McGill initiative in
Computational Medicine

Introduction to UNIX

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McGill initiative in Computational Medicine

<u>Mission</u> : aims to deliver inter-disciplinary research programs and empower the use of data in health research and health care delivery

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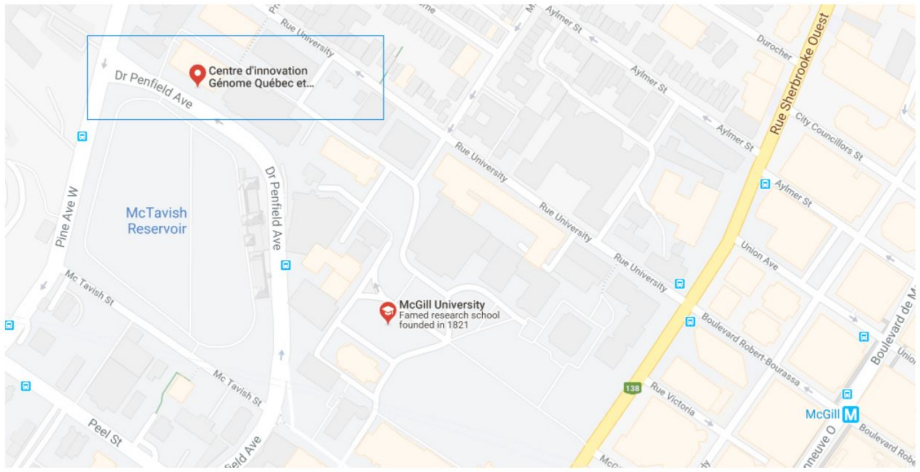

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Workshop outline

1
- Introduction to the UNIX operating system
- Files and processes
- Directory Structure
- The Terminal

2
- Basic Commands
- Directory Management
- File Management
- Redirecting output
- File permissions

3
- Text processing
- Pipes

4
- Variables
- Connecting to a remote server
- How to transfer files to and from a server

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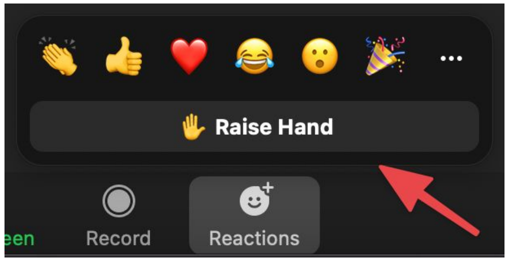
This is an interactive workshop!

- If possible try to follow along in your own computer.
- Feel free to interrupt or raise your hand to ask questions.
- I will not be checking the chat that much, but feel free to ask questions there / write results / error messages.
- We can check error messages if I ask if there are questions or during the breaks.



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Workshop material is available at:

https://github.com/McGill-MiCM/MiCM_Intro_Unix_Fall2022

Please go to the page and download the material.

Part I: What is UNIX?

1

Introduction to the UNIX operating system
Files and processes
Directory Structure
The Terminal

Dennis Ritchie (standing) and Ken Thompson (seating) at Bell Labs, 1960’s

UNIX Operating system

- Multi-user, multi-tasking and interactive system.

Characterized by:

- Resource-efficient
- Hierarchical file system
- Compatibility (files, devices, processes)
- Plain files to store data

Parts

The Kernel

- The core of the operating system
- Manages processes' time, memory and resources
- Handles file storage
- Responds to system calls

The shell

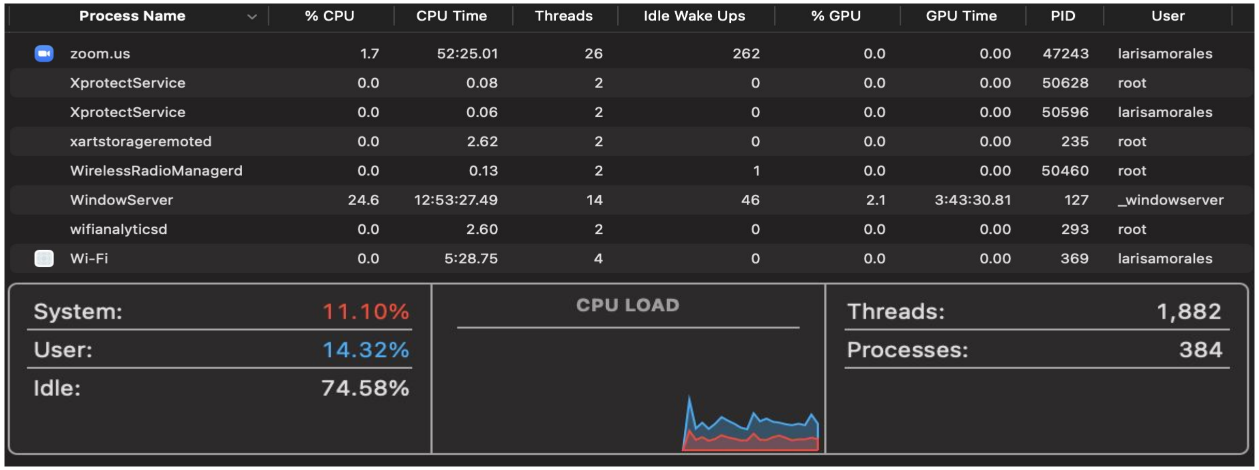
- Let's the user communicate with the kernel.
- Command line interpreter (CLI)
- Executes the instructions requested by the user (commands/programs)

The programs

- Let's the user navigate the operating system
- And perform specific actions

In UNIX everything is a file or a process!

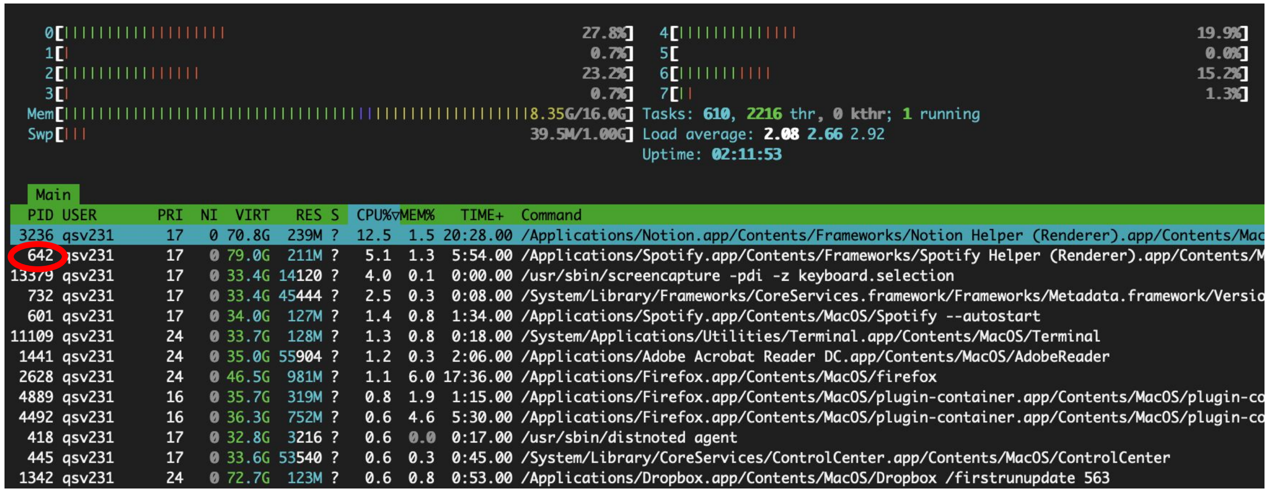
Processes



Process Name	% CPU	CPU Time	Threads	Idle Wake Ups	% GPU	GPU Time	PID	User
zoom.us	1.7	52:25.01	26	262	0.0	0.00	47243	larisamorales
XprotectService	0.0	0.08	2	0	0.0	0.00	50628	root
XprotectService	0.0	0.06	2	0	0.0	0.00	50596	larisamorales
xartstorageremoted	0.0	2.62	2	0	0.0	0.00	235	root
WirelessRadioManagerd	0.0	0.13	2	1	0.0	0.00	50460	root
WindowServer	24.6	12:53:27.49	14	46	2.1	3:43:30.81	127	_windowserver
wifianalyticsd	0.0	2.60	2	0	0.0	0.00	293	root
Wi-Fi	0.0	5:28.75	4	0	0.0	0.00	369	larisamorales

