BIO609 Introduction to UNIX/Linux and Bash Scripting

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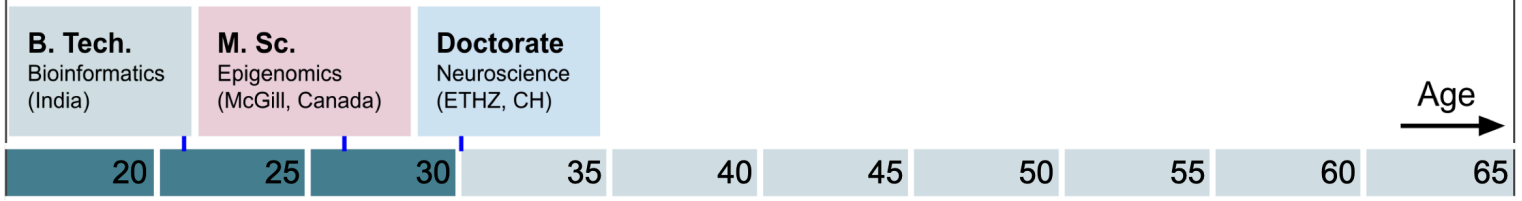
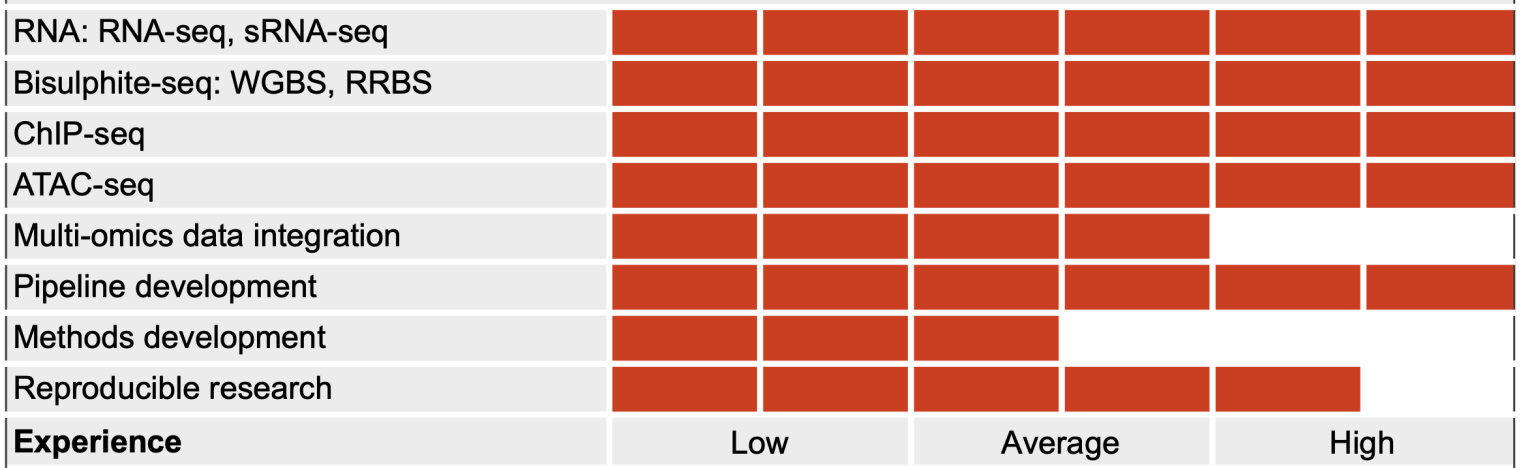
Deepak Tanwar (embedded bioinformatics scientist)

Deepak is a bioinformatician at the URPP Evolution in Action. Deepak has a strong background in multi-omics research and has expertise in reproducible data analysis, benchmarking, and methods development.

