

Summer Particle Astrophysics Workshop 2022: Introduction to Unix Command Line Interface (CLI) and tools for scientific computing

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May 3, 2022

Most of these slides were made for the 2020 McGill Physics Hackathon Coding workshops by Marcus Merryfield (MM) & Laurent MacKay (LM). And 2021 slides from Sabrina Berger (McGill).



About Me



- Completed Undergrad in Honours Experimental Physics from Carleton University (2019)
 - Bachelors Thesis project on measuring Cherenkov Radiation from DEAP-3600 Acrylic
- Completed Master's Degree in Particle Physics from Carleton University (2021)
 - Master's Thesis project was on building a small-scale R&D liquid argon detector using Silicon Photomultipliers for readout (Argon-1)
 - Also did work on DEAP-3600 data analysis and R&D for future dark matter detectors (ARGO)
- Currently finishing first year of PhD at McGill University working on nEXO photodetector R&D and the Light-only-liquid Xenon detector (LoLX)
 - Main research focus is on light readout from LXe detectors, signal analysis, and studying background rejection techniques for future LXe detectors
- Checkout my personal website for my full CV and information on research!
www.davidgallacherphysics.com

Workshop Outline

Part 1: Learn the basics of the command line (CLI)

- What is Linux?
- Tutorial 1: Navigating the Filesystem
- Tutorial 2: File Permissions
- Tutorial 3: The Builtin Software Library

Part 2: Shell Scripting

- What is a shell?
- Tutorial 1: Your shell profile
- Tutorial 2: Using shell scripts
- Tutorial 3: ssh

Part 3: Containers (Time Permitting)

- What is a container?
- Tutorial 1: Using a container

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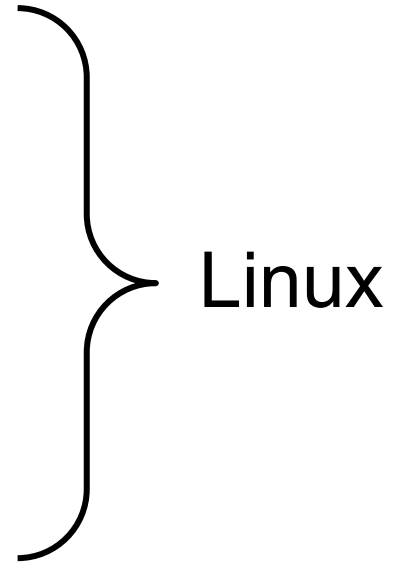
- What is a shell?
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Part 3: Containers (Time Permitting)

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What is Linux?

- Collection of Open Source Unix-like Operating Systems
 - Linux → Linux Is Not UNIX
- Unix Filesystem
 - Everything is a file (Everything)
 - Every file has a place. You don't have to put it there, but you should.
- Large library of software tools
- A shell scripting environment
 - Navigate the filesystem
 - Combine the software tools to accomplish complex tasks



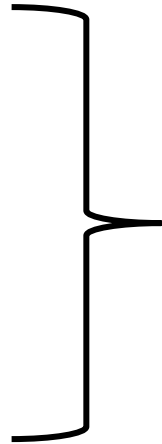
What is Linux?

- Collection of open source unix-like operating systems
 - Linux → Linux Is Not UNIX



Linux Developer: Linus Torvalds

- Software Library
- Kernel
- UNIX Filesystem



Linux Distribution (Ubuntu, Fedora, Debian, Arch,...)

Why you should use Linux?

1. Its free and open source!
 - a. Many flavors (distributions) to choose from, almost all of them are free.
 - b. Ubuntu - Good all around option with long-term support options, CentOS/RHL for scientific computing, Lubuntu - Lightweight Ubuntu version, great for bringing old PC's to life
2. When it works, it works!
 - a. Can be left running for months/years without any issues.
 - b. No need to reboot after installing software!
3. Runs on any hardware
 - a. Can run full-scale desktop Linux options or ultra-lightweight linux for single-board-computers (SBCs) like Raspberry PI

The Most Useful Linux Troubleshooting Advice

Google:

Error Message/file + [Linux Distribution Name]

Check out the top 2-3 results, see what they agree on.

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Tutorial 1: Navigating the Filesystem

1. `Open Terminal (Mac) or Ctrl + Alt +T (Windows/Ubuntu)`
 - a. It may look like nothing, but it can do almost everything.
2. Check out your home folder

`ls`

(Lists the contents of your home folder)

`ls -a`

(Includes “hidden” files, i.e., files whose name starts with ‘.’)

(Files and Directories will probably be colored differently)

Tutorial 1: Navigating the Filesystem

1. Move into a new directory (e.g. Downloads)
`cd Downloads`

```
lmackay@ubuntu:~$ cd Downloads/  
lmackay@ubuntu:~/Downloads$ ls
```

Username

Machine name

Current folder

Tutorial 1: Navigating the Filesystem

1. Move into a new directory (e.g. Downloads)

```
cd Downloads
```

```
lmackay@ubuntu:~$ cd Downloads/  
lmackay@ubuntu:~/Downloads$ ls
```

2. Is there anything there?

```
ls
```

(maybe not)

```
ls -a
```

(you will notice '.' and '..')

3. What does .. mean?

```
cd ..
```

4. `pwd` (what is the present working directory?)

Linux Shorthand:

. → Current Directory

.. → Parent Director

~ → Home Folder

Tutorial 1: Navigating the Filesystem

1. Try using an absolute file path
`cd /home/[username]/Downloads`
2. You can use ~ as a shortcut for your home folder
`cd ~/Documents`

Let's start playing around with files:

1. Copy a file into your Documents folder (commands are equivalent)
absolute paths: `cp /home/[username]/.bashrc /home/[username]/Documents/`
relative paths: `cp ../.bashrc ./`
2. You can copy a file to a new filename
`cp ~/.bashrc ./dummyfile`

Tutorial 1: Navigating the Filesystem

1. Make a new directory:

```
mkdir dummydir
```

2. Move your dummyfile into dummydir:

```
mv dummyfile dummydir
```

3. Check that it worked:

```
ls dummyfile
```

(should return ls: cannot access 'dummyfile': No such file or directory)

```
ls dummyfolder/dummyfile
```

(should not give an error)

Tutorial 1: Navigating the Filesystem

Let's make a sample Python file with *nano* (*also check out vim and emacs*).

1. Open your file (notice the .py ending): `nano test.py`
2. Add some lines

```
print('Hello McDonald Institute!')
```

3. To save and exit:
 - a. Ctrl+x - To exit
 - b. Then type "y" to save changes ("n" to not save")
4. Run your python file: `python test.py`

Tutorial 1: Navigating the Filesystem

Let's clean up after ourselves

1. `rm ./bashrc`
(deletes the `.bashrc` file we copied into Documents)
2. `rm -r dummydir`
(recursively deletes anything inside `dummydir` and then deletes `dummydir`)

Tutorial 1: Navigating the Filesystem

Summary of Commands:

1. `ls` lists contents of current directory
2. `ls /path/to/dir` lists contents of a specific directory
3. `cd /path/to/dir` changes current directory
4. `cp` copies files
5. `mv` moves/renames files/directories
6. `mkdir` makes directory
7. `rm` deletes files/directories

Specific options for all of these commands can be found using the `--help` flag

More detailed instructions can be found using `man` (e.g., try `man ls` or `man echo`)

Activity 1: Navigating the Filesystem

1. Make two directories: *testing* and *EIEIOO_Scripts*
2. Make two sample python scripts in the *testing* directory
3. Move one script to *EIEIOO_Scripts*
4. Copy the other script to *EIEIOO_Scripts*
5. Delete the *testing* folder
6. Run your python scripts

```
physuser@b77ad2eae59:~/EIEIOO_Scripts$ ls  
test.py  test2.py
```

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Tutorial 2: File Permissions

Lets have a look at the root folder again:

```
ls -l /
```

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx   1 root root      7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x   3 root root 4096 Oct 20 10:38 boot
```



What is all this stuff?

Tutorial 2: The Linux Filesystem

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x   3 root root    4096 Oct 20 10:38 boot
```



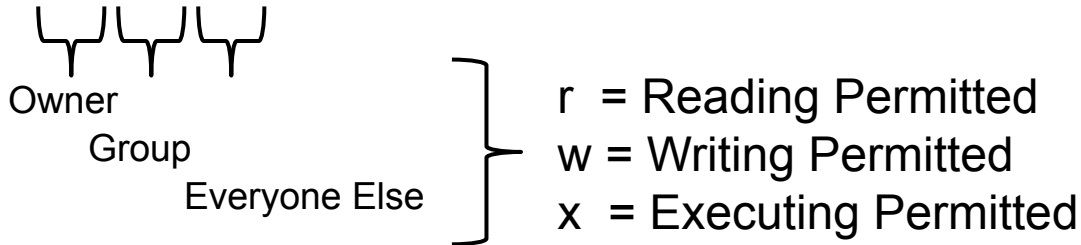
The first character tells you what type of file: - (regular file), d (directory), l (link)

Tutorial 2: File Permissions

The next nine characters gives you three different sets of “permissions” for the file

- Three different levels of control over the file

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x   3 root root    4096 Oct 20 10:38 boot
```



Tutorial 2: File Permissions

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x   3 root root    4096 Oct 20 10:38 boot
```



Number of links/directories inside a link/directory

Tutorial 2: File Permissions

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x   3 root root    4096 Oct 20 10:38 boot
```



Owner of the file

You can modify who owns a file with: `chown [username] [filename]`

Tutorial 2: File Permissions

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x   3 root root    4096 Oct 20 10:38 boot
```



Group that owns the file

You can add users to a group using: `usermod -aG [groupname] [username]` (or `chgrp -options GROUP FILE`)

Tutorial 2: File Permissions

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x    3 root root     4096 Oct 20 10:38 boot
```



Size of the file in bytes. Try using `ls -lh` for human readable sizes.

Tutorial 2: File Permissions

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x   3 root root    4096 Oct 20 10:38 boot
```


Date of last modification

Tutorial 2: File Permissions

```
lmackay@ubuntu:/$ ls -l
total 970048
lrwxrwxrwx    1 root root          7 Oct 20 10:30 bin -> usr/bin
drwxr-xr-x    3 root root    4096 Oct 20 10:38 boot
```



Filename

Tutorial 2: File Permissions

Ok so we have seen how to give ourselves ownership (`chown`) or group membership (`usermod -aG`).