System:	11.10%
User:	14.32%
Idle:	74.58%

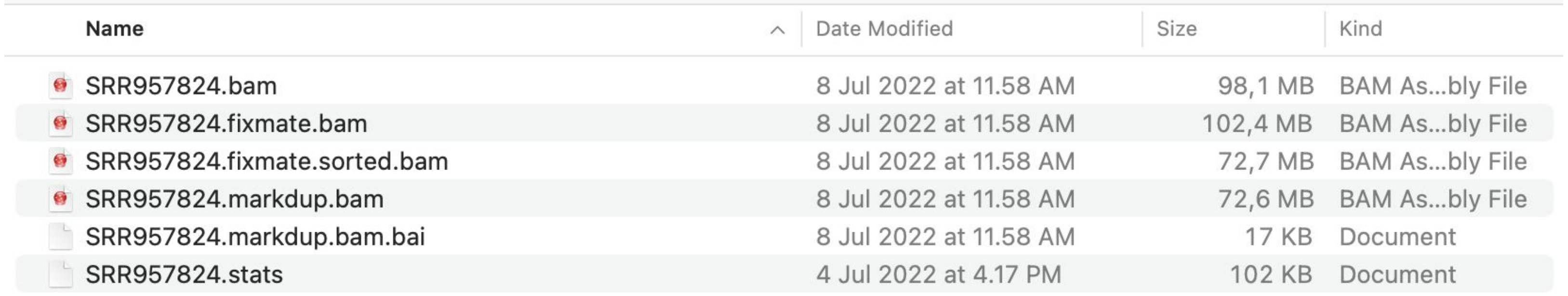
Threads:	1,882
Processes:	384



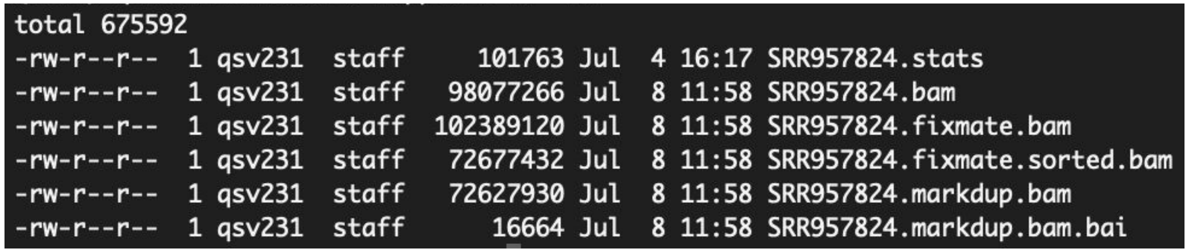
```
  0[|||||||||||||||||||                              27.8%]   4[||||||||||||||                                  19.9%]
  1[|                                                 0.7%]   5[                                                 0.0%]
  2[|||||||||||||||                                  23.2%]   6[|||||||||||                                     15.2%]
  3[|                                                 0.7%]   7[||                                               1.3%]
Mem[||||||||||||||||||||||||||||||||||||||||||||||||||8.35G/16.0G] Tasks: 610, 2216 thr, 0 kthr; 1 running
Swp[|||                                          39.5M/1.00G] Load average: 2.08 2.66 2.92
                                                              Uptime: 02:11:53

 Main
  PID USER      PRI  NI  VIRT   RES S  CPU%▽MEM%   TIME+  Command
 3236 qsv231     17   0 70.8G  239M ?  12.5  1.5 20:28.00 /Applications/Notion.app/Contents/Frameworks/Notion Helper (Renderer).app/Contents/Mac
  642 qsv231     17   0 79.0G  211M ?   5.1  1.3  5:54.00 /Applications/Spotify.app/Contents/Frameworks/Spotify Helper (Renderer).app/Contents/M
13379 qsv231     17   0 33.4G 14120 ?   4.0  0.1  0:00.00 /usr/sbin/screencapture -pdi -z keyboard.selection
  732 qsv231     17   0 33.4G 45444 ?   2.5  0.3  0:08.00 /System/Library/Frameworks/CoreServices.framework/Frameworks/Metadata.framework/Versio
  601 qsv231     17   0 34.0G  127M ?   1.4  0.8  1:34.00 /Applications/Spotify.app/Contents/MacOS/Spotify --autostart
11109 qsv231     24   0 33.7G  128M ?   1.3  0.8  0:18.00 /System/Applications/Utilities/Terminal.app/Contents/MacOS/Terminal
 1441 qsv231     24   0 35.0G 55904 ?   1.2  0.3  2:06.00 /Applications/Adobe Acrobat Reader DC.app/Contents/MacOS/AdobeReader
 2628 qsv231     24   0 46.5G  981M ?   1.1  6.0 17:36.00 /Applications/Firefox.app/Contents/MacOS/firefox
 4889 qsv231     16   0 35.7G  319M ?   0.8  1.9  1:15.00 /Applications/Firefox.app/Contents/MacOS/plugin-container.app/Contents/MacOS/plugin-co
 4492 qsv231     16   0 36.3G  752M ?   0.6  4.6  5:30.00 /Applications/Firefox.app/Contents/MacOS/plugin-container.app/Contents/MacOS/plugin-co
  418 qsv231     17   0 32.8G  3216 ?   0.6  0.0  0:17.00 /usr/sbin/distnoted agent
  445 qsv231     17   0 33.6G 53540 ?   0.6  0.3  0:45.00 /System/Library/CoreServices/ControlCenter.app/Contents/MacOS/ControlCenter
 1342 qsv231     24   0 72.7G  123M ?   0.6  0.8  0:53.00 /Applications/Dropbox.app/Contents/MacOS/Dropbox /firstrunupdate 563
```

PID (process identifier) $\rightarrow$

Files



Name	Date Modified	Size	Kind
SRR957824.bam	8 Jul 2022 at 11.58 AM	98,1 MB	BAM As...bly File
SRR957824.fixmate.bam	8 Jul 2022 at 11.58 AM	102,4 MB	BAM As...bly File
SRR957824.fixmate.sorted.bam	8 Jul 2022 at 11.58 AM	72,7 MB	BAM As...bly File
SRR957824.markdup.bam	8 Jul 2022 at 11.58 AM	72,6 MB	BAM As...bly File
SRR957824.markdup.bam.bai	8 Jul 2022 at 11.58 AM	17 KB	Document
SRR957824.stats	4 Jul 2022 at 4.17 PM	102 KB	Document