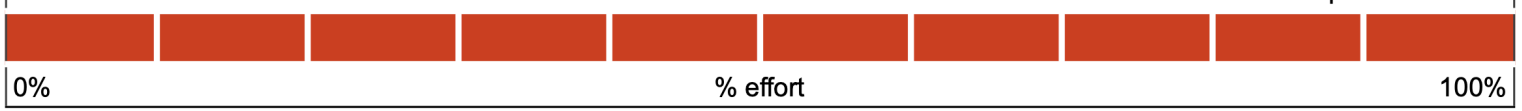
Education timeline



Multi-omics experience



Distribution of time between bench work and computational work



UNIX

Ken Thompson

Dennis Ritchie

W wikipedia.org/wiki/History_of_Unix

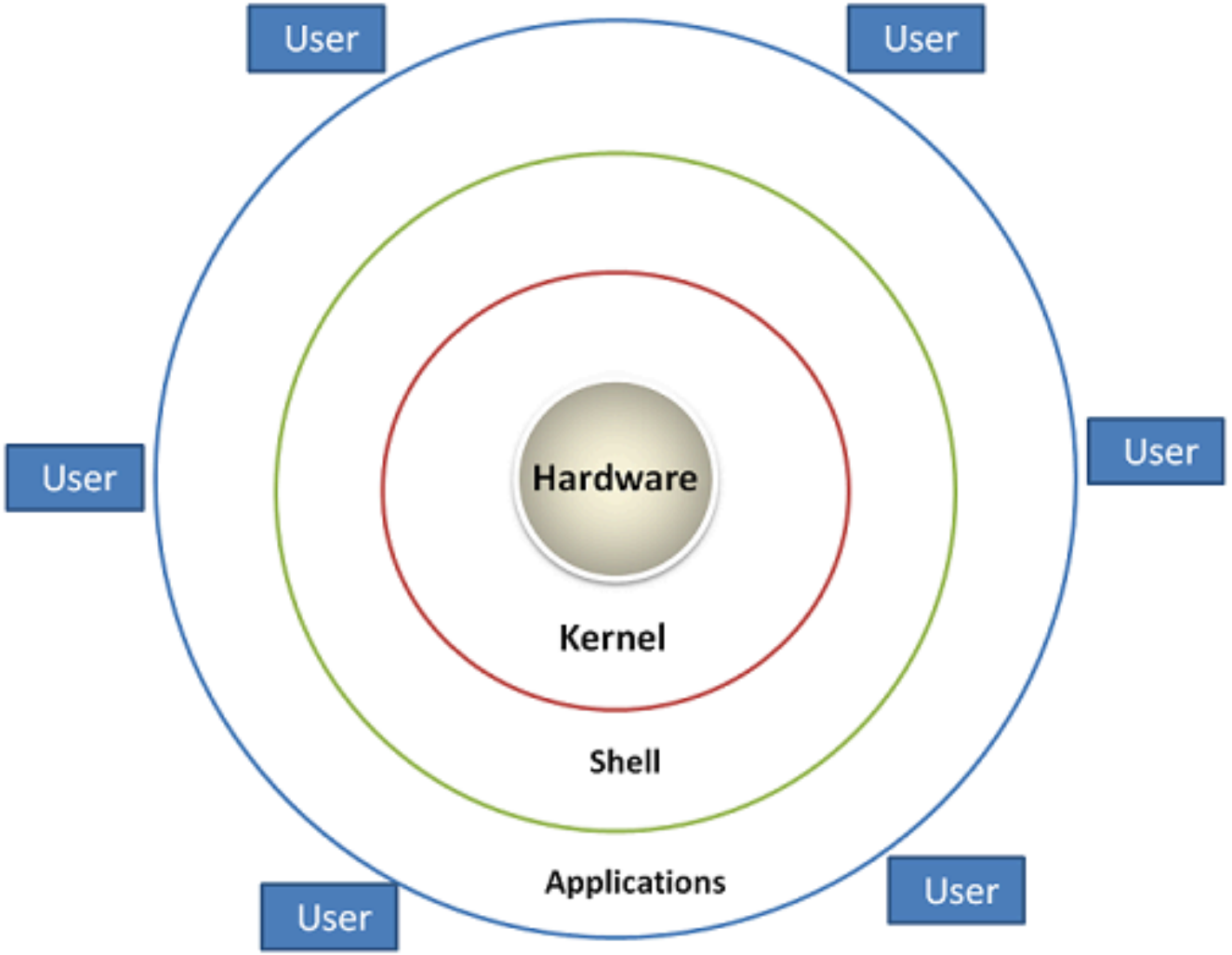
Linus Torvalds

helsinkitimes.fi



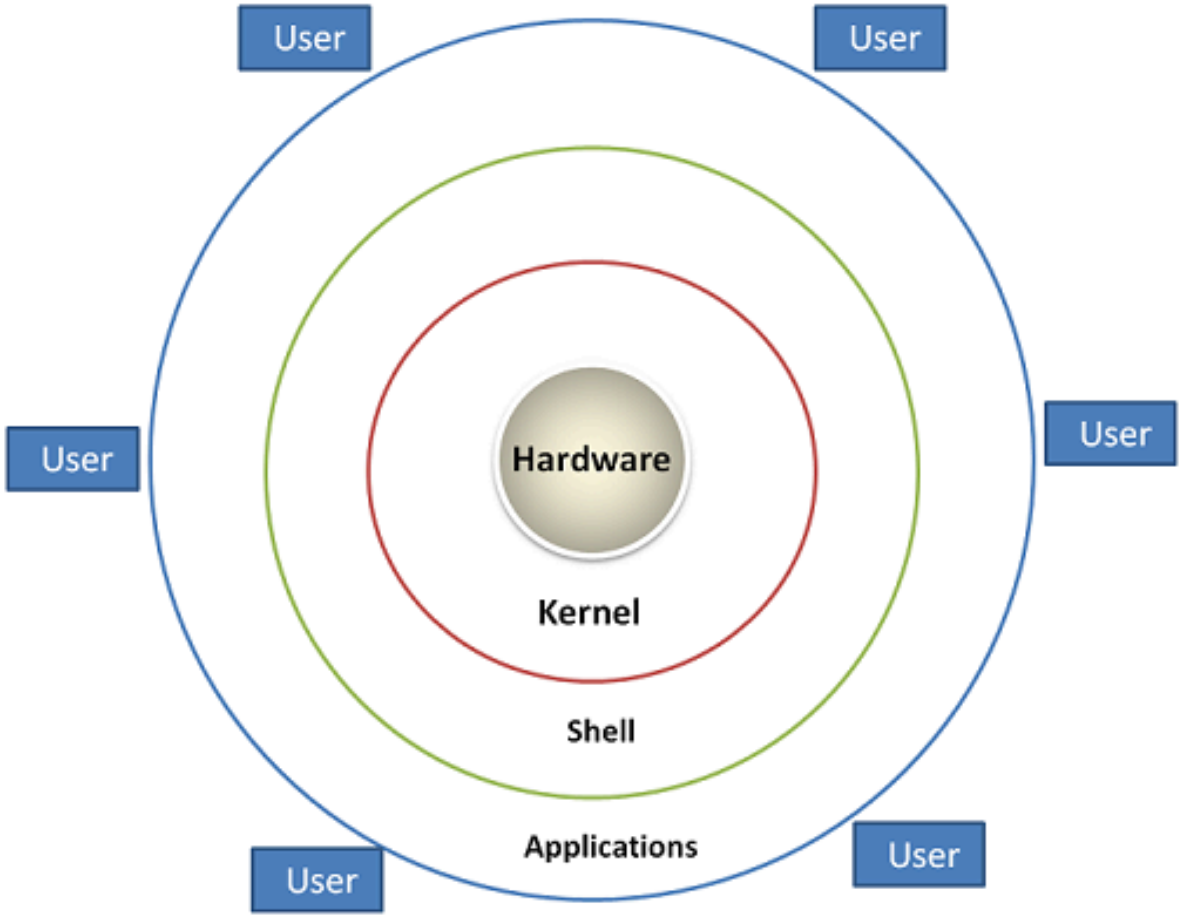


iOS



Linux System Architecture

Linux System Architecture: A Layered Approach



Linux System Architecture

Hardware Layer (Core)

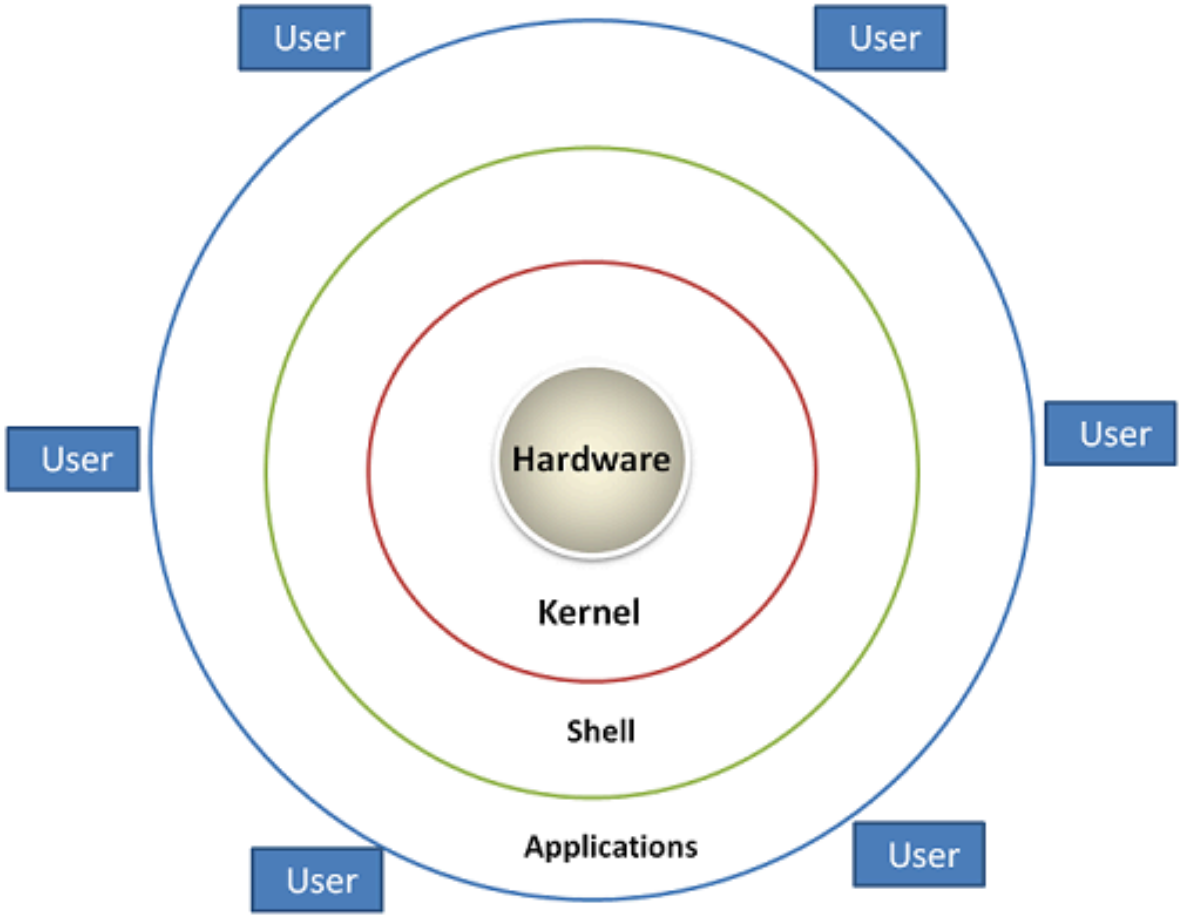
Location: Center of the architecture

Components:

- CPU
- Memory (RAM)
- Storage devices
- Input/output devices

Role: Physical foundation of the system

Linux System Architecture: A Layered Approach



Linux System Architecture

Kernel Layer

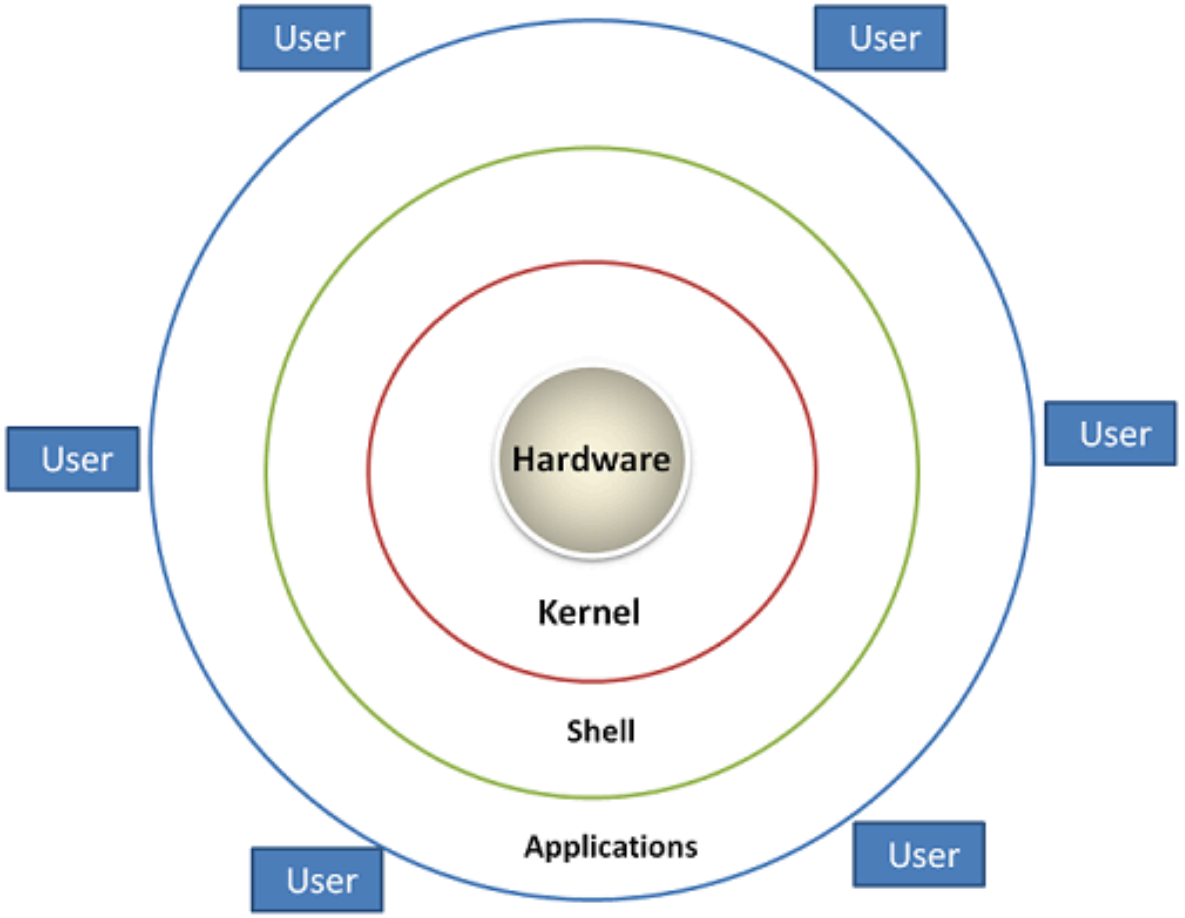
Location: First ring around hardware

Functions:

- Memory management
- Process scheduling
- Device driver management

Key point: Direct interface with hardware

Linux System Architecture: A Layered Approach



Linux System Architecture

Shell Layer

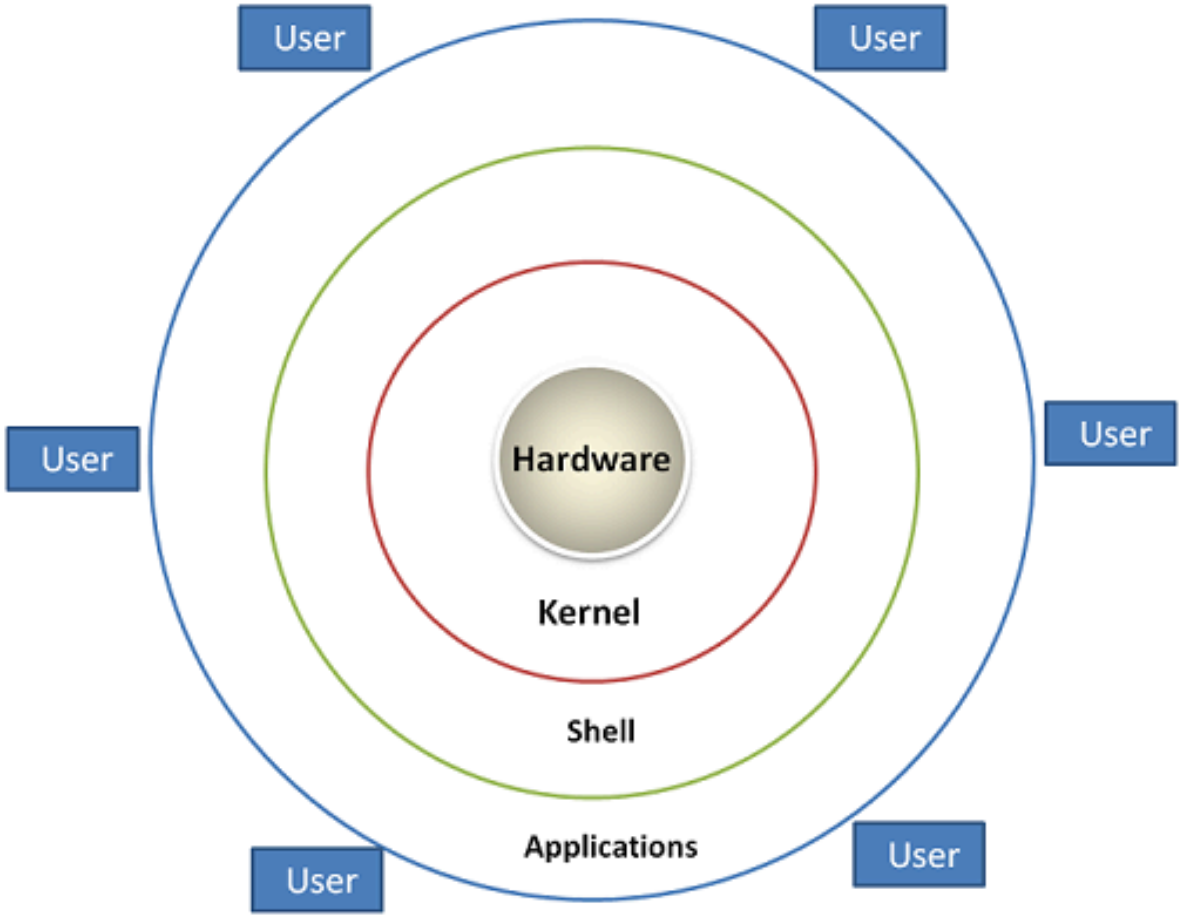
Location: Second ring around hardware

Purpose:

- Command interpretation
- Script execution
- User interface to kernel services

Types: `Bash`, `sh`

Linux System Architecture: A Layered Approach



Linux System Architecture

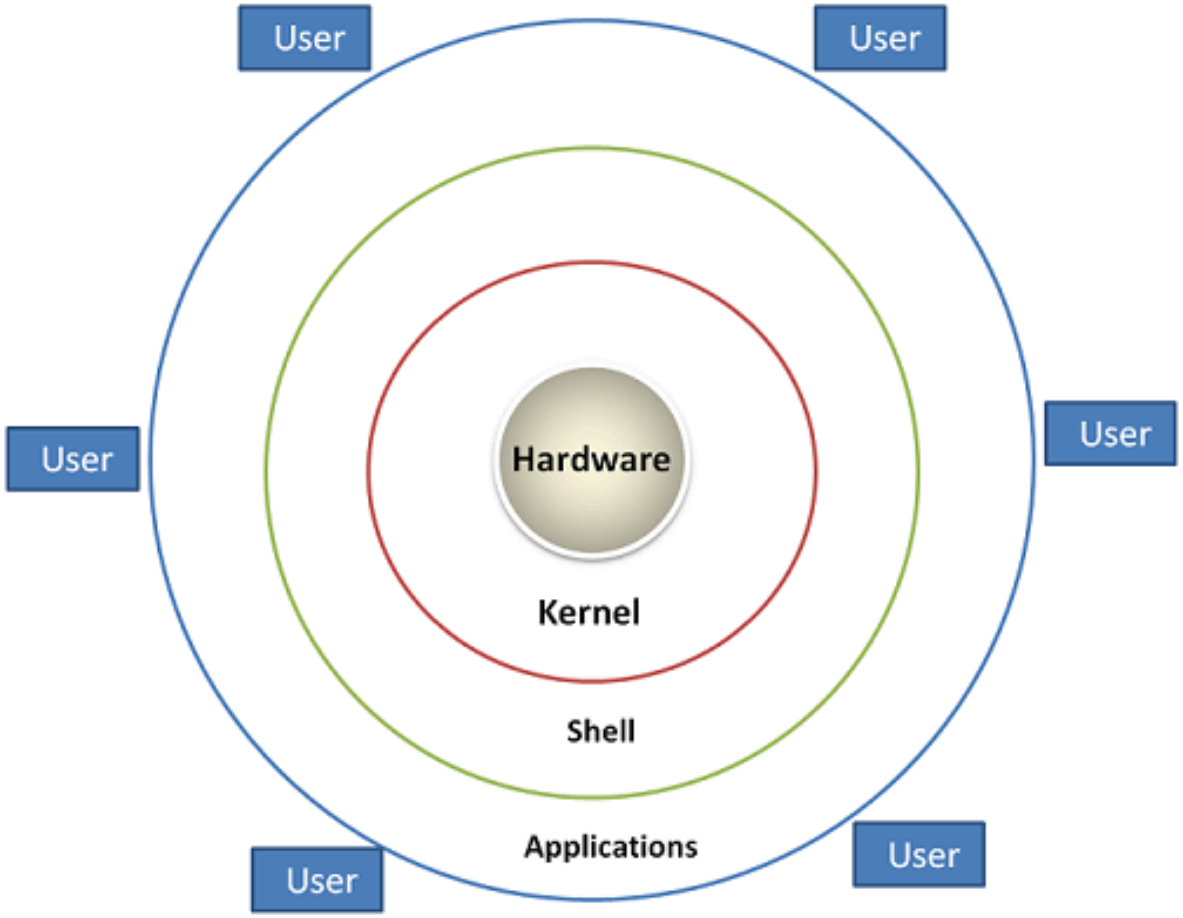
Applications Layer

Location: Outermost ring before users

Contains:

- User applications
- System utilities
- Development tools
- Graphical interfaces

Linux System Architecture: A Layered Approach



Linux System Architecture

Users (External Layer)