What about everyone else? Can we modify the owner/group permissions?

```
chmod u=rwx,g=rx,o=r [filename]
```

u = user = owner

g = group

o = other = everyone else

Everyone can read, write, and execute: `chmod 777 <filename>`

Tutorial 2: File Permissions

Ok so we have seen how to give ourselves ownership (`chown`) or group membership (`usermod -aG`).

What about everyone else? Can we modify the owner/group permissions?

```
chmod u=rwx,g=rx,o=r [filename]
```

u = user = owner

g = group

o = other = everyone else

Different Permutations:

0 – no permission

1 – execute

2 – write

3 – write and execute

4 – read

5 – read and execute

6 – read and write

7 – read, write, and execute

Tutorial 2: File Permissions

The dangerous but useful: `chmod 777 <filename>`

Everyone can read, write, and execute this file.

Exercise 2: File Permissions

1. Change one of your sample Python files permissions so that you get the following error when you try to run it:

```
python: can't open file 'test.py': [Errno 13] Permission denied
```

2. Figure out how to successfully run it again

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Tutorial 3: The Builtin Software Library

1. Let's find where python is:

```
whereis python
```

For me, there are multiple python versions installed.

2. `cd /usr/lib/python3`

Let's check out the Python versions installed here.

Tutorial 3: The Builtin Software Library

1. Lets see how many python files there are

```
find . -name '*.py'
```

Look 'here' for files whose name matches the pattern *.py (*=wildcard)
(Ok, that's a lot of files!)

2.

```
grep -r --include '*.py' '= list()'
```

Recurse down the filesystem, looking inside files that end with .py searching for '= list()'

Tutorial 3: The Builtin Software Library

1. Now to count them up

```
grep -r --include '*.py' '= list()' | wc -l
```

The character | “pipes” the output of `grep` into `wc` which counts the number of words it is (or in this case lines due to `-l`)

2. Ok now lets try to repeat that with `my_list = []`

```
grep -r --include '*.py' '= []' | wc -l
```

You will get an error:

The `[]` characters are special and must be “escaped”

```
grep -r --include '*.py' '= \[\]' | wc -l
```

Tutorial 3: The Builtin Software Library

Great!

So how many instances did you find?

More generally, `grep` is extremely useful for finding strings (or a `RegExp`) in text files when you can't remember which file its in.

Also very useful - piping outputs into `grep`.

For example:

`Ifconfig` - Returns a long list of all your network interfaces. ('ip a' instead on some linux systems)

`Ifconfig | grep "inet"` - "|" is for "piping" the output of the left-hand side, as input into the right-hand side (Read more [here](#)), "inet" is your IP address

Tutorial 3: The Builtin Software Library

Some commands I commonly use:

`find`: find files

`grep`: search for strings/patterns inside text files

`top` or `htop` (fancy version): similar to task manager

`df -h`: check how much free disk space is available on your system

`du -h`: Check how much space is used in the current directory

Tip: Google “How to do <blank> command line linux”

Exercise 3: The Builtin Software Library

Determine how many times 'import' is used in your Python3 installation. For me, it's 18!

Lastly, what about a job I need to quit?

Ok now we started a rogue process which will never finish and will eat up our hard drive. What do we do?

Use the pid to kill the process!

```
kill 25879
```

If you do not remember the pid, use `jobs -l` to find the jobs currently running in a given shell.

Check for tasks+PIDs running on your computer with `ps -aux`, to search for a specific task, pipe to grep! `ps -aux | grep "taskname"`

```
n$ jobs -l
[1]+ 25879 Running                  while sleep 1; do
    date >> curr_time;
done &
```

Shell Scripting

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What is the shell?

We've been working in the 'terminal' or 'command-line interface' these are examples of shell programs.

Shell programs take keyboard inputs and turn them into instructions for the computer

Examples include: Mac Terminal, Windows PowerShell, Linux Terminals

Different Shell types are around: bash (Bourne again shell), csh (C-Shell), zsh (Z-shell, default on Mac)



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Tutorial 1: Shell Profiles

You may have noticed that my shell has colour highlighting and other quality of life features

Your shell has default options that you can configure.

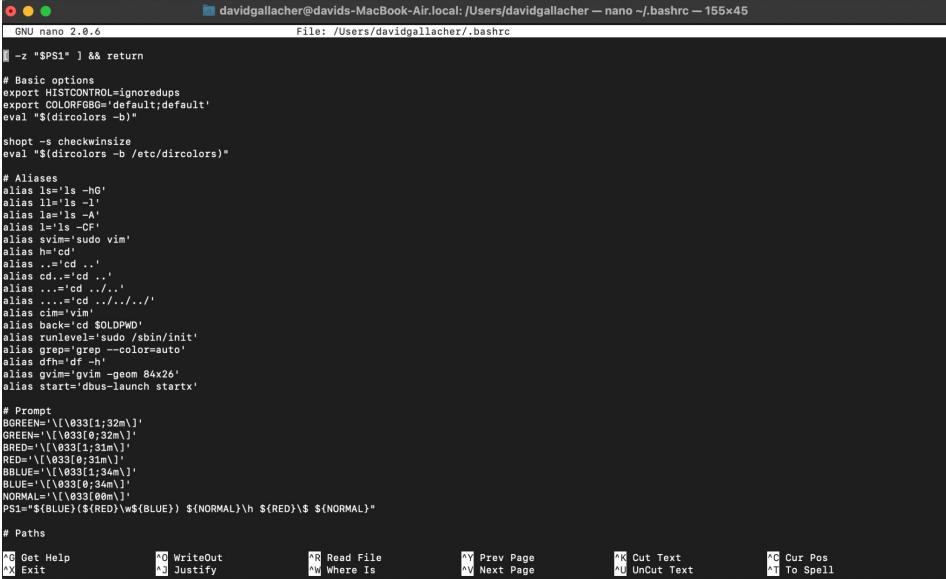
Take a look at your shell profile~

```
Nano ~/.bashrc
```

```
nano ~/.bash_profile
```

Or on Mac

```
nano ~/.zprofile or nano ~/.zshrc
```



```
GNU nano 2.0.6 File: /Users/davidgallacher/.bashrc
|-z "$PS1" ] && return

# Basic options
export HISTCONTROL=ignoredups
export COLORFGBG='default;default'
eval "$(dircolours -b)"

shopt -s checkwinsize
eval "$(dircolours -b /etc/dircolours)"

# Aliases
alias ls='ls -hG'
alias ll='ls -l'
alias la='ls -A'
alias lc='ls -CF'
alias svim='sudo vim'
alias h='cd'
alias ..='cd ..'
alias cd..'='cd ..'
alias ..='cd ../..'
alias ...='cd ../../..'
alias cim='vim'
alias back='cd $OLDPWD'
alias runlevel='sudo /sbin/init'
alias grep='grep --color=auto'
alias dfh='df -h'
alias gvim='gvim -geom 84x26'
alias start='dbus-launch startx'

# Prompt
BGREEN='\[\033[1;32m\]'
GREEN='\[\033[0;32m\]'
BRED='\[\033[1;31m\]'
RED='\[\033[0;31m\]'
BBLUE='\[\033[1;34m\]'
BLUE='\[\033[0;34m\]'
NORMAL='\[\033[00m\]'
PS1="$BBLUE)$(RED)\w$(BLUE) ${NORMAL}\h $(RED)\$ ${NORMAL}"

# Paths
^G Get Help      ^O WriteOut     ^R Read File    ^V Prev Page    ^U Cut Text
^X Exit          ^J Justify      ^W Where Is     ^N Next Page    ^_ UnCut Text
^C Cur Pos      ^T To Spell
```

Tutorial 1: Shell Profiles

Interactive shells (What happens when you open the terminal) call `~/.bashrc` before starting

This is a useful place to set any variables we may want to use in CLI, as well as calling any scripts we may want to run before starting a CLI session

Let's do an example, open your terminal and call:

```
nano ~/.bashrc
```

We will add a new variable and a print statement.