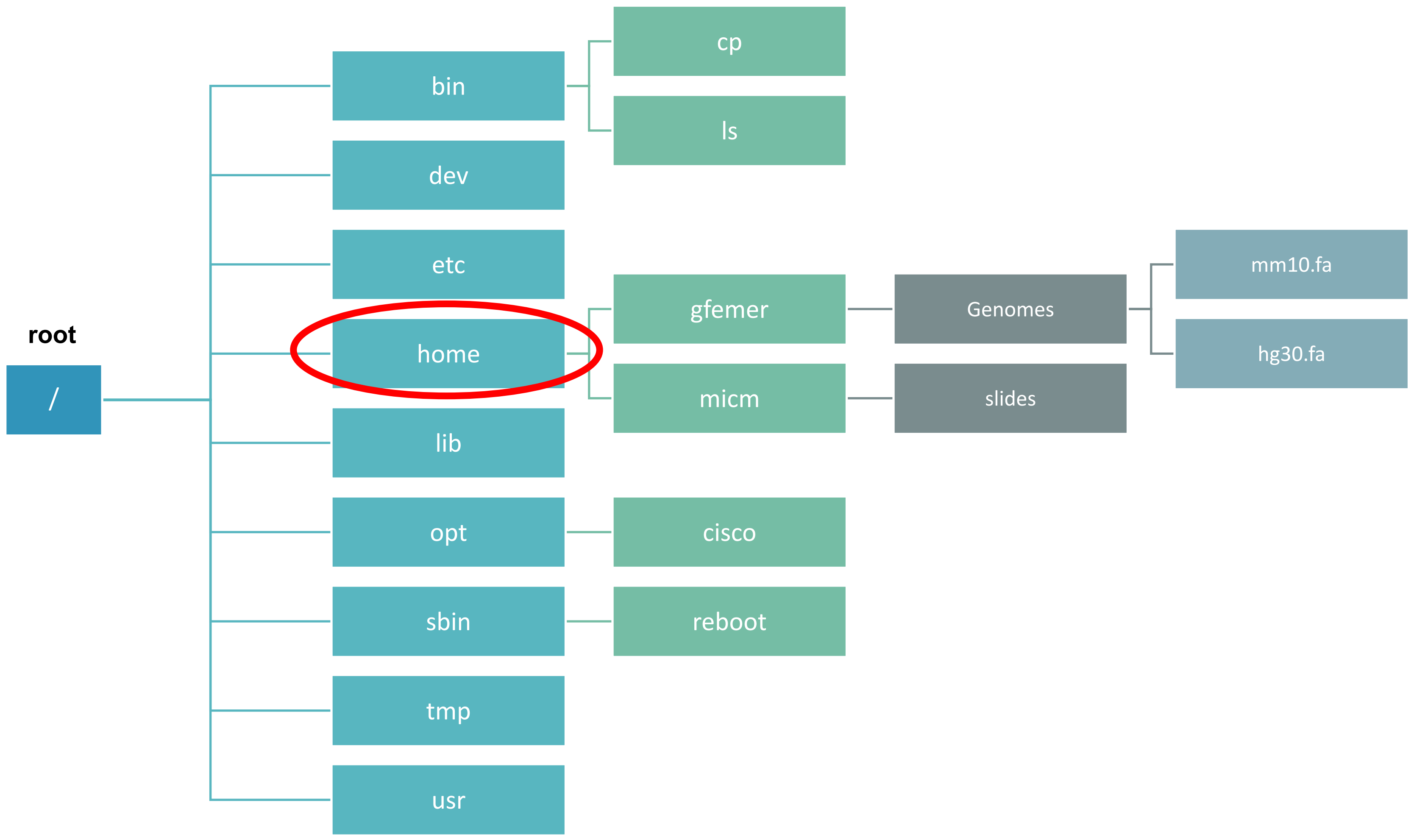


```
total 675592
-rw-r--r--  1 qsv231  staff     101763 Jul  4 16:17 SRR957824.stats
-rw-r--r--  1 qsv231  staff   98077266 Jul  8 11:58 SRR957824.bam
-rw-r--r--  1 qsv231  staff  102389120 Jul  8 11:58 SRR957824.fixmate.bam
-rw-r--r--  1 qsv231  staff   72677432 Jul  8 11:58 SRR957824.fixmate.sorted.bam
-rw-r--r--  1 qsv231  staff   72627930 Jul  8 11:58 SRR957824.markdup.bam
-rw-r--r--  1 qsv231  staff      16664 Jul  8 11:58 SRR957824.markdup.bam.bai
```

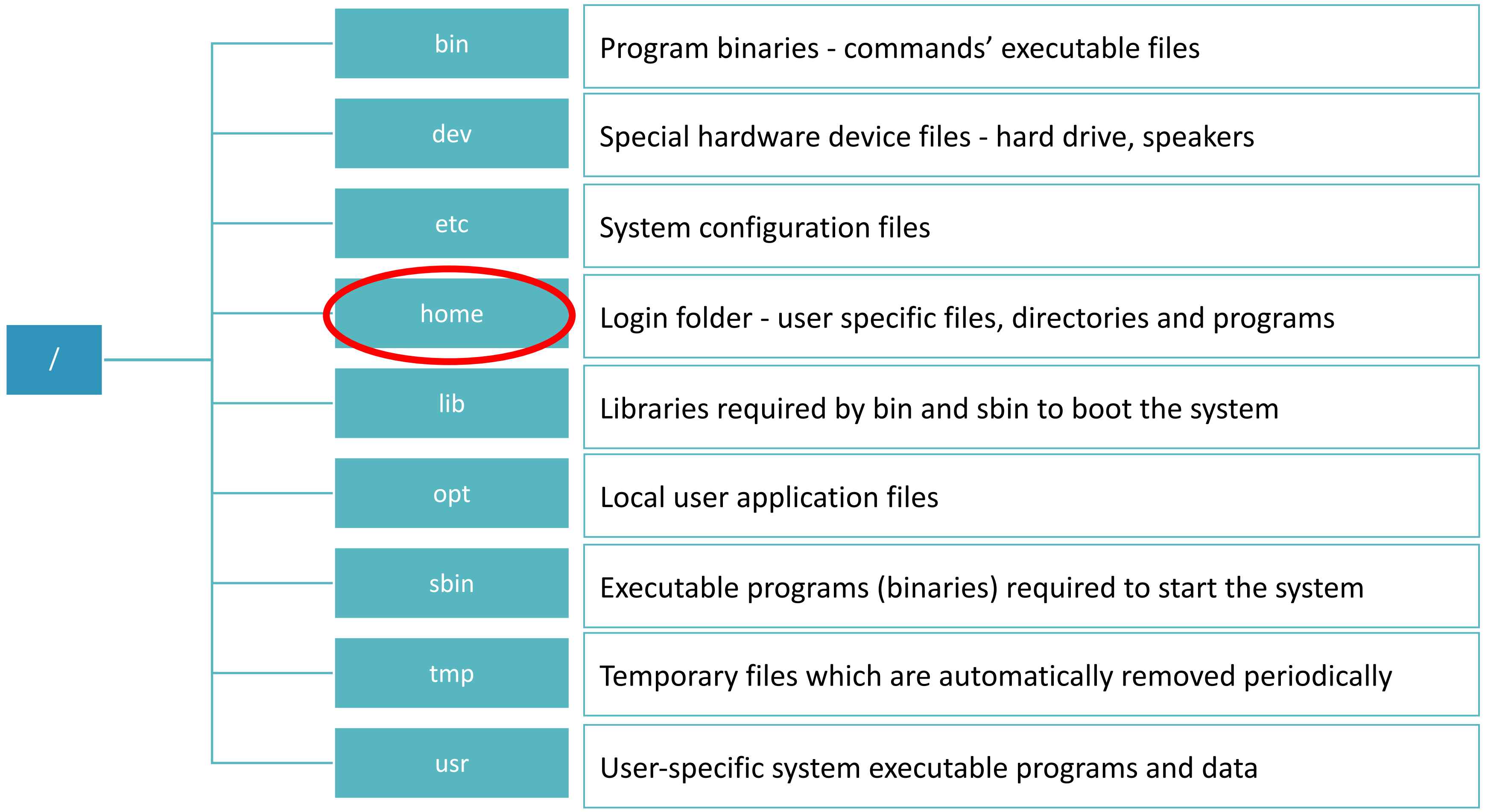
Examples of files:

- Any document (report, essay, presentation, sequence data file pdf, etc.)
- A computer program
- Binary Files
- A directory (folder)