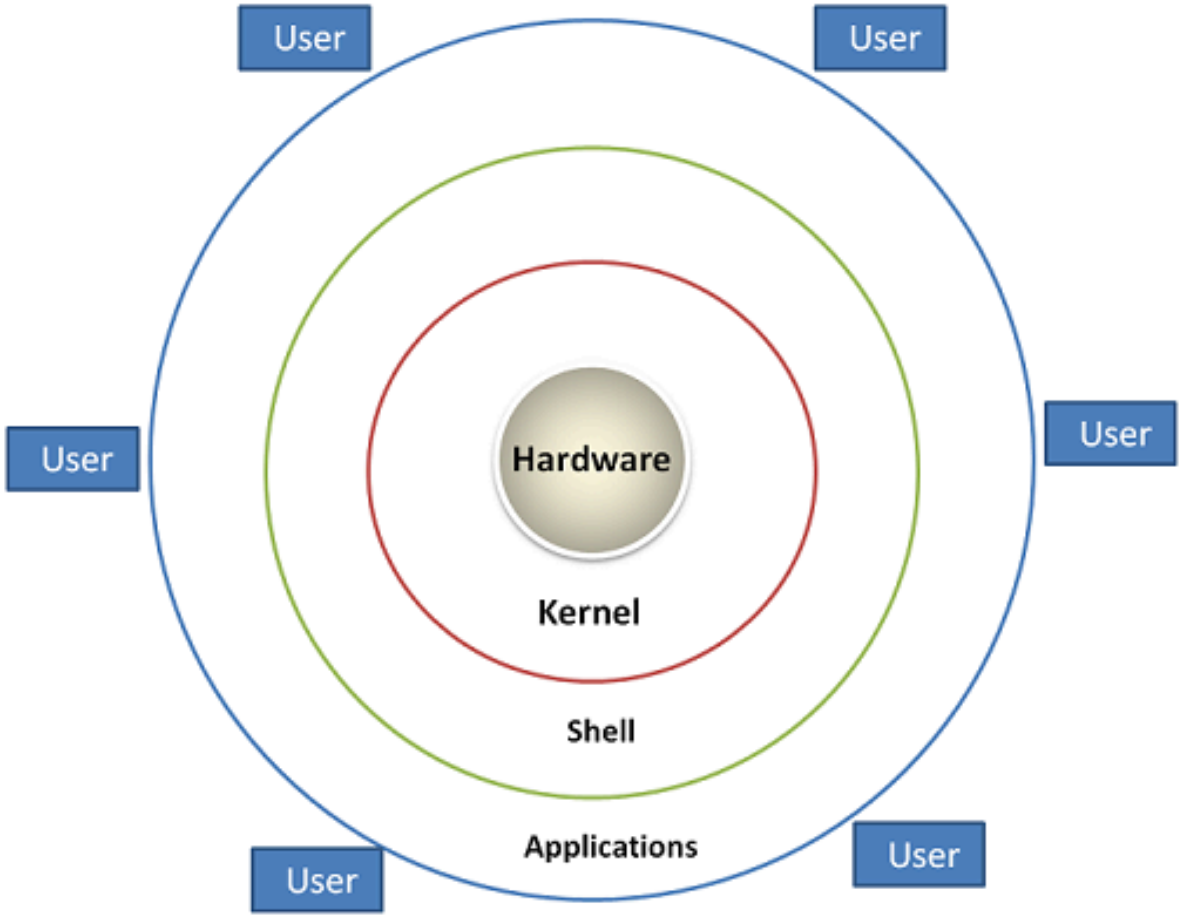
Location: Surrounding the system

Interaction:

- Multiple users can access simultaneously
- Each user has defined permissions
- Users interact through applications

Key point: Direct interface with hardware

Linux System Architecture: A Layered Approach



Linux System Architecture

Interaction Flow

User initiates action through application

Application communicates with shell

Shell interprets and sends to kernel

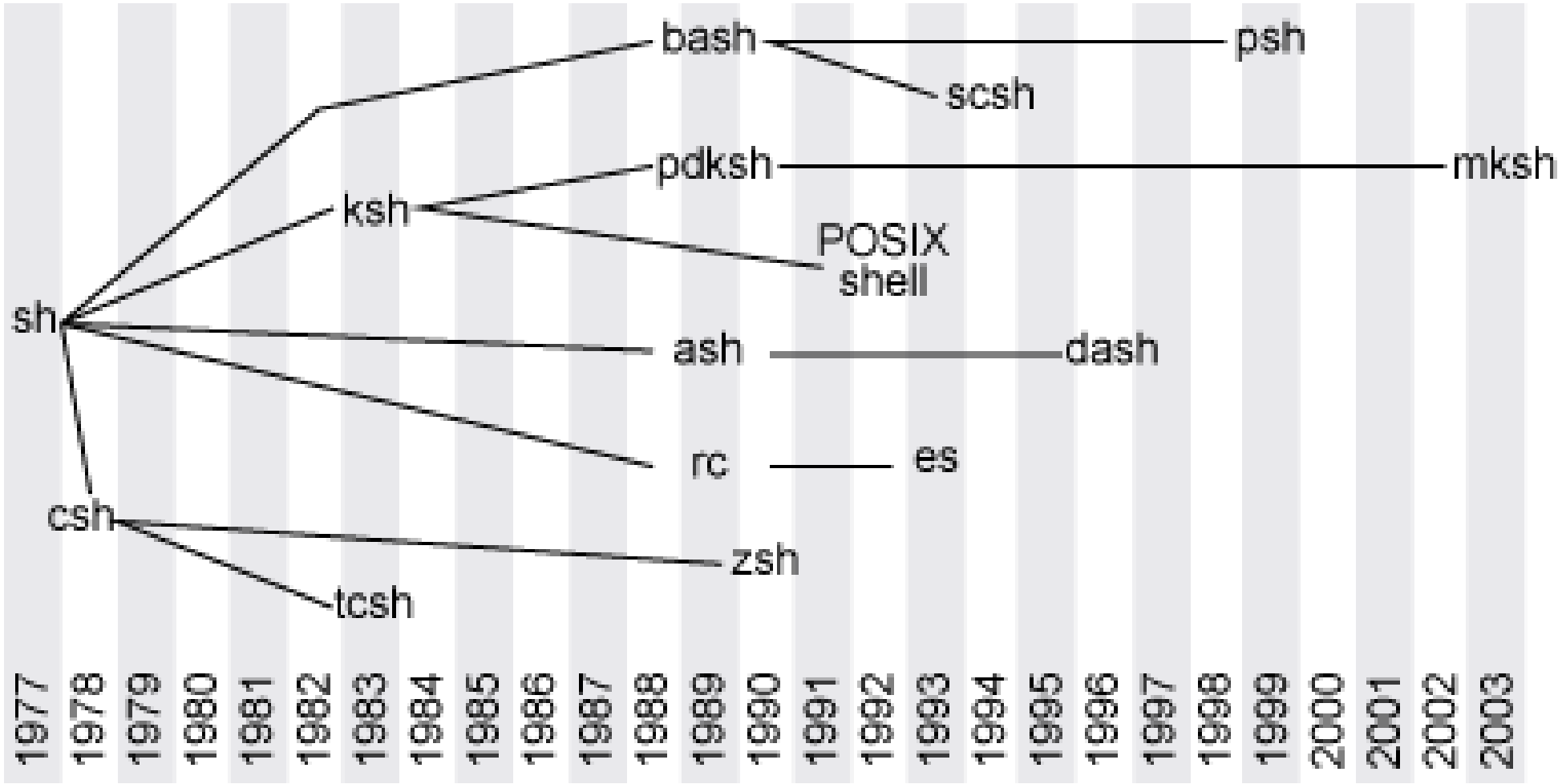
Kernel manages hardware resources

Results flow back through layers to user

KERNEL VERSUS SHELL

KERNEL	SHELL
A computer program which acts as the core of the computer's operating system and has the control over everything in the system	A computer program which works as the interface to access the services provided by the operating system
Core of the system that controls all the tasks of the system	Interface between the kernel and user
Does not have types	Has types such as Bourne shell, C shell, Korn Shell, Bourne Again Shell, etc.