Add the following lines:

`MYVAR="Hello McDonald Institute!"` - this sets a variable within the `bashrc` script, which can be called later on

`export MYVAR` - Tells the shell to remember this variable, now we can call it from the CLI, this is now an “environment variable”

`echo $MYVAR` - “echo” prints the argument to the command line, this will print the contents of `MYVAR`

Exit and save (Ctrl+x then ‘y’)

Tutorial 1: Shell Profiles

Now we need to re-load the `~/.bashrc` script, we can either do that by opening a new terminal or by resourcing the script

```
source ~/.bashrc
```

We should see our print statement with the variable contents

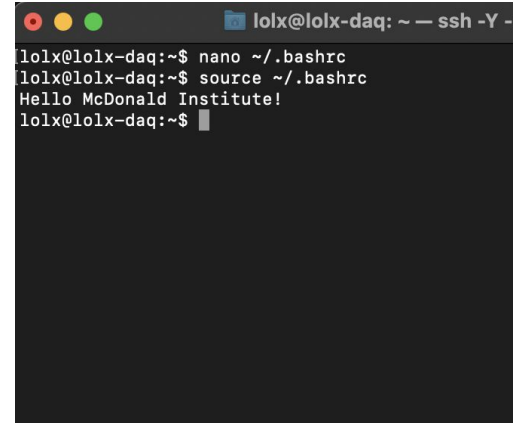
Next let's print the statement from the terminal to check if it was exported properly

```
echo $MYVAR
```

 - Print the contents of this environment variable!

Lastly we can assign “aliases” to commands, so that we can invoke them later-on. Very handy for long commands you don't want to type out!

See [here](#) for details on making aliases.



```
lolx@lolx-daq: ~ — ssh -Y -
lolx@lolx-daq:~$ nano ~/.bashrc
lolx@lolx-daq:~$ source ~/.bashrc
Hello McDonald Institute!
lolx@lolx-daq:~$
```


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Tutorial 2: Shell Scripts

We just saw our first example of a shell script, a set of command-line instructions we can call from a script instead of manually

This opens lots of doors for us!

Shell scripts typically end in “.sh” and can be called like:

```
bash myscript.sh
```

Or `sh myscript.sh`

Or `./myscript.sh` - This option requires some additional steps!

Tutorial 2: Shell Scripts

Let's make a shell script and test it out

From the terminal do:

```
nano myscript.sh
```

Let's add the following lines

```
#This script creates a variable and prints it! - Comments in Shell scripts are prepended with '#'
```

```
var=100 - Make a variable called var, and set it to 100 (Careful here, 'var = 100' returns an error!)
```

```
echo $newvar
```

Save the script and run it with `bash myscript.sh`

Tutorial 2: Shell Scripts

Now we will expand the test script to do more things

We can call programs and other commands from the shell script.

Anything you can do in the command line interface, you can do in a shell script!

Tutorial 2: Shell Scripts

We can pass arguments to our scripts as well

Bash supports up to 9 arguments directly from the command line

Let's modify our script, add the following lines:

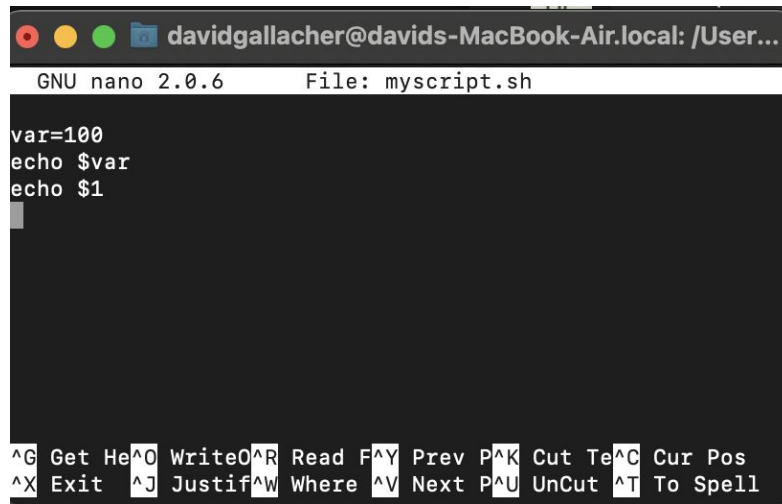
`echo $1` - This prints the first command-line argument, similarly, `$0-$9` print any other arguments.

`$0` is reserved for the script name (myscript.sh)

Save and exit, and then call the script, this time passing an argument:

```
bash myscript.sh "Hello McDonald Institute"
```

```
(base) (~) davids-MacBook-Air $ nano myscript.sh
(base) (~) davids-MacBook-Air $ bash myscript.sh "Hello McDonald Institute"
100
Hello McDonald Institute
(base) (~) davids-MacBook-Air $
```



```
GNU nano 2.0.6 File: myscript.sh
var=100
echo $var
echo $1
```

Our script so far!

Tutorial 2: Shell Scripts

Lastly, we will call python from our shell script and save the output to a variable that gets printed in a formatted message

Add the following lines to your script:

```
pythonVersion=$(python -version)
```

```
printf "The python version currently installed is : %s \n" "$pythonVersion"
```

Then we can save the file and call it again, this time we call it directly:

```
./myscript.sh "Hello McDonald Institute"
```

Tutorial 2: Shell Scripts

... Then we can save the file and call it again, this time we call it directly:

```
./myscript.sh "Hello McDonald Institute"
```

This will return an error! We need to set the file permissions to make this script “executable”, and we need to tell the shell what scripting language to use.

First, add this line to the very start of your script:

```
#!/usr/bin/env bash
```

-This is called “shebang” and tells the computer which interpreter to use to understand the instructions in the rest of the file, here we’re using bash

Now we need to make it executable:

```
chmod u+=x myscript.sh
```

Now we should be able to call it directly!

```
./myscript.sh
```

Tutorial 2: Shell Scripts

Lots of options for automating tasks in shell scripts:

Some examples that I've used in physics before:

- Script that analyzes data using a python script then sends the output to another script
- Create a for-loop in the bash script to process many data files and rename their outputs and sync to cloud
- Script that runs continuously in the background and looks for new data files being written, then analyzes them automatically
- Much more..

Lots of power in shell scripts for making your life easier!

Google is your best friend, if you're thinking of automating a task try searching “do `task` in bash script”

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Tutorial 3: SSH - The secure shell

SSH or “Secure Shell” is a network communication protocol. It allows you to obtain a virtual terminal or “shell” from a remote machine.

Using SSH you can connect to a machine with an SSH-server and run command-line-interface instructions over the network

Widely used in physics for connecting to computing clusters, remote workstations, experimental equipment etc..

SSH is an encrypted network protocol, all traffic is encrypted and secure!

Tutorial 3: SSH - The secure shell

SSH works in two parts, a client and a server

A client runs on your PC and communicates with an SSH server running on the remote machine over the network

This can be done directly in a Mac/Linux Terminal, on Windows in Powershell or by using a GUI for SSH like Putty

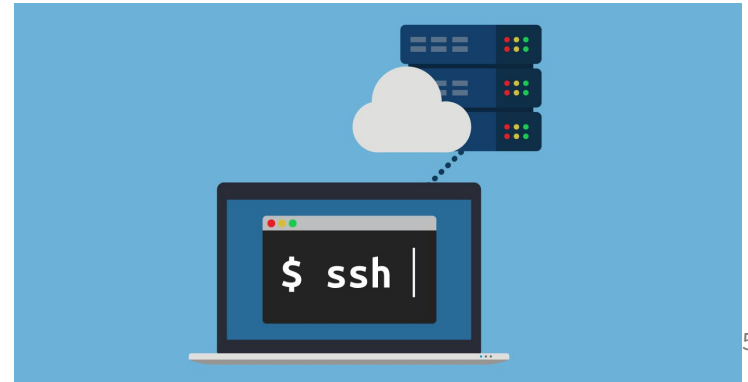
Example:

```
ssh -Y username@remote-address.com
```

Remote addresses can be IP addresses or domain names!