File system structure

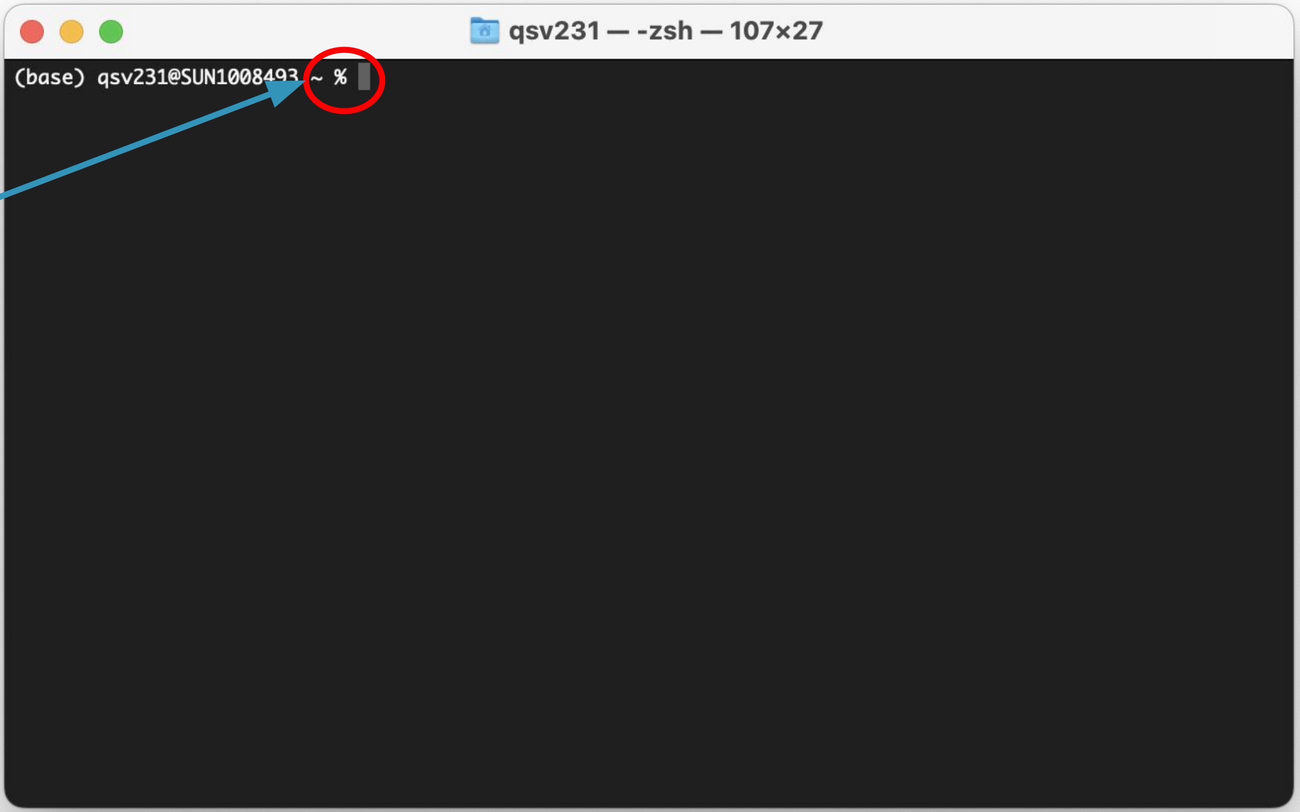


File system structure



/	
bin	Program binaries - commands' executable files
dev	Special hardware device files - hard drive, speakers
etc	System configuration files
home	Login folder - user specific files, directories and programs
lib	Libraries required by bin and sbin to boot the system
opt	Local user application files
sbin	Executable programs (binaries) required to start the system
tmp	Temporary files which are automatically removed periodically
usr	User-specific system executable programs and data

The terminal



```
(base) qsv231@SUN1008493 ~ %
```

The prompt
- % or $

A terminal is **a text input and output environment** that provides a command-line interface using a shell program.

What is a UNIX Command?

- A UNIX command is a **program** inbuilt with UNIX OS that can be invoked in several ways.
- UNIX commands work interactively from a UNIX terminal.
- The commands are used for several purposes including getting information, manipulating data, displaying and linking files, network communication, and more.
- Not all UNIX Commands are universal.

Syntax of a UNIX command

Command -[Options] [Argument(s)]

```
$   ls   -lt   ~/Onedrive
```

- **The command** tells the computer what sort of operation is being done.
- **The options** assign more specific functions to the command, or add additional actions to the command.
  - Usually single letters
  - Options are preceded with a hyphen
  - Multiple options can be combined with no spaces or separators
- **The arguments** are any piece of additional information that might be necessary to execute the command.
  - If more than one argument, they must be separated by a space.

Other concepts

- Data streams
  - STDIN: Standard input. It takes text as input.
  - STDOUT: Standard output. The text output of a command is stored in the stdout stream.
  - STDERR: Standard error. Whenever a command faces an error, the error message is stored here.

  → stdin takes as input text typed in in the terminal and stdout and stderr are normally printed out in the terminal.

- In UNIX, folders are called **directories**

Questions / Issues with installations?

Part II: Basic commands and working with files and directories

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2

Basic Commands
Directory Management
File Management
Redirecting output
File permissions
Hands on 1 exercise

Keyboard shortcuts

Ctrl+A	Go to the start of the line
Ctrl+E	Go to the end of the line
Ctrl+C	Stop the current process
q	Exit a child process (less, more, etc)
[Tab]	Autocomplete file/dirname or command

Basic commands

top	man	history	clear
See active processes and the resources they're using	Shows the manual page of a command	List your previous commands	Clear your terminal window

`% top`	`% man ls`
	`% man cd`
	`% man htop`
		`% history`	`% clear`

Working with directories

ls	pwd	mkdir	cd
Prints the content of the current directory	Shows the current directory	Creates a new directory	Access a directory
`% ls`	`% pwd`	`% mkdir test1`	`% cd test1`

Special characters

.	..	~	*
Current directory	Parent directory	Home directory	Match any and all characters
`% ls .`	`% ls ..`	`% ls ~`	`% ls *`

Understanding pathnames

- A path is a unique location to a file or a folder in a file system of an OS.
- A path to a file is a combination of / and alpha-numeric characters.

Absolute path

An **absolute path** is defined as specifying the location of a file or directory from the root directory(/).

To write an absolute path-name:

- Start at the root directory (/) and work down
- Write a slash (/) after every directory name (last one is optional)
- You can use the shortcut ~ to reference the path to the home directory.

Relative path

A **relative path** is defined as the path related to the present working directly(pwd).

- It starts at your current directory and **never starts with a /**
- You can use the shortcuts for the current (.) or parent (..) directory as reference and specifies the path relative to it.

Working with files

cp	mv	rm	rmdir	ln
Copy a file	Move a file or rename it	Removes file(s)	Removes an empty directory	Creates link to a file or directory (symbolic or hard)
`% cp f1.txt f1_copy.txt`	`% mv f1_copy.txt f1.txt`	`% rm cars.csv`	`% rmdir data/`	`% ln -s cars.csv cars_sl.csv`

Display contents of a file

head	tail	more	less
Print the first N lines of a file	Print the last N lines of a file	View contents of a file	View contents of a file
% head -3 cars.csv	% tail -3 cars.csv	% more cars.csv	% less cars.csv

File Management

cat	nano	touch	wc
Concatenate files and print the contents of a file(s) to the terminal	text editor if arguments given open a file to edit/create.	Creates a new empty file	Count words, characters lines and bytes
% cat cars_aa.txt cars_bb.txt	% nano f2.txt	% touch f1.txt	% wc cars.csv