Evolution of shells in Linux

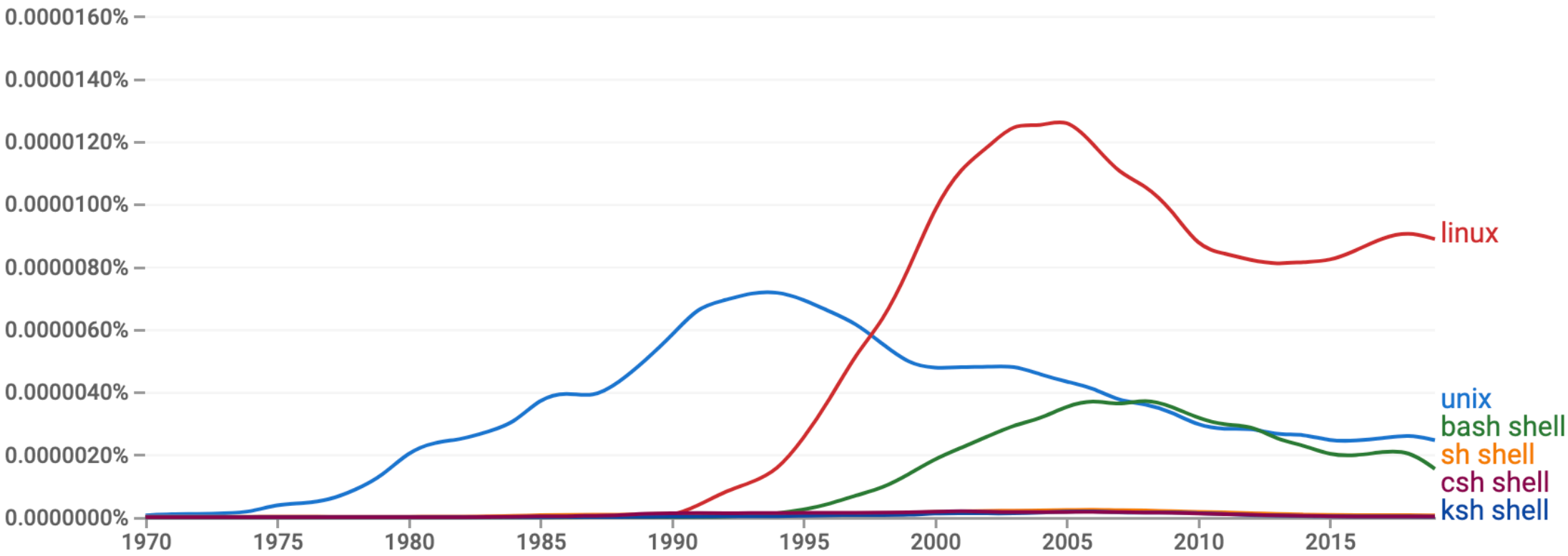


developer.ibm.com/tutorials/l-linux-shells

Google Books Ngram Viewer

unix,linux,bash shell,sh shell,ksh shell,csh shell

1965 - 2019 | English (2019) | Case-Insensitive | Smoothing of 3

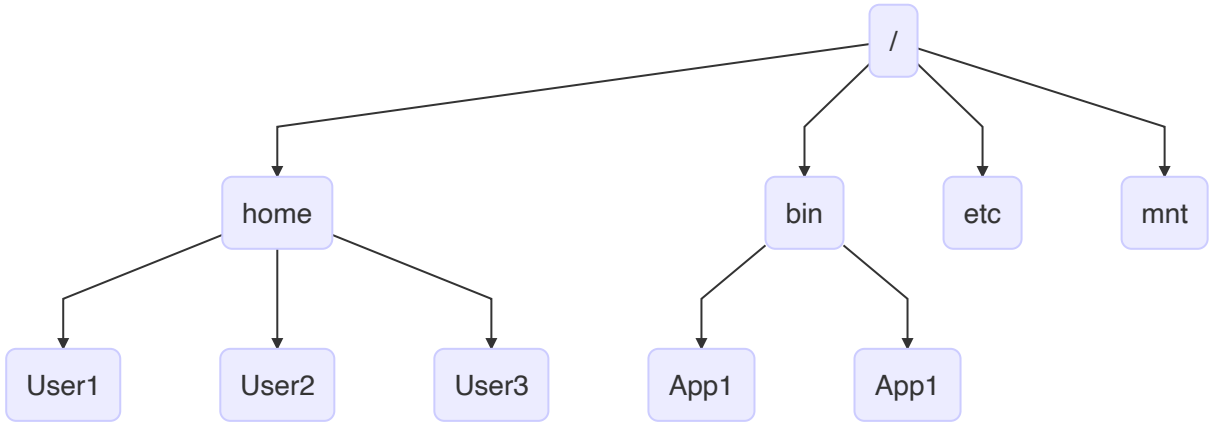


Bourne again shell

Bourne again shell

Directory structure and Bash

Directory structure



Linux command-line has a structure

student@biodocker:~$

PROMPT

Linux command-line has a structure

student@biodocker:~$ command option argument

PROMPT	`ls`	`-l`	`/`

Linux command-line has a structure

student@biodocker:~$ command option argument

PROMPT	`ls`	`-l`	`/`

Name two folders that you see after running the above command.

Exercise

Enter into the `Docker` container. `./login_student.sh`

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List the files. `ls`

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Display the content in "long listing format" + "sort by modification time". `ls -l -t`

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Display the content in "long listing format" + "sort by modification time" + "reverse the order of sorting". `ls -l -t -r`

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Print the working directory using `pwd` command. `pwd`

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Check your user name by `whoami` command. `whoami`

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Enter into the `Docker` container. `./login_student.sh`

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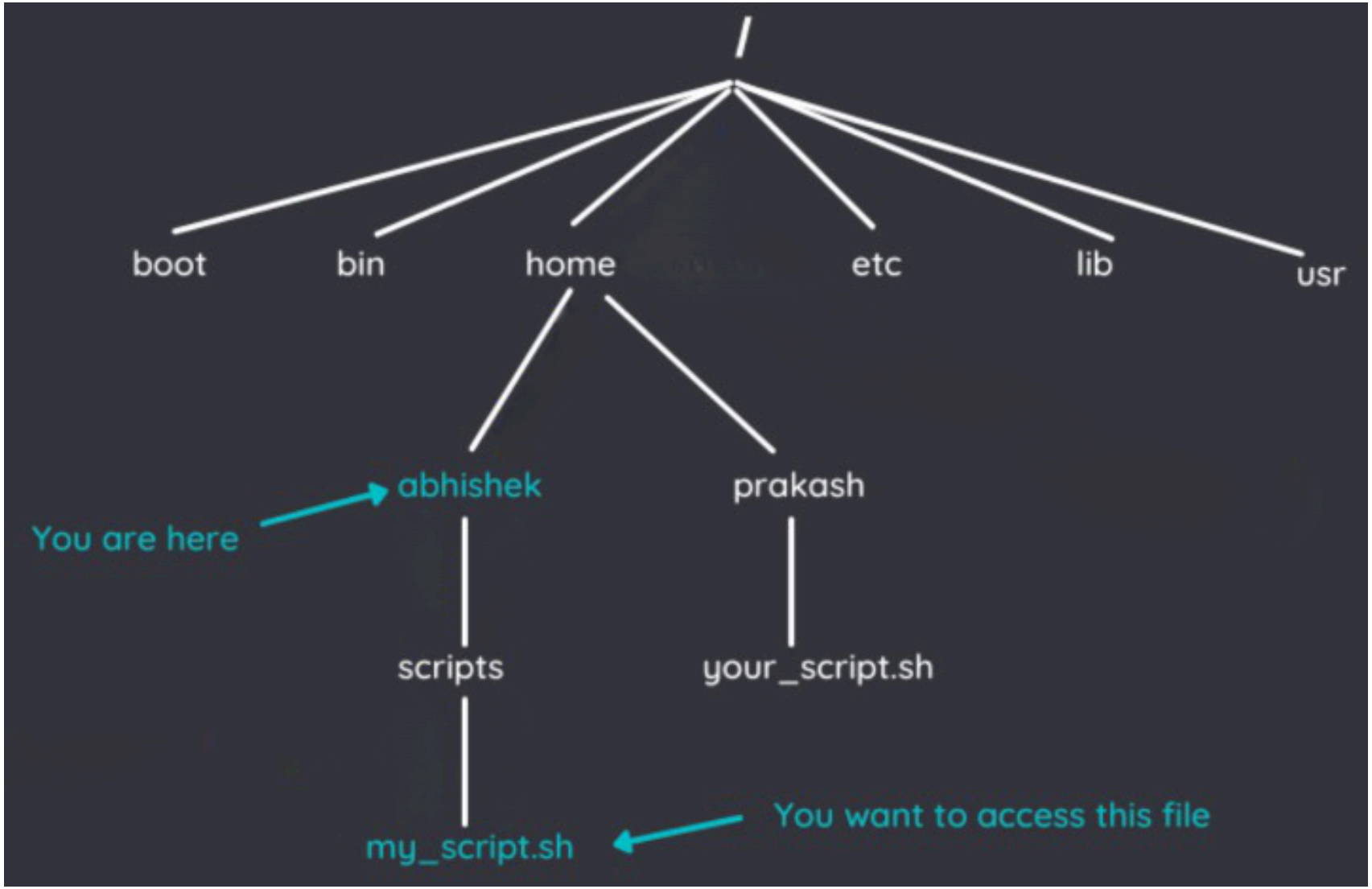
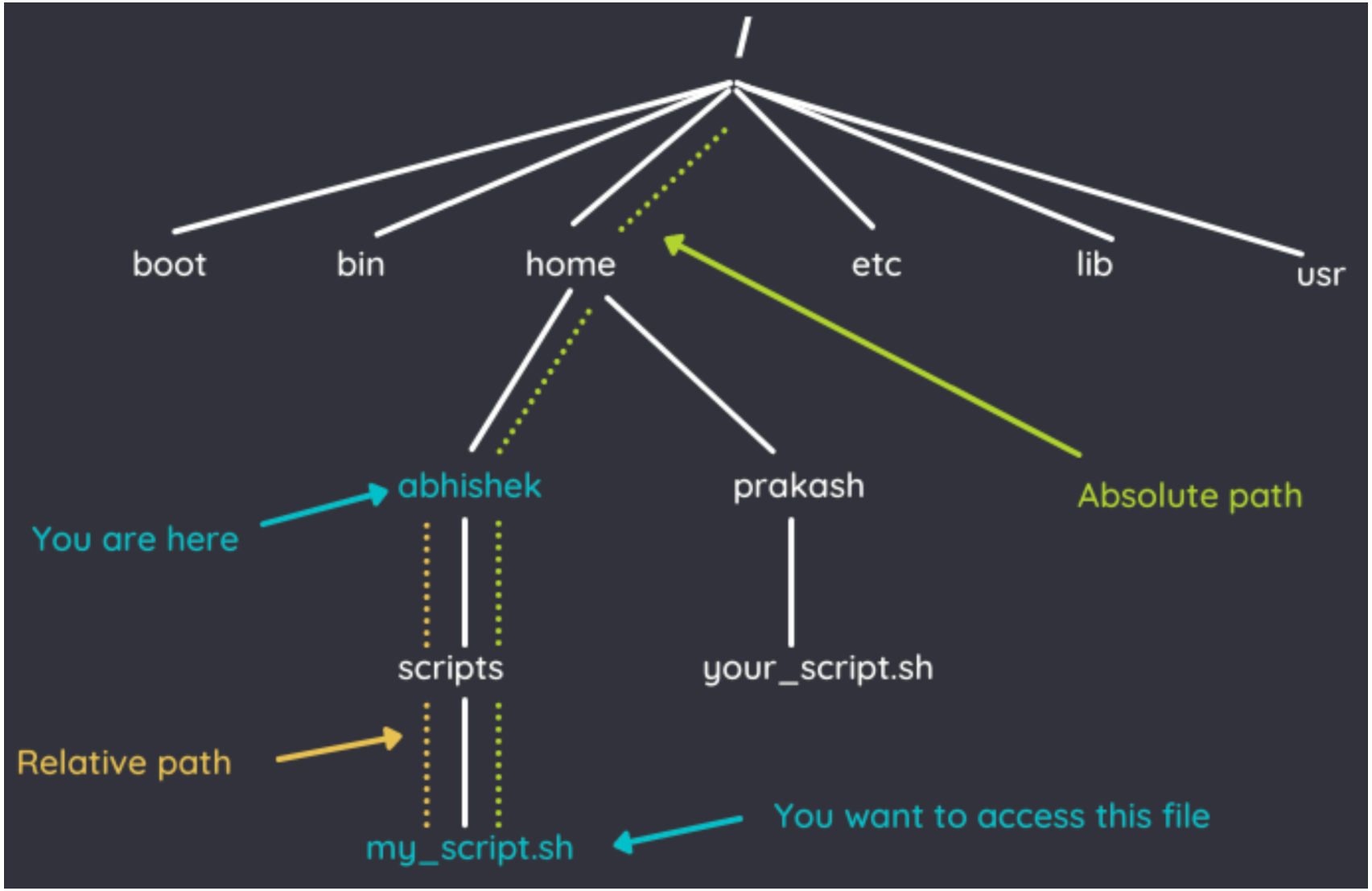
Most command names are abbreviations of their function.