PuTTY



Tutorial 3: SSH - The secure shell

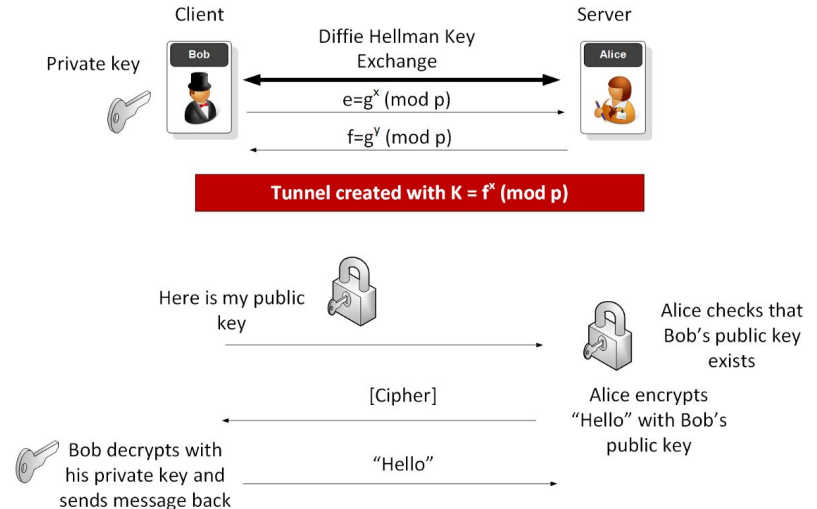
SSH requires you to log in to the target machine, this can be done in 2 ways

1. Password authentication

- You enter the password for the user you are trying to obtain a shell from
- Susceptible to attacks! Password authentication left open on a public IP can be a serious security flaw

2. Key-exchange

- You copy your “public” key to the server, which it uses to verify connections later
- For an in-depth overview of key-exchange see [this great video!](#)



Tutorial 3:

Now we will make an ssh public key, copy it to a remote server and establish a connection

Let's first check if a key exists by running in the terminal:

```
ls -la ~/.ssh/
```

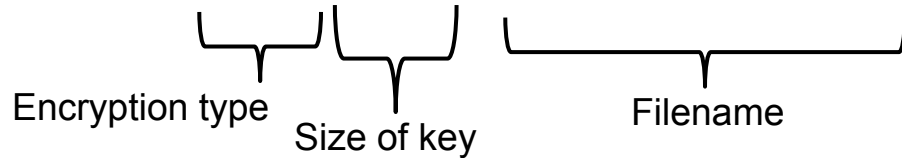
```
(base) (~) dauids-Air $ ls -la ~/.ssh/
total 64
drwxr-xr-x  9 davidgallacher  staff  288B 17 Mar 14:11 .
drwxr-xr-x+ 74 davidgallacher  staff  2.3K 29 Apr 16:09 ..
-rw-r--r--  1 davidgallacher  staff  416B 17 Sep  2021 config
-rw-----  1 davidgallacher  staff  2.6K 20 Jul  2021 id_rsa
-rw-r--r--  1 davidgallacher  staff  593B 20 Jul  2021 id_rsa.pub
-rw-r--r--  1 davidgallacher  staff  9.2K 25 Mar 16:51 known_hosts
drwx-----  2 davidgallacher  staff   64B 28 Apr 18:11 socket
-rw-----  1 davidgallacher  staff  3.4K 16 Sep  2021 test-key
-rw-----  1 davidgallacher  staff  754B 13 Sep  2021 test-key.pub
(base) (~) dauids-Air $
```

I already have two keys, “id_rsa” (private and public) and “test-key”

Tutorial 3: SSH - The secure shell

Let's make a new key:

```
ssh-keygen -t rsa -b 4096 -f "~/.ssh/my_new_key"
```



This will prompt you for a password for your key, you can leave it blank (Hit enter) or make a password. **Some servers require you to have password protected ssh keys!**

You will see a random-art image representing your new key

```
[Enter passphrase (empty for no passphrase):
[Enter same passphrase again:
Your identification has been saved in my_new_key.
Your public key has been saved in my_new_key.pub.
The key fingerprint is:
SHA256:0ejmxJWuLLR1H/xY9kgZ0rA1RDvuKHPNj7E0K75ipIA davidga
The key's randomart image is:
+----[RSA 4096]-----+
|
|  oo
|  o..
|  o*
| . +o.o
| . S...o
|E oo.o.*o =
| . + oB.=.B o
| . =.= oo=0 .
| . **o..+ .
+----[SHA256]-----+
```

Tutorial 3: SSH - The secure shell

Now that we have created an ssh key, we can connect to a remote server without password authentication

But first the server needs to know our key!

Two ways of doing this:

1. For some systems that have password authentication + key exchange options
 - `ssh-copyid -i "~/ssh/my_new_key.pub" user@remote-address` - copies our public key to the server to store, need passwords!
2. Other systems will require you to send your plaintext public key (Contents of `~/ssh/my_new_key.pub`) to the system administrators to store manually. No password access to the server.

Lots of power to simplify things, including using the SSH config file, [see here](#) for more information on setting up your own configurations.

Tutorial 3: SSH - The secure shell

What if we need to copy files that we made on a remote machine to a local machine?

Here are two options:

`scp` - ‘Secure copy’, copy data from a remote location to local, or vice-versa, is encrypted by default

- Can specify address and port for transfer
- Example to copy from remote to a local directory, through port ‘2205’ on remote host
 - `scp -P 2205 username@remote_host:/path/to/file/to/copy /path/to/local/directory/to/store`
- Example to copy a local file to a remote directory, through port ‘2205’ on remote host
 - `scp -P 2205 /path/to/local/file/to/copy/file.txt username@remote_host:/path/to/remote/directory/to/store`

`rsync` - “Remote Sync”, tool for copying files, or synchronizing a remote directory to a local one

- Faster than `scp`, but not encrypted by default (Can encrypt with an `ssh` tunnel)
- Example to sync two directories between remote and local
 - `rsync -avrtz username@remote_host:/home/username/dir1 /place/to/sync/on/local/machine`

Google and GNU/Linux manual pages are your best friends when using command-line tools!

Tutorial 3: SSH - The secure shell

Lots of doors open with ssh connections

- Running remote commands on other PCs
- Connecting to remote instruments to control (Raspberry Pi's and other SBC's are ideal for this!)
- Connect to computing clusters to perform large scale computing tasks (Such as the Digital Research Alliance clusters, formerly Compute Canada)
- Access a computer on your home network from the office, or vice-versa, to work remotely

Containers

Workshop Outline

Part 1: Learn the basics of the command line (CLI)

- What is Linux?
- Tutorial 1: Navigating the Filesystem
- Tutorial 2: File Permissions
- Tutorial 3: The Builtin Software Library

Part 2: Shell Scripting

- What is a shell?
- Tutorial 1: Your shell profile
- Tutorial 2: Using shell scripts
- Tutorial 3: ssh

Part 3: Containers (Time Permitting)

- **What is a container?**
- Tutorial 1: Using a container

What is a container?

Containers are software development tools that are growing in usage in scientific research

Containers package together the application with the required libraries and dependencies to run on any operating system or hardware

Similar to virtual machines (VMs) but differ in important ways

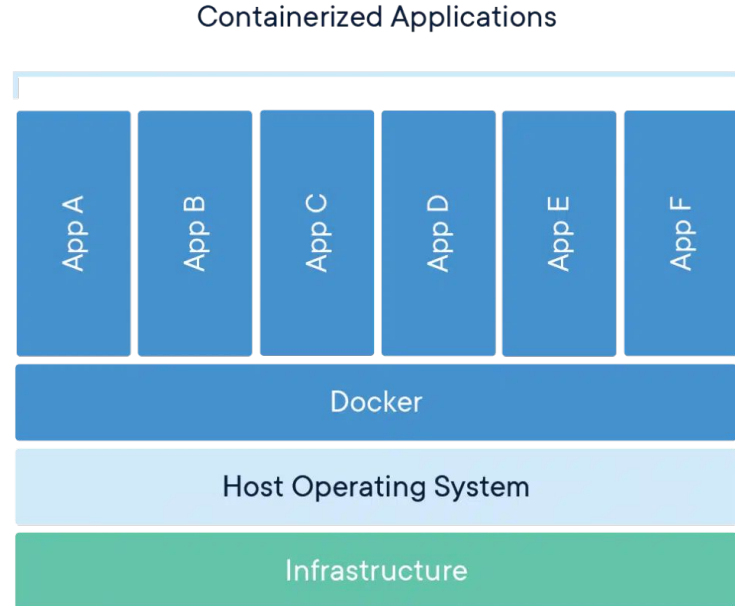


Image from Docker ([link](#))

Container vs VM

VM's are instances of operating systems that run separate from the main OS on the hardware

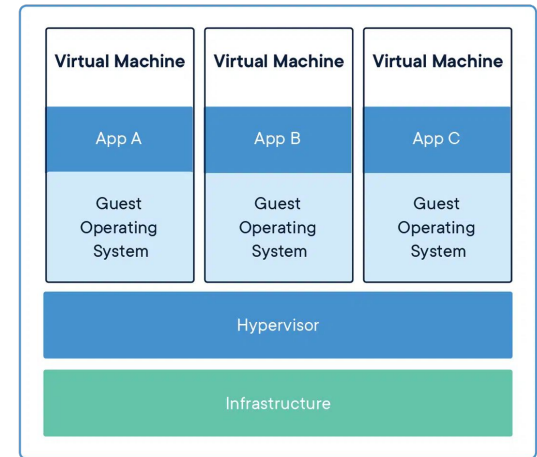
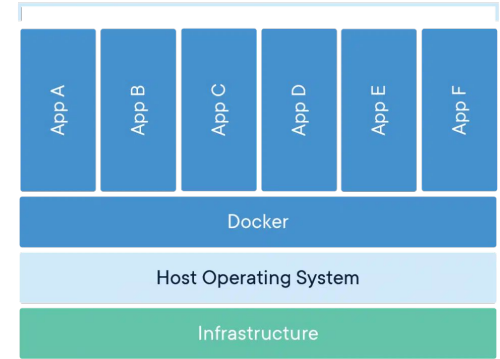
For example, you can run a Windows VM on a Mac in order to run Windows specific software

VM's are large (Several GB's) and contain everything required for an operating system to work

Containers are lightweight (MB's) and contain only what's required for a specific application to run.