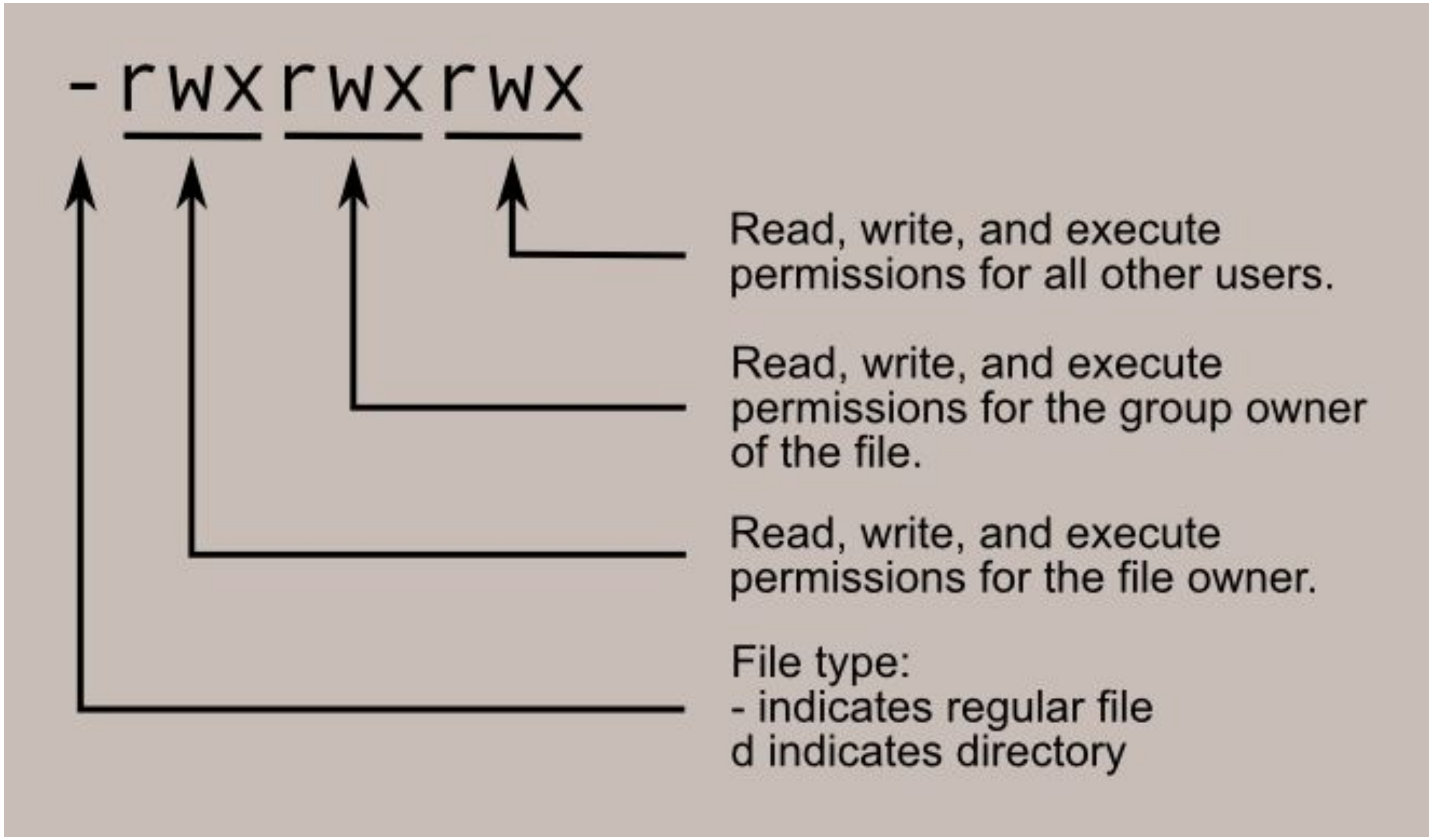
Compressed File management

gzip	gunzip	tar	zcat
Compress a file	Decompress a file	Bundle files with compression (optional)	Print the contents of a zipped file(s) to the terminal
`% gzip cars.csv`	`% gunzip *`	`% tar –cvzf cars.tgz *csv`	`% zcat f1.txt.gz`

Redirect output

>	>>	<
Will send the output of the command to a NEW file	Will APPENND the output of the command to a file	Redirect output of one command as input to another command
% ls folder1 > files.txt	% ls folder1 >> files.txt	% head -1 <(cat files.txt)

File permissions


-rwxrwxrwx
Read, write, and execute permissions for all other users.
Read, write, and execute permissions for the group owner of the file.
Read, write, and execute permissions for the file owner.
File type:
- indicates regular file
d indicates directory

Adapted from https://linuxcommand.org/lc3_lts0090.php

Managing permissions

- To display information about the permissions of a file we use **ls -l**

```
% ls -l cars.tgz
-rwxr-xr-x 1 user  group file_size day month  year cars.tgz
```

- To change the permissions we use the **chmod** command.
- There are two ways of using chmod: the symbolic and the absolute.

Symbolic

- u, g, o, and a
- + (to add)
- - (to remove)
- = (to set)

```
% chmod u = rwx,go-wx file.txt
```

Absolute

- one digit from 0-7 per user type (u,g,o)
- 0: no permission
- 7: all the permissions

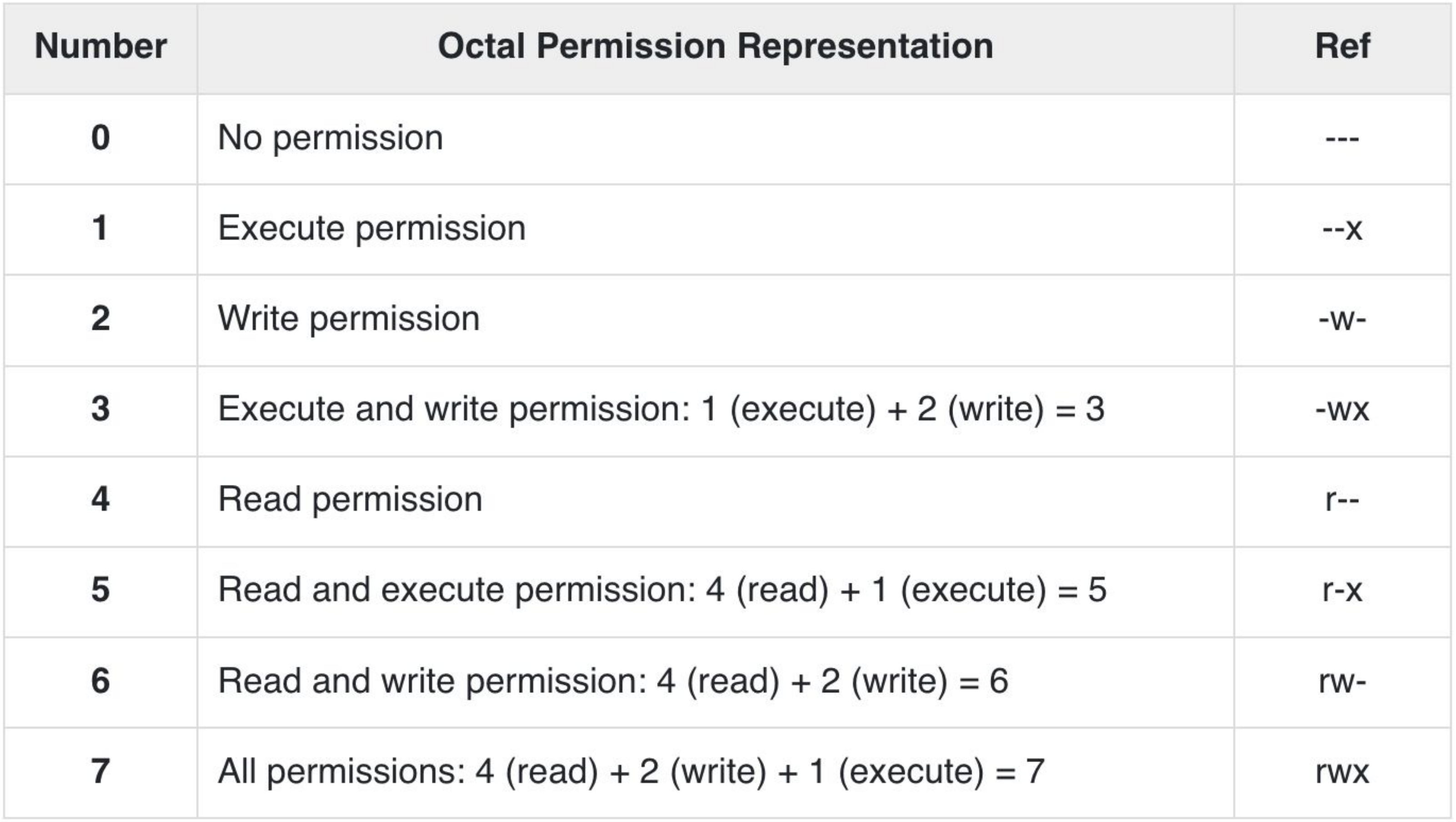
```
% chmod 744 file.txt
```

chmod

Change file(s) permissions

```
% chmod o-x
cars.csv
```

Absolute permissions



Number	Octal Permission Representation	Ref
0	No permission	---
1	Execute permission	--x
2	Write permission	-w-
3	Execute and write permission: 1 (execute) + 2 (write) = 3	-wx
4	Read permission	r--
5	Read and execute permission: 4 (read) + 1 (execute) = 5	r-x
6	Read and write permission: 4 (read) + 2 (write) = 6	rw-
7	All permissions: 4 (read) + 2 (write) + 1 (execute) = 7	rwx

https://www.tutorialspoint.com/unix/unix-file-permission.htm

Hands on 1

1. Go to the exercises directory inside the Intro to Unix folder you downloaded.
2. Create a directory called folder1 under data/ho1
3. Access the directory you just created
4. Create two files: f1.txt and .f2.txt
5. Write the numbers from 1 to 10 in f1.txt (one number per line)
6. Write the following sequence in .f2.txt (one letter per line)
   - **a a b b b c c c c d d d d d**
7. List all the contents of the directory (including .f2.txt) – hint look at the manual of `ls`
8. Change the name of .f2.txt to f2.txt
9. Write the first 10 lines of f1.txt and all the lines in f2.txt to a new file f3.txt
10. Change the permissions of f1.txt so that only the user can read and write the file
11. Count the number of lines in file f3.txt
12. Go back to the data directory and create a symbolic link to folder1

Part III: Text processing

Workshop outline

3

Text processing
Pipes
Hands on 2 exercise

Pipes

- A way to connect the end of something with the start of something else.
- Pipes will take the output of a command and give it to the following command as input.
- Pipes are very useful for text processing and filtering.
- They are specified with the control operator “ | ”

```
% cat cars.csv | head -10
```

