Reproducible Research

Practices & Tools

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Introductions

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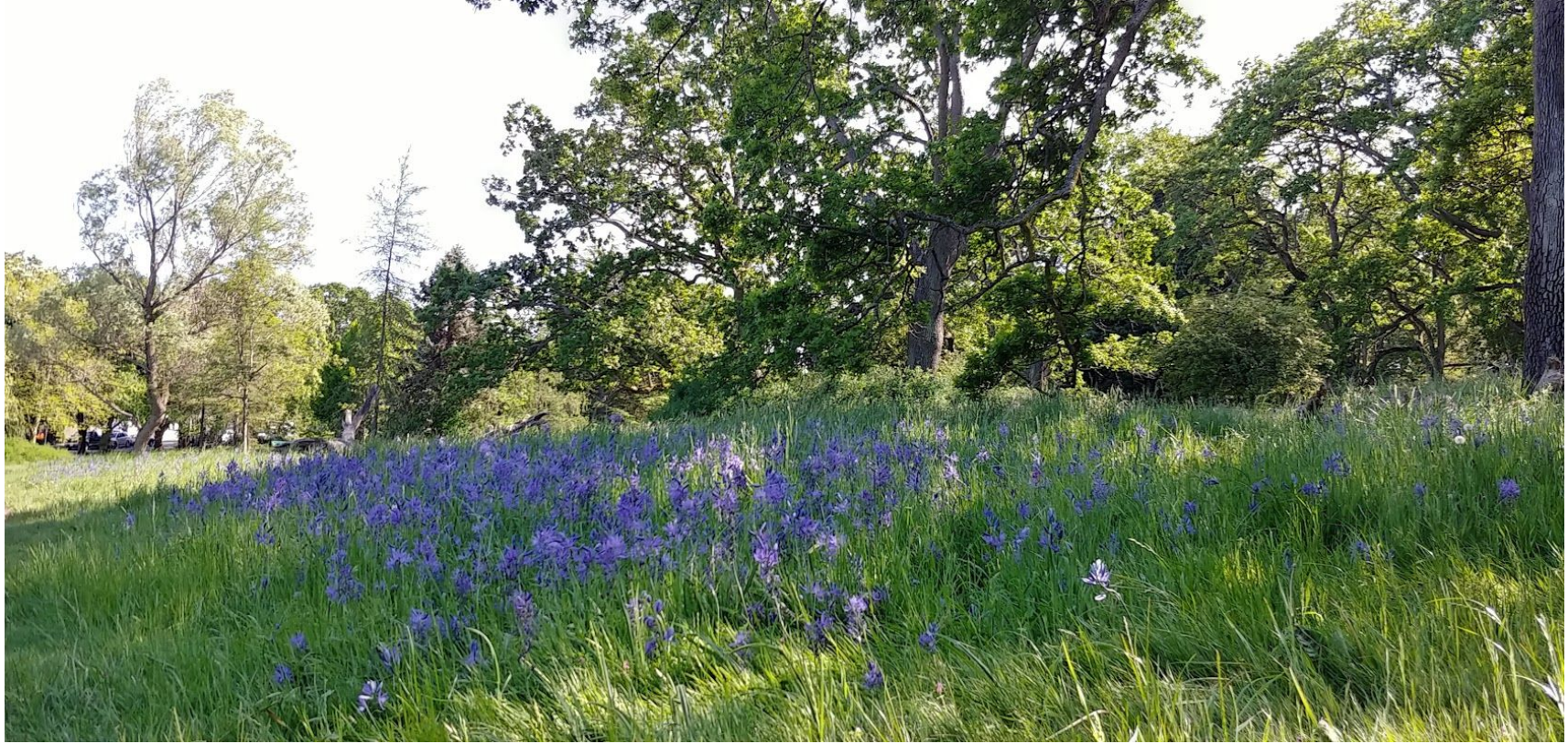


We acknowledge and respect the Lək̓ʷəŋən (Songhees and Xwsepsum/Esquimalt) Peoples on whose territory the University of Victoria stands, and the Lək̓ʷəŋən and W̱SÁNEĆ Peoples whose historical relationships with the land continue to this day.