Containers run like applications on the host OS and virtualize resources

Containerized Applications



Images from Docker ([link](#))

Containers for Scientific Computing

Containers have a lot of value in scientific computing, here are some common considerations for scientific software

- Research often uses custom software packages where scientists are developers
- Creating cross-platform reliable software with idiosyncratic differences from different compiler versions, hardware and OS's is a challenge
- Usability is a major consideration for scientific software, we need tools that will work reliably with minimal upkeep, so we can spend our time doing science instead of solving software related bugs
- Reproducibility, Some simulation software (GEANT4 or ROOT for example) will have different implementations of **physics**, depending on what version you use! So we need to specify exact versions for use in order to reproduce our results

Containers can address all of these points!

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- Tutorial 3: ssh

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- Tutorial 1: Using a container

Tutorial 1: Using a container

The most popular container engine is Docker

We will use this for the tutorial, you can download docker here: <https://www.docker.com/get-started/>

We will follow the sample tutorial here ([link](#))

This will also allow us to test out our command-line interface techniques



Tutorial 1: Using a container

To run our first container, we simply type:

```
docker run hello-world
```

```
(base) (~) davids-Air $ docker run hello-world
Unable to find image 'hello-world:latest' locally
latest: Pulling from library/hello-world
7050e35b49f5: Pull complete
Digest: sha256:10d7d58d5ebd2a652f4d93fdd86da8f265f5318c6a73cc5b6a9798ff6d2b2e67
Status: Downloaded newer image for hello-world:latest

Hello from Docker!
This message shows that your installation appears to be working correctly.

To generate this message, Docker took the following steps:
 1. The Docker client contacted the Docker daemon.
 2. The Docker daemon pulled the "hello-world" image from the Docker Hub.
    (arm64v8)
 3. The Docker daemon created a new container from that image which runs the
    executable that produces the output you are currently reading.
 4. The Docker daemon streamed that output to the Docker client, which sent it
    to your terminal.

To try something more ambitious, you can run an Ubuntu container with:
$ docker run -it ubuntu bash

Share images, automate workflows, and more with a free Docker ID:
https://hub.docker.com/

For more examples and ideas, visit:
https://docs.docker.com/get-started/
```



Tutorial 1: Using a container

To run our first container, we simply type:

```
docker run hello-world
```

```
(base) (~) davids-Air $ docker run hello-world
Unable to find image 'hello-world:latest' locally
latest: Pulling from library/hello-world
7050e35b49f5: Pull complete
Digest: sha256:10d7d58d5ebd2a652f4d93fdd86da8f265f5318c6a73cc5b6a9798ff6d2b2e67
Status: Downloaded newer image for hello-world:latest
```

```
Hello from Docker!
This message shows that your installation appears to be working correctly.
```

To generate this message, Docker took the following steps:

1. The Docker client contacted the Docker daemon.
2. The Docker daemon pulled the "hello-world" image from the Docker Hub.
(arm64v8)
3. The Docker daemon created a new container from that image which runs the executable that produces the output you are currently reading.
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To try something more ambitious, you can run an Ubuntu container with:
\$ docker run -it ubuntu bash

Share images, automate workflows, and more with a free Docker ID:
<https://hub.docker.com/>

For more examples and ideas, visit:
<https://docs.docker.com/get-started/>



Since we didn't have "hello-world" image installed, docker downloaded it for us before running as a container

Tutorial 1: Using a container

Now we will install another container from Docker's repository of containers (See [here](#) for more containers)



```
docker pull alpine
```

Then we can see all the images we've installed from docker

```
docker images
```

```
(base) (~) davids-Air $ docker pull alpine
Using default tag: latest
latest: Pulling from library/alpine
9981e73032c8: Pull complete
Digest: sha256:4edbd2beb5f78b1014028f4fbb99f3237d9561100b6881aabbf5acce2c4f9454
Status: Downloaded newer image for alpine:latest
docker.io/library/alpine:latest
(base) (~) davids-Air $ docker images
REPOSITORY          TAG          IMAGE ID          CREATED          SIZE
alpine              latest       3fb3c9af89a9     4 weeks ago     5.32MB
hello-world         latest       46331d942d63     6 weeks ago     9.14kB
docker101tutorial   latest       6ad88b1adc44     5 months ago    27.2MB
alpine/git           latest       4ee6a3b79e0c     5 months ago    27.1MB
(base) (~) davids-Air $
```

Tutorial 1: Using a container

Now we will install another container from Docker's repository of containers (See [here](#) for more containers)



```
docker pull alpine
```

Then we can see all the images we've installed from docker

```
docker images
```

```
(base) (~) davids-Air $ docker pull alpine
Using default tag: latest
latest: Pulling from library/alpine
9981e73032c8: Pull complete
Digest: sha256:4edbd2beb5f78b1014028f4fbb99f3237d9561100b6881aabbf5acce2c4f9454
Status: Downloaded newer image for alpine:latest
docker.io/library/alpine:latest
(base) (~) davids-Air $ docker images
REPOSITORY          TAG             IMAGE ID        CREATED         SIZE
alpine               latest         3fb3c9af89a9   4 weeks ago    5.32MB
hello-world         latest         46331d942d63   6 weeks ago    9.14kB
docker101tutorial   latest         6ad88b1adc44   5 months ago   27.2MB
alpine/git           latest         4ee6a3b79e0c   5 months ago   27.1MB
(base) (~) davids-Air $
```

Tutorial 1: Using a container



Alpine is a lightweight linux distro, available as a docker container

We can use alpine + docker to run linux command-line instructions

```
docker run alpine ls -l
```

When we call “run” we’re telling docker to create the container for the “alpine” image that we pulled earlier, and issue the command ‘ls -l’

Tutorial 1: Using a container

We can also use and “interactive” flag to keep the container running after issuing the command, try:

```
docker run -it alpine /bin/sh
```

Then run:

```
echo “Hello McDonald Institute”
```

We can exit with “exit” or CTRL+C



```
[(base) (~/.mcdonald_institute_summer_workshop_2022) davids-Air $ docker run -it alpine /bin/sh
[/ #
[/ #
[/ # ls
bin dev etc home lib media mnt opt proc root run sbin srv sys
[/ # echo "Hello World"
Hello World
[/ # exit
(base) (~/.mcdonald_institute_summer_workshop_2022) davids-Air $
```

Tutorial 1: Using a container



Lastly, let's check our tasks to see if any containers are running:

```
docker ps
```

You should see an empty line, since none of the containers we started were running as “Daemons”, which tells the container to run continuously in the background

To see what containers we've run recently, we can append an -a or “all”

```
docker ps -a
```

```
((base) ~/mcdonald_institute_summer_workshop_2022) davids-Air $ docker ps -a
CONTAINER ID   IMAGE          COMMAND                  CREATED        STATUS              PORTS          NAMES
489de7610038   alpine        "/bin/sh"               9 minutes ago Exited (0) 9 minutes ago
a762a6ef467f   alpine        "echo 'Hello McDonal..." 13 minutes ago Exited (0) 13 minutes ago
fa44a217009c   alpine        "ls -l"                 17 minutes ago Exited (0) 17 minutes ago
ced271379bc6   hello-world   "/hello"                41 hours ago  Exited (0) 41 hours ago
```

Tutorial 1: Using a container



We've used some phrases without explaining in detail, here are some definitions (Copied from [here](#))

- *Images* - The file system and configuration of our application, which are used to create containers. To find out more about a Docker image, run `docker inspect alpine`. In the demo above, you used the `docker pull` command to download the **alpine** image. When you executed the command `docker run hello-world`, it also did a `docker pull` behind the scenes to download the **hello-world** image
- *Containers* - Running instances of Docker images — containers run the actual applications. A container includes an application and all of its dependencies. It shares the kernel with other containers, and runs as an isolated process in user space on the host OS. You created a container using `docker run` which you did using the `alpine` image that you downloaded. A list of running containers can be seen using the `docker ps` command.
- *Docker daemon* - The background service running on the host that manages building, running and distributing Docker containers.
- *Docker client* - The command line tool that allows the user to interact with the Docker daemon.
- *Docker Store* - A [registry](#) of Docker images, where you can find trusted and enterprise ready containers, plugins, and Docker editions.

Containers Closing Remarks



Containers are very useful tools for running specific applications/custom software on arbitrary systems

Loads of applications (Especially web-apps) available as containers

Scientific software (Custom simulation packages, version dependent effects etc..) are fertile ground for containers

Some further steps:

- Make your own image to learn more about Docker ([link](#))
- Look for an image of a software you're considering using

Workshop Closing Remarks

Command-line interface tools are powerful and plentiful!

Making use of existing tools, and doing some research on what's possible before starting a project or a new task can make your life much easier! Less time spent on software wrangling = More time for science

Google and online manuals are your best friends for learning, and talk to your colleagues and collaborators about the tools they like best!

A word of caution, be very careful copying and pasting commands from online forums, malicious actors exist and a seemingly benign looking set of commands can become a serious security issue!