Text processing commands

cut	paste	sort	uniq
Cut textfiles on specific columns	Paste two files column-wise	Order contents of file	Get unique entries
`% cut –f1 happiness.complete.tsv > col1.txt`	`% paste col1.txt happiness.complete.tsv`	`% sort happiness.dup.csv`	`% sort happiness.dup.csv | uniq -c`

Pattern matching with grep

grep

Search a pattern in a file

```
% grep Male
happiness.csv
```

```
Country Gender Mean
N=
AT Male 7.3 471
AT Female 7.3 570
AT Both 7.3 1041
BE Male 7.8 468
BE Female 7.8 542
BE Both 7.8 1010
BG Male 5.8 416
BG Female 5.8 555
BG Both 5.8 971
```

Some useful options:

- -v (reverse)
- -i (case insensitive)
- -c (outputs the count)
- -E (Regular expressions)
- -f (from file)
- -w (the exact word)

Some pattern hacks:

- ^ (line starts with)
- $ (line ends with)

Examples

- All lines that start with a letter

```
% grep ^S countries.txt
```

- Lines that do not start with a letter

```
% grep -v ^S countries.txt
```

- Lines with a country from the list

```
% grep -f countries.txt happiness.complete.csv
```

Pattern substitution with sed

Command or streamline editor with multiple text processing functionalities.

sed

Search a pattern in a file and substitutes with another

```
% sed s/Male/M/g
happiness.csv
```

> Basic syntax to replace a pattern:
sed ‘s/*search*/*replace*/’ file

- /g – replace all occurrences
- /1,/2,… - specifying which occurrence to replace
- /I – Ignore case

> Sed can also delete lines
sed ‘*n*d’ file

Options

- -e to run multiple commands

```
% sed -e 's/a/A/' -e 's/b/B/' file.txt
```

Examples

- Delete the first line

```
% ls -l | sed 1d
```

- Replace capital A and B for lowercase a and b

```
% sed -e 's/A/a/g' -e  's/B/b/g' happiness.complete.txt | head
```

- Convert csv to tab separated

```
% sed 's/,/\t/g' happiness.csv | head
```

Hands on 2

1. Go to the directory data/ho2 and list the files in it in long format.
2. Count how many lines start with a "," in the file happiness.csv
3. Convert the file happiness.complete.csv into a tab-delimited file and store it as happiness.complete.tsv
4. Using the file happiness.complete.tsv
   a. Count how many unique countries are listed
   b. Count how many entries of each gender are
   c. Replace all spaces with "_" within the same file
   d. Replace "**Female**" for "**F**", "Male for "**M**" and "**Both**" for **B** and look at the first 10 lines
   e. Write a new file with all the "**Both**" entries from the countries in the file countries.txt

Part IV: UNIX variables, accessing a server and transferring files

Workshop outline

Variables in UNIX
How to connect to a server
Running and monitoring jobs
How to copy files to and from a server

Variables

- A variable is a character string to which we assign a value.
- Used to store information
  - number, text, file name, etc
- The variable name can only contain:
  - Letters (a to z or A to Z)
  - Numbers (0 to 9) *not at the beginning
  - Underscore (“_”)

Defining variables

- Variables are defined as:

```
% variable_name=variable_value
```

```
% NAME="Zara Ali"

% VAR1="Zara Ali"
% VAR2=100
```

- Variables of this type are called **scalar variables**. A scalar variable can hold only one value at a time.

Access variables

- To access the value stored in a variable, prefix its name with the dollar sign (**$**)

```
% NAME="Zara Ali"
%  echo $NAME
```

- You can access variables inside a string (“”)

```
% echo “My name is $NAME”
```

- You can use variables as arguments to commands:

```
% data_dir="exercises/data"
% cd $data_dir
```

echo

Prints something to the terminal (stdout)

```
% echo “Hello World”
```

Types of variables

- When the shell is running, 3 types of variables are present:

`Local`	`Environment`	`Shell`
Variable that is present within the current instance of the shell. It is not available to programs that are started by the shell. They are set at the command prompt.	Available to any child process of the shell. Some programs need environment variables in order to function correctly.	A special variable that is set by the shell and is required by the shell in order to function correctly.

Shell variables

- Shell environment variables required by the shell to function.

`$USER`	`$HOME`	`$PATH`	`$PWD`
Stores the name of the current user	Has the path to the user's home	Contains all the directories where executable files are stored	Contains the path of the current directory

Environment variables

- Variables that apply to both the current shell and to any subshells that it creates

```
% export MY_NAME=Georgette

% echo $MY_NAME
```

Local variables

- Are only available to the current process (current shell, current script, etc.)
- They disappear when the process is done

```
% MY_NAME_LOCAL=Georgette

% echo $MY_NAME_LOCAL
```

Environment vs local variables

```
% export MY_NAME=LARISA
% MY_NAME_LOCAL=larisa
% nano my_name.sh
```

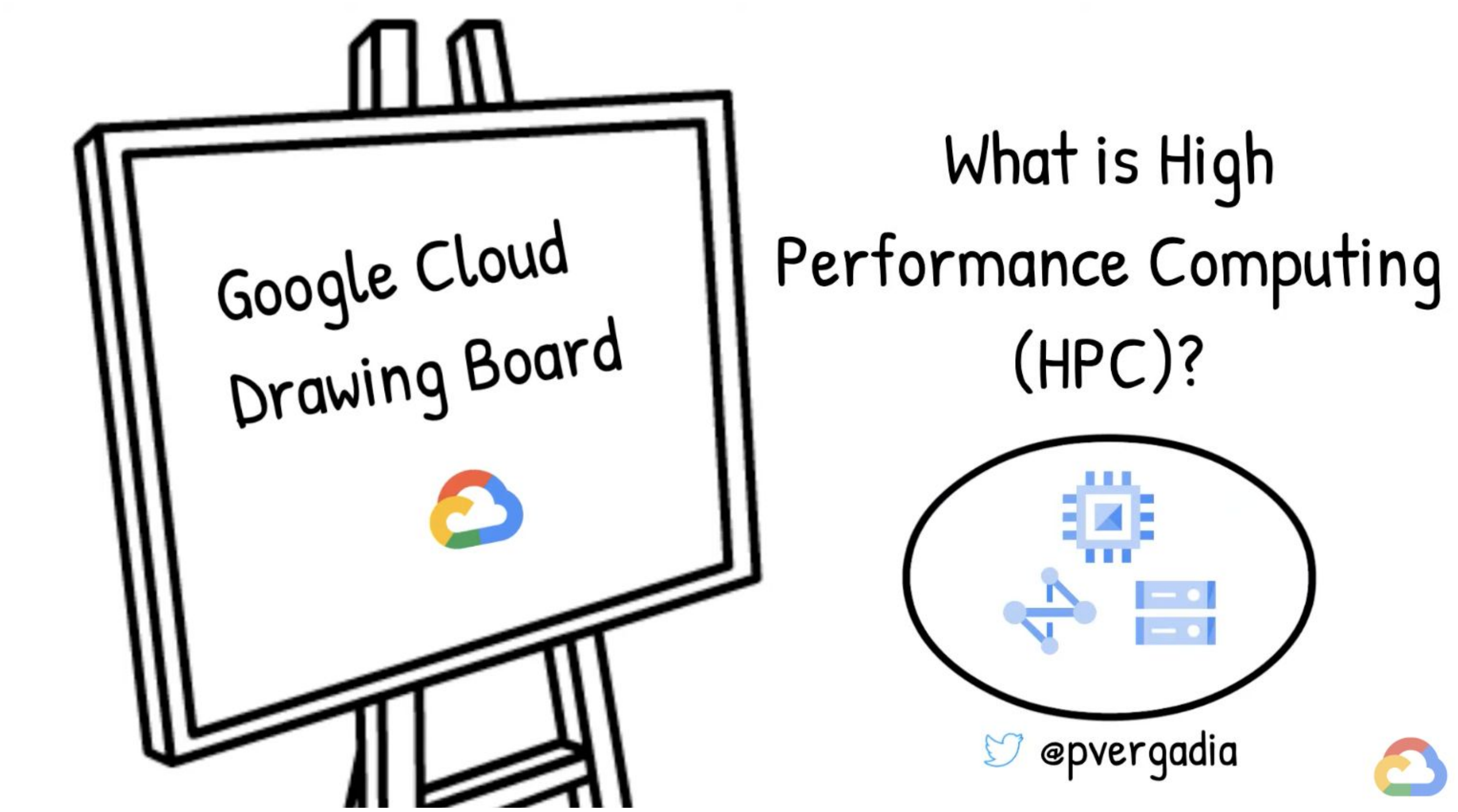
```
#!/bin/sh
echo "My name is ${MY_NAME}"
echo "My name is ${MY_NAME_LOCAL}"
```

```
% chmod u+x my_name.sh
% ./my_name.sh
```

Variables

- **Shell variables** are needed for the correct functioning of the shell. Be careful about creating a variable with the same name (in uppercase letters).
- **Environment variables** only apply to the current shell and subprocesses (scripts, programs, etc), when you open a new shell it will no longer exist. They are rarely used.
- **Local variables** exist only in the context that you created them. Useful for bash scripts to make it look more readable and when you need to use something multiple times in the same shell.