Learning Objectives

This hands-on session will provide researchers with tools and techniques to make their research process more transparent and reusable in remote computing environments.

In this workshop, you'll learn about:

- Organizing your file directories
- Writing readable metadata with readme files
- Automating your workflows with scripts
- Capture and share your computational environment

NEW for 2025!

- Using large language models (GenAI) to assist with the above

Workshop Outline

Introduction to reproducibility

- Reproducibility “crisis”
- Elements of reproducible research
- Tools for reproducibility

Exercises

1. Organizing and Documenting Data and Code
2. Automating Workflows
3. Capturing Computational Environments

What is Reproducibility?

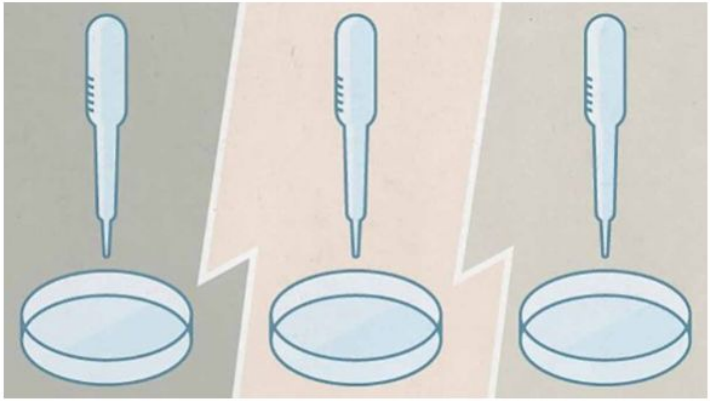
A quality of research involving some element of computation.

When the code and data are assembled in a way that another group can recreate your analyses and achieve the same result.

nature

SPECIAL | 18 OCTOBER 2018

Challenges in irreproducible research



Science moves forward by corroboration – when researchers verify others' results. Science advances faster when people waste less time pursuing false leads. No research paper can ever be considered to be the final word, but there are too many that do not stand up to further study.

There is growing alarm about results that cannot be reproduced. Explanations include increased levels of scrutiny, complexity of experiments and statistics, and pressures on researchers. Journals, scientists, institutions and funders all have a part in tackling reproducibility. Nature has taken substantive steps to improve the transparency and robustness in what we publish, and to promote awareness within the scientific community. We hope that the articles contained in this collection will help. show less

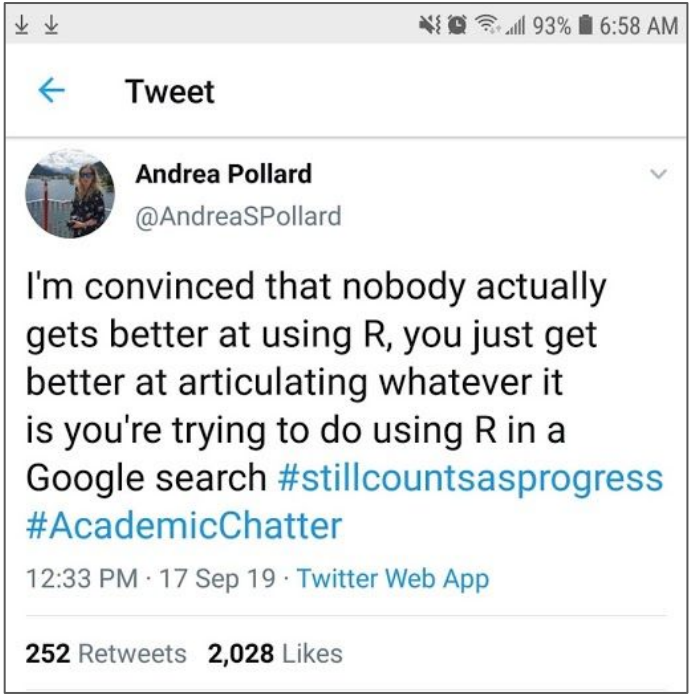
IS THERE A REPRODUCIBILITY CRISIS?

- ❏ Yes, significant crisis
- ❏ Yes, slight crisis
- ❏ No crisis
- ❏ Don’t know

Who has ever tried to reproduce **your own** OR someone else's results?