Check multiple sources before running commands from the internet! If you're unsure, reach out to colleagues for help.

Always think before you 'sudo'

MCGILL PHYSICS

HACKATHON

**See you in the fall at the
McGill Physics
Hackathon?**



Questions?

You can also email me after at david.gallacher@mail.mcgill.ca

Resources

- [How to install git on any OS](#)
- [A nice ELI5 git series](#)
- ["What is git" from Atlassian](#)
- [Basic git tutorial](#)
- [Reference for adding local git projects to the cloud](#)
- [An in-depth summary of remote branches](#)
- [Tutorial on how to deal with merge conflicts](#)
- [SSH Beginner Guide](#)

Backup

Tutorial extra: Networked Computing

Open a secure connection to a shell instance on a remote machine:

```
ssh [username]@[remote machine]
```

e.g., `lmacka3@mimi.cs.mcgill.ca` ([register here](#))

[Do what you need to do on the remote machine]

Close the shell:

```
exit
```

Tutorial extra: Networked Computing - Copying Files

You may need some of your files on remote machine. Use `scp [source] [target]!`

Lets make a dummy file: `touch ~/foo`

Copy the file to a remote machine:

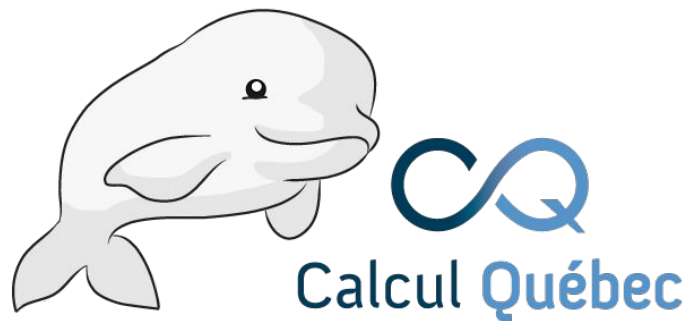
```
scp ~/foo lmacka3@mimi.cs.mcgill.ca:/home/cnd/lmacka3
```

You may need to use ssh to figure out the remote path you are copying to.

[You can also use rsync to transfer only new files](#)

Demonstration extra: Networked Computing - Copying Files

I will now share my terminal to demonstrate copying some files on Compute Canada's Beluga.



Workshop Outline

Part 1: Learn the basics of the command line (CLI)

- What is Linux?
- Tutorial 1: Navigating the Filesystem
- Tutorial 2: File Permissions
- Tutorial 3: The Builtin Software Library

Part 2: Understand how to use *git*

- **What is git?**
- Tutorial 1: Set up your first git repository
- Tutorial 2: Make a branch
- Tutorial 3: Check out an old version of your code

What *is* Git?



- Git is what is known as a Version Control System (VCS)
- By using git, you can keep track of **what** changed in a coding project, **when** it changed, **who** changed it, and **why** (if you're keeping good commit messages!)
- Particularly useful in collaborative projects, where multiple people are making changes at once. If anything in your changes conflicts (known as “**merge conflicts**”), changes can be made (sort of) gracefully
- In some ways, git is like a philosophy of how collaboration in code should be done

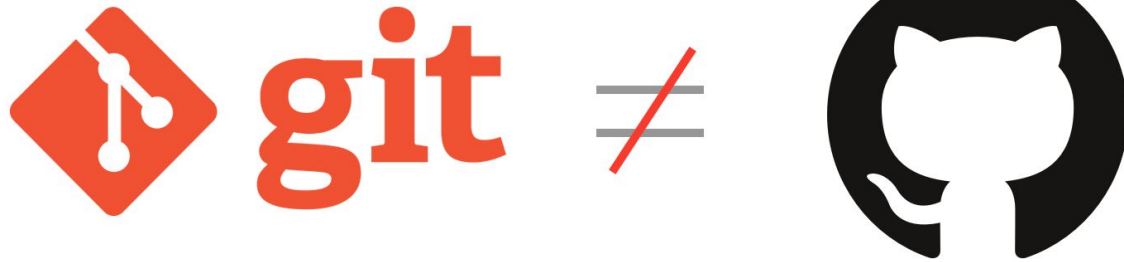
GitHub: working collaboratively online



- GitHub is an online service for hosting projects managed with git online
- Expands on the branching of git with useful collaborative features
 - **Issues**
 - **Pull requests**
 - **Wikis, projects, ...**



Note: *GitHub* \neq *git*!



- Very common misunderstanding
- *git* is the original VCS code, and doesn't have online hosting on its own
- *GitHub* is an online cloud hosting service with extra features for git projects

Workshop Outline

Part 1: Learn the basics of the command line (CLI)

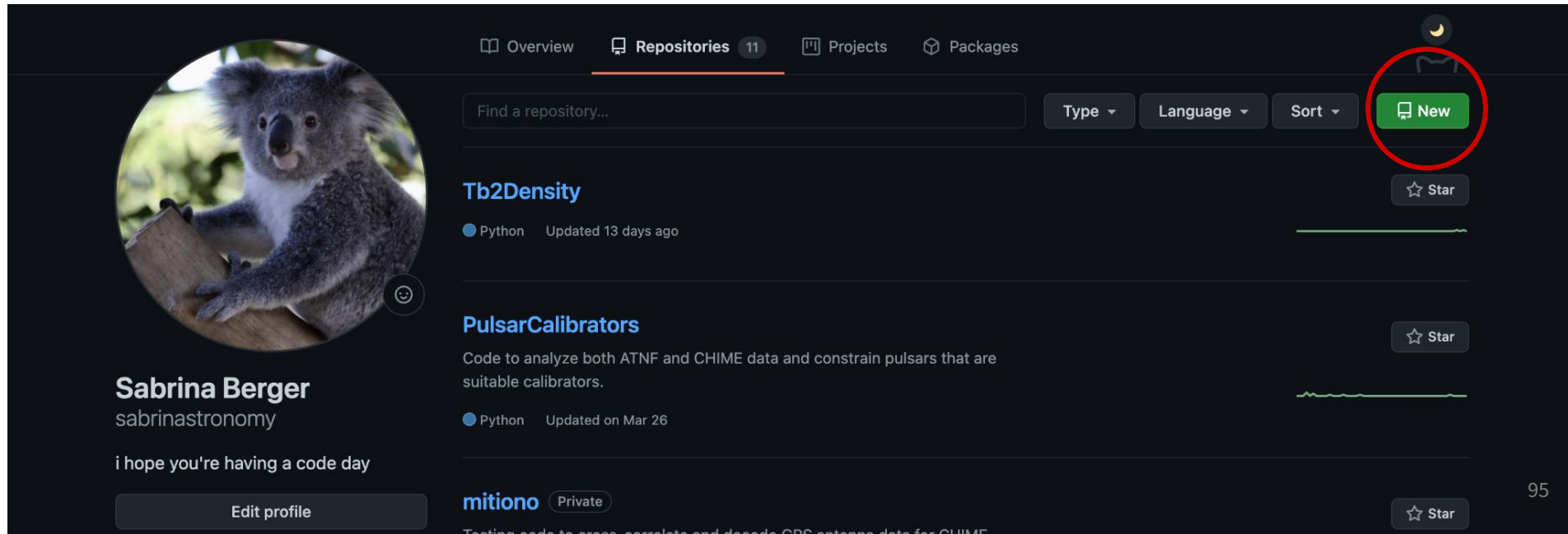
- What is Linux?
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Tutorial 1: Making a repository

- Hopefully everyone's made a GitHub account to follow along with this tutorial -- if you haven't, you can quickly to follow along!



The screenshot shows the GitHub profile page for Sabrina Berger (sabrinastronomy). The 'Repositories' tab is active, showing a list of repositories. The 'New' button is circled in red. The profile picture is a koala holding a piece of wood. The bio reads 'i hope you're having a code day'. The repositories listed are 'Tb2Density' (Python, updated 13 days ago) and 'PulsarCalibrators' (Python, updated on Mar 26). A 'mitiono' repository is partially visible at the bottom, marked as 'Private'.

Overview Repositories 11 Projects Packages

Find a repository... Type Language Sort **New**

Tb2Density ☆ Star

Python Updated 13 days ago

PulsarCalibrators ☆ Star

Code to analyze both ATNF and CHIME data and constrain pulsars that are suitable calibrators.