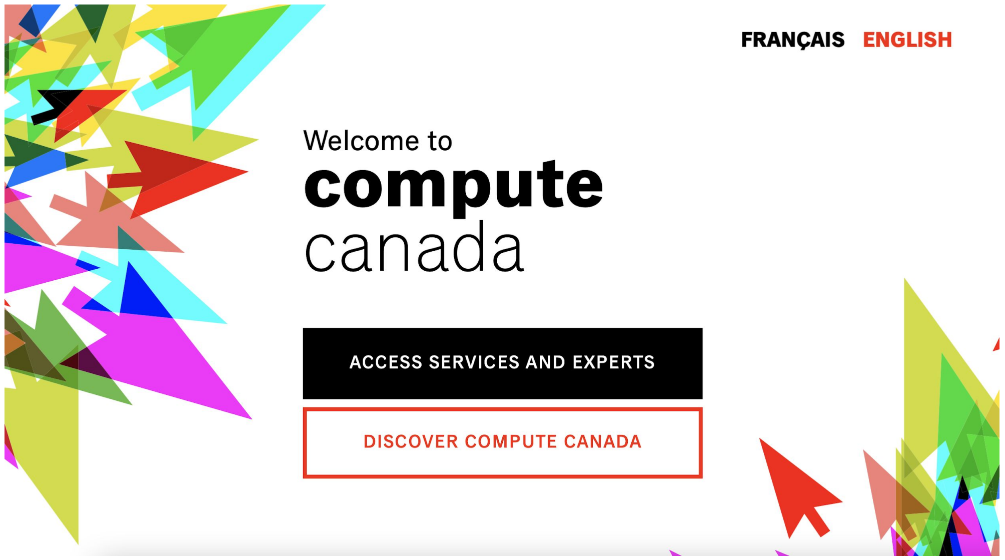
HPC servers


Google Cloud Drawing Board
What is High Performance Computing (HPC)?
@pvergadia

https://www.youtube.com/watch?v=nIBu1EFYmBU

Academic resources

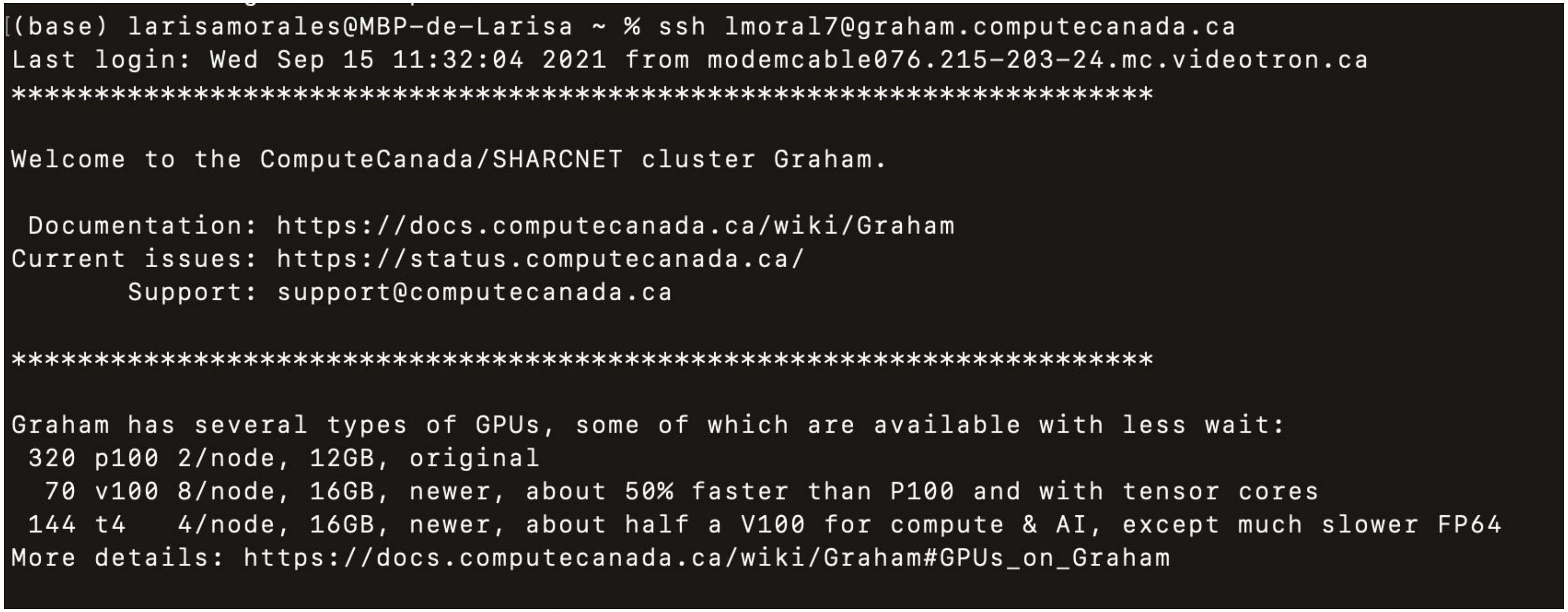
- General purpose clusters
  - Beluga
  - Graham
  - Cedar
  - Narval
- Large parallel jobs
  - Niagara
- GPU cluster
  - Helios
- Cloud computing service
- Storage
  - Nextcloud
- File transfer
  - Globus
- Database servers



https://www.computecanada.ca/research-portal/accessing-resources/available-resources/

Connect to a cluster

```
ssh user@cluster.computecanada.ca
```



```
(base) larisamorales@MBP-de-Larisa ~ % ssh lmoral7@graham.computecanada.ca
Last login: Wed Sep 15 11:32:04 2021 from modemcable076.215-203-24.mc.videotron.ca
*********************************************************************

Welcome to the ComputeCanada/SHARCNET cluster Graham.

 Documentation: https://docs.computecanada.ca/wiki/Graham
Current issues: https://status.computecanada.ca/
       Support: support@computecanada.ca

*********************************************************************

Graham has several types of GPUs, some of which are available with less wait:
 320 p100 2/node, 12GB, original
  70 v100 8/node, 16GB, newer, about 50% faster than P100 and with tensor cores
 144 t4   4/node, 16GB, newer, about half a V100 for compute & AI, except much slower FP64
More details: https://docs.computecanada.ca/wiki/Graham#GPUs_on_Graham
```