HOW DID IT GO?

http://gph.is/1PaRTrX



Question Asked 9th Mar, 2020

Maggie Sabay
Grand Canyon University

I forgot to collect descriptive data and I have closed data collection for my dissertation. What should I do?

I am a novice writer working on my dissertation. As I started setting up data for analysis, I realized that I did not collect descriptive data. This was anonymous and there is no way to collect descriptive data at this time. Any suggestions on way forward?

r/GradSchool • 8 yr. ago
by ChaosCon

Join

How do I deal with my adviser's shitty codes and other such rantings

Hey guys -

I'm partly looking for advice, but mostly just some solidarity. Lately I've become extremely disheartened with one of my advisers. From my perspective, at least, it appears as though everything he does is for the advancement of his own career without any regard for his students. In no particular order

1. Code quality is *awful*. We're an algorithm development group (so we're not just writing one-off programs to process data), but the twenty-odd years of accumulated crufty code is *unintelligible* without a guide (my adviser). Things like meaningless variable names (`x = xx`), convoluted data structures in the name of "speed" with zero profiling data, comments that *lie*, etc. When I've pointed out how difficult this makes things (alongside other faculty!), I was told "You should see $PRIOR_STUDENT's code! *His* is a mess!" and "The fact that you graduate from this lab will get you a job much more easily than focusing on good code."

OUTLOOK | 29 March 2022

Breaking into the black box of artificial intelligence

Scientists are finding ways to explain the inner workings of complex machine-learning models.