Python Updated on Mar 26

mitiono Private ☆ Star

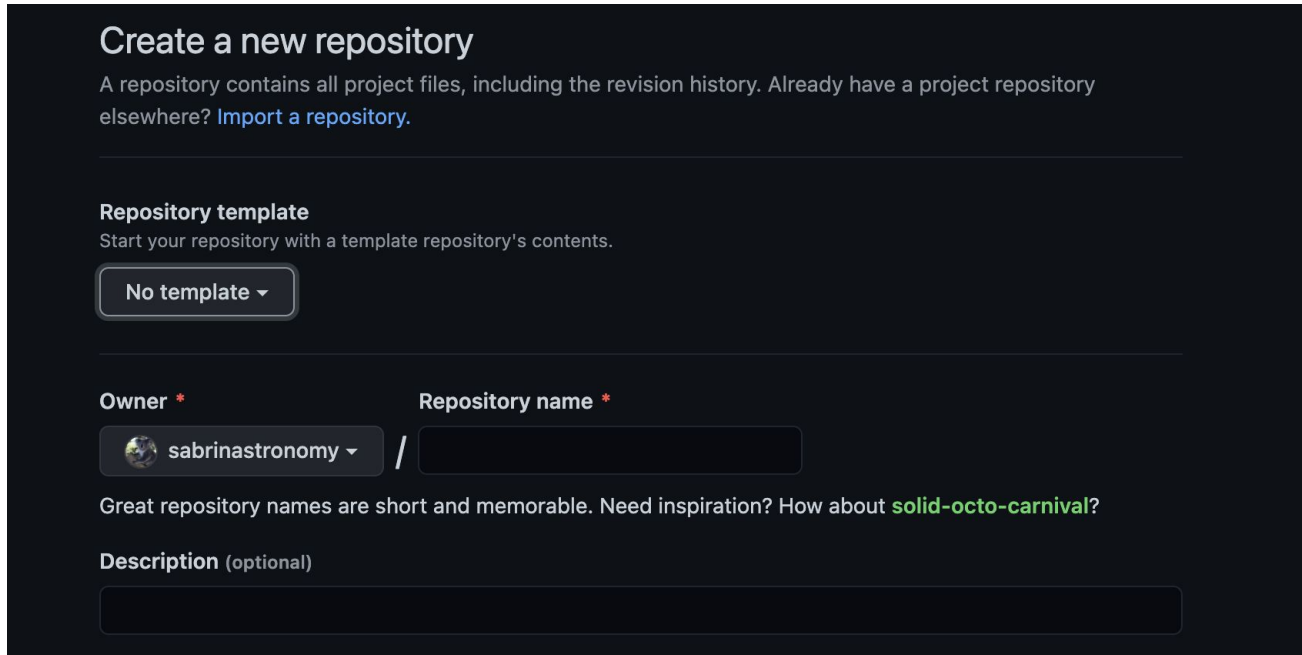
Testing code to cross-correlate and decode GPS antenna data for CHIME

Sabrina Berger
sabrinastronomy

i hope you're having a code day

Edit profile

Follow the instructions to create a repository (don't worry about any of the extra features for now).



The screenshot shows the GitHub 'Create a new repository' interface. At the top, it says 'Create a new repository' and explains that a repository contains all project files and revision history. Below this, there is a section for 'Repository template' with a 'No template' dropdown menu. The 'Owner' field is set to 'sabrinastronomy' and the 'Repository name' field is empty. A tip suggests repository names should be short and memorable, with an example 'solid-octo-carnival?'. At the bottom, there is an optional 'Description' text area.

Create a new repository


A repository contains all project files, including the revision history. Already have a project repository elsewhere? [Import a repository.](#)

Repository template

Start your repository with a template repository's contents.

No template ▾

Owner * **Repository name ***

 sabrinastronomy ▾ /

Great repository names are short and memorable. Need inspiration? How about [solid-octo-carnival?](#)

Description (optional)

Now we want to *git clone* the repository we just made on to our local machines (wherever we'd like!)

Tutorial 1: Making a repository (Summary)

- We can **clone** (*git clone*) GitHub repos to our local machine, which will copy over all the git history from the online project (**./git** folder!)
 - **Note:** this makes a **remote branch** called **origin** which is attached to the cloud, this can be a confusing detail if you accidentally make a local branch and then try and merge it into origin
- We can also create a git repository locally (*git init*), which creates a **./git** folder locally. We can then push to GitHub later
 - IMO, this workflow is confusing, and I recommend starting *all* personal coding projects with repositories on GitHub

Important basic git commands

- `git --help`
 - Gives a helpful list of git commands! Can also do ``git {command} --help`` for specifics on commands
- `git config --global user.name "{username}"`
- `git config --global user.email {email}`
 - **Note:** these are *git* associated names/emails, so they don't have much to do with GitHub! Just useful for identifying yourself in local git projects
- `git status`
 - Shows you current changes
- `git log`
 - Shows you the commit history for your project
- `git fetch`
 - Updates information stored in the local **./git** folder, such as new remote branches

Making our first commit

- The most basic git workflow consists of three important steps:
 - a. Use ``git add {file}`` to “add” a new file, or to “add” changes to an already existing file
 - You can use “wildcard” operators with this! E.g. ``git add *.py`` to add .py file changes
 - b. Once you’re happy with your additions, use ``git commit -m “{useful message}”`` to add a commit with a helpful commit message explaining your changes
 - c. Finally, we need to push our changes to the cloud. We’ll do this with the command ``git push origin master``
 - Note that the *origin* here specifies the remote cloud, and *master* is the branch we’re committing to. By default, GitHub repos start with only a master branch

Pulling from remote

- To pull in any changes from collaborators, just use `git pull` in the relevant directory
 - This won't do anything for us now, since we just made this repo for ourselves... But it's VERY important to pull the most recent version of the repository before you start making changes!
 - Ideally if everyone was working on their own branches and being responsible about workflow, this wouldn't be an issue... But nobody's perfect :)

Summary

- Step 0: PULL changes that might have been made by collaborators
- Step 1: ADD our changes
- Step 2: COMMIT changes with a message (-m)
- Step 3: PUSH changes to the cloud
- **NOTE:** all the while we can check the STATUS of our additions!

Exercise 1:

1. Create a GitHub repository on your account
2. Move the files from *EIEIOO_Scripts* to the cloned repository and make your first commit.
3. Then change `test2.py` to print “One day Github will save me from the coding monsters”.
4. Push your changes to GitHub

Workshop Outline

Part 1: Learn the basics of the command line (CLI)

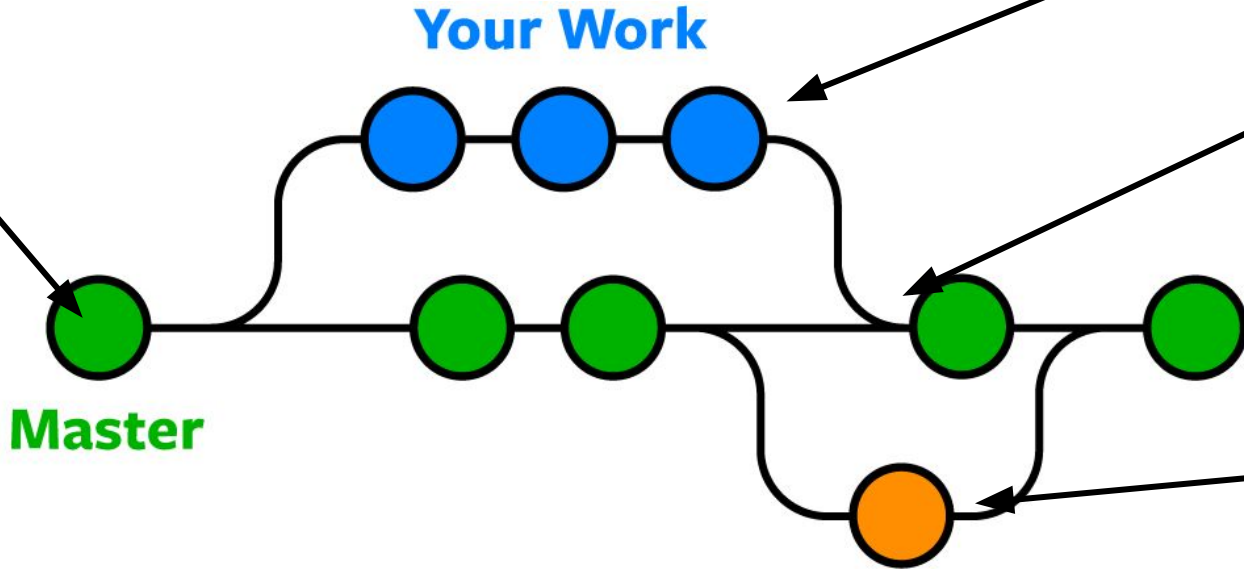
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- What is git?
- Tutorial 1: Set up your first git repository
- **Tutorial 2: Make a branch**
- Tutorial 3: Check out an old version of your code

Tutorial 2: Make a Git branch

Start with some original version of the code base



Master

Your Work

Someone Else's Work

You want to code a new feature in the code without breaking the stable code base, so you make your own branch!

Merge your changes into the master branch once they're stable!

Others can write features in tandem!