Path to navigate



Path to navigate



Some important symbols/ commands

Symbols/ Commands	Descriptions
`.`	current directory
`..`	directory up in heirarchy
`cd` or **`cd ~`** or **`cd ~/`**	change directory to home directory

Some important symbols/ commands

Symbols/ Commands	Descriptions
`touch`	create a file
`*`	list out all the files
List`?`	any file that begins with List followed by 1 character

Exercise

Make a folder in your home directory: test. Enter into the test folder. Create some files using `touch` command: test1.txt, test2.txt, abc.txt, DEF.txt, 1file.txt, and bcd.txt. Display all files, display all test files using `?`, and display files starting with a.

Exercise

Make a folder in your home directory: test. Enter into the test folder. Create some files using `touch` command: test1.txt, test2.txt, abc.txt, DEF.txt, 1file.txt, and bcd.txt. Display all files, display all test files using `?`, and display files starting with a.

```
cd ~/ # go to home directory

mkdir test # make a test directory

cd test # change directory

touch test1.txt test2.txt abc.txt DEF.txt 1file.txt bcd.txt # create files

ls # display all files

ls test?.txt # display all test files

ls a* # display all files starting with a
```

Some important symbols/ commands

Symbols/ Commands	Descriptions
`[abc]*`	any file that begins with either ‘a’ or ‘b’ or ‘c’ and ending with any number of characters
`[[:upper:]]*`	any file that begins with an uppercase letter
`[![:upper:]]*`	any file that does notbegins with an uppercase letter
`[[:digit:]]*`	any file that begins with digit
`[![:digit:]]*`	any file that does not begins with digit
`[a-d]???`	any file that begins from a range of a-d and followed by exactly 3 character

Some important symbols/ commands

Symbols/ Commands	Descriptions
`echo`	display argument
`$*`	stored variables
`history`	display history of your activity

Exercise

Print "Hello World!". Store "Hello World!" in a varaible named `hello`. Display the history of your activity.

Exercise

Print "Hello World!". Store "Hello World!" in a varaible named `hello`. Display the history of your activity.

```
echo "Hello World!" # print

hello="Hello World!" # store into a variable
echo $hello # print content of variable

history # display history of your activity
```

Some important symbols/ commands

Symbols/ Commands	Descriptions
`mkdir`	make a directory
`rmdir`	remove a directory
`rm`	remove files/ directories
`cp`	copy files/ directories
`mv`	move files/ directories
`wget`	download file from internet

Some important symbols/ commands

Symbols/ Commands	Descriptions
`less`, `more`, `head`, `tail`, `cat`	show content
`grep`, `cut`, `uniq`, `sort`	search or extract or modify or sort
`tr`	string manipulation
`wc`	count

Some important symbols/ commands

Symbols/ Commands	Descriptions
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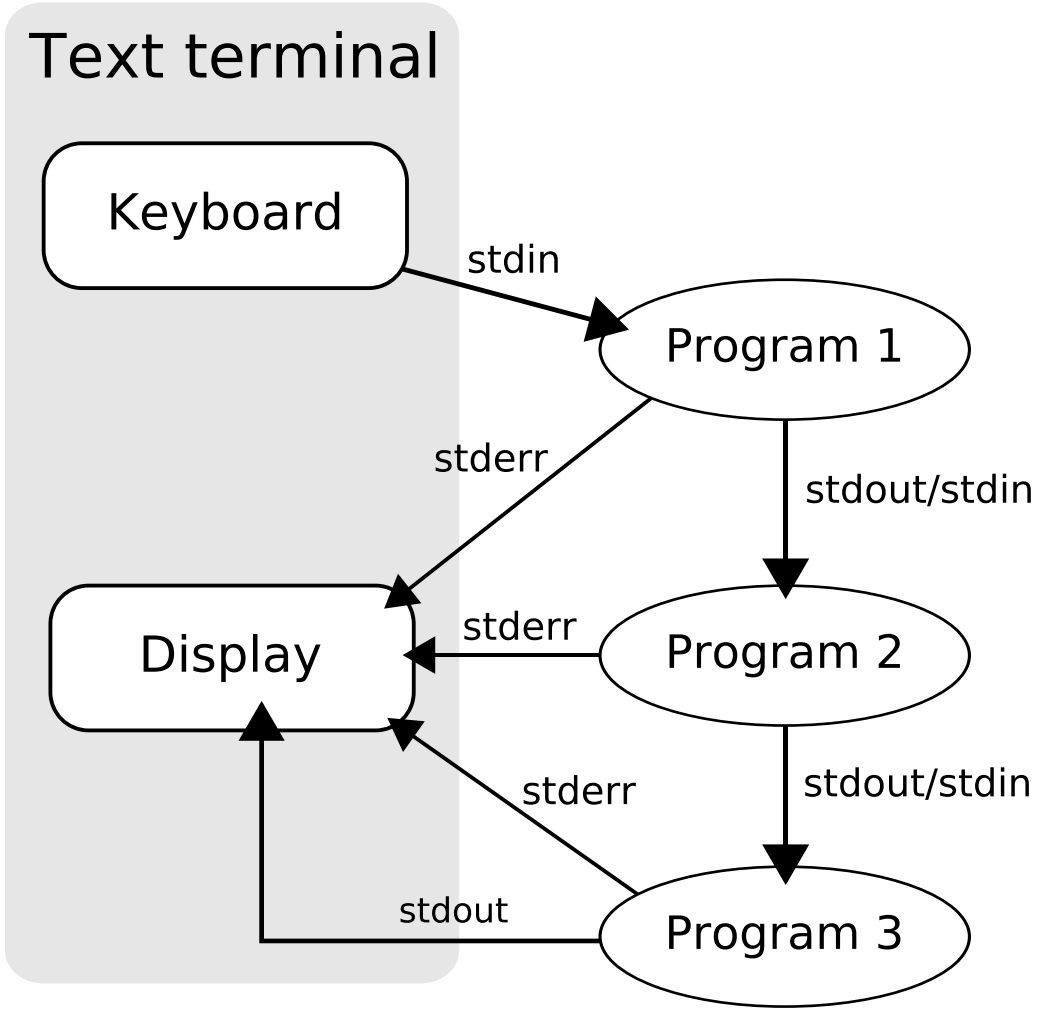
arabidopsis.org/download_files/Genes/TAIR10_genome_release/TAIR10_gff3/TAIR10_GFF3_genes.gff

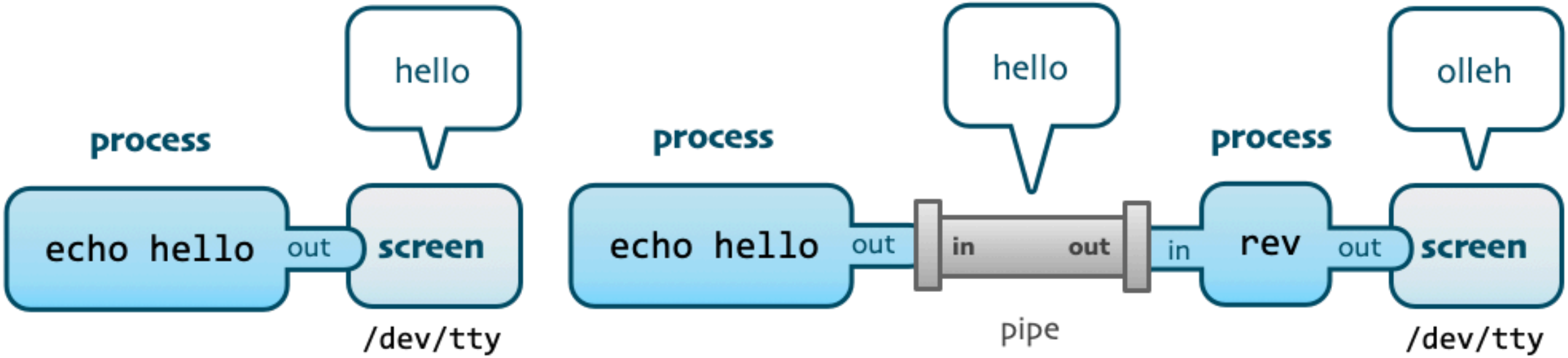
Redirection

STDIN, STDOUT, and STDERR

STDIN, STDOUT, and STDERR



Pipes


process
hello
echo hello
out
screen
/dev/tty
process
hello
echo hello
out
in
out
pipe
process
olleh
in
rev
out
screen
/dev/tty

Redirection

Symbols/ Commands	Descriptions
`>`	Standard output redirection
`<`	Standard Input redirection
`2>`	Standard error redirection
`&>`	Standard output and error redirection
`>>`	Standard output redirection
`<<`	Standard input redirection
|	Redirection using pipes