By Neil Savage

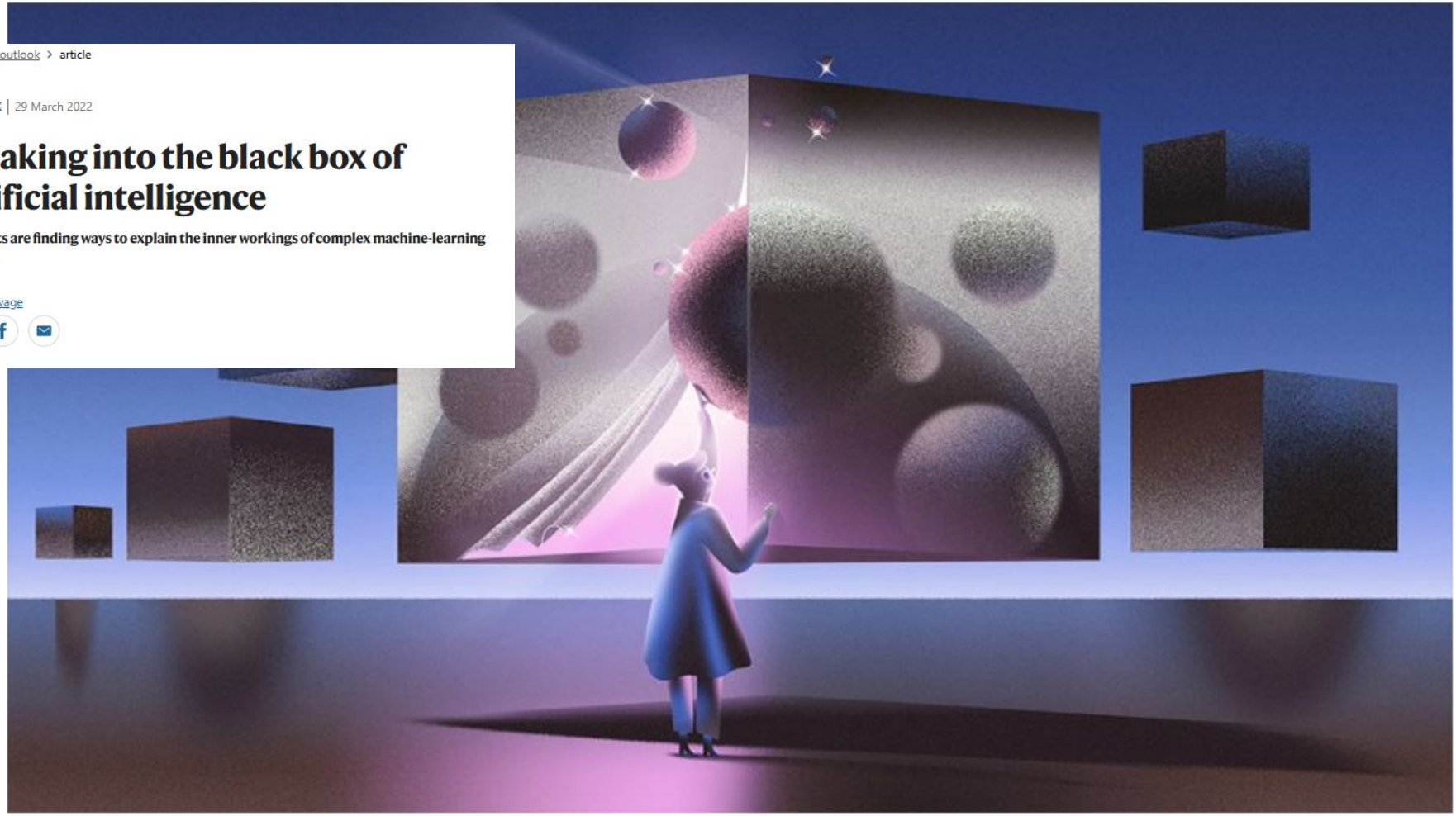


Illustration: Sandro Rybak

January 27 2025

Open Science at the generative AI turn: An exploratory analysis of challenges and opportunities

Mohammad Hosseini, Serge P. J. M. Horbach, Kristi Holmes, Tony Ross-Hellauer

Check for updates

Author and Article Information

Quantitative Science Studies (2025) 6: 22–45.

https://doi.org/10.1162/qss_a_00337 **Article history**

• Supporting Research Data Management and data sharing documentation, data analysis and curation. • Detecting errors or inconsistencies in datasets. • Creating synthetic datasets.	**Open Research Data**	• Generating fabricated datasets that support specific hypotheses and falsely validate fake papers. • Worsening reproducibility and integrity by enabling the use of unvalidated mathematical and statistical methods.

For eg.

- Subject classification
- Metadata tagging
- Code documentation
- Dataset documentation (e.g. READMEs)

“An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship.”

Buckheit and Donoho (1995) paraphrasing Jon Claerbout

Scientific method in the 21st century...

Most researchers are not formally trained as programmers, but increasingly need to deal with:

- Size and complexity of modern datasets
- Complexity of modern data analysis
- Sophistication and continuing advancement of software

Spectrum of reproducibility

High Reproducibility: studies which provide the code, data, and full computational environment necessary to reproduce the results of the study

Medium Reproducibility: studies which provide the code and data but not the computational environment in which the code can be run

Low Reproducibility: studies which describe algorithms and results

Iceberg of reproducibility

Documentation

1

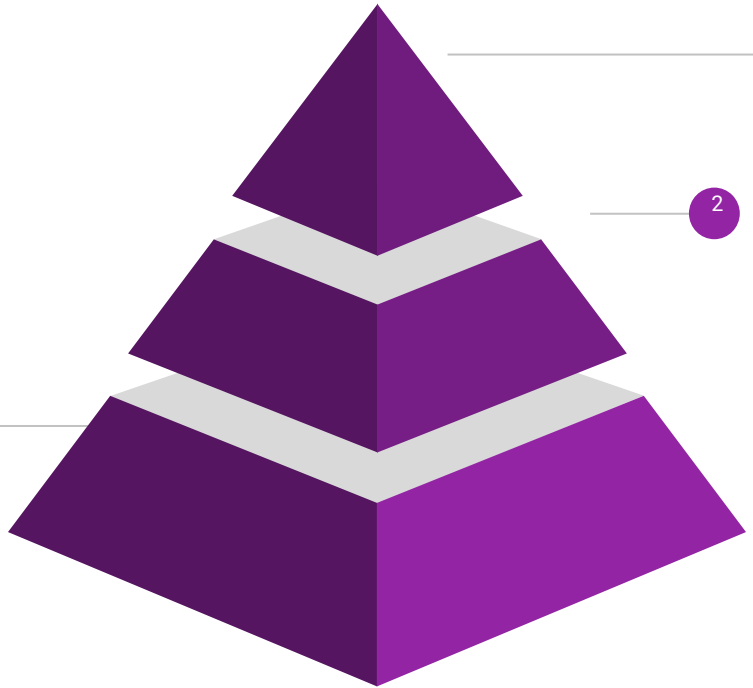
Usually written in separate effort from the study, describing the algorithms, results, environment