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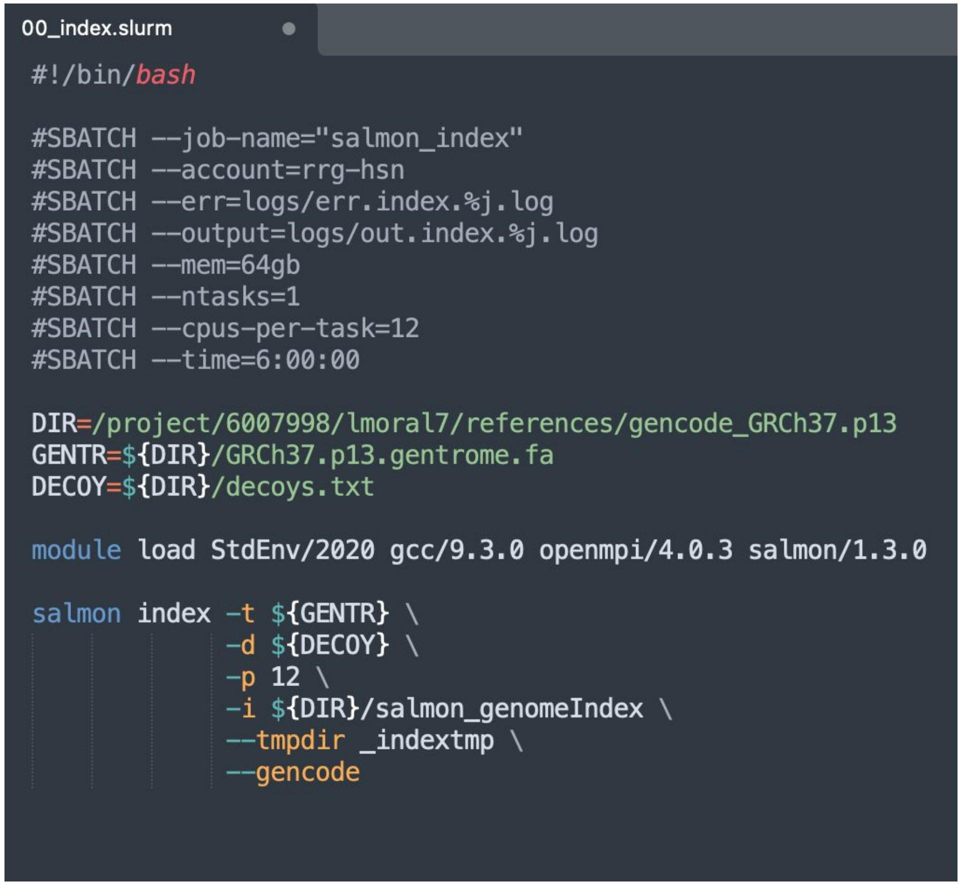
Jobs

The clusters in Compute Canada use the SLURM workload manager to handle to submissions and monitoring.



00_index.slurm

```
#!/bin/bash

#SBATCH --job-name="salmon_index"
#SBATCH --account=rrg-hsn
#SBATCH --err=logs/err.index.%j.log
#SBATCH --output=logs/out.index.%j.log
#SBATCH --mem=64gb
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=12
#SBATCH --time=6:00:00

DIR=/project/6007998/lmoral7/references/gencode_GRCh37.p13
GENTR=${DIR}/GRCh37.p13.gentrome.fa
DECOY=${DIR}/decoys.txt

module load StdEnv/2020 gcc/9.3.0 openmpi/4.0.3 salmon/1.3.0

salmon index -t ${GENTR} \
             -d ${DECOY} \
             -p 12 \
             -i ${DIR}/salmon_genomeIndex \
             --tmpdir _indextmp \
             --gencode
```

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Job submission and monitoring

sbatch job_script.slurm	Submit a job using a job script
squeue -u ${USER}	List all the processes of $USER
scancel [PID]	Cancel a process using its process ID (PID)
scancel -u ${USER}	Cancel all processes that belong to $USER

One way to transfer files to and from a server

scp

copies files between hosts on a network

```
% scp [source] [target]
```

We need to tell scp to connect to the source/target computer and where to find the file(s)

```
user@cluster.computecanada.ca:[absolute path to file(s)]
```

- Not needed for the computer you are running it from.

```
% scp gfemer@narval.computecanada.ca:/home/gfemer/storage/testcopyfile.txt .
```

```
% scp mytestscript.sh gfemer@narval.computecanada.ca:/home/gfemer/storage/
```

In summary

- HPC can help solve problems that your personal computer could never do or would take too long
- It can reduce the computing time by running jobs in parallel
- As part of McGill you can have access to Compute Canada's resources.
- Processes run as jobs that need to be submitted with a script
- You can transfer files to and from a server using scp.

What we have learned

1

Introduction to the UNIX operating system
Files and processes
Directory Structure
The Terminal

2

Basic Commands
Directory Management
File Management
Redirecting output
File permissions

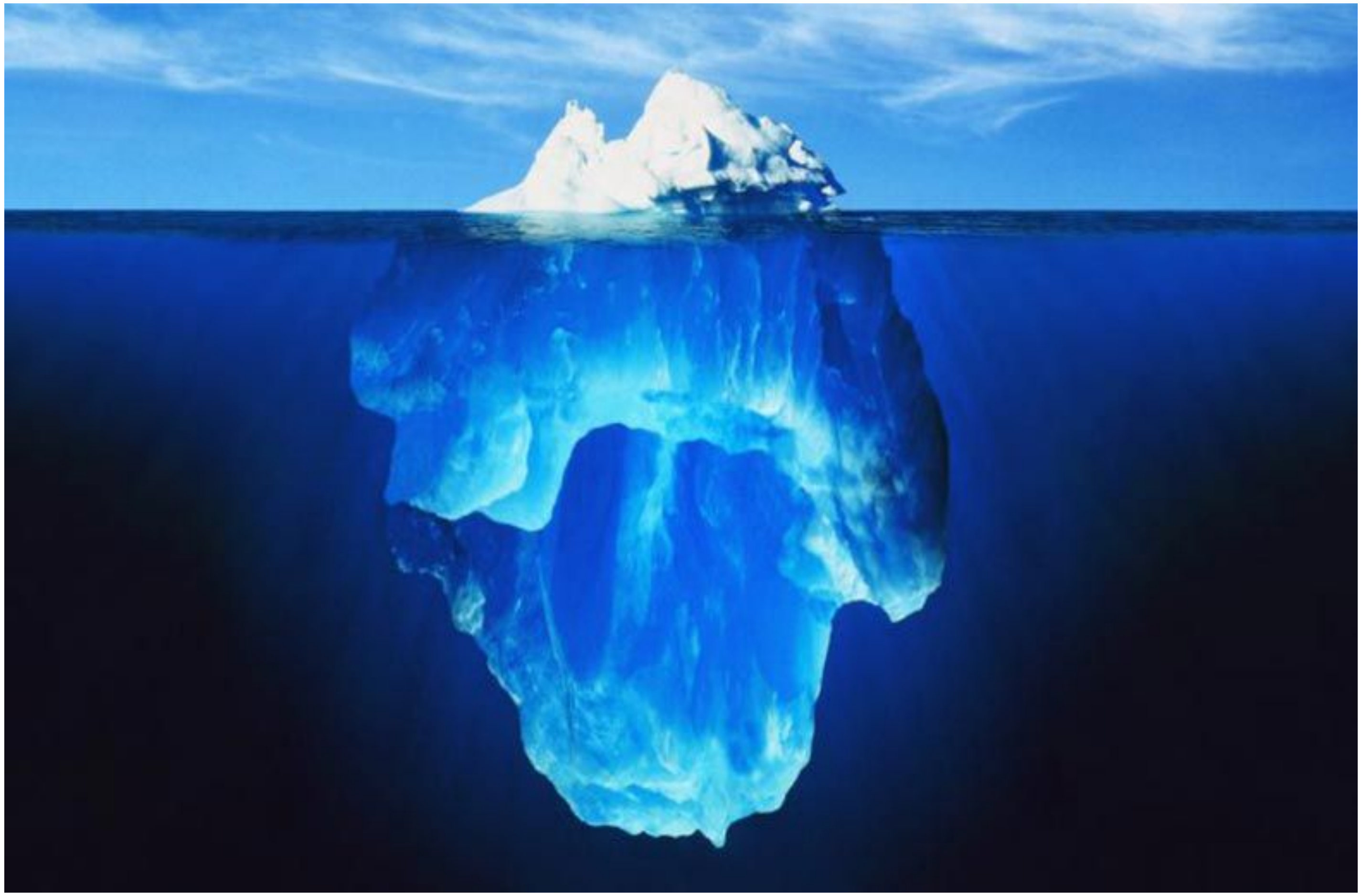
3

Text processing
Pipes

4

Variables
Connecting to a remote server
How to transfer files to and from a server

This is really just the tip of the iceberg!



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Big thanks to:

- MiCM team
  - MiCM Student Society
  - Prof. Guillaume Bourque
  - Prof. Celia Greenwood

Thanks for your attention!

Keep an eye for the workshops offered by the MiCM!

workshop-micm@mcgill.ca
https://www.mcgill.ca/micm/

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Datasets references

Hands on 1 – Cars dataset
https://perso.telecom-paristech.fr/eagan/class/igr204/datasets
Hands on 2 – Happiness surveys dataset
https://perso.telecom-paristech.fr/eagan/class/igr204/datasets