Bash scripting

Text editors

- `nano`
- `vim`
- `emacs`

Bash scripts

```
#!/bin/bash

# This script will print ...

echo "Hello World!"
```

```
# shebang line

# a comment

# code
```

Bash scripts

```
#!/bin/bash

# This script will print ...

echo "Hello World!"
```

```
# shebang line

# a comment

# code
```

```
#!/bin/bash

# This script will print my name

name="Deepak Tanwar"

echo "Hello $name!"
```

```
# shebang line

# a comment

# store name in a variable

# print name
```

Bash script

Using nano, write a script to print your name.

```
nano name.sh # create a file using nano

#!/bin/bash
echo "Deepak Tanwar"

# close the file with ctrl + x
```

Bash script

Using nano, write a script to print your name.

```
nano name.sh # create a file using nano

#!/bin/bash
echo "Deepak Tanwar"

# close the file with ctrl + x
```

Redirect output as STDOUT: `name.stdout`.

```
bash name.sh > name.stdout
```

Bash script

Redirect output as STDERR: `name.stderr`.

```
bash name.sh 2> name.stderr
```

Bash script

Redirect output as STDERR: `name.stderr`.

```
bash name.sh 2> name.stderr
```

Append `name.stdout` with your favourite animal.

```
echo "Tiger" >> name.stdout
```

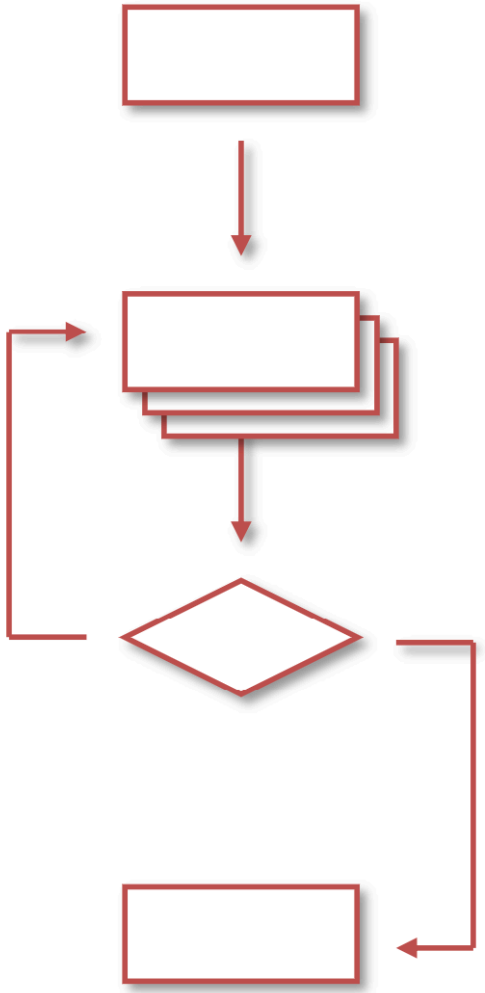
Bash script

Append `name.stderr` with your favourite food.

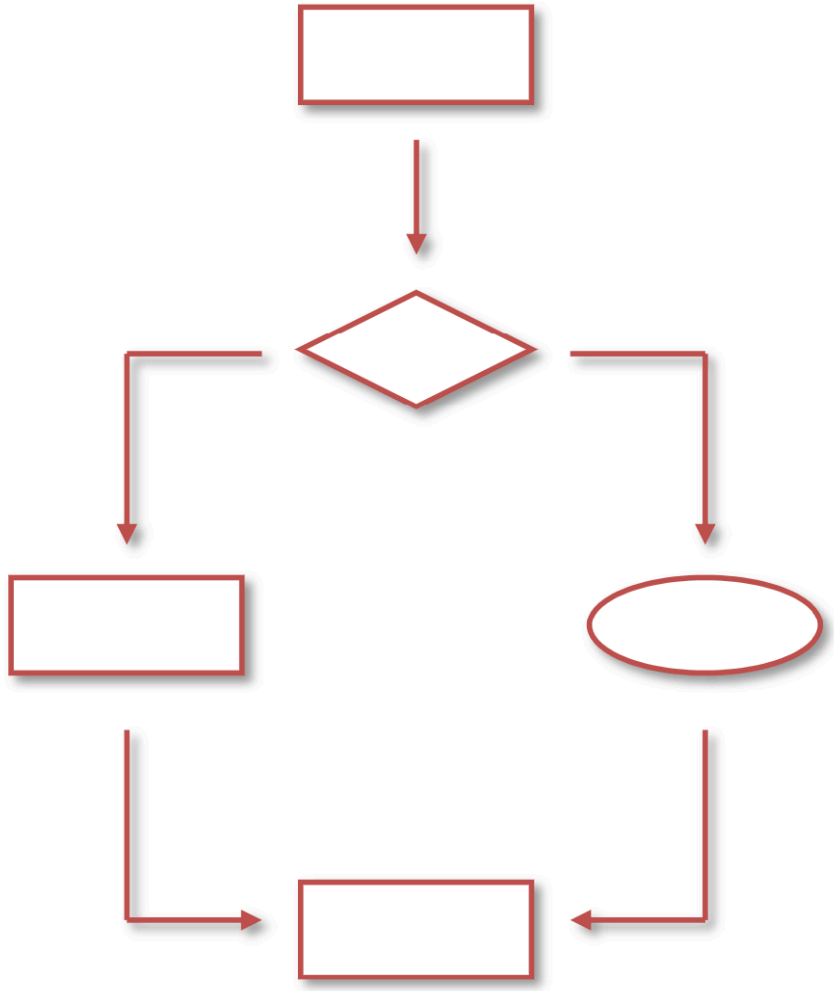
```
echo "Fondue" 2>> name.stderr
```

Flow control

repetition



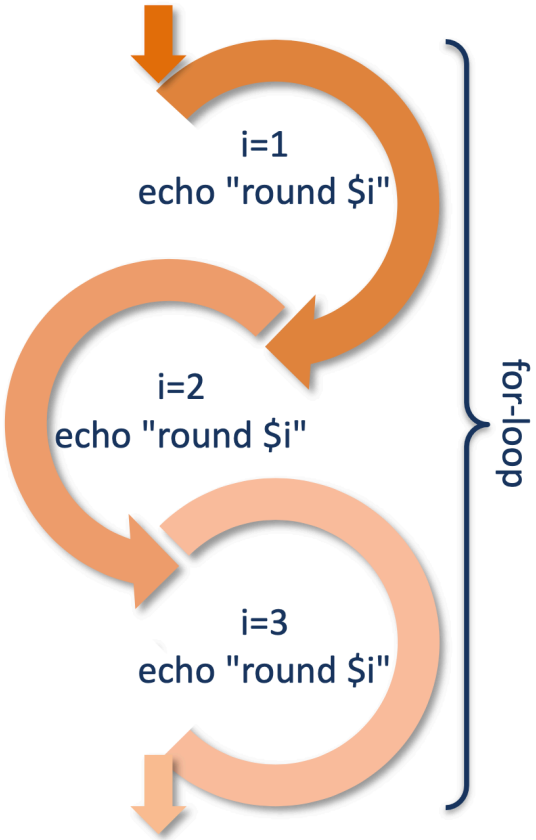
selection



for loop

```
for VARIABLE in 1 2 3
do
  command1
done
```

- Can be used to repeat certain tasks



- Examples:

```
#!/bin/bash
for i in 1 2 3
do
  echo "round $i"
done
```

```
#!/bin/bash
for i in {1..3}
do
  echo "round $i"
done
```

```
round 1
round 2
round 3
```

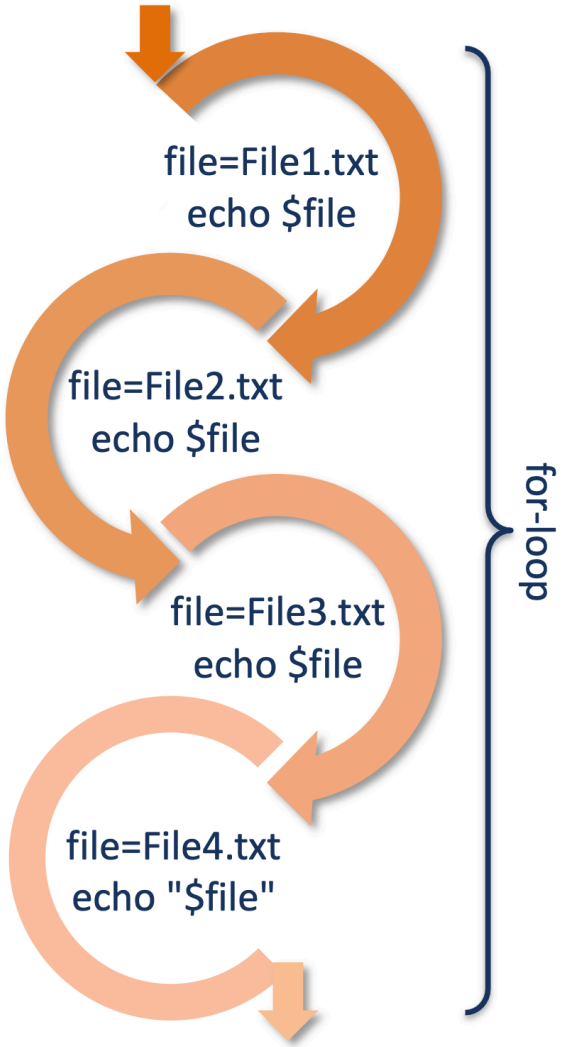
for loop

- Examples:

Go through all files in a folder:

```
#!/bin/bash
for file in /home/user/*
do
  echo $file
done
```

```
File1.txt
File2.txt
File3.txt
File4.txt
```



while loop

- Can also be used to repeat certain tasks:

```
while [[ something ]]
do
  command
done
```

- Example:

```
#!/bin/bash
count=0
while [[ $count -lt 4 ]]
do
  echo $count
  let count+=1
done
echo "done"
```

```
0
1
2
3
done
```

if-else

```
if [[ someting ]]
then
   command1
elif [[ something ]]
then
   command2
else
   command3
fi
```

if-else

Boolean operators:

- **-e FILE**: True if file exists

```
#!/bin/bash
if [[ -e log.txt ]]
then
  echo "log file exist"
else
  echo "log file doesn't exist"
fi
```

Setting path and permissions

Setting path

```
export PATH="/path/to/dir:$PATH"
```

Setting path

```
export PATH="/path/to/dir:$PATH"
```

```
export PATH="/path/to/dir:$PATH" >> ~/.bash_profile
```

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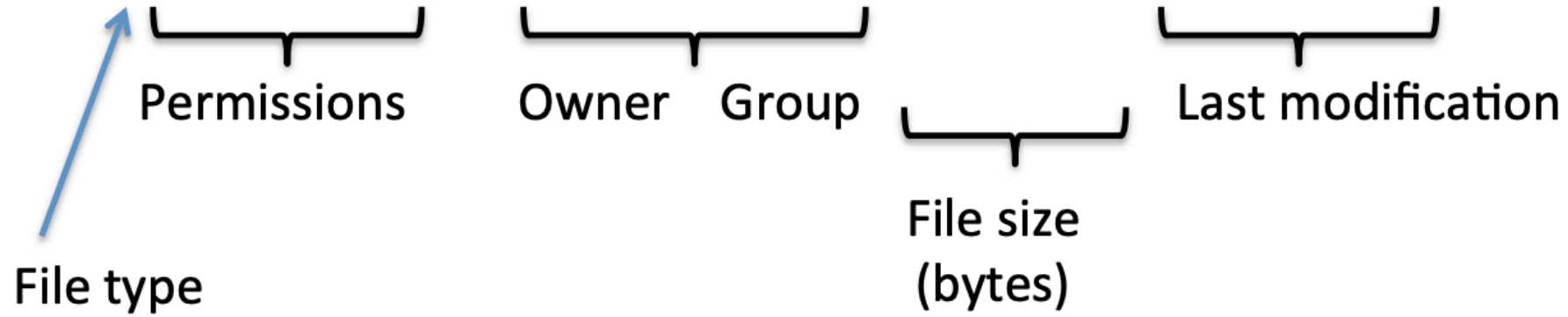
```
export PATH="/path/to/dir:$PATH" >> ~/.bash_profile
```

```
export PATH="/path/to/dir:$PATH" >> ~/.bashrc
```

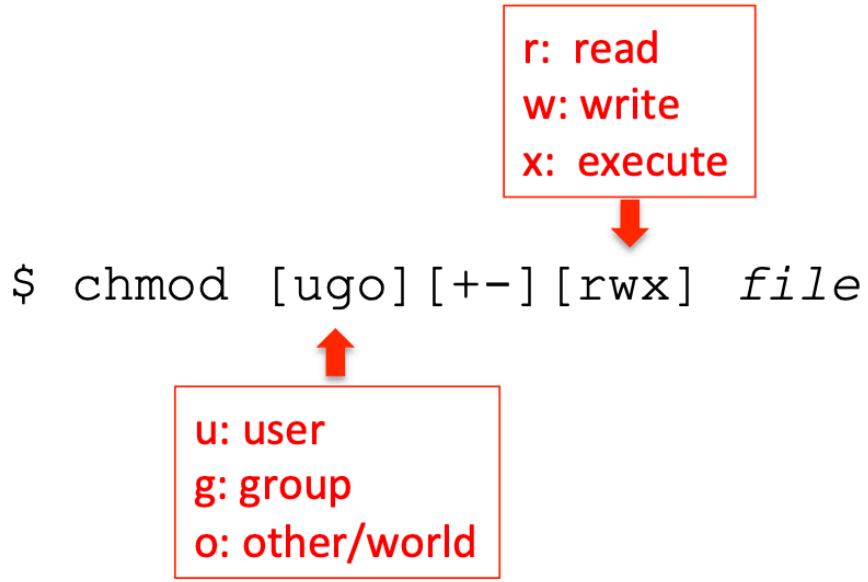
Permissions and changing permissions

```
$ ls -l
```

```
-rw-r--r--    1 swyder   staff       6677 30 Okt 22:02 At.gff
-rw-r--r--@   1 swyder   staff    3723486 28 Okt 17:30 CheatSheetguideUNIX.pdf
drwxr-xr-x   11 swyder   staff        374 11 Nov 16:13 FASTAS
-rw-r--r--    1 swyder   staff         21 30 Okt 22:04 indA.txt
```



Permissions and changing permissions



Make a file executable (for you)

```
$ chmod +x file
chmod ug+rx my_file
```

Setting exact permission (only reading, for you)

```
$ chmod =r file
```

Removing permissions (for you)

```
$ chmod -wx file
```

Permissions and changing permissions

Owner	Group	Other
r w x	r w x	r - x
4+2+1	4+2+1	4+0+1
7	7	5

r: read
w: write
x: execute

chmod 775 *file*

Power of &&

Do a **task2** only after **task1** is completed

Power of &&

Do a **task2** only after **task1** is completed

Not working example

```
echo "Hello"; echo "World"
```

Power of &&

Do a **task2** only after **task1** is completed

Not working example

```
echo "Hello"; echo "World"
```

Working example

```
echo "Hello" && echo "World"
```

Testing your knowledge

Problem 1

PFAM is a domain database. It also includes domains that have already been computed for all proteomes. The most recent version is available here: https://ftp.ebi.ac.uk/pub/databases/Pfam/releases/Pfam35.0/proteomes/. Each file represents a proteome, which is recognized by its taxonomy ID. The ID `9606` belongs to a human. Each of these files is tab-delimited, with the domain ID in the sixth column. Using `wget`, download the human proteome file. After downloading, run a single line of `bash` commands to determine the number of domain types (unique domains) in the human genome. You may use as many commands as you want, connected together in `pipes`.

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```

```
zcat 9606.tsv.gz | cut -f 6 | grep -v "#" | sort| uniq | wc -l
```

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```

```
6680
```

Problem 2

Download the covid19 fasta file from https://ftp.ebi.ac.uk/pub/databases/Pfam/releases/Pfam_SARS-CoV-2_2.0/ using `wget` command.

1. How many proteins are there?
2. How many amino acids are there?
3. Take only the protein sequences, and convert them to lower case.

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```
cat covid-19.fasta | grep ">" | wc -l
```

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```

```
cat covid-19.fasta | grep -v ">" | wc -c
```

```
cat covid-19.fasta | grep -v ">" | tr [:upper:] [:lower:]
```

Problem 3

PFAM is a domain database. It also includes domains that have already been computed for all proteomes. The most recent version is available here: https://ftp.ebi.ac.uk/pub/databases/Pfam/releases/Pfam35.0/proteomes/. Each file represents a proteome, which is recognized by its taxonomy ID. The ID `9606` belongs to a human. Each of these files is tab-delimited, with the domain ID in the sixth column.

1. Make a directory in your home folder `software/bin`.
2. Change directory to `software/bin`.
3. Write a `bash` script that take an input: taxonomy ID.
4. If file does not exist, Script should download the proteome file for the input taxonomy ID.
5. Script should run a single line of `bash` commands to determine the number of domain types (unique domains) in the genome.
6. Run step 5 **only if** step 4 is finished.
7. Save your file as `count_uniq_domains`
8. Add your script to `PATH`
9. Go to your home folder.
10. Create a `bash` script that will run `count_uniq_domains` (without specifying path). This script should store `STDOUT` and `STDERR`.

Problem 3

```
# 1 and 2

cd ~/
mkdir software
cd software
mkdir bin
```

Problem 3

```
# 3, 4, 5, 6, and 7

nano count_uniq_domains

#!/bin/bash

txid=$1
txid2=$txid.final.tsv.gz

if [ -e $txid2 ]
        then
zcat $txid2 | grep -v "#" | cut -f 6 | sort| uniq| wc -l
        else
wget https://ftp.ebi.ac.uk/pub/databases/Pfam/releases/Pfam35.0/proteomes/$txid.tsv.gz &&\
 mv $txid.tsv.gz $txid2 &&\
 zcat $txid2 | grep -v "#" | cut -f 6 | sort| uniq| wc -l
fi
```

Problem 3

```
# 8

chmod +x count_uniq_domains

export PATH="~/software/bin/:$PATH"
```

```
# 9

cd ~/
```

```
# 10

nano run.sh

#!/bin/bash

count_uniq_domains 9696 > STDOUT 2>STDERR

## close the file with ctrl + x

bash run.sh
```

Resources

https://github.com/urppeia/BIO609_2016

https://github.com/urppeia/BIO609_2017

https://github.com/urppeia/BIO609_2018

https://github.com/urppeia/bio609

https://github.com/urppeia/BIO609_2021

Instructor and Course evaluation

bit.ly/bio609_2024

Thank you for your attention!