2

Scripting and automation

Used to make the computational/analysis components of the study easily re-runnable. May capture some information on how the computational environment is set up or used

3



Platform and environment

Captures the configuration of the computation environment (software, operating system)

Tatman, VanderPlas, and Dane (2018)

Iceberg of reproducibility

Documentation

Usually written in separate effort from the study, describing the algorithms, results, environment

Scripting and automation

Used to make the computational/analysis components of the study easily re-runnable. May capture some information on how the computational environment is set up or used

Platform and environment

Captures the configuration of the computation environment (software, operating system)

Adapted from *Tatman, VanderPlas, and Dane (2018)*

photo: Andreas Weith

Sharing ≠ Reproducible

Could someone else:

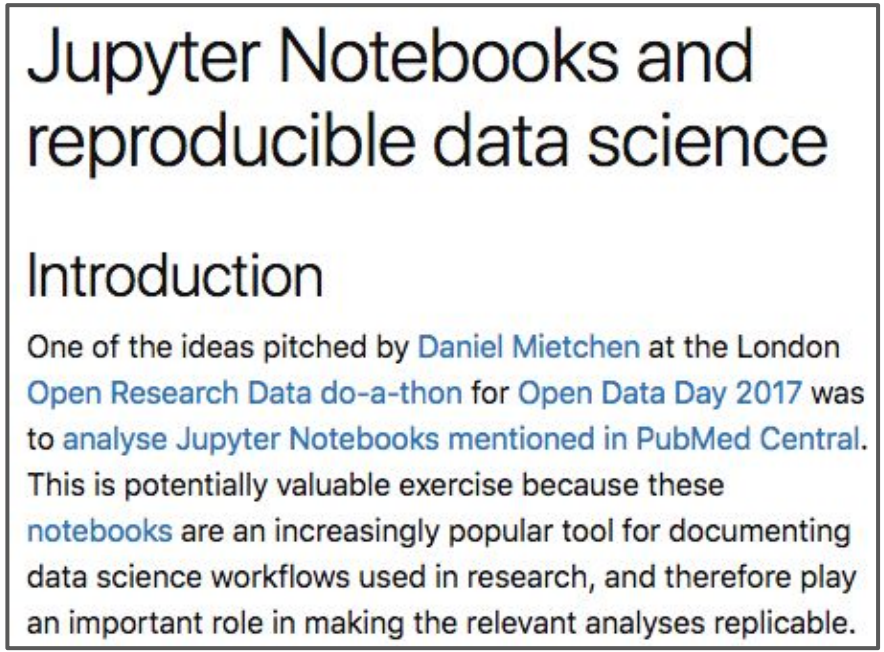
- open it ?
- understand it ?
- run it ?
- reuse it ?

Consider...

- Organization and documentation of files
- Different technical skills & experience of reusers
- Range of computing environments
- Impacts of proprietary software & licensing restrictions

Testing reproducibility

- Queried Europe PMC for “jupyter OR ipynb”
- “My initial thought was that analysing the validity of the notebooks would simply involve searching the text of each article for a notebook reference, then downloading and executing it … **It turned out that this was hopelessly naive**…”



Jupyter Notebooks and reproducible data science

Introduction

One of the ideas pitched by Daniel Mietchen at the London Open Research Data do-a-thon for Open Data Day 2017 was to analyse Jupyter Notebooks mentioned in PubMed Central. This is potentially valuable exercise because these notebooks are an increasingly popular tool for documenting data science workflows used in research, and therefore play an important role in making the relevant analyses replicable.

https://markwoodbridge.com/2017/03/05/jupyter-reproducible-science.html

Challenge 1 = workflows are not portable

- A single step in your workflow could rely on multiple dependencies
- Documentation takes a lot of time and still can be imprecise
- Links break and code rots

Challenge 2 = so many components

- Complex data analysis involves many inputs and outputs

- Annotated code, readme files, and other documentation are helpful but still separated from the data, analysis, and results

Challenge 3 = collaborators have different skills + computer setups

“A scientist unwilling to disenfranchise their collaborators could certainly elect to use more widely used tools, accepting frustration with inefficiency as the price for collaboration.

However, the price is often paid in reproducibility as well when those widely used, lowest-common denominator tools conflict with reproducibility goals”

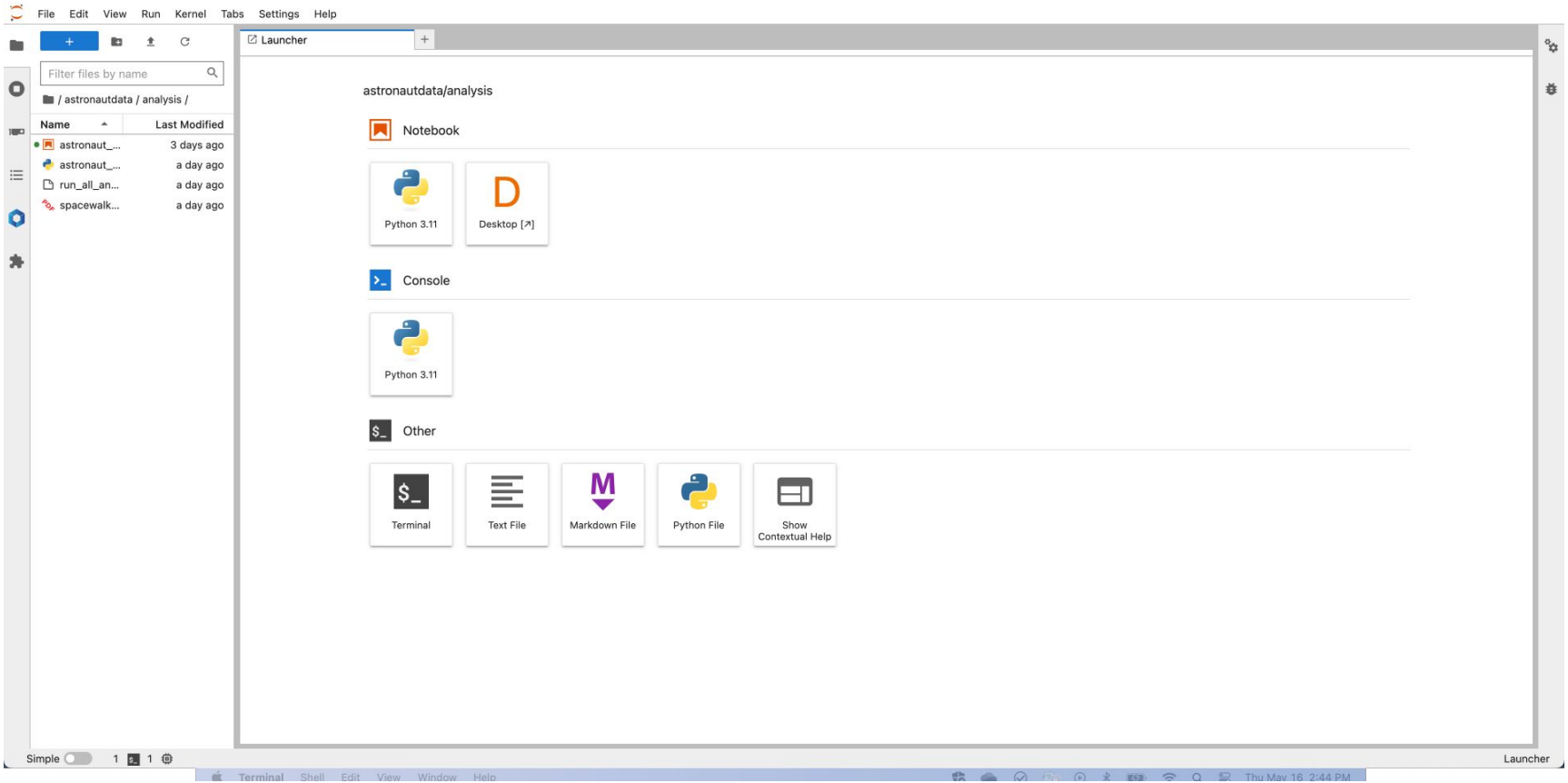
from Kathryn Huff (2018). Lessons Learned. In *The practice of reproducible research.*

Challenge 4 = Computational environments change with time

- Software of all levels requires updates to remain usable
- Research software challenging to maintain
- Loss of backwards compatibility
- For what amount of time should functionality be preserved?
- Hardware also changes

Discussion break

Today’s computing environment



Activity scenario

You've recently joined a new lab and have inherited the last post-doc's work with all their data on astronauts...

Exercise 1

1. Import the dataset into Jupyter notebook

```
$ git clone https://github.com/saehuber/reproducibility-workshop-202
```

2. Review and organize files following best practices

3. Draft a readme using this template

Organize your files

- Create **one repository** that holds all your related research files

```
Basic directory

|--astro_dataset
```

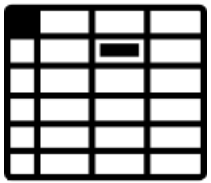
Think about the workflow….

- How were files be created?
- In what format?
- In what order?
- With what stability?

For example…

Questionnaire
(physical)

Scan
(.pdf)



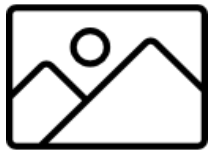
Spreadsheet
(.csv)

Journal Article
(.txt)

Interview
(.mp3)

Transcript
(.txt)

NVIVO
(.nvp)



Figures
(.jpeg)

Codes,
annotations
(.txt)

Organize your files

- Create one repository that holds all your related research files

- **Organize your files to distinguish your data, code, and results**

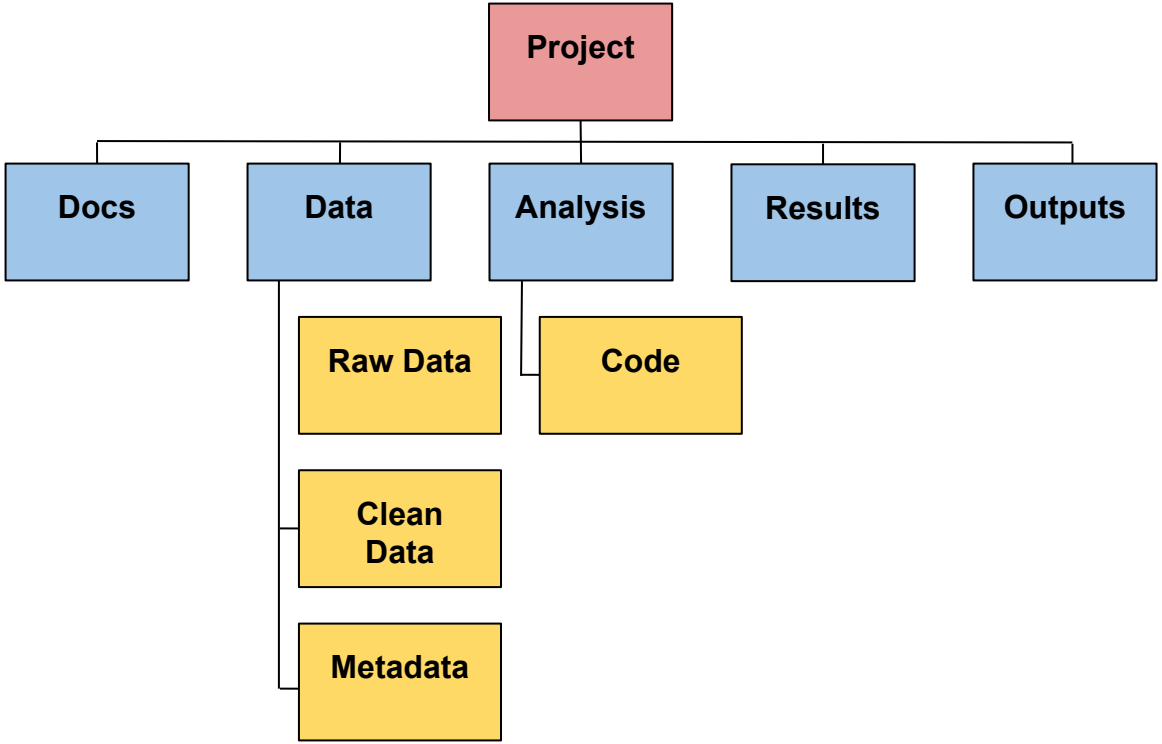
```
Basic directory

|--astro_dataset
```

Filesystem

A filesystem organizes a computer's files and directories into a tree structure:

- The first directory in the filesystem is the root directory.
- Each directory can contain more files and child directories.



Organize your files

- Create one repository that holds all your related research files

- Organize your files to distinguish your data, code, and results
  - **Separate input and output data**

```
Basic directory

|--astro_dataset
|    | -- data_raw
|    |    | -- launch_dat.csv
|    |    | -- transcripts.csv
```

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|    | -- data_clean
|    |    | -- clean_launch_dat.csv
|    |    | -- coded_transcripts.csv
```

Organize your files

- Create one repository that holds all your related research files

- Organize your files to distinguish your data, code, and results
  - Separate input and output data
  - **Separate scripts from data**

```
Basic directory

|--astro_dataset
|    | -- data_raw
|    |    | -- launch_dat.csv
|    |    | -- transcripts.csv
|    | -- data_clean
|    |    | -- clean_launch_dat.csv
|    |    | -- coded_transcripts.csv
|    | -- src
|    |    | -- analysis_launch_dat.R
|    |    | -- process_launch_dat.R
```

Organize your files

- Create one repository that holds all your related research files

- Organize your files to distinguish your data, code, and results
  - Separate input and output data
  - Separate data from scripts
  - **Separate results from data and scripts**

```
Basic directory

|--astro_dataset
|    | -- data_raw
|    |    | -- launch_dat.csv
|    |    | -- transcripts.csv
|    | -- data_clean
|    |    | -- clean_launch_dat.csv
|    |    | -- coded_transcripts.csv
|    | -- results
|    |    | -- t-test_results.txt
|    |    | -- fig1_freq.jpg
|    |    | -- fig2_distribution.jpg
|    | -- src
|    |    | -- analysis_launch_dat.R
|    |    | -- process_launch_dat.R
```

Organize your files

- Create one repository that holds all your related research files

- Organize your files to distinguish your data, code, and results
  - Separate input and output data
  - Separate data from scripts
  - Separate results from data and scripts

- **Use clear and explicit file names**

```
Basic directory

|--astro_dataset
|    | -- data_raw
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|    |    | -- transcripts.csv
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|    |    | -- clean_launch_dat.csv
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|    |    | -- fig1_freq.jpg
|    |    | -- fig2_distribution.jpg
|    | -- src
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Organize your files

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- Organize your files to distinguish your data, code, and results
  - Separate input and output data
  - Separate data from scripts
  - Separate results from data and scripts

- Use clear and explicit file names

- Include a **readme file** in your main directory

```
Basic directory

|--astro_dataset
|    | -- data_raw
|    |    | -- launch_dat.csv
|    |    | -- transcripts.csv
|    | -- data_clean
|    |    | -- clean_launch_dat.csv
|    |    | -- coded_transcripts.csv
|    | -- results
|    |    | -- t-test_results.txt
|    |    | -- fig1_freq.jpg
|    |    | -- fig2_distribution.jpg
|    | -- src
|    |    | -- analysis_launch_dat.R
|    |    | -- process_launch_dat.R
|    | -- README.txt
```

How to write a README

readme template

Project-level Description

Provide a description of your dataset, highlighting its purpose and features.

Attribution

Acknowledge contributors, include a main contact, and cite sources.

License

Specify the project's license to clarify how others can use your code.

Installation / Methodology

