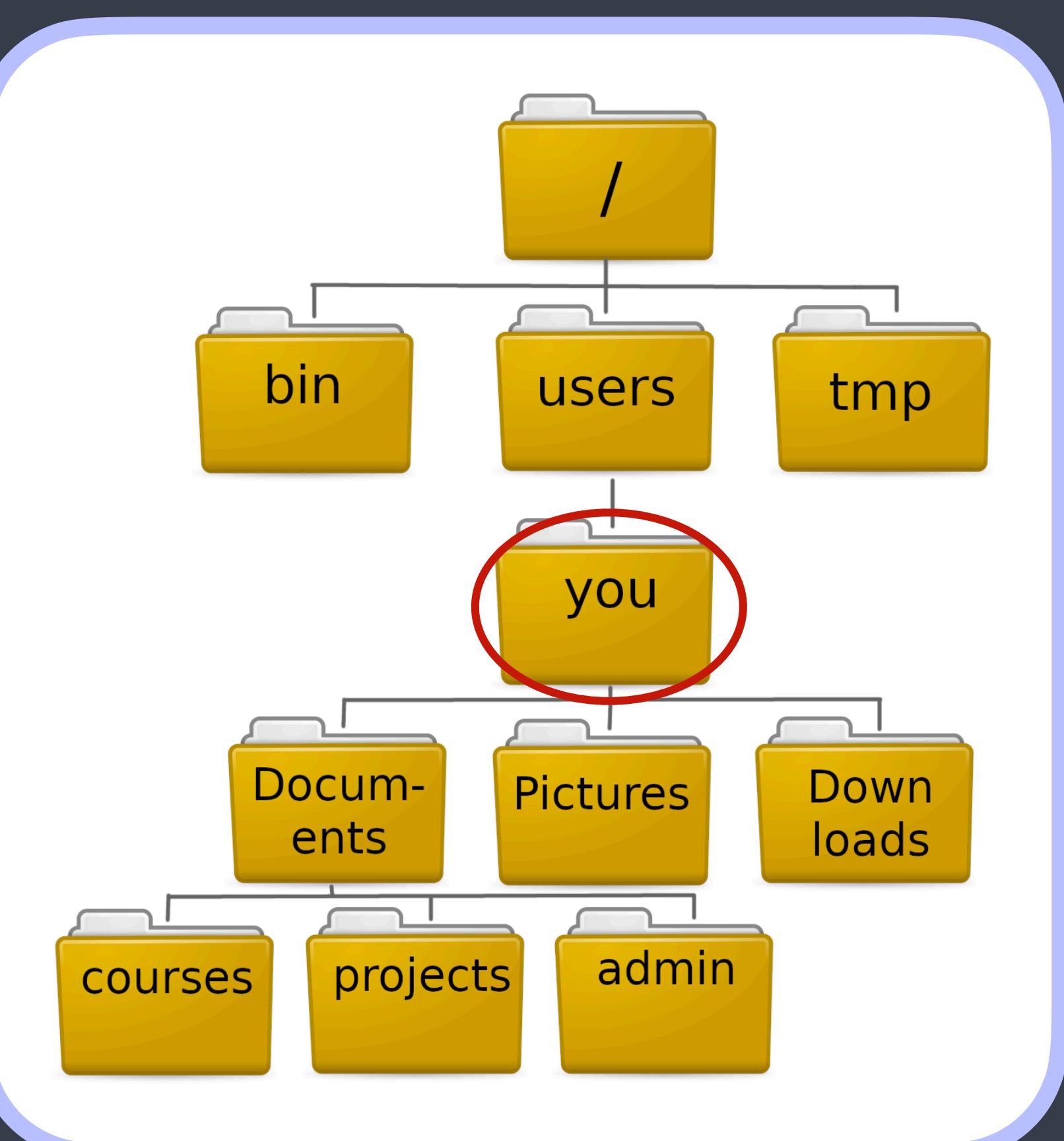
- To **list all contents of a directory**, including other directories, use the command:

```
$ ls
```

- ls will list what is in your current **wd**.
- You can list other directories by specifying the **path** to them:

```
$ ls /home/Users/
```

- ls has many useful options such as **-l**, **-t** and **-h**, **-F**. Try it out!



CHANGING DIRECTORIES

- From your **wd**, you can easily move into any subdirectory:

```
$ cd Documents
```

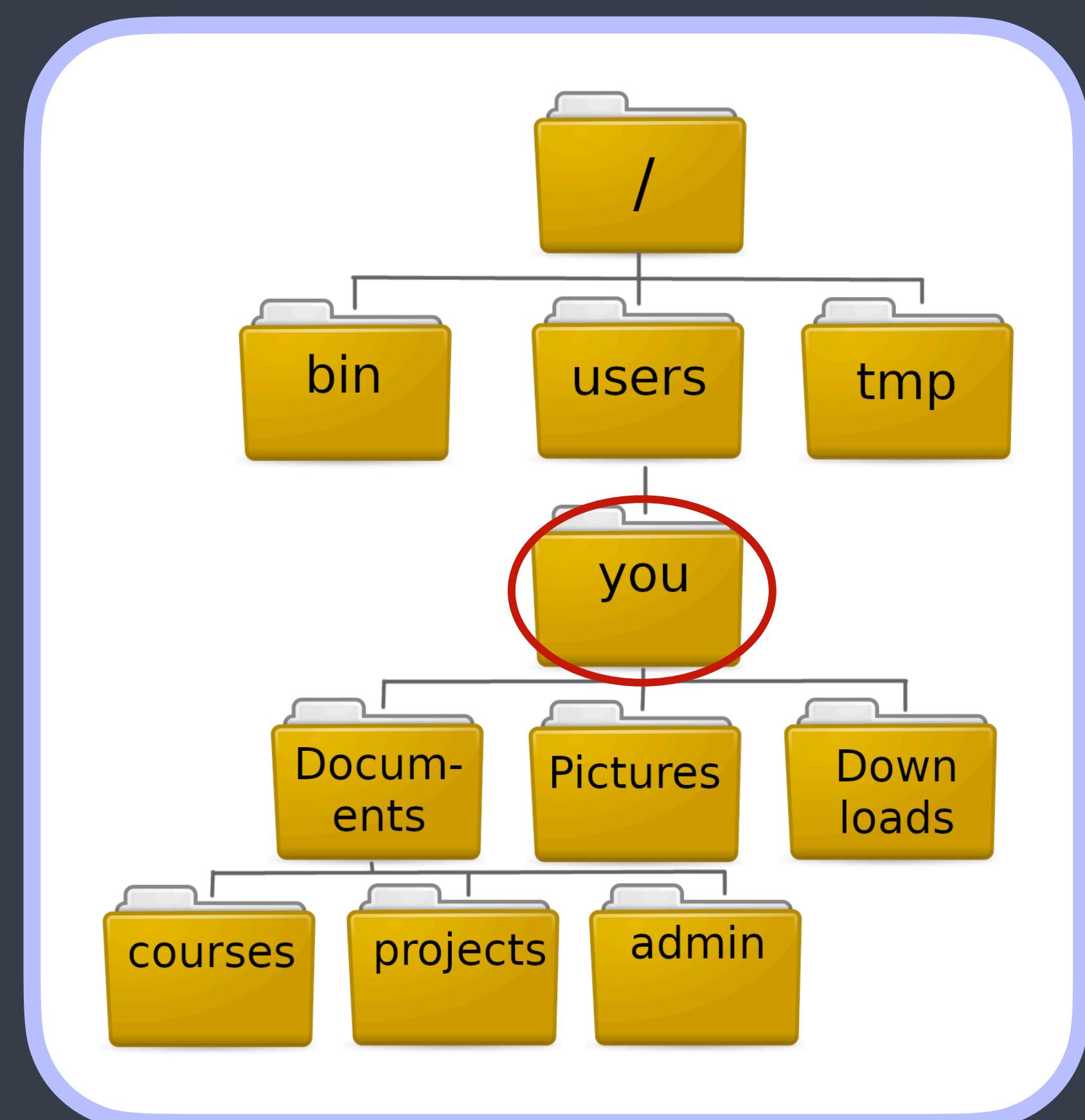
- You can also move several directories down:

```
$ cd Documents/courses
```

- To move 'up' in the directory tree you need to use `'..'`. Each time you write this, you go one level up.

```
$ cd ../../tmp
```

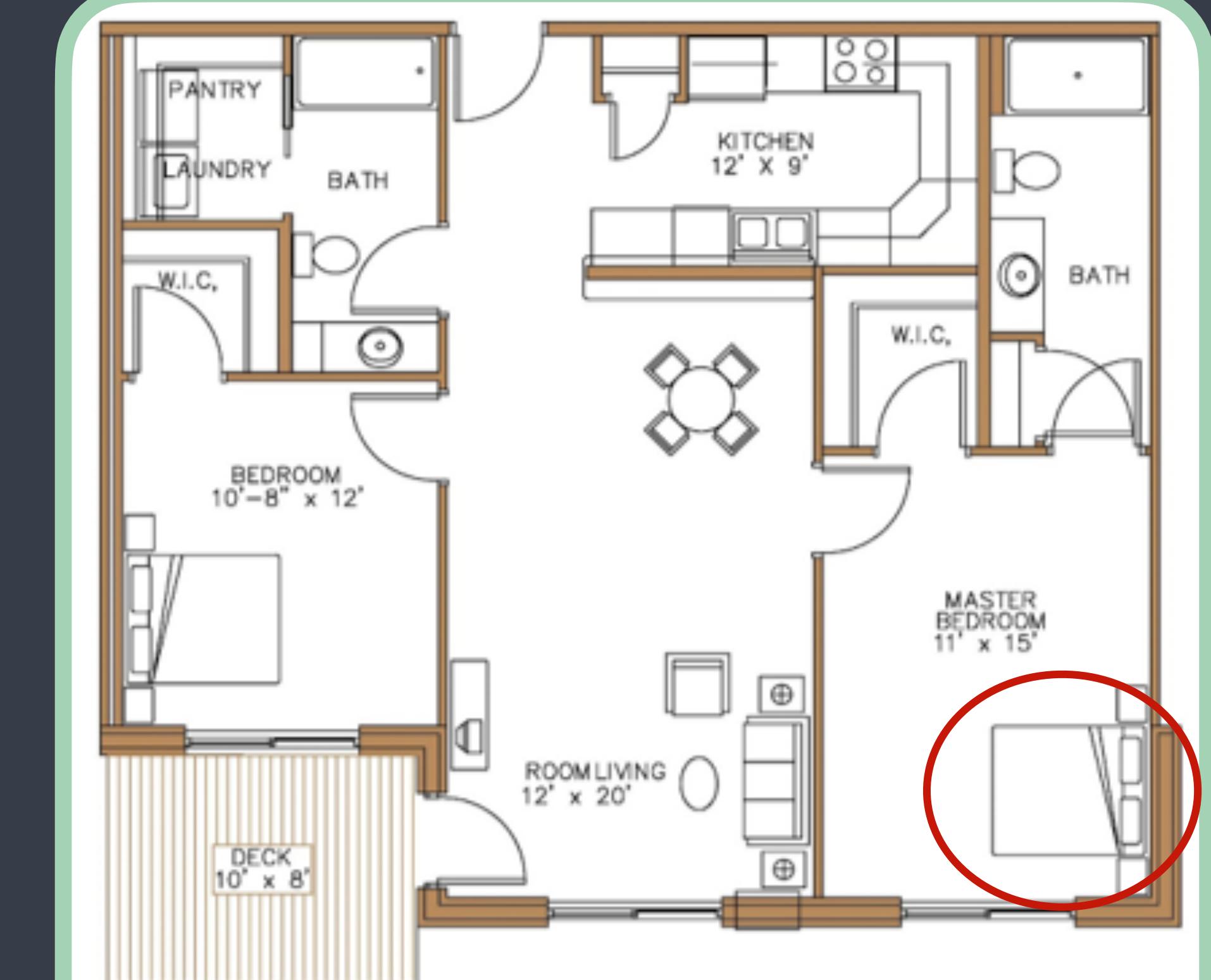
- '**cd**' without any arguments brings you back to your home directory. Try it out!



PATHS

- Each file and directory exist in one specific place on your computer. One could say they have an address.
- This ‘address’ is called their **path**. It is an instructions how to find the file or directory.
- Following the example from earlier, the path to your bed would be:

/entrance/living_room/Bedroom/bved.txt



Two Bedroom 1,003 sq.ft.

PATHS

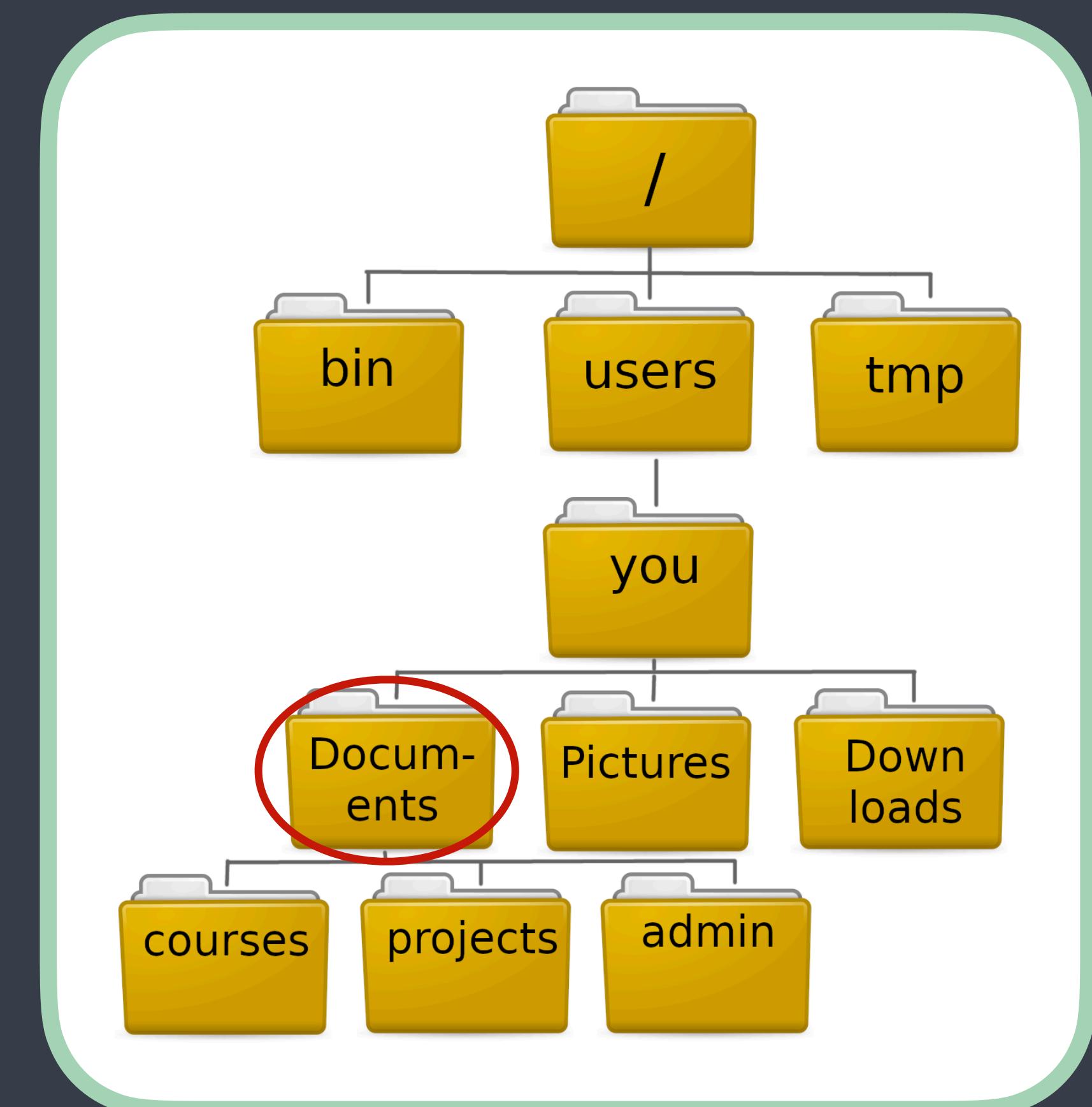
- Paths can be full/absolute or relative.
- Full paths always start at the root. Since ~ represent the path to your home directory it naturally includes the root. So

/home/user/[you]/Documents

and

~/Documents

- Are the same place and the same path.
- Full paths are always unambiguous since they describe the entire 'journey' starting from the root.



PATHS

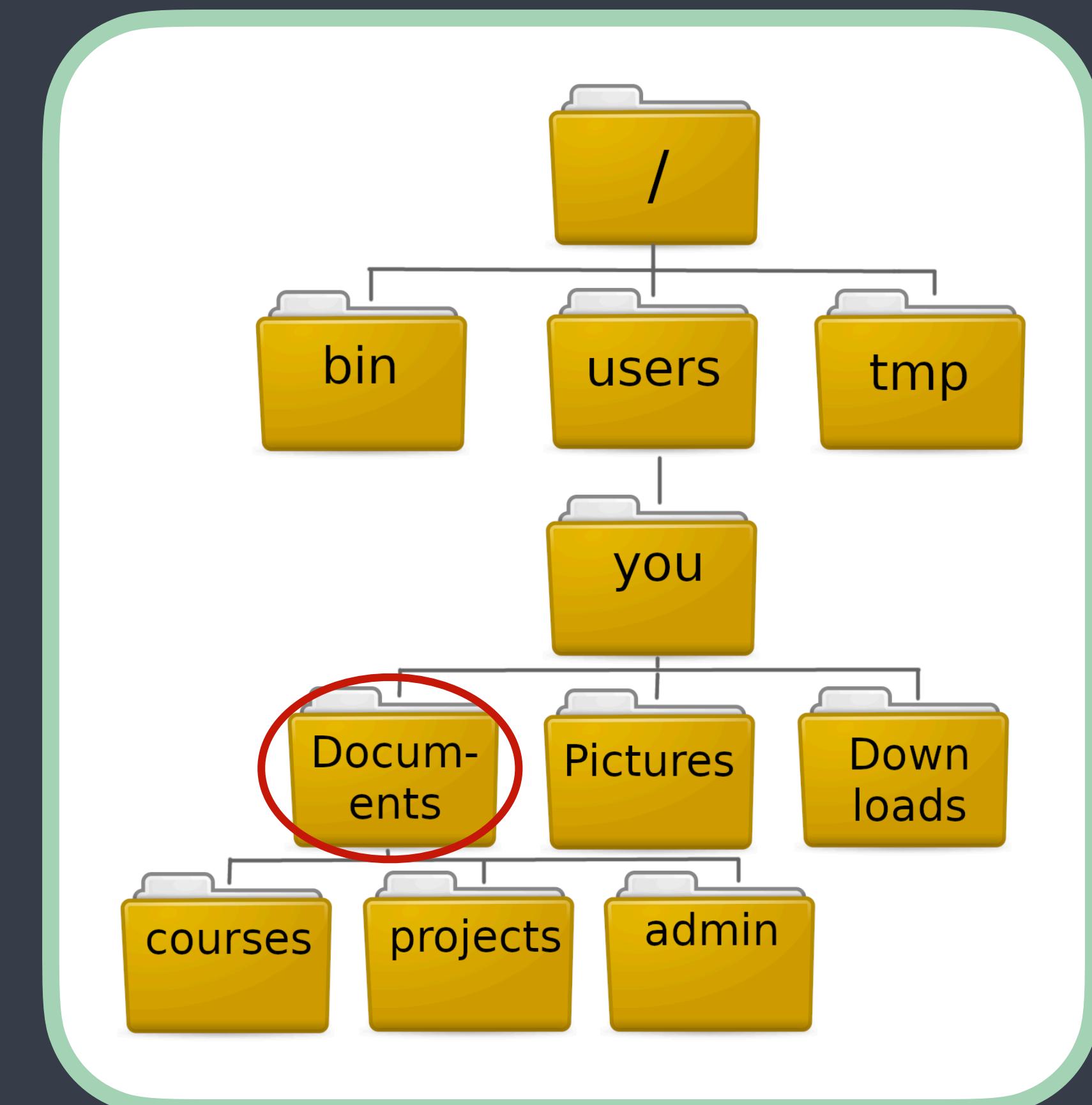
- A **relative paths** is an address relative to the current working directory.
- If my working directory is 'Documents', I can address this presentation as:

courses/Just-Bash-It-main/Commandline_ Workshop.pptx

- Relative paths can include going up the directory tree:

../Pictures/summer2022/Bornholm

- This notation does not make sense for full paths as they start from the root and go strictly downwards.



MOVING FILES AND DIRS

- For this part, lets go into the '*Examples*' folder of the github repo.
- You can move files (and directories) from one place into another with **mv**:

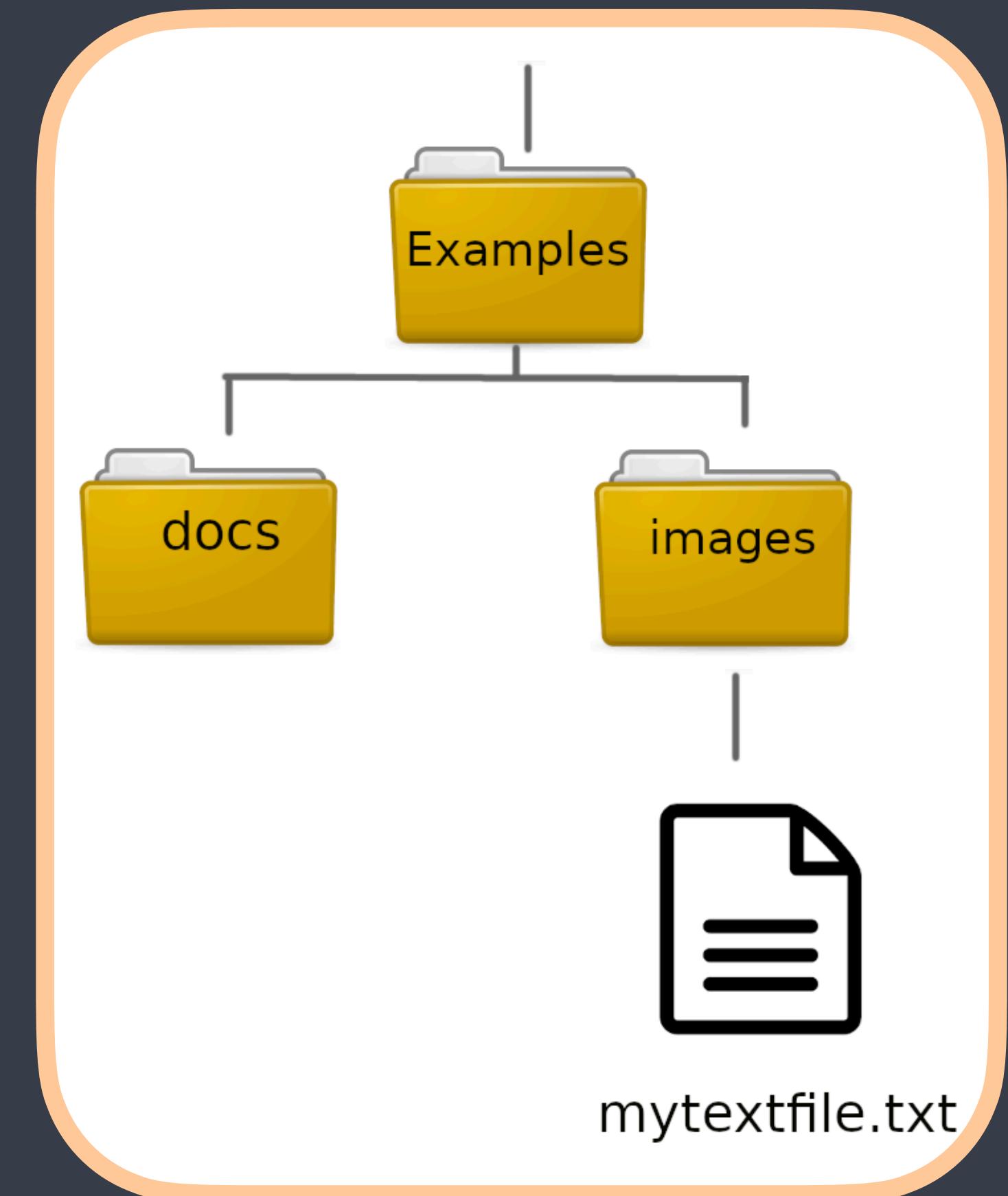
```
$ mv mytextfile.txt ..docs
```

- **mv** can also be used for renaming:

```
$ mv mytextfile.txt my_text_file.txt
```



- Do not try to move or remove your home directory or other system critical dirs. This may have unintended consequences.



COPY AND REMOVE

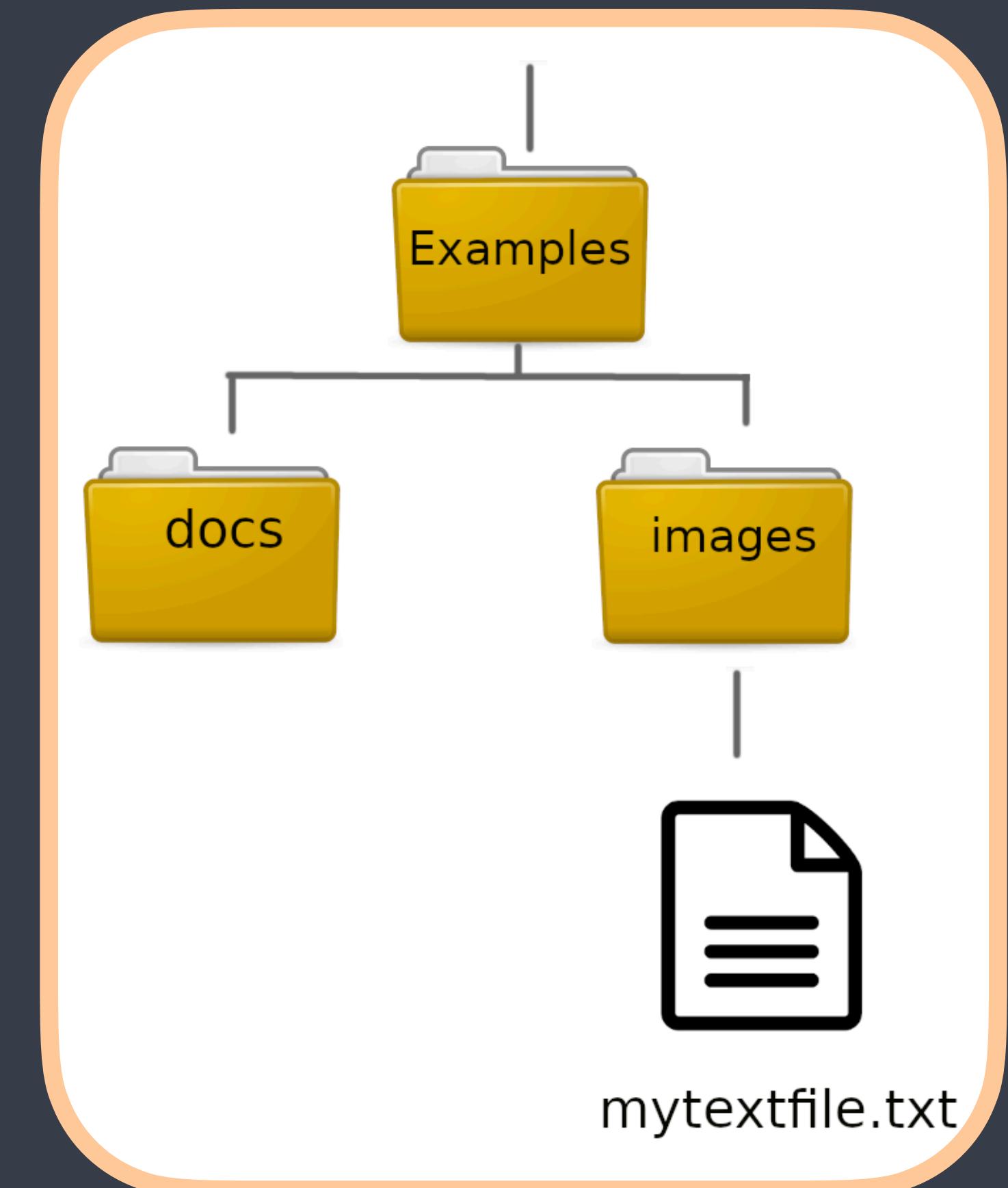
- Files can also be duplicated with the **cp** command:

```
$ cp my_text_file.txt text_copy.txt
```

- To copy a directory (and all its contents!) you need the **-r** flag
- To remove files and dirs, use **rm**

```
$ rm text_copy.txt
```

- Unlike in many graphical file managers, **rm** **is permanent!** You cannot recover a removed file and you will not be asked whether you are sure you want it gone.



COMMANDS

We interact with the computer by issuing **commands** to it. You have already tried some like **cd**, **ls**, **pwd**.

Some commands can stand by themselves like **pwd**, but often they have arguments and options/flags:



The command:

List contents

The options/ flags:

Long format &
Human-readable size

The argument:

Path to the directory
to work on

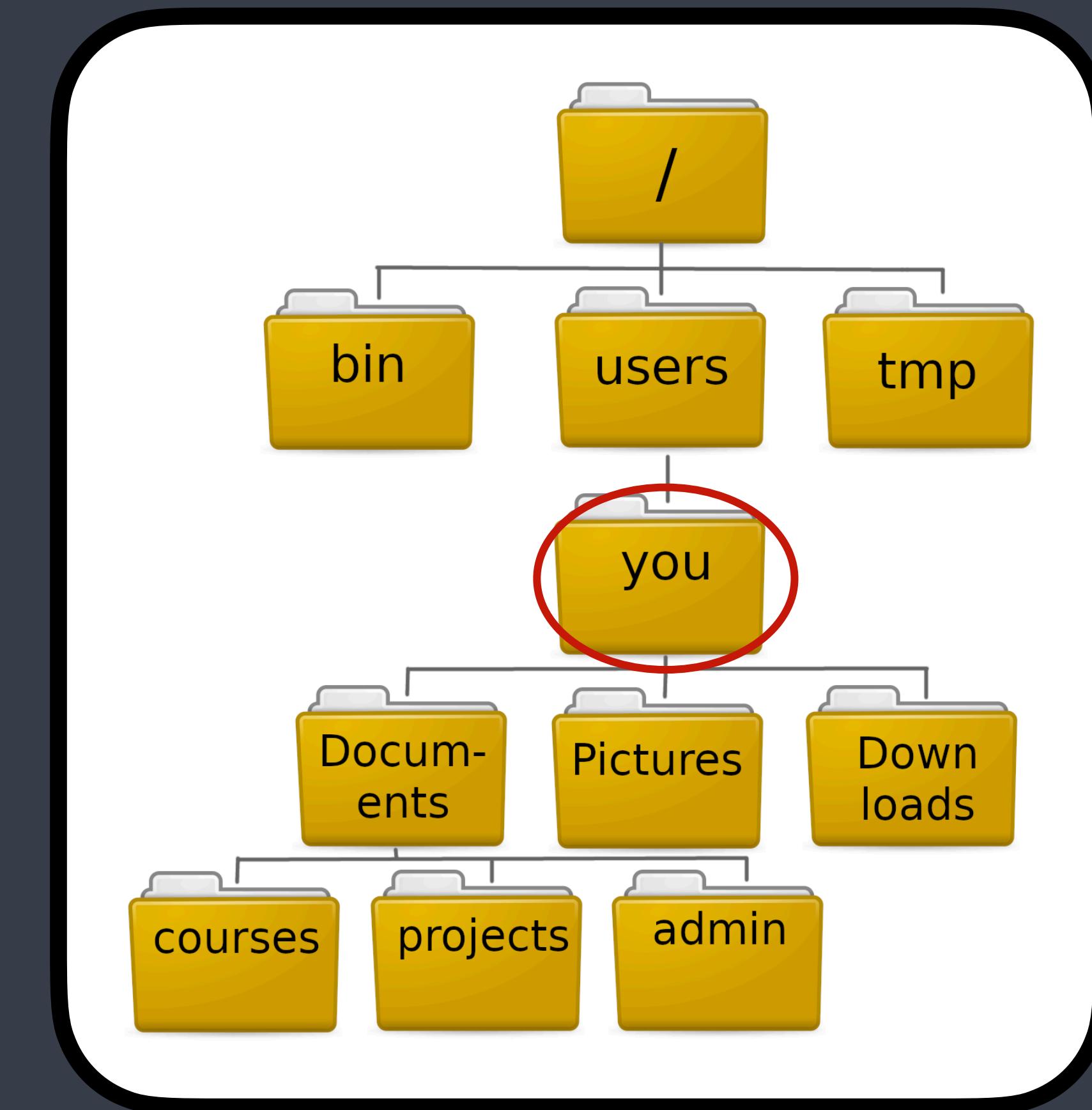
WHEN THINGS GO WRONG

Assuming I am in my home directory and I write:

```
$ cd courses
```

What will happen?

```
henrike@henrike-Swift-SF314-42: ~
henrike@henrike-Swift-SF314-42: ~ 56x24
henrike@henrike-Swift-SF314-42:~$ pwd
/home/henrike
henrike@henrike-Swift-SF314-42:~$ ls
Desktop  Downloads  Pictures  snap      Videos
Documents  Music    Public     Templates
henrike@henrike-Swift-SF314-42:~$ ls Documents/
courses  planets1.xcf  tap-fix.sh
henrike@henrike-Swift-SF314-42:~$ cd courses
bash: cd: courses: No such file or directory
henrike@henrike-Swift-SF314-42:~$
```



WHEN THINGS GO WRONG

1

Don't panic!

2

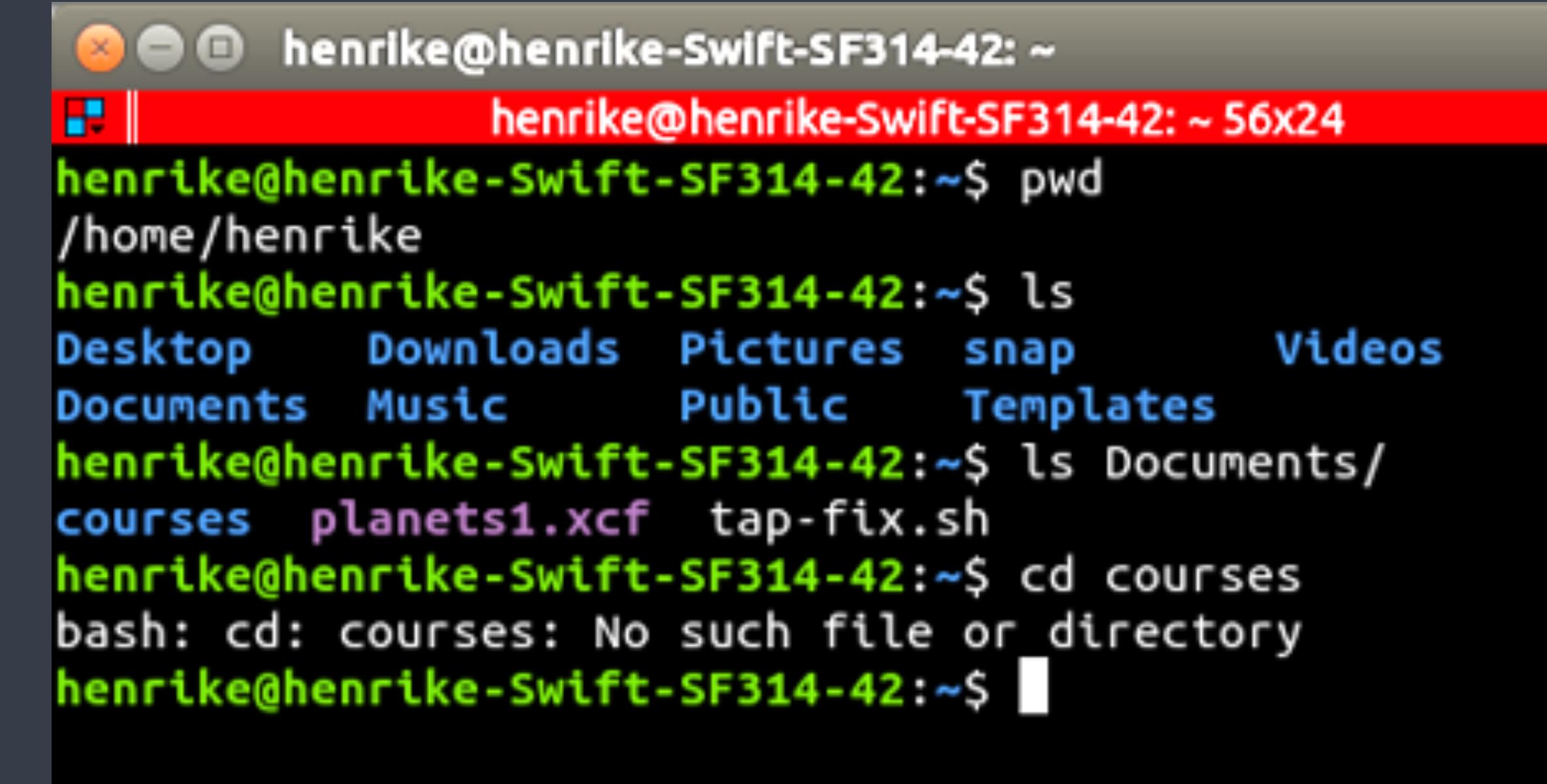
Read the error message

3

Try to correct your error

4

If lost, google or read the help page



```
henrike@henrike-Swift-SF314-42: ~
henrike@henrike-Swift-SF314-42: ~ 56x24
henrike@henrike-Swift-SF314-42:~$ pwd
/home/henrike
henrike@henrike-Swift-SF314-42:~$ ls
Desktop    Downloads  Pictures  snap      Videos
Documents  Music     Public    Templates
henrike@henrike-Swift-SF314-42:~$ ls Documents/
courses   planets1.xcf  tap-fix.sh
henrike@henrike-Swift-SF314-42:~$ cd courses
bash: cd: courses: No such file or directory
henrike@henrike-Swift-SF314-42:~$
```

GETTING HELP

- Many commands have a help page, i.e. a **manual**. You can call it with **man**:

```
$ man ls
```

- The **man** page includes:

- A description of what the command does
- Explanation for arguments
- Usage examples (the syntax of the command, what goes where)

- Commands that do not have a man page often have a help instead, option **(-)help** or **(-)h**

```
henrike@henrike-Swift-SF314-42: ~
henrike@henrike-Swift-SF314-42: ~ 56x24
LS(1) User Commands LS(1)

NAME
    ls - list directory contents

SYNOPSIS
    ls [OPTION]... [FILE]...

DESCRIPTION
    List information about the FILEs (the current
    directory by default). Sort entries alphabeti-
    cally if none of -cftuvSUX nor --sort is speci-
    fied.

    Mandatory arguments to long options are manda-
    tory for short options too.

    -a, --all
            do not ignore entries starting with .

    -A, --almost-all
            do not list implied . and ..
```

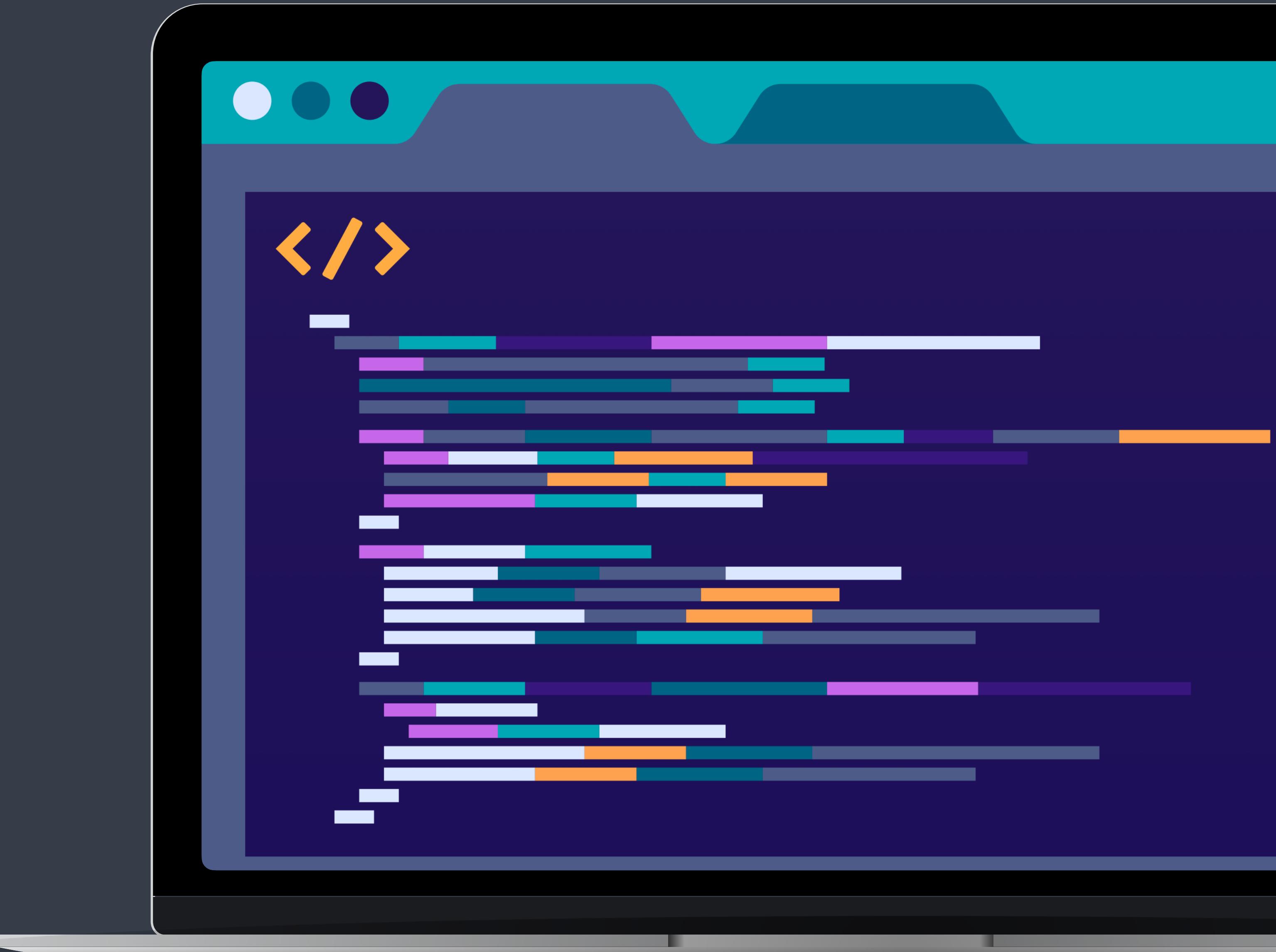
ge ls(1) line 1/297 7% (press h for help or q to quit)

CHEAT SHEET 1

```
pwd # print working dir  
cd # go to home dir  
cd [path] # change dir (remember path)  
ls # list dir content  
man [cmd] # get info about command  
[cmd] --help # view the help for command
```

WHERE & WHAT

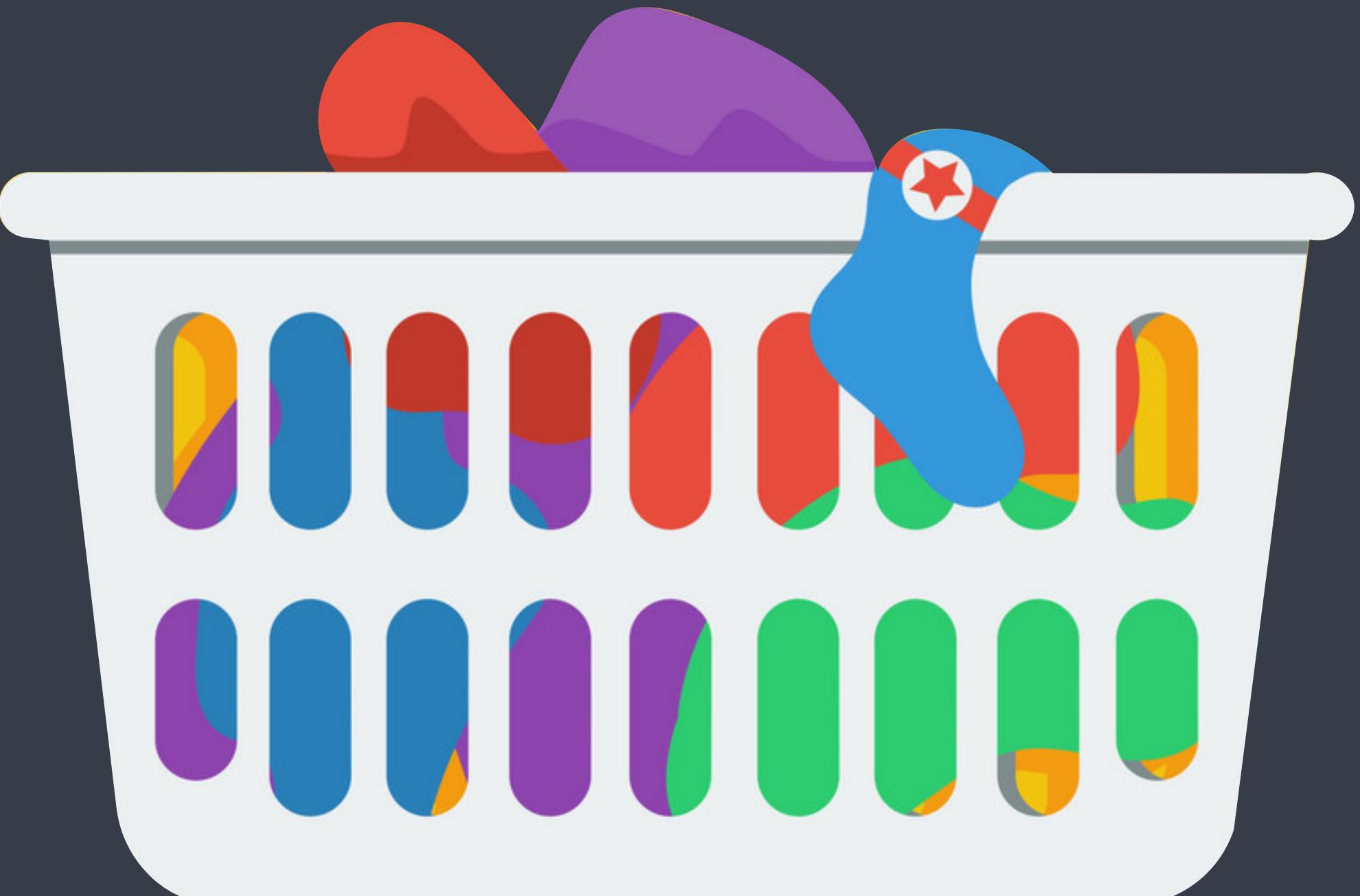
2. PROJECT ORGANIZATION & BACKUP



IS YOUR COMPUTER A LAUNDRY BASKET?

Why should I care about directory structure and file naming?

- Not nice to not “work” in a mess.
- If your computer crashes it is MUCH easier to recover work if files/directories are structured.
- If you apply a command (bash, R, Python) to a group of files/directories, naming is important!
- Large files should be stored smartly to save space.



DO'S and DON'TS



Consistent and Logical Directory Structure and Naming



Consistant & Non-redundant File Naming



**Version Control System
git/GitHub & Back-up**



Clean and Update Your Computer Regularly



Don't Use Symbols or Spaces in File/Directory Names



Don't store multiple copies of file, instead point to it (path).

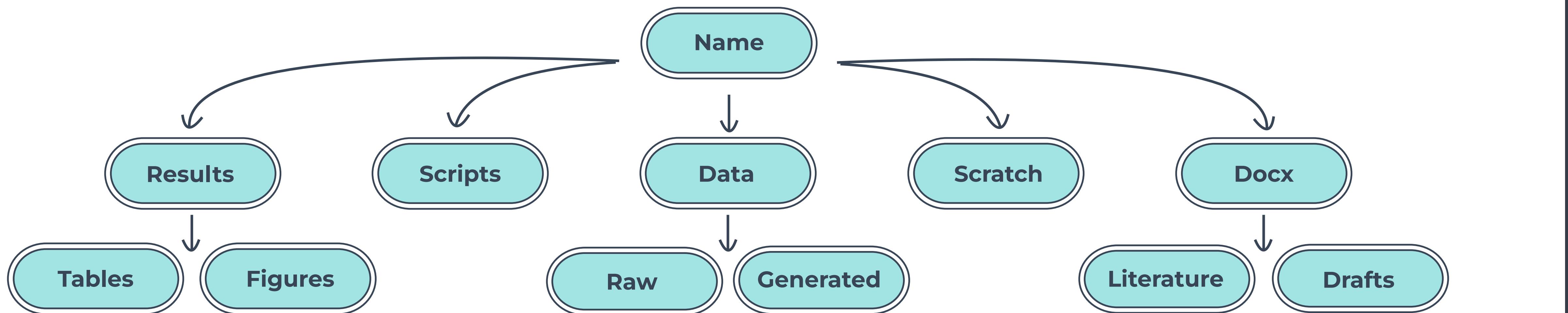
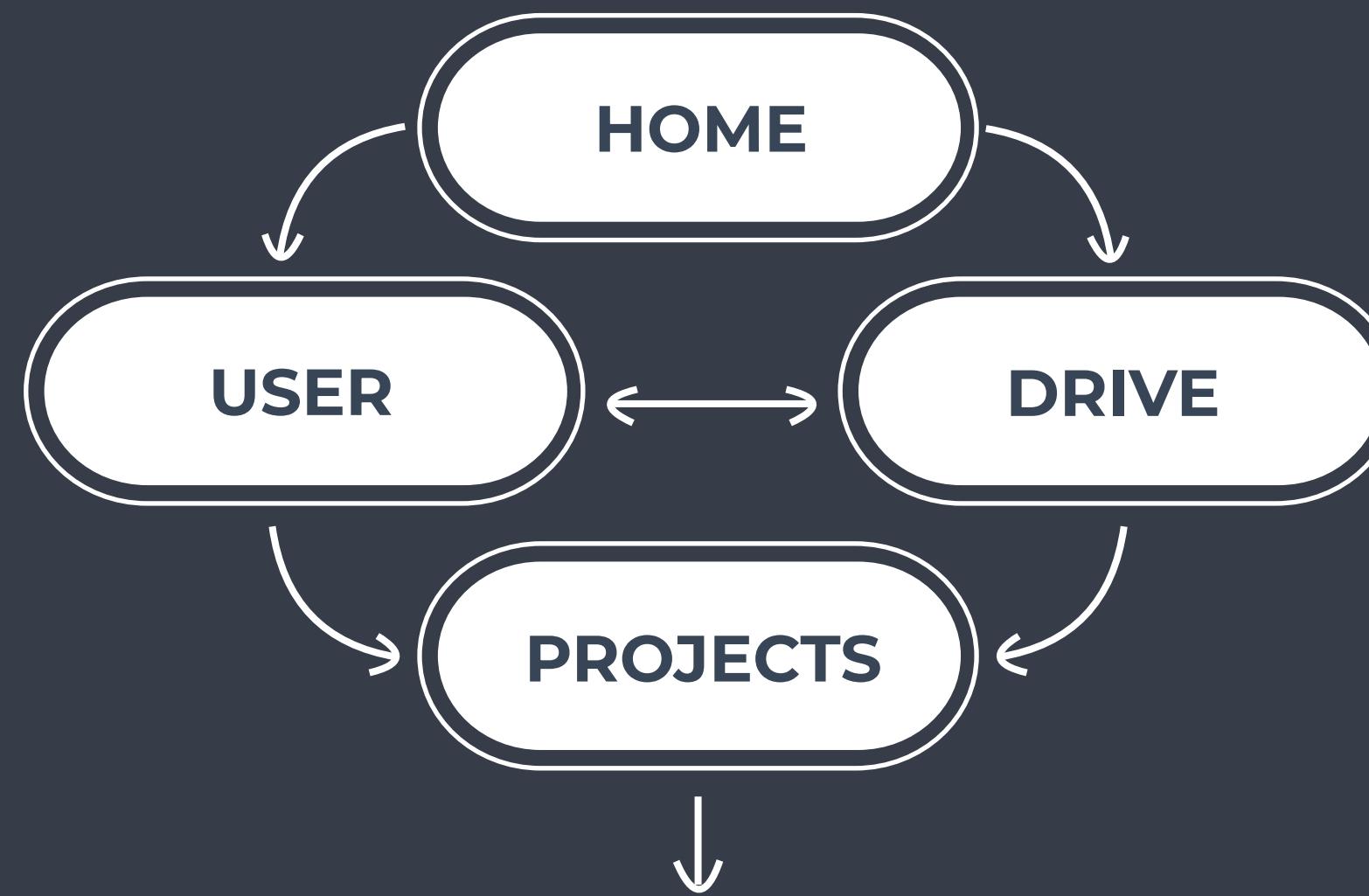


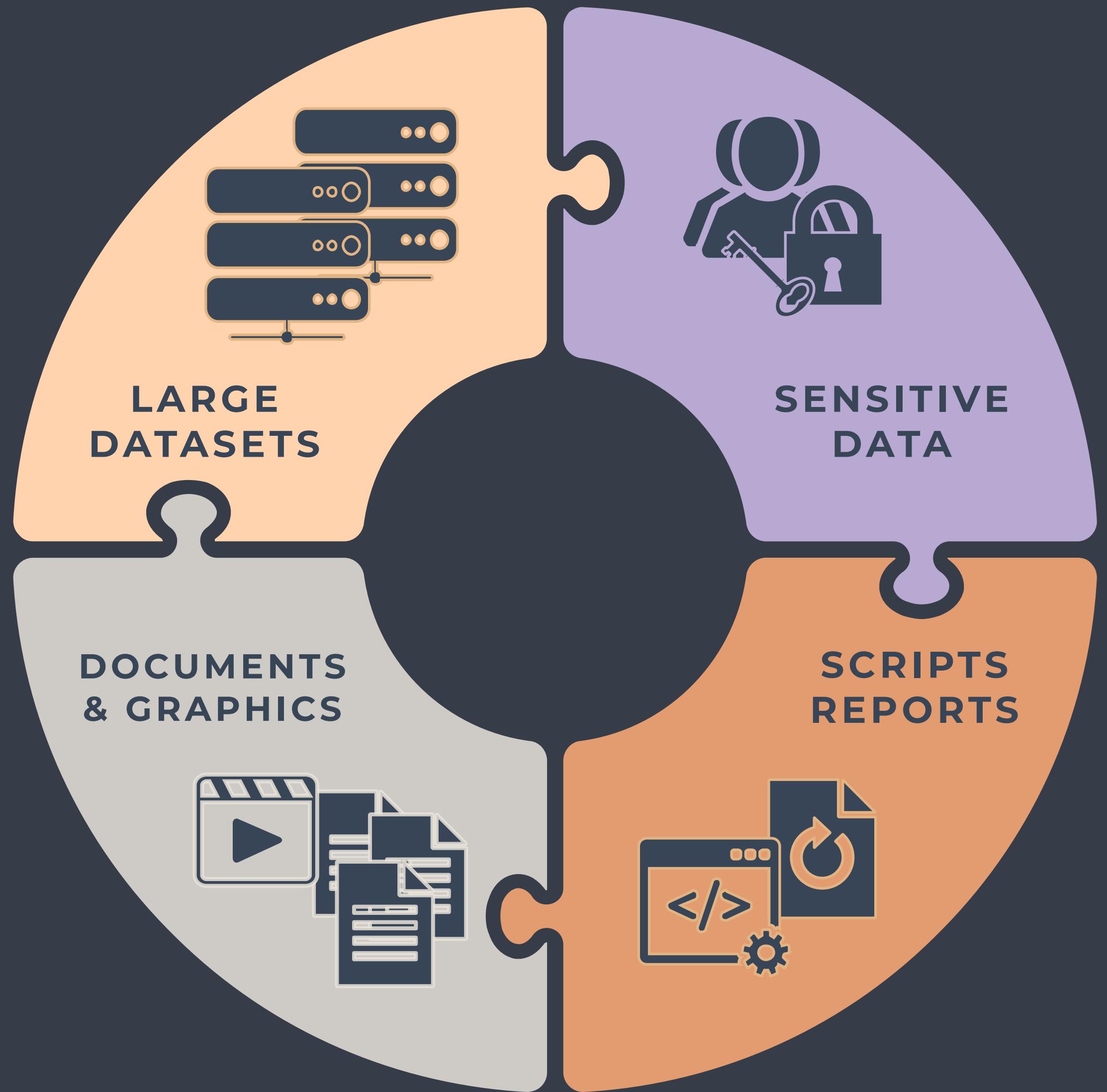
Don't Store Large Data/Files on Your Local Computer



Don't Store Sensitive Datasets on Your Computer

A SUGGESTION FOR STRUCTURE





BACKUP

- BIG DATA & SENSITIVE DATA:
 - Your own KU drives (S-drive)
 - ERDA & SIF (KU data storage)
 - Lab or department server
 - Lab or department cloud solution
- SCRIPTS, MARKDOWNS:
 - git/GitHub**
(KU drives)
- DOCX, EXCEL, POWERPOINT:
 - Google Drive
 - Dropbox
 - (KU drives)

GIT & GITHUB

Git is a version control software, created by Linus Torvalds for the management of the Linux kernel.

Other clients exist.

<https://git-scm.com>

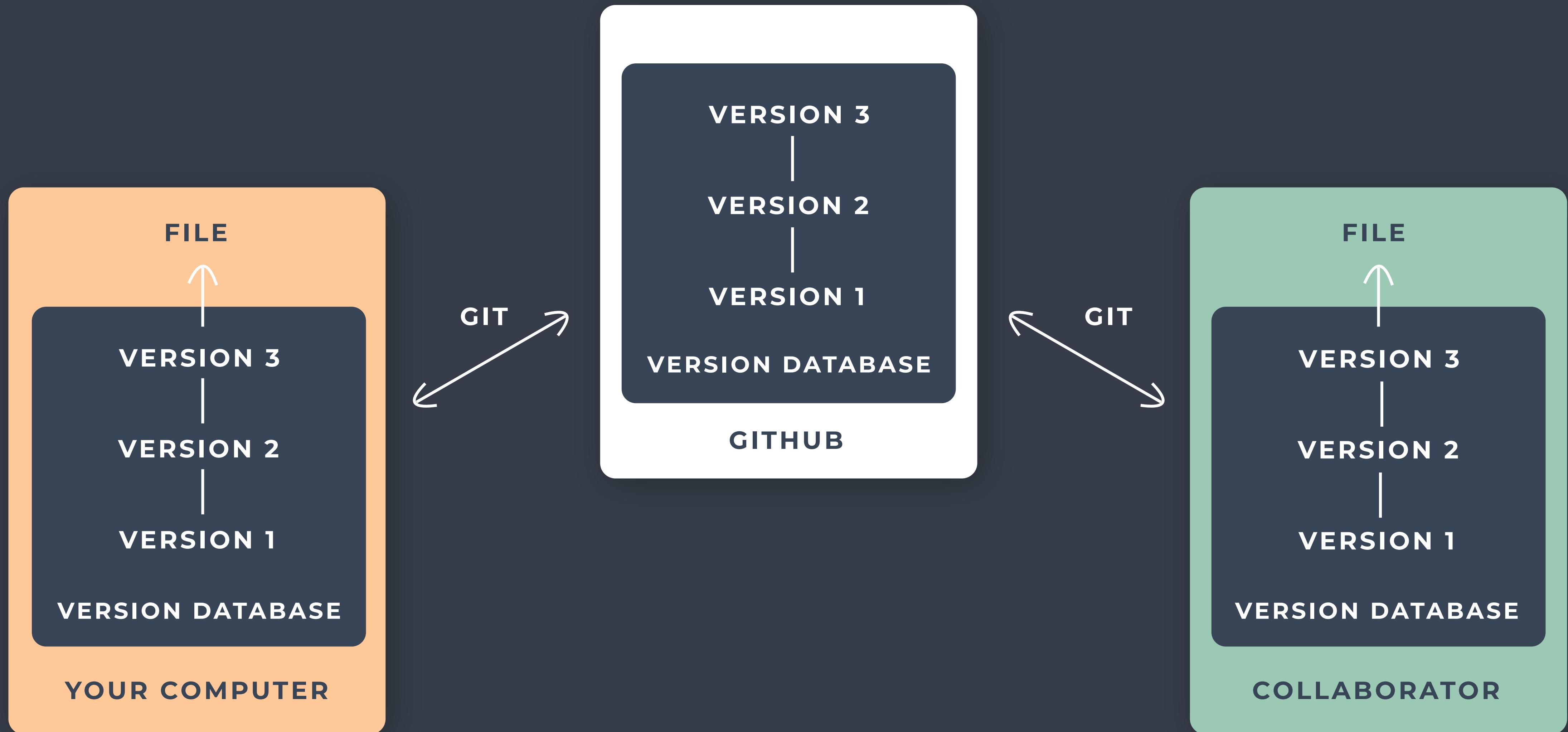


GitHub is a web-based hosting service for version control that uses git

Other services exist.

<https://github.com>

WHAT IS A VERSION CONTROL SYSTEM?

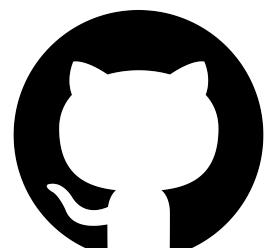


GIT WORKS FROM THE COMMAND LINE

Git is used from the command line to edit directories & files in a version controlled way

A git command always begins with git

Git enables a local computer to interact with a cloud service (GitHub) to back up your work



Sounds cool, yes!
Take our 'Introduction to git & GitHub' Workshop and learn how to git

git clone [your repository]

Username: [your user]

Password: [your password]

git status (status of the repo)

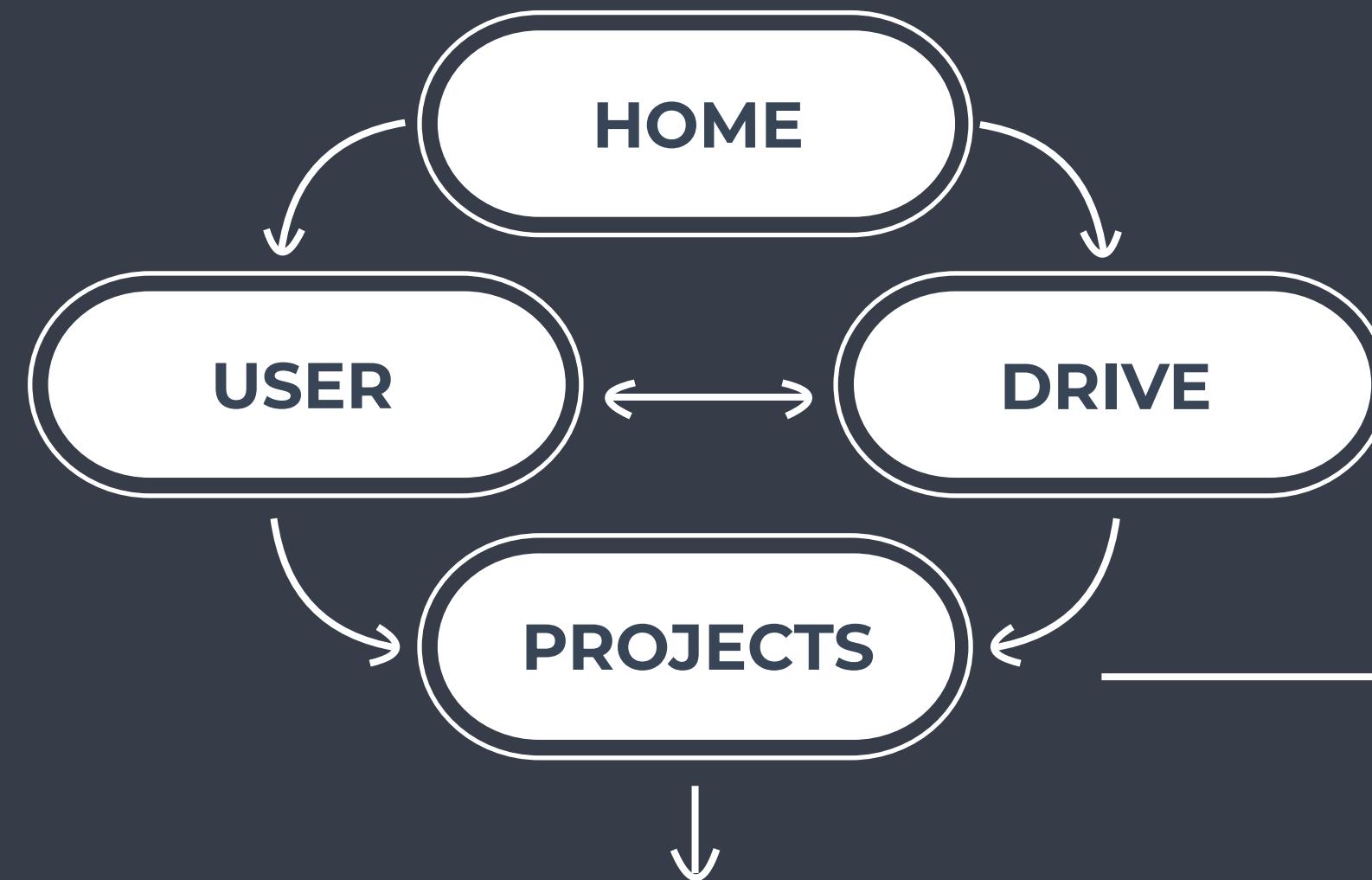
git add (add new files or changes)

git commit -m (commit the changes)

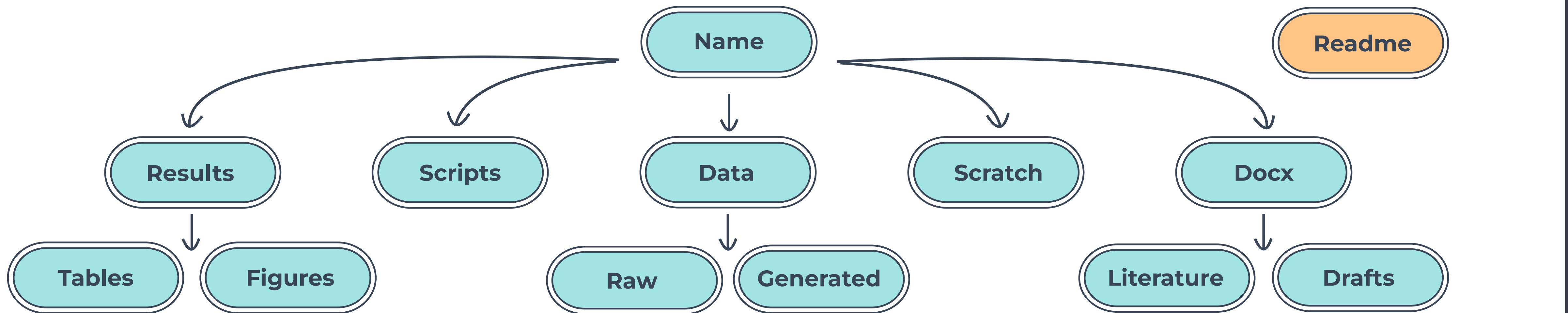
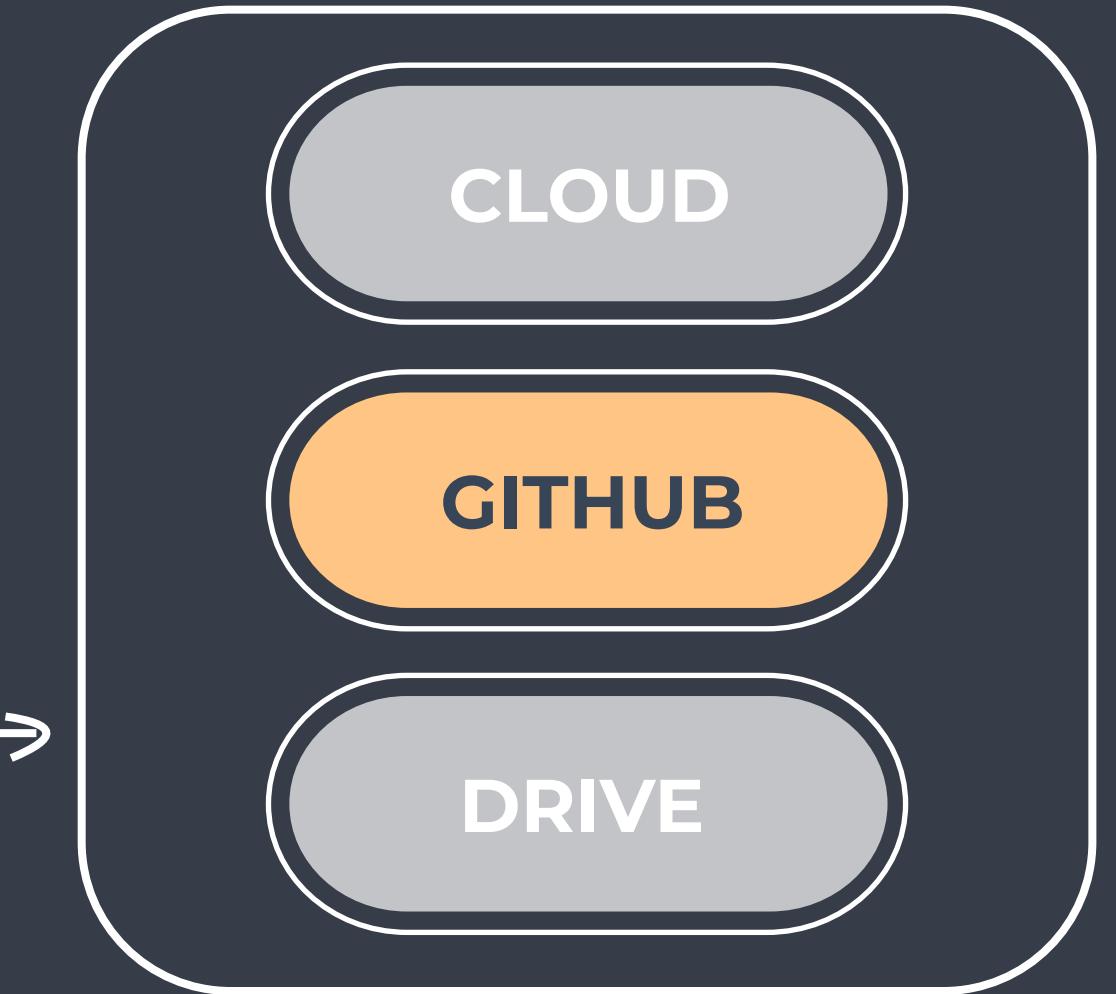
git push (push the changes to GitHub)

A SUGGESTION FOR STRUCTURE

LOCAL COMPUTER

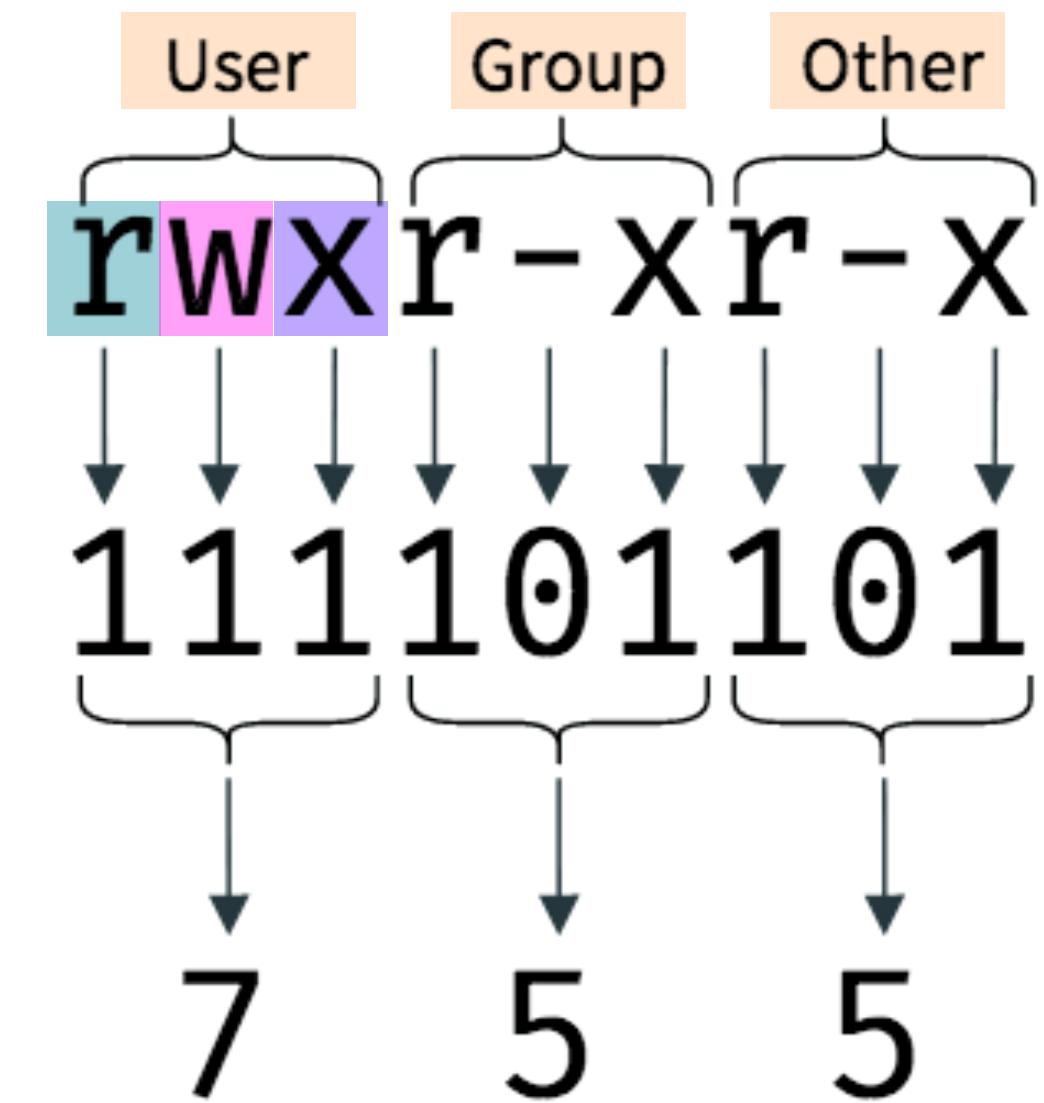


EXTERNAL BACKUP



USERS, GROUPS & PERMISSIONS

- Files & directories have **permission settings**
- Permissions denote who can **read**, **write** (edit) and **execute** a file/dir
- Permissions can be changed **IF** you are a system administrator (sys admin).
 - **Private computer** : You are sys admin
 - **KU computer** : You may be the system admin
 - **Shared KU drives** : You are not sys admin
 - **HPCs, Servers & Clouds** : You are **not** sys admin



```
chmod +rwx [filename]  
chmod -wx [directoryname]
```

CHEAT SHEET 1

```
pwd # print working dir  
cd # go to home dir  
cd [path] # change dir (remember path)  
ls # list dir content  
man [cmd] # get info about command  
[cmd] --help # view the help for command
```

WHERE & WHAT

```
touch [name] # make a file  
mkdir [name] # make a dir  
rm (-r) [name] # remove a file or dir  
  
cp [name] # copy a file/dir  
mv [name] [path] # move file/dir
```

FILE/DIR BASICS

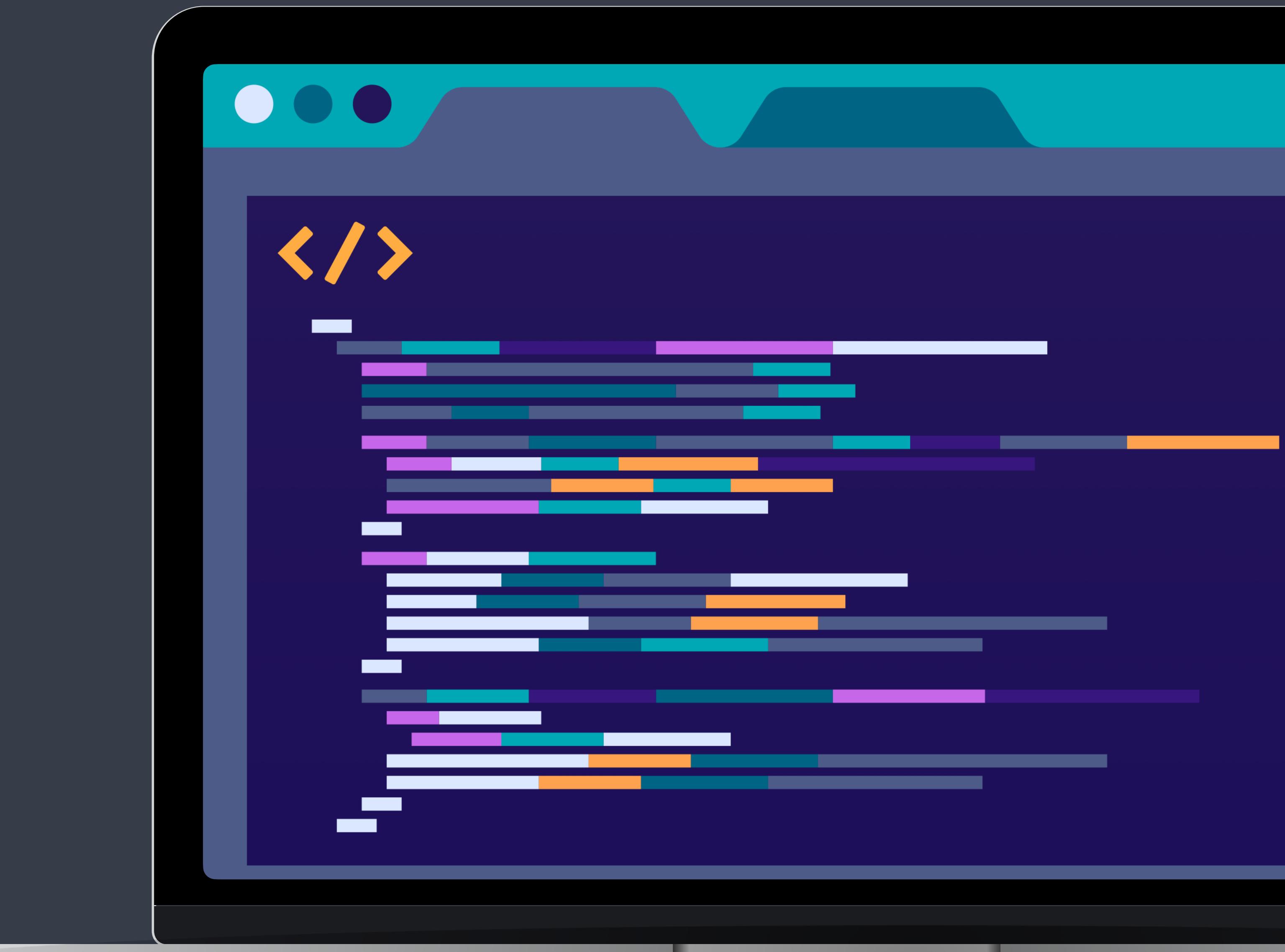
```
* # select everything  
/ # forward slash paths  
\ # escape character (don't use for now)  
.. # one dir up/back  
. # current dir  
- # denotes a flag/argument
```

SPECIAL CHARACTERS

```
ls -lh * # all sizes  
ls -lh [name] # file/dir size  
du -sh # total size  
  
chmod +rwx [name] # add a permission  
chmod -rwx [name] # remove a permission
```

SIZE & PERMISSION

3. WORKING WITH FILES



VIEWING FILES



- Many roads lead to Rome... For viewing files we can use:
- **less [file]**:
 - Prints N first lines of file. You can change the default N. Interactive viewing.
 - Exit with **q**
- **cat [file]**:
 - (concatenation), prints all lines of file. Interactive viewing.
 - Exit with **ctrl + c**
- **head/tail [file]**:
 - Prints **n first / last** lines of file. You can change the default **n**. Static viewing.

VIEW - SUBSET & RENAME

echo

```
echo 'Hello, World!'
```

**less
&
cat**

```
less myfile.txt
```

Patient	Age	Sex	Smoker	Grade
ID1	61	Female	No	G2
ID2	58	Female	Yes	G3
.

```
less myfile.txt > myfile_new.txt
```

**head
&
tail**

```
head -n 20 myfile.txt
```

```
head -n 20 myfile.txt > myfile_small.txt
```

EDITING FILES

- **Nano** [file] :

- Simple and easy to use
- Limited functionality
- Exit with **Ctrl + x (Y + enter)**

- **VIM or VI** [file] :

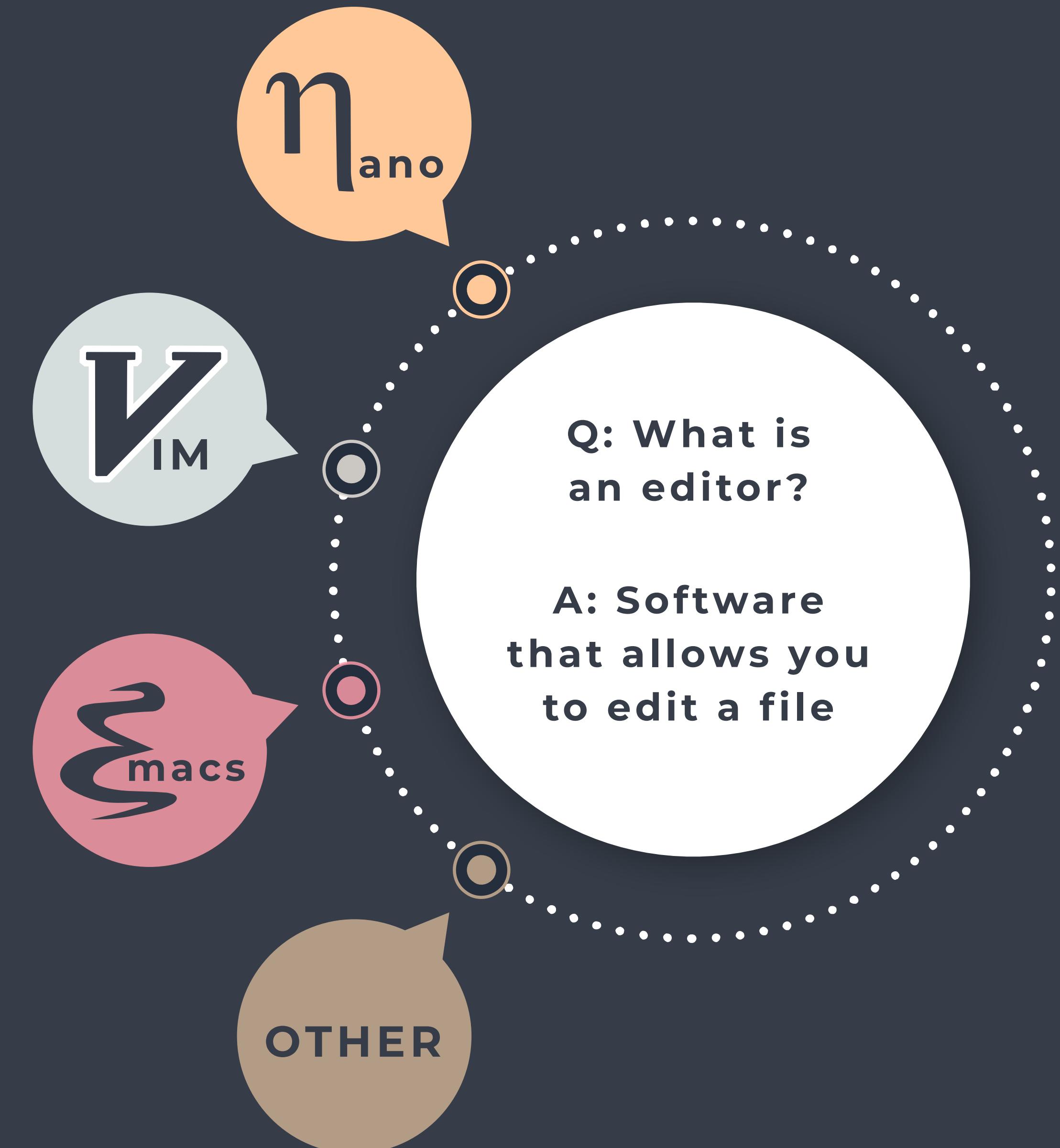
- Many functionalities, i.e. complex
- Keyboard shortcuts
- Exit with **:q (:w or :q!)**

- **EMACS** [file] :

- Oldest editor
- Keyboard shortcuts, **Ctrl, Alt/Esc + [L]**
- Exit with **Ctrl + x (Ctrl + s)**

- **OTHER** [file] :

- There are many other editors ...



COMPRESSED FILES

.GZ

**Standard gzip (GNU zip) compression.
May contain multiple files & directories**

.TAR

**An archive of multiple files put
together inside a single file.**

.TAR.GZ

**A compressed archive of multiple files
put together inside a single file.**

`gunzip -k [file.gz]`

`gzip -dk [file.gz]`

`unzip [file.zip]`

`tar -xf [file.tar.gz]`

`tar -tf [file.tar]`



CHEAT SHEET 2

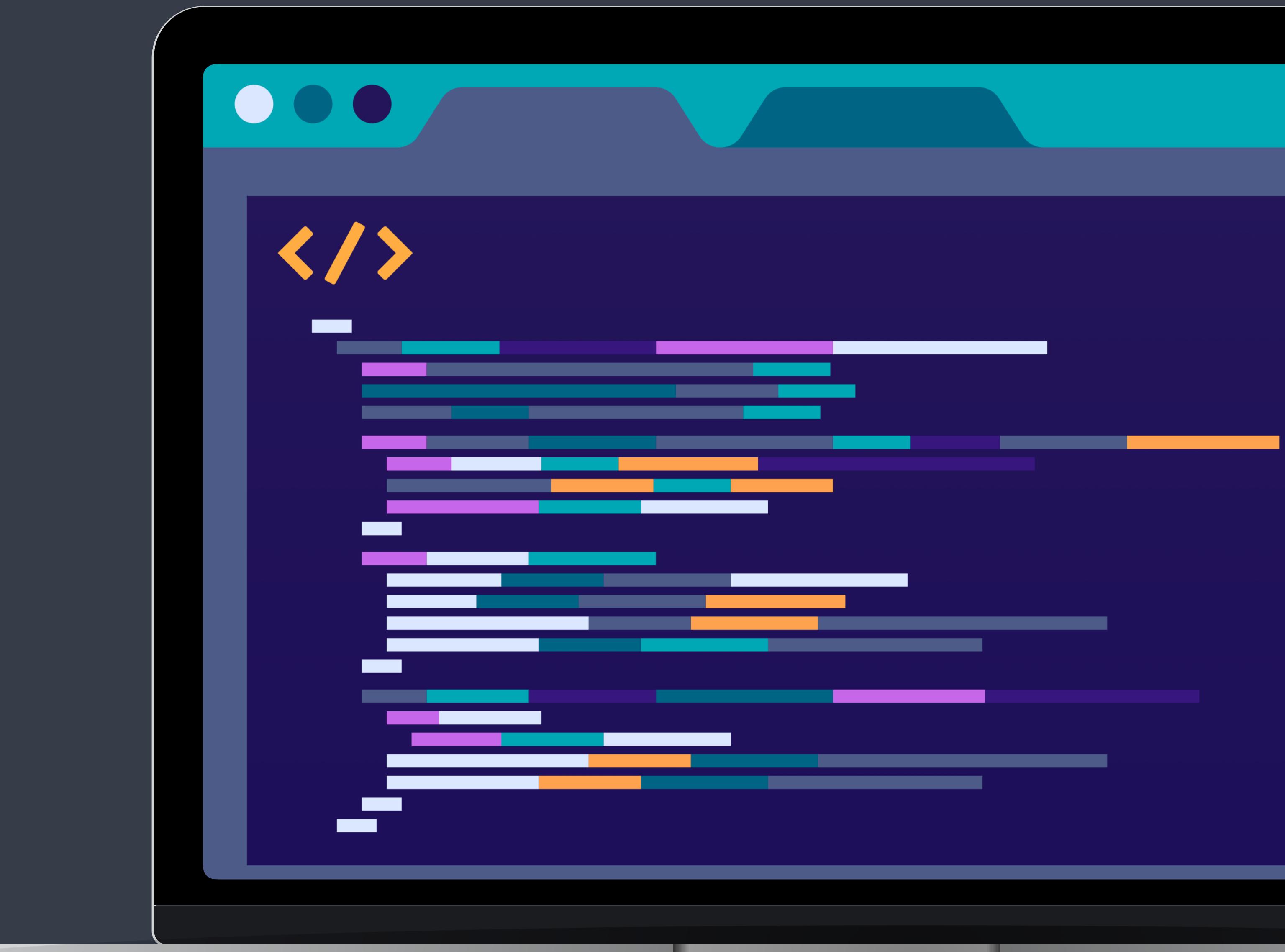
View Files

```
less [file] # view file content  
cat [file] # view file content (full)  
head / tail -n 10 [file] # view n first/last lines  
nano [file] # https://www.nano-editor.org/dist/latest/cheatsheet.html  
vim | vi [file] # https://vim.rtorr.com/
```

Compressed Files

```
tar -[f] [file] # .tar files  
gzip -[f] [file] # decompress (.tar).gz files  
unzip -[f] [file] # decompress .zip files  
zless -[f][file] # view .gz file w/o decompression  
  
others: zcat, zmore, gzcat
```

4. MORE BASH COMMANDS



FROM FILE NAVIGATION TO MANIPULATION

- FILES & DIRECTORIES:

- Move & Copy
- Make & Remove
- Open & Read
- Edit & Save
- Subset & Rename
- View & Change Permissions



NAVIGATE THE TERMINAL
&
FILE MANAGEMENT

- FILES:

- Sort
- Count Lines & Entries
- Merge & Concatenate
- Find & Replace Patterns
- Cut & Paste
- Insert & Delete



FILE MANIPULATION,
WRANGLING, SUMMATION

BASH COMMANDS

Sort
Sort a file/column
Number, character, mixed

Sort

grep

Search & Extract
pattern in file

Report unique entries only
awk is tool & a command

uniq

find

Search for pattern in file &
directory name(s).

awk

paste

sed

Paste corresponding or
subsequent lines of files

cut

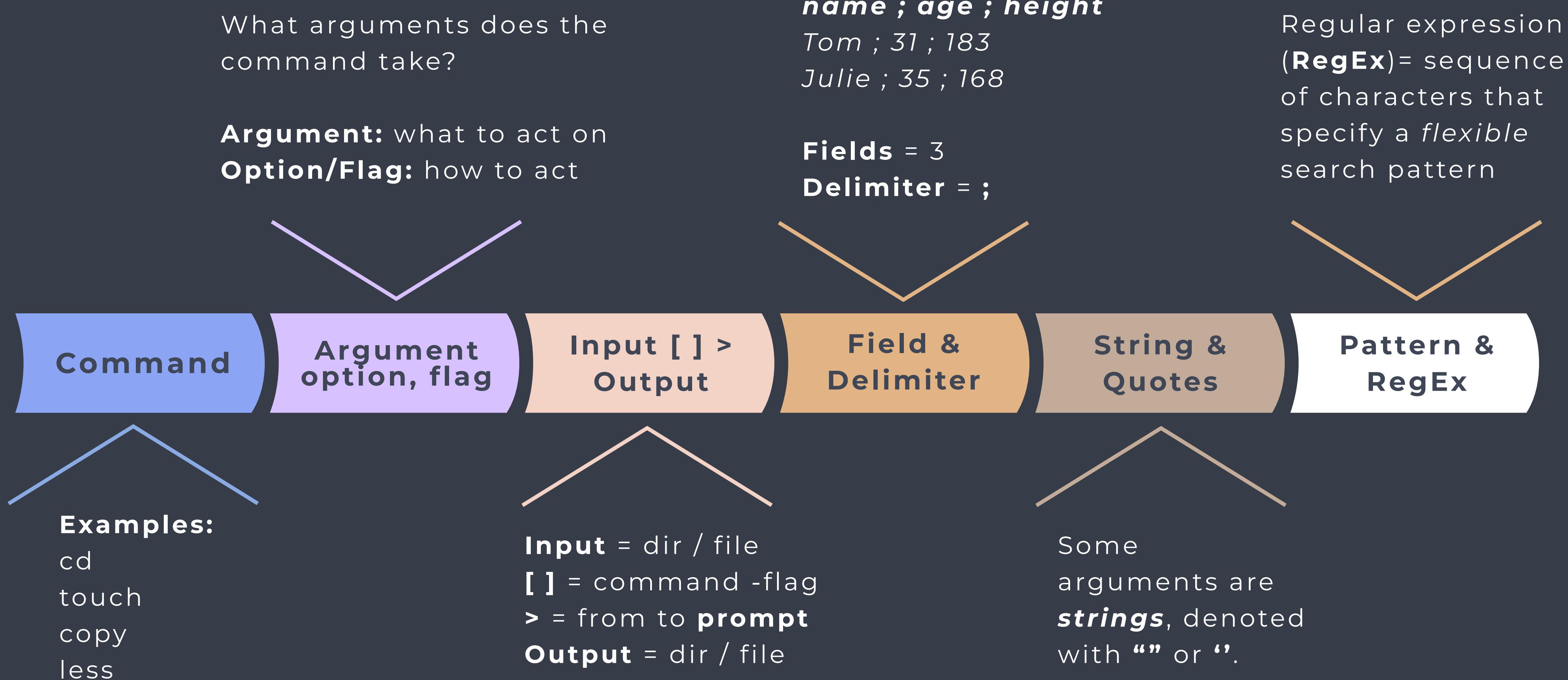
wc

Select field of each line

Count lines & words

Find and replace,
insertion or deletion

A LITTLE TERMINOLOGY



CHEAT SHEET 2

View Files

```
less [file] # view file content  
cat [file] # view file content (full)  
head / tail -n 10 [file] # view n first/last lines  
nano [file] # https://www.nano-editor.org/dist/latest/cheatsheet.html  
vim [file] # https://vim.rtorr.com/
```

Compressed Files

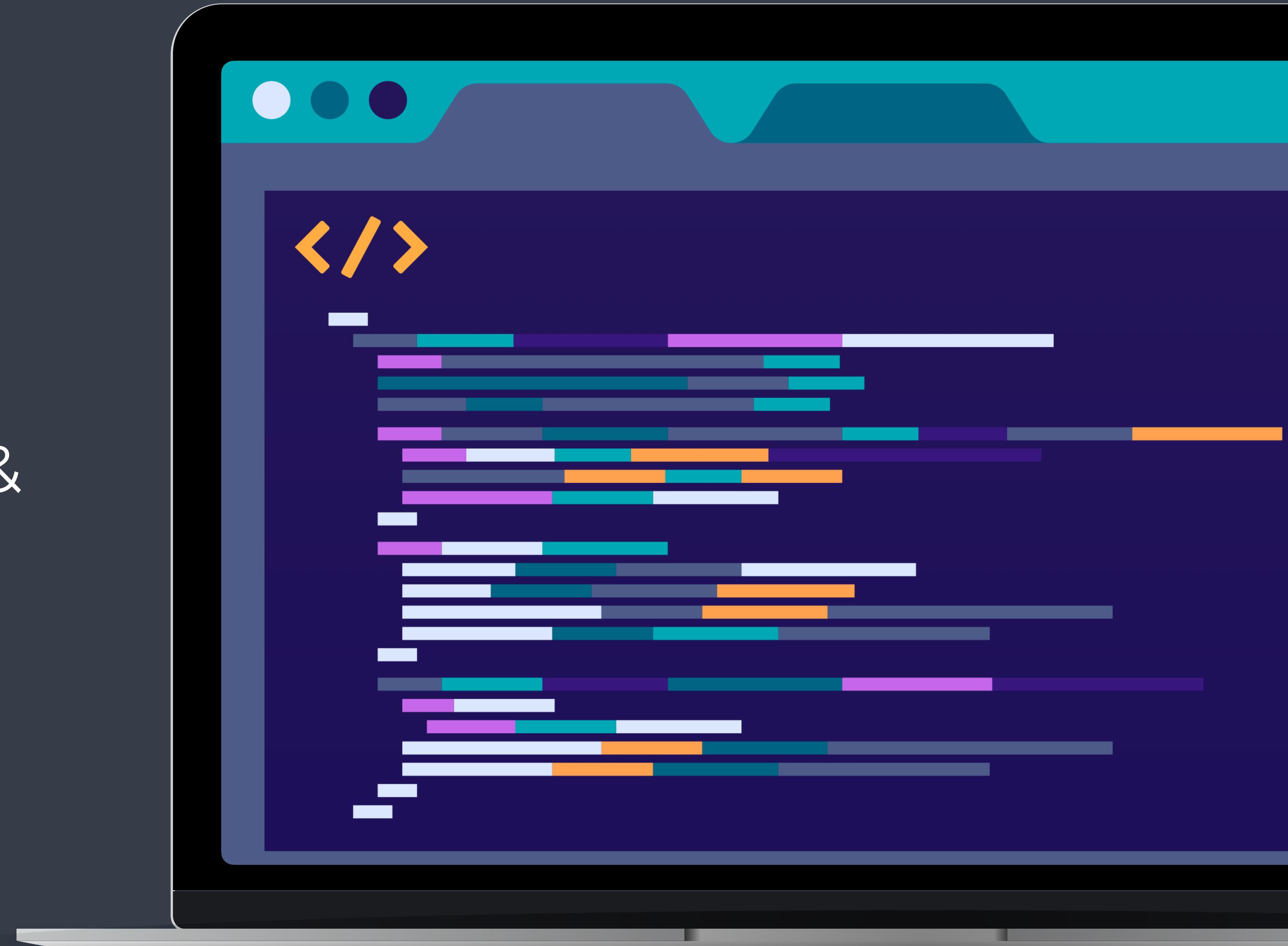
```
tar -[f] [file] # .tar files  
gzip -[f] [file] # decompress (.tar).gz files  
unzip -[f] [file] # decompress .zip files  
zless -[f] [file] # view .gz file w/o decompression  
  
others: zcat, zmore, gzcat
```

Manipulating Files

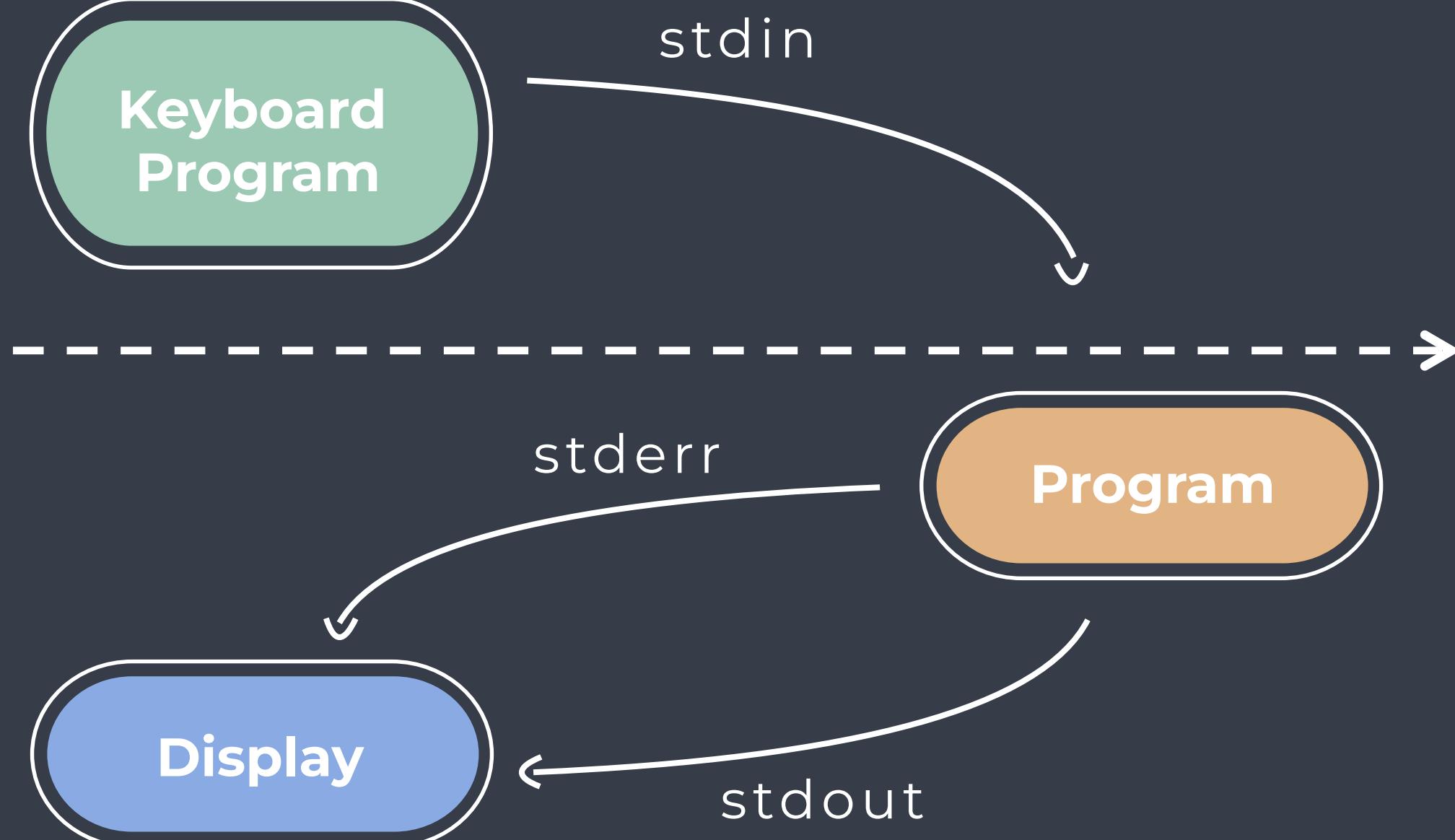
```
wc -[f] [file] # Count lines, characters, bits  
sort -[f] [file] # Sort file (by field/column)  
uniq -[f] [file] # Return unique values  
cut -[f] [file]: # Extract field/column  
paste -[f] [files]: # Merge file lines
```

```
sed -[f] 'command' [file] # Insertion, deletion, ...  
grep -[f] ['pattern'] [file] # Search for pattern  
awk '{pattern}' [file] # Search, replace, extract, ...  
find -[f] [path] ['pattern'] # Search pattern in file name
```

5. REDIRECTION & PIPES

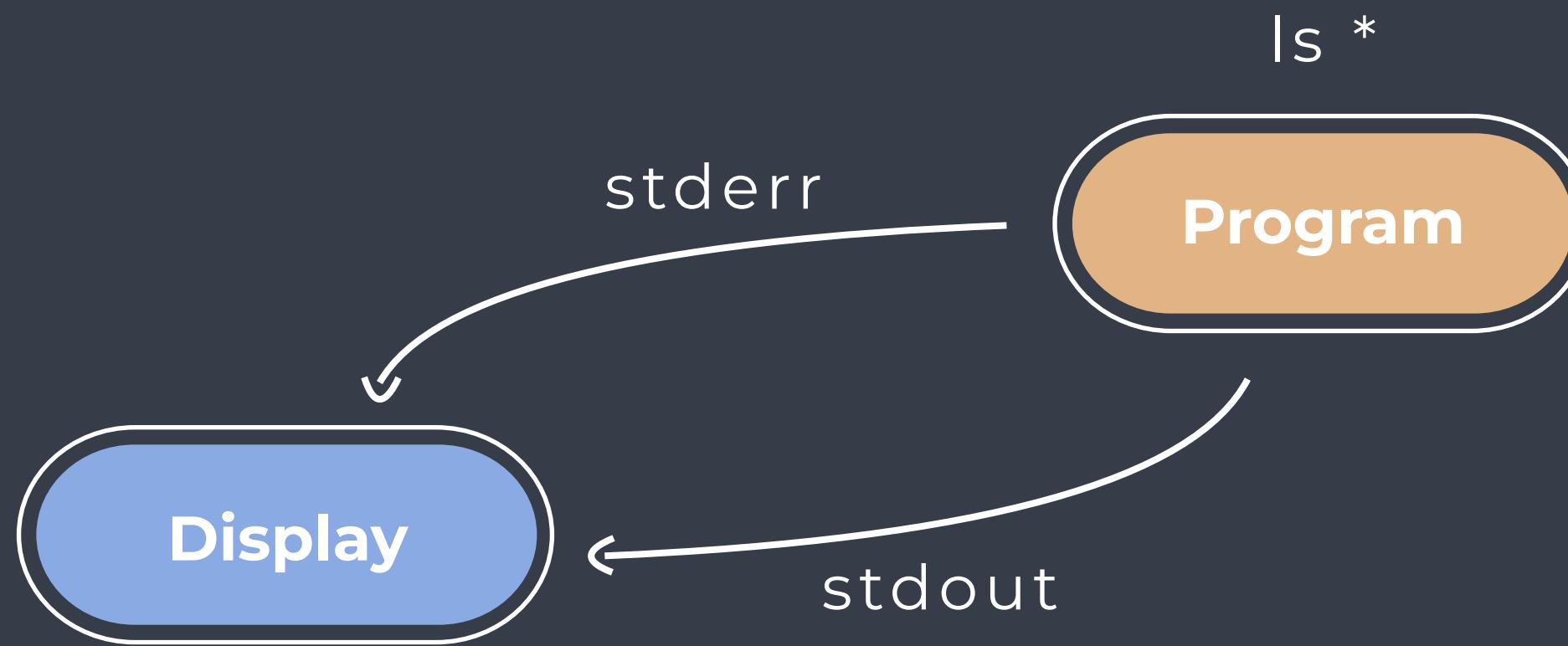


A TALE OF THREE STREAMS



- Data in unix always moves along one of **three (data) streams**:
 - **stdin** (Standard In) – the stream along which input to commands moves
 - **stdout** (Standard out) - the output of commands moves along this stream
 - **stderr** (Standard error) – error messages move via this stream
- Each of the streams can be redirected separately.

A TALE OF THREE STREAMS



Your terminal

```
BashFigure1.jpeg
Commandline_Workshop.pptx
Data
Examples
Just_Bash_It_Exercises.md
Just_Bash_It_Exercises.Rmd
Just_Bash_It_Presentations.md
Just_Bash_It_Presentations.Rmd
LICENSE
README.md
```

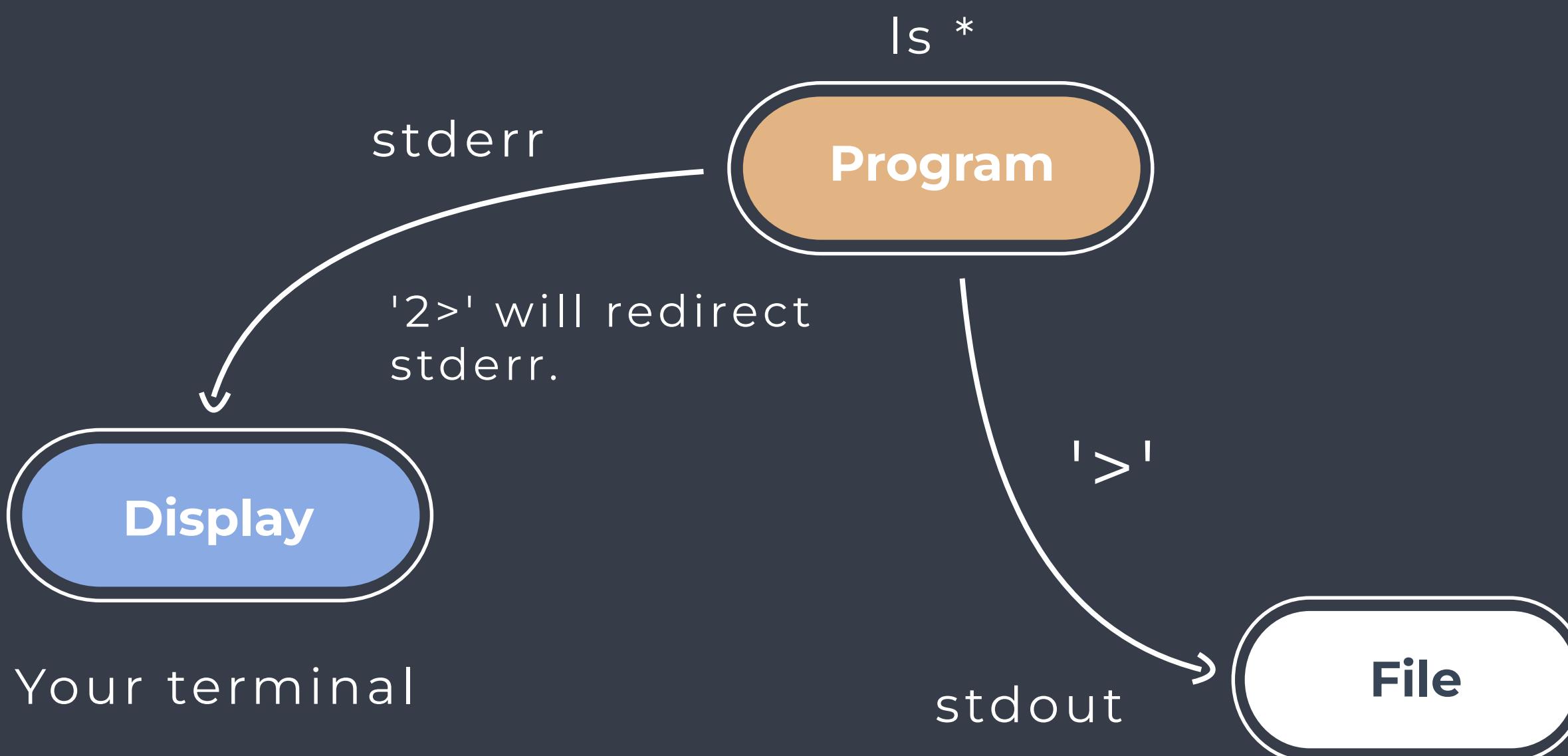
- **stdout** (standard out) - the output of commands moves along this stream

- **stderr** (standard error) – error messages move via this stream

- By default **stdout** points to the display, your terminal window

A TALE OF THREE STREAMS

But **stdout** and **stderr** can be **redirected** to i.e. a file:



Redirect stdout:

```
$ ls > list_results.txt
```

Redirect stderr:

```
$ ls 2 > err.txt
```

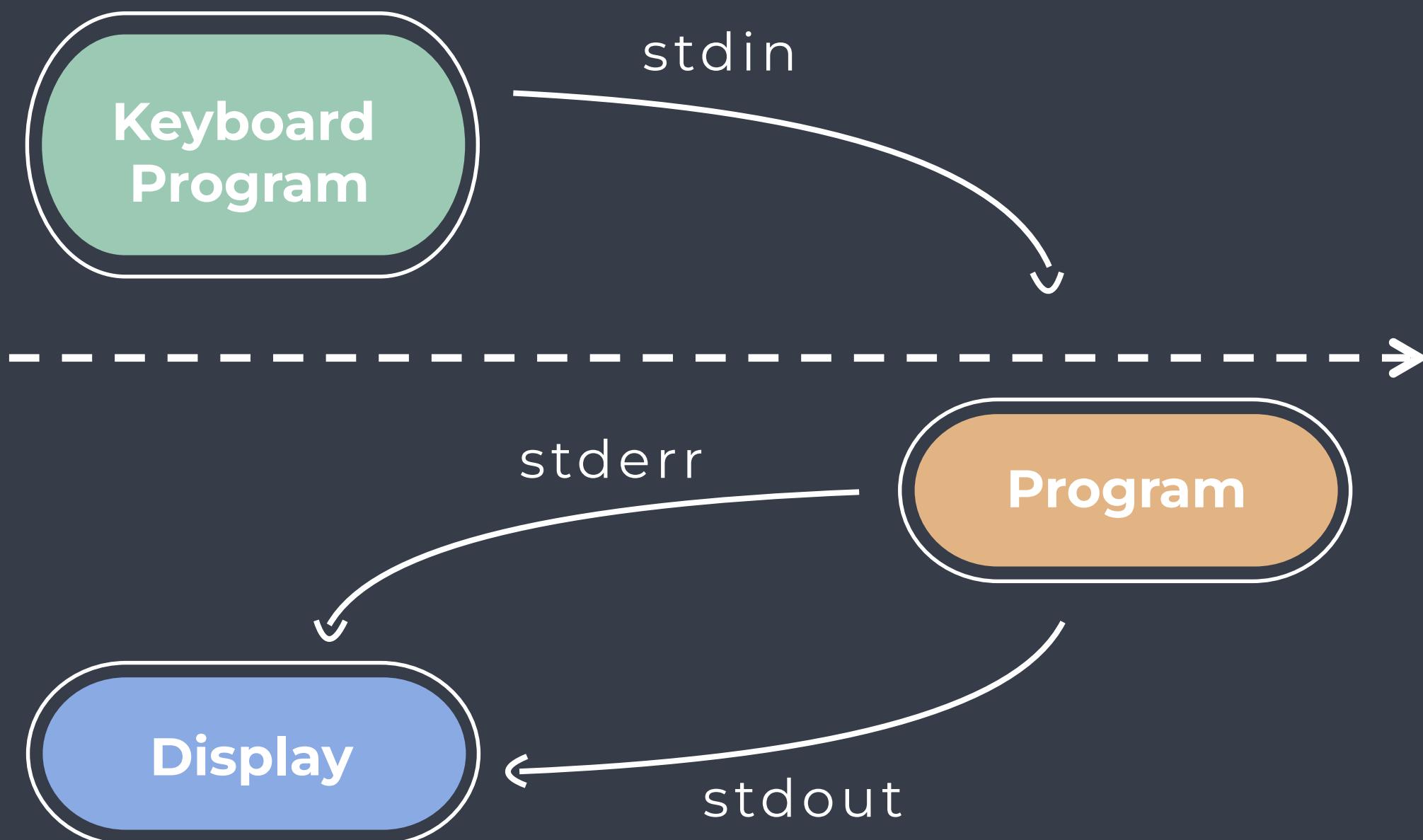
Redirect both into different files:

```
$ ls 2 > err.txt > list_results.txt
```

Redirect both into the same file:

```
$ ls & > both
```

A TALE OF THREE STREAMS



- Many commands require input data to work on, i.e. **wc** works on a file.
- Usually input data comes from the keyboard, i.e. the name of the file to word count.
- But it can also come directly from another program!

CHAINING (PIPING) COMMANDS



File1.txt 10 → sort
File2.txt 5
File3.txt 8

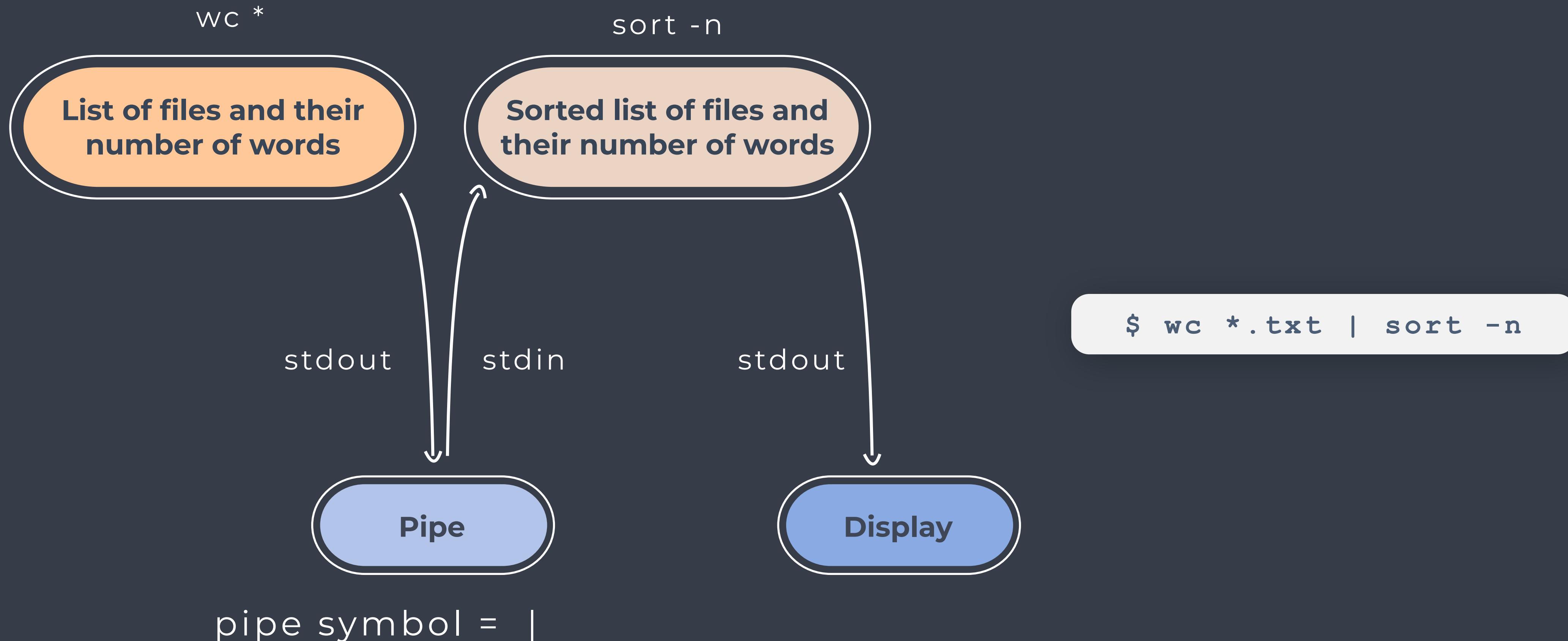
```
$ wc *.txt > file_lengths
```



```
$ sort -n file_lengths
```

But now we have an intermediate file we don't need!

CHAINING (PIPING) COMMANDS



CHAINING (PIPING) COMMANDS

Some examples:

- Take the second column and count how often each element occurs:

```
$ cut -d ',' -f 2 patients.txt | sort | uniq -c
```

- Get only lines containing 'Herlev' and sort by age:

```
$ grep 'Herlev' patients.txt | sort -t ',' -n -k5
```

- If we don't want the entire line we could also cut out the age column before sorting:

```
$ grep 'Herlev' patients.txt | cut -d ',' -f 5 | sort -n
```

```
Last login: Thu Sep 29 17:30:26 on ttys000
[kgx936@SUN1007442 ~ % cd Desktop/HeaDS/GitHub_repos/Just-Ba
[kgx936@SUN1007442 docs % head patients.txt
patient_ID,technique,hospital,conv_days,age,satisfaction
402109,A,Rigshospitalet,15,68,3
092070,A,Rigshospitalet,13,74,5
994082,B,Herlev,27,76,2
843094,A,Herlev,30,65,5
369360,B,Rigshospitalet,21,68,5
688213,B,Rigshospitalet,29,77,3
197347,A,Herlev,25,65,5
759063,B,Rigshospitalet,16,75,4
121219,B,Herlev,27,68,4
kgx936@SUN1007442 docs %
```

CHEAT SHEET 2

View Files

```
less [file] # view file content  
cat [file] # view file content (full)  
head / tail -n 10 [file] # view n first/last lines  
nano [file] # https://www.nano-editor.org/dist/latest/cheatsheet.html  
vim [file] # https://vim.rtorr.com/
```

Compressed Files

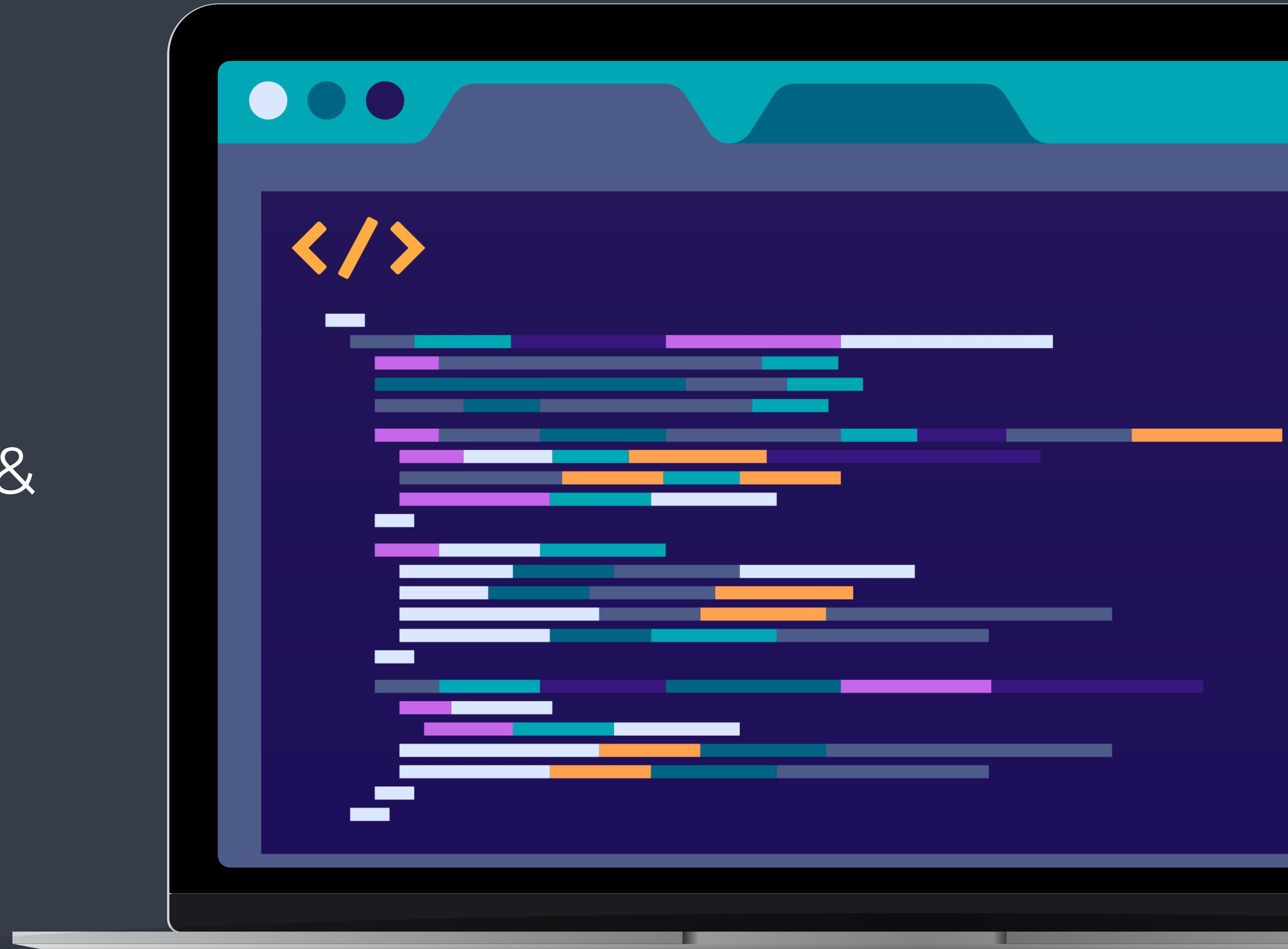
```
tar -[f] [file] # .tar files  
gzip -[f] [file] # decompress (.tar).gz files  
unzip -[f] [file] # decompress .zip files  
zless -[f][file] # view .gz file w/o decompression  
  
others: zcat, zmore, gzcat
```

Manipulating Files

```
wc -[f][file] # Count lines, characters, bits  
sort -[f][file] # Sort file (by field/column)  
uniq -[f][file] # Return unique values  
cut -[f][file]: # Extract field/column  
paste -[f][files]: # Merge file lines
```

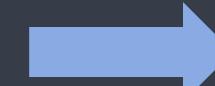
```
sed -[f]'command'[file] # Insertion, deletion, ...  
grep -[f]['pattern'][file] # Search for pattern  
awk '{pattern}'[file] # Search, replace, extract, ...  
find -[f][path]['pattern'] # Search pattern in file name
```

6. SHELL SCRIPTS & LOOPS



WRITING SCRIPTS

```
(base) henrike@henrike-ThinkPad-X390:~/Documents/Heads_center_management/courses/Just-Bash-It/Examples/docs$ cut -f 3 -d ',' patients.dat | sort | uniq -c
      1 herlev
      9 Herlev
      1 hospital
     10 Rigshospitalet
(base) henrike@henrike-ThinkPad-X390:~/Documents/Heads_center_management/courses/Just-Bash-It/Examples/docs$ head -n 1 patients.dat > herlev.dat
(base) henrike@henrike-ThinkPad-X390:~/Documents/Heads_center_management/courses/Just-Bash-It/Examples/docs$ grep 'Herlev' patients.dat | sort -n -k 5 -t ',' >> herlev.dat
```



```
x - my_script.sh (~/Documents/Heads_center_management/courses)
Open + ~/Documents/Heads_center_management/courses/Just-... Save
my_script.sh
1 cut -f 3 -d ',' patients.dat | sort | uniq -c
2 head -n 1 patients.dat > herlev.dat
3 grep 'Herlev' patients.dat | sort -n -k 5 -t ',' >>
herlev.dat
```



- Save your commands for later use!
- Re-run anytime, always same result
- Check your script if you don't remember the steps of an analysis
- Back-up your scripts on i.e. github, KU drive, ect.

```
(base) henrike@henrike-ThinkPad-X390:~/Documents/Heads_center_management/courses/Just-Bash-It/Examples/docs$ bash my_script.sh
      1 herlev
      9 Herlev
      1 hospital
     10 Rigshospitalet
(base) henrike@henrike-ThinkPad-X390:~/Documents/Heads_center_management/courses/Just-Bash-It/Examples/docs$ █
```

COMMAND LINE INPUT

- Add **arguments** when you execute your script, these will be passed to it.
- Useful if you want to i.e. specify the file you want to run the script on.
- A script is called with **bash** (or simply **sh**).
- The **first argument** after the script name will be **\$1** inside the script.
- The **second argument** will be **\$2** and so on.

```
# Comment line script 1
# Usage: sort_this.sh file_name

sort $1 -n
```

```
$ bash sort_this.sh patients.txt
```

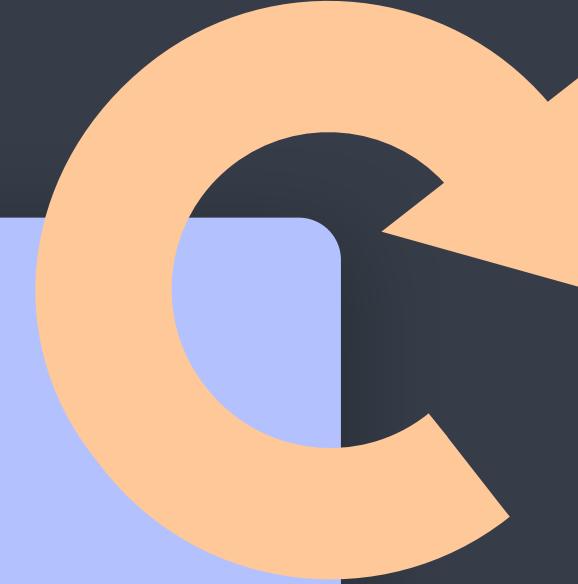
```
$ bash sort_this.sh my_textfile.txt
```

```
# Comment line script 2
# Usage: cut_col file_name column_number

cut -d ',' -f $2 $1
```

```
$ bash cut_col patients.txt 3
```

LOOP IN BASH



```
#example of a for loop in bash

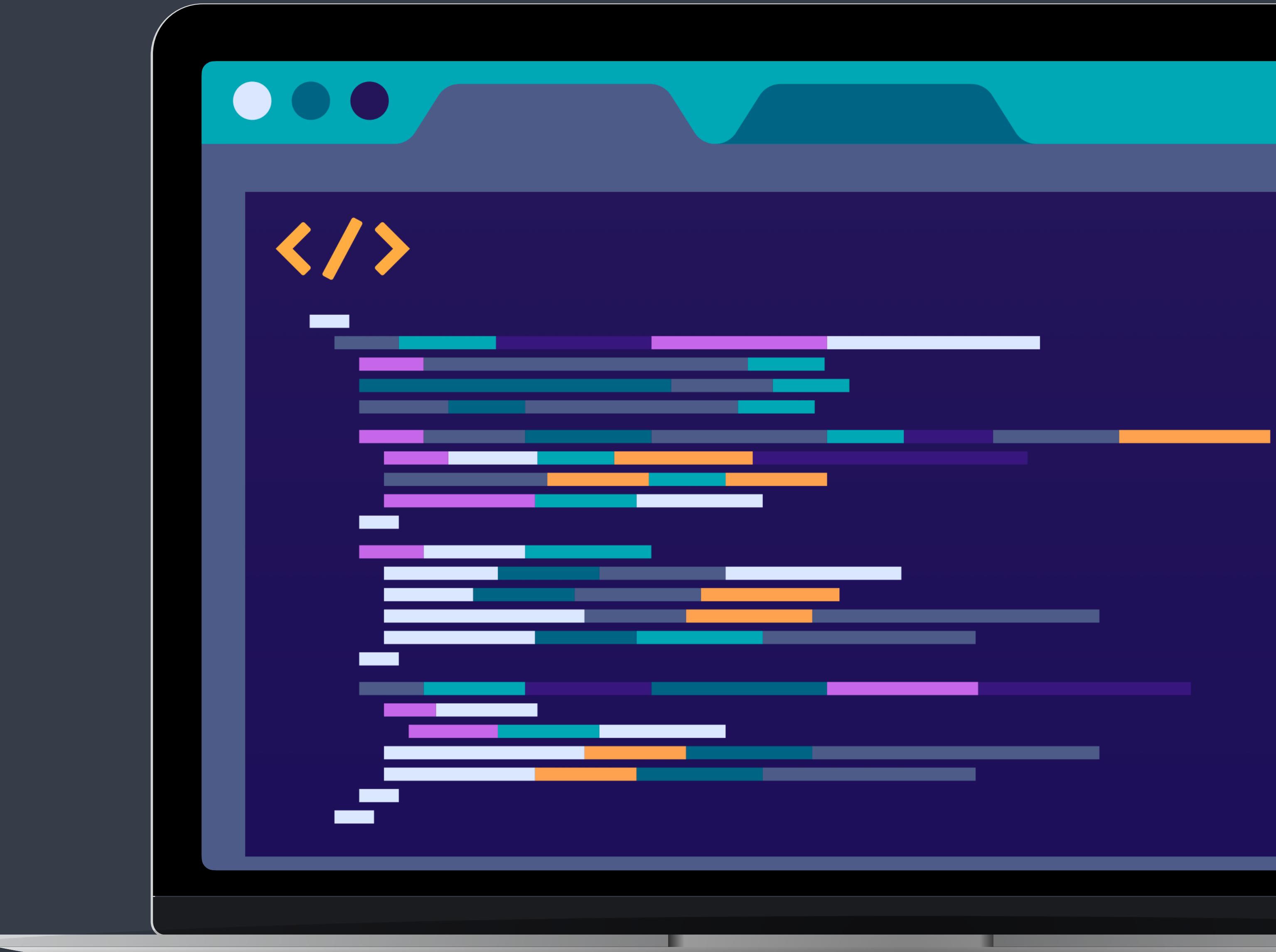
for file in *.txt
do
    echo $file
    wc $file
done

#the general syntax of a for loop is:

for [iterator] in [generator]
do
    commands
done
```

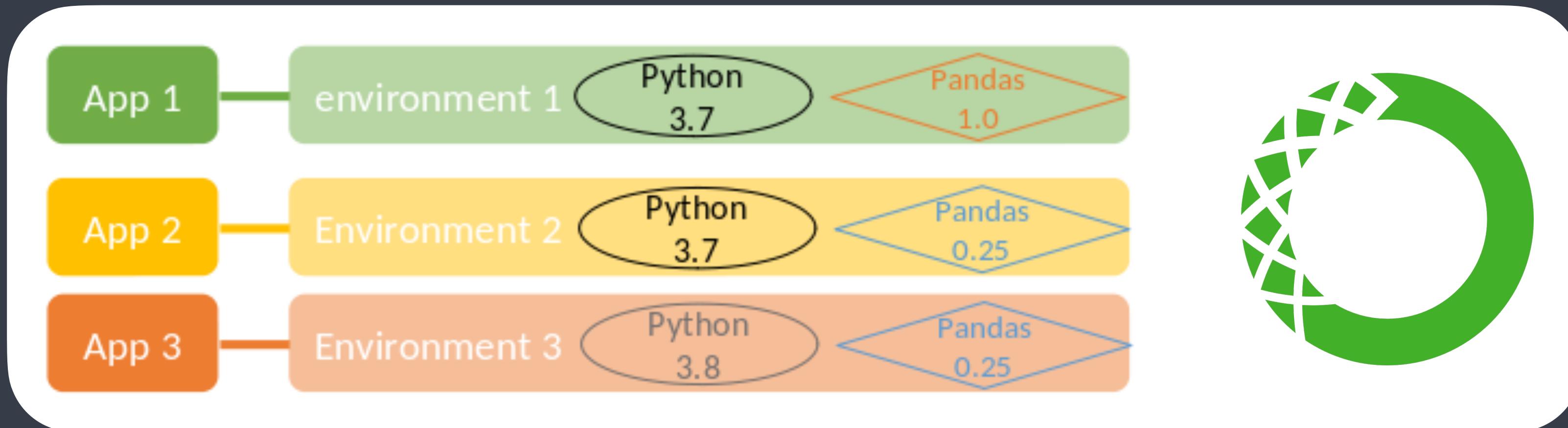
- Loops allow you to repeat the same action several times, once for each file for example.
- Many bash commands can be run on several files, i.e.
 \$ wc *.txt
- However, a loop is useful if you want to execute several commands for each file.

7. SOFTWARE INSTALLATION UPKEEP & MORE



CONDA®

- **Conda** is an open source package & environment management system.
- Many softwares exist as conda packages, you can use conda to install them and their dependencies.
- **An environment** is a specific combination of packages in a specific version.
- If you do not update the packages, running an analysis in the same environment will give the same result.



PROS

Comprehensive, many options
Environment management
Well documented

CONS

Can be overwhelming



Homebrew

- **Homebrew** - source software package management system, for OSX, Ubuntu (Linux).
- NOT an environment manager, package manager only.
- Creates separate directories for libs and configurations, adds symlinks to *user/local*.
- Manage all installed softwares via the terminal, install, check, update, remove...

PROS

Easy to use
Good documentation
Commands a few and logical

CONS

Packages, NOT environments

APT-GET

- **apt-get** is a command-line tool for handling packages in Linux (Ubuntu, ‘Windows’).
- APT = *Advanced Packaging Tool*
- Upgrade and remove of packages along with their dependencies.
- NOT an environment manager, package manager only.

PROS

Works like any linux command
No installation (is default)
Robust to OS updates

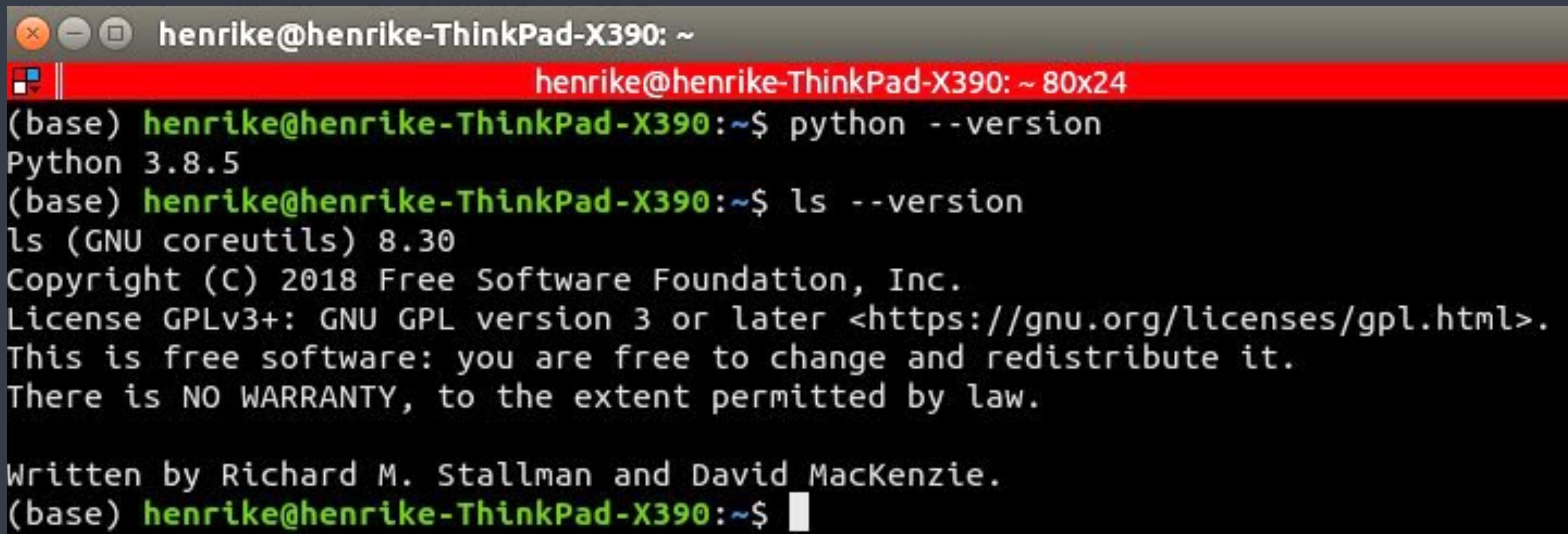
CONS

Packages, NOT environments

SOFTWARE VERSION

You can generally check the version of installed software with:

```
[name of software] --version
```



The screenshot shows a terminal window with a dark background and light-colored text. The title bar reads "henrike@henrike-ThinkPad-X390: ~". The terminal prompt "(base)" appears in green. The user runs two commands: "python --version" which outputs "Python 3.8.5", and "ls --version" which outputs the GNU coreutils version information, including the copyright notice from 2018 and the GPL license details.

```
henrike@henrike-ThinkPad-X390: ~
(base) henrike@henrike-ThinkPad-X390:~$ python --version
Python 3.8.5
(base) henrike@henrike-ThinkPad-X390:~$ ls --version
ls (GNU coreutils) 8.30
Copyright (C) 2018 Free Software Foundation, Inc.
License GPLv3+: GNU GPL version 3 or later <https://gnu.org/licenses/gpl.html>.
This is free software: you are free to change and redistribute it.
There is NO WARRANTY, to the extent permitted by law.

Written by Richard M. Stallman and David MacKenzie.
(base) henrike@henrike-ThinkPad-X390:~$
```

KEEPING THINGS UP TO DATE

Update your software with the same tool you used to install it:

- Installed with **conda**: (update only the current environment)

```
conda update -all
```



- Installed with **homebrew** (updates a software):

```
brew upgrade [software]
```



- Installed with **apt-get**:

```
apt-get update (apt-get dist-upgrade)
```



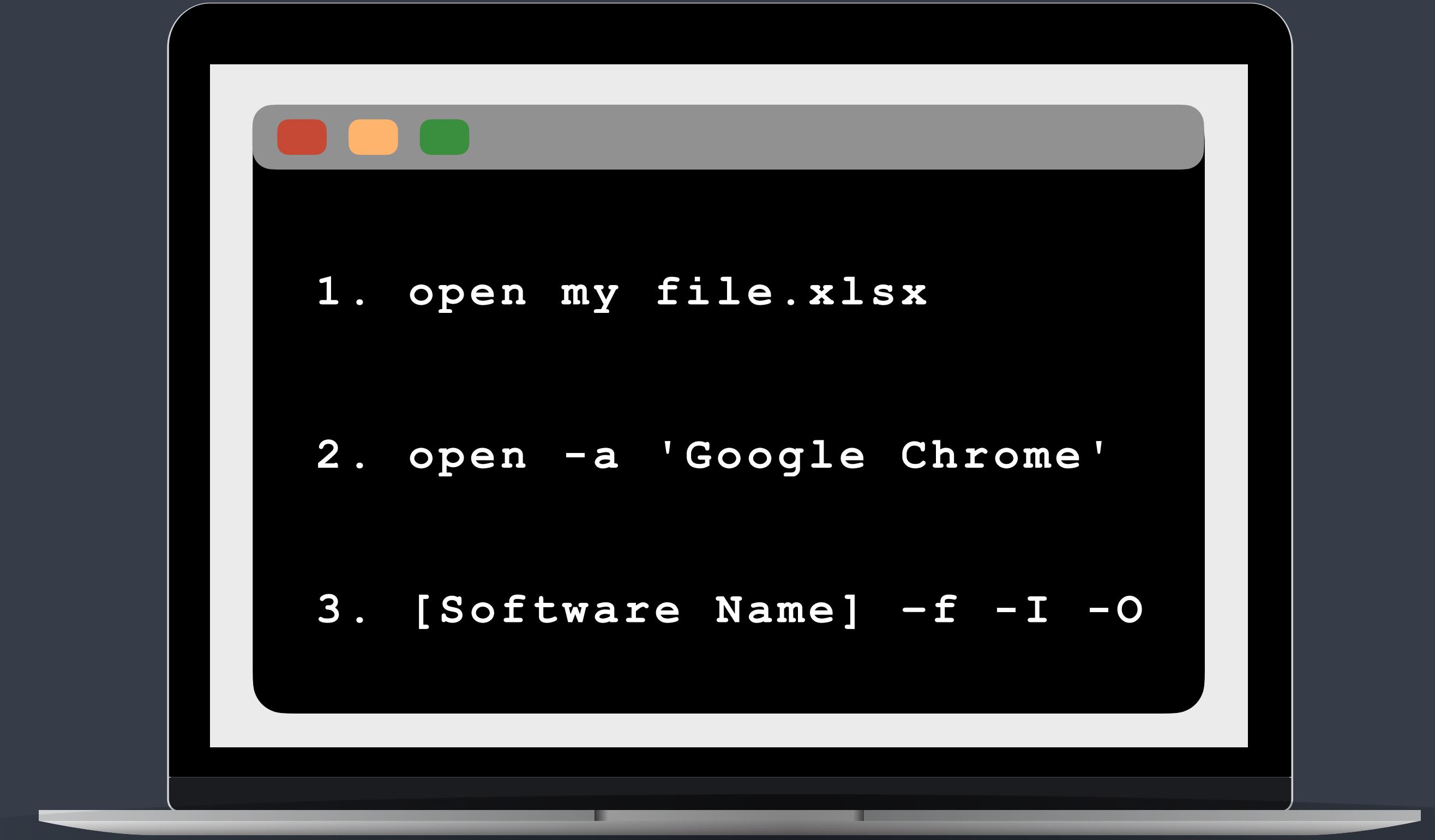
- With **Windows App store**:

*Update via
Windows App store*



LAUNCHING APPS, OPENING FILES & RUNNING SOFTWARE

1. Some, but not all **files** can be **opened** without specifying an app.
3. Many **apps** can be **launched** with open -a.
5. Some **softwares** are designed to run on both the command line and in a GUI, while others are specific to one of these.



CONFIGURATION FILES

- Configuration files (config files) are used to specify parameters and settings your OS and software.
- Types of config files; system-wide, program-specific, user-specific.
- Extension will pertain to what is configured.
- Rarely permission to change system-wide files.
- Software-specific files you can usually edit.
- **N.B** config files are ‘hidden’, i.e. ls -la (or similar) to see them.

BASH SHELL



`.profile`
`.bashrc`
`.bash_profile`

`.profile`
`.bashrc`
`.bash_profile`

Z SHELL (BASH +)

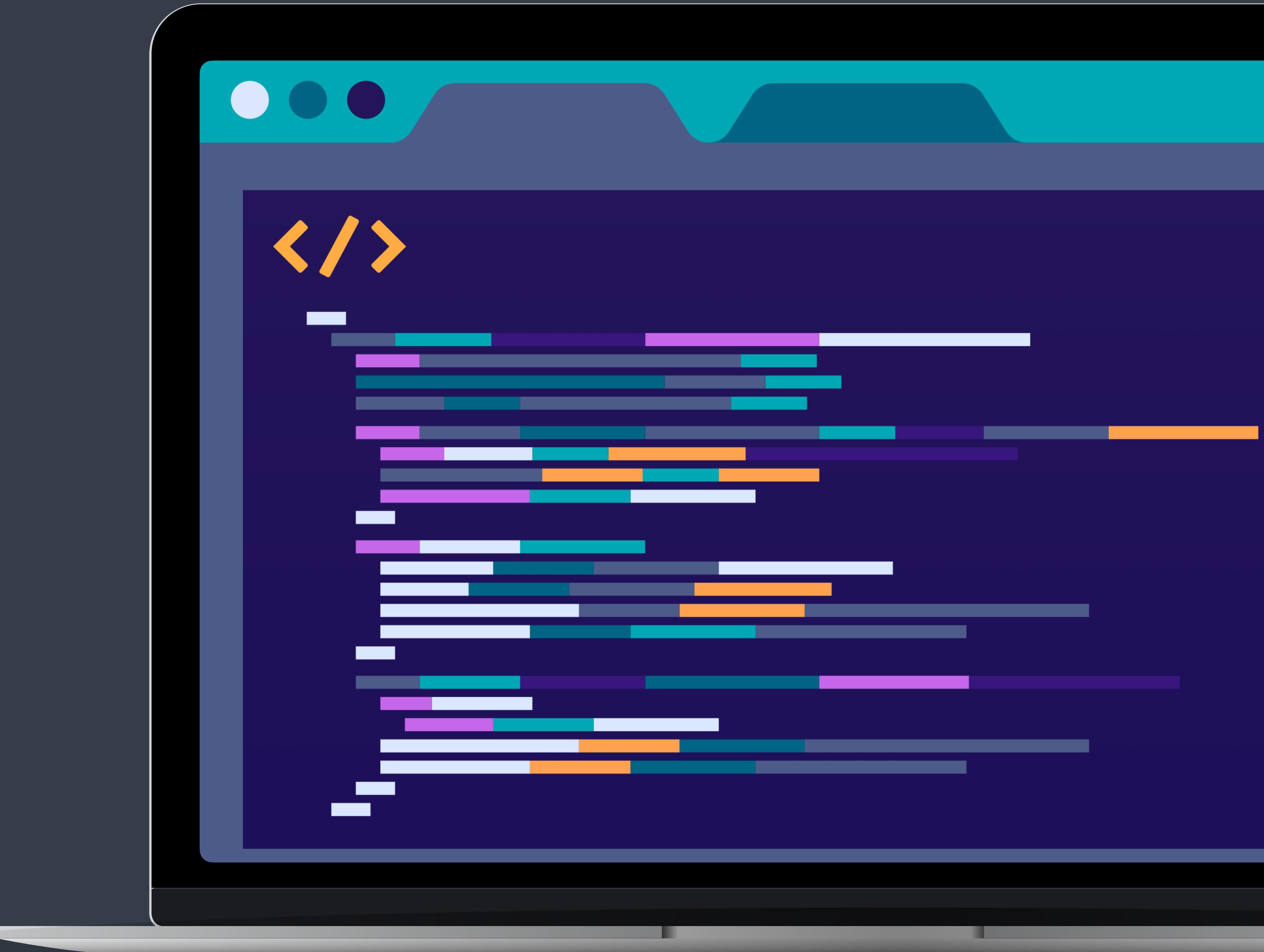


`.zprofile`
`.zshrc`
`.zsh_profile`

CYGWIN (WINDOWS)



8. WORKFLOW LANGUAGE & COMPUTE POWER



WORKFLOW LANGUAGES

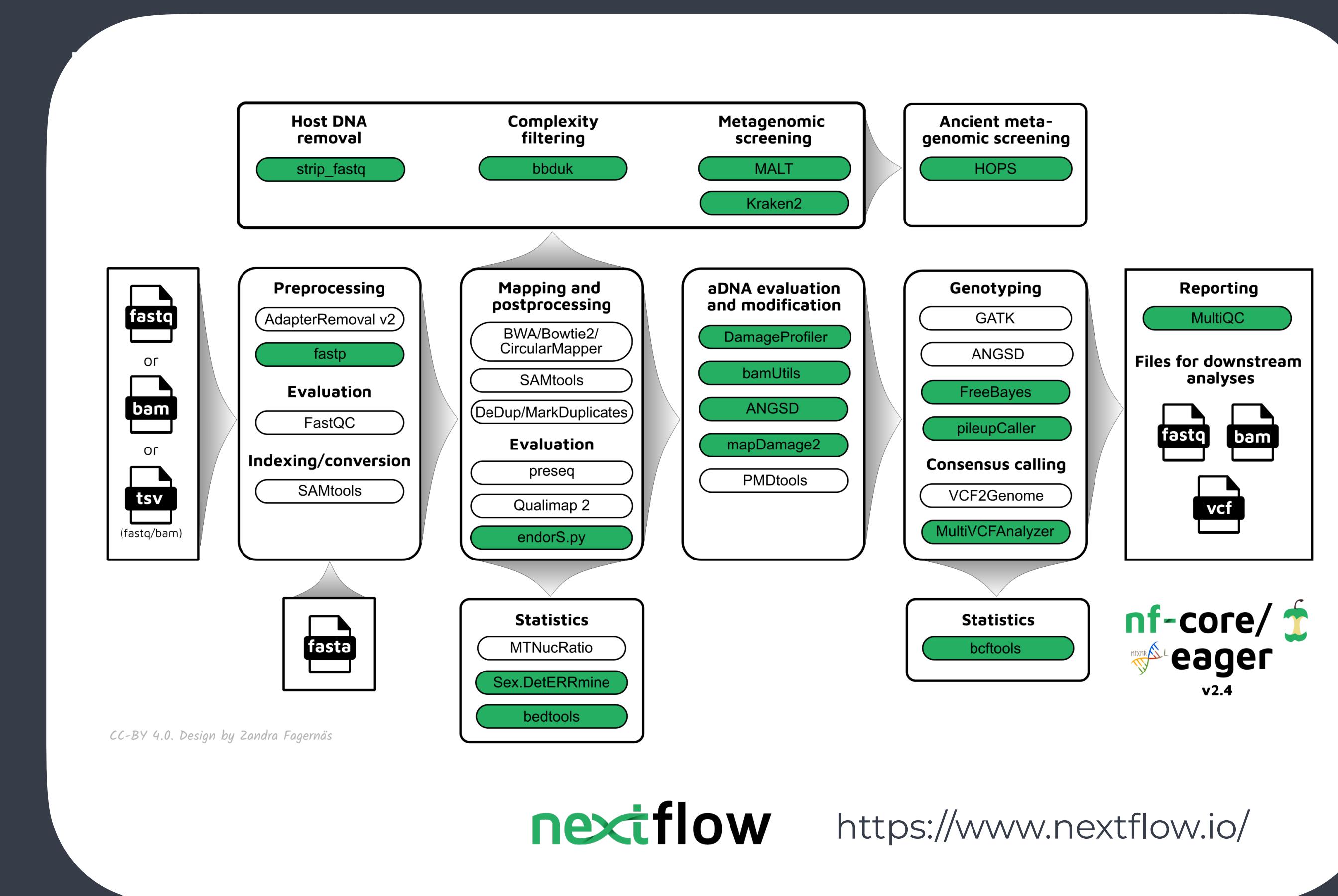
. Workflow languages:

- . Tools to create reproducible pipelines - more robust than bash scripts.
- . Workflow languages allow you to:
 - . Control the flow of your pipeline
 - . Restart at various defined points.
 - . Ensure previous commands have. executed without error.
 - . Logging & Reporting of your job.



snakemake

<https://snakemake.readthedocs.io/en/stable/>



HIGH PERFORMANCE COMPUTING (HPC)