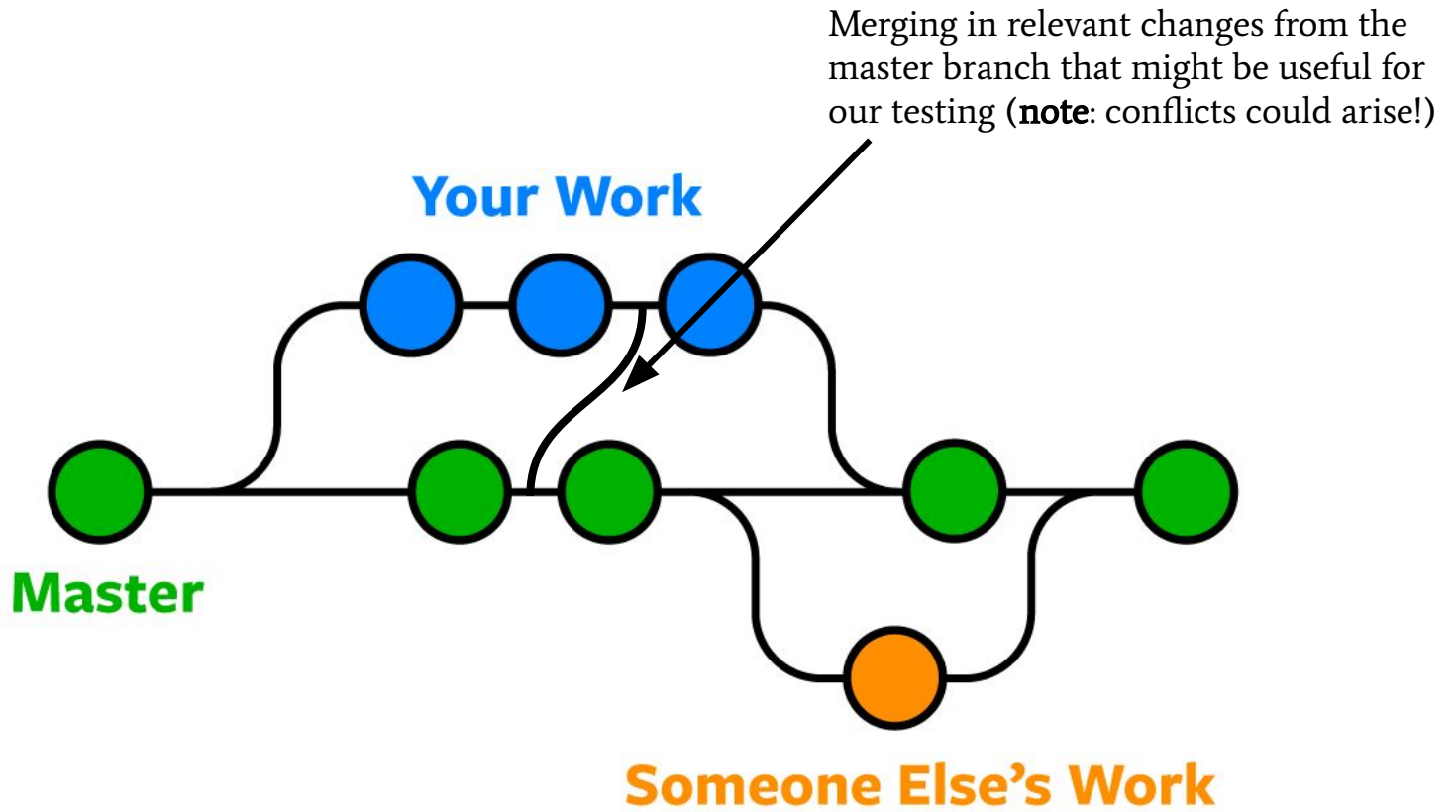
Making our own branch

- We can take a look at the available branches with ``git branch``
 - Can do ``git branch -r`` for remote branches, ``git branch -a`` for all branches
- Make our own branch with ``git branch {branch name}``

- NOTE: ``git branch {branch name}`` only makes a branch *locally!* Later, we'll see how to get this branch on GitHub
- The branch command only *made* the branch. Now if we want to **checkout** to our new branch -- i.e. move to the space where we'll make our changes
 - ``git checkout {branch name}``
 - **NOTE:** we can checkout to a new branch in one command! ``git checkout -b {new branch}``
- Now we can safely make our changes without interfering in the stable master branch!
- Once we've ADDED and COMMITTED our changes, we can PUSH!
 - **NOTE:** we have to do ``git push --set-upstream origin {our branch}`` -- this is because our branch has only been local, until now: we're making our branch sync with the cloud with **--set-upstream**

Merging in changes from other branches

- Usually a good practice to compare differences between branches first
 - ``git diff {one-branch} {other-branch}`` to compare
- Now, say we're working on our own feature branch, and there are some useful changes on another part of the code base in ***origin/master*** we want on our branch
 - First: ``git pull`` to update your local branches with changes from the cloud (***origin***)
 - Next: ``git merge {other-branch}`` to put those changes in your current branch!



Exercise 2: Make your own branch

Create and push a new branch to your online GitHub repository for EIEI00_Scripts. Call the branch “trying_new_things”.

Making a pull request

- When you're working in a collaboration, and you're ready to incorporate your changes into the master branch, you can make a pull request!

sabrinastronomy / summerschool

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Label issues and pull requests for new contributors [Dismiss](#)

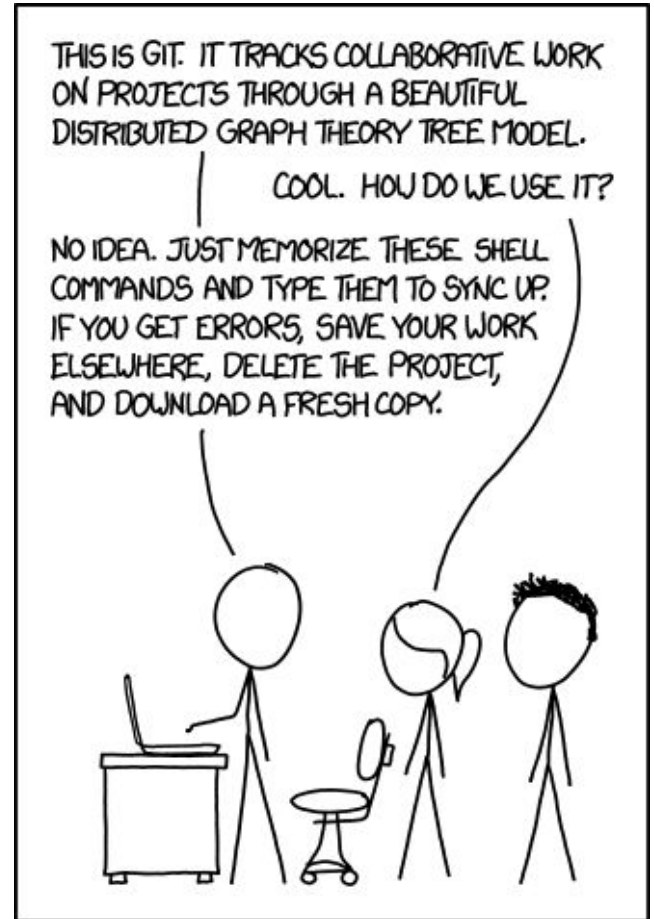
Now, GitHub will help potential first-time contributors [discover issues](#) labeled with [good first issue](#)

Filters Labels 9 Milestones 0 **New pull request**

- Pull requests are a super useful way of keeping major code changes organized
- Rule of thumb: **master** branch should ALWAYS be deployable
 - This is why pull requests exist: typically if you're a part of a collaboration, there will be other people working on the code base with you. Usually there'll be one/a few people who manage most of a given repository, and making a pull request allows you to give them a chance to view your code, review it, suggest changes, and then finally accept the merge into master once it's deemed ready
- Workflow goes something like
 - Propose a new feature
 - Checkout a new branch to start working on your feature (make sure nobody interferes with your work so you don't get merge conflicts)
 - Keep pushing changes to your branch until things are stable/finished, then make a pull request

Dealing with merge conflicts

- Despite best efforts to keep organized, issues *will* arise!
- Merge conflicts are the part of git that will, at some point in your coding life, make you scream at your computer
- We can fix these problems pretty easily, in fact! Try not to resort to saving your changes locally, and re-downloading the whole repo



Workshop Outline

Part 1: Learn the basics of the command line (CLI)

- What is Linux?
- Tutorial 1: Navigating the Filesystem
- Tutorial 2: File Permissions
- Tutorial 3: The Builtin Software Library

Part 2: Understand how to use *git*

- What is git?
- Tutorial 1: Set up your first git repository
- Tutorial 2: Make a branch
- **Tutorial 3 (Final): Checkout an old version of your code**

Going back to an old commit when your new code breaks!

- You can get a log of all previous commits with
 - ``git log``
- This should return your previous commits along with their corresponding hash, e.g.,

```
(base) sabrinaberger@sabrinaastronomy summerschool % git log
commit 5d29d753054e787005f0202364e286d1211032db (HEAD)
```

- You can revert to a previous commit with
 - ``git checkout <commit hash> .``

```
$ cat merge.txt
<<<<<<< HEAD
this is some content to mess with
content to append
=====
totally different content to merge later
>>>>>>> new_branch_to_merge_later
```

The important parts of a merge conflict will show up in our conflicted files:

- <<<<<<< HEAD
- =====
- >>>>>>> new_branch_to_merge_later

Think of the “=====” as the conflict divider. The content between HEAD and the divider is our content, and the content between the divider and the new_branch_to_merge_later is the content we tried to merge in. By reconciling the differences on these lines of code in a text editor, once you’re happy with the outcome, you can add/commit/push as usual!

Final Exercise

Restore your local *EIEIOO_Scripts* to its original commit before you modified the file.

Great job on all the tutorials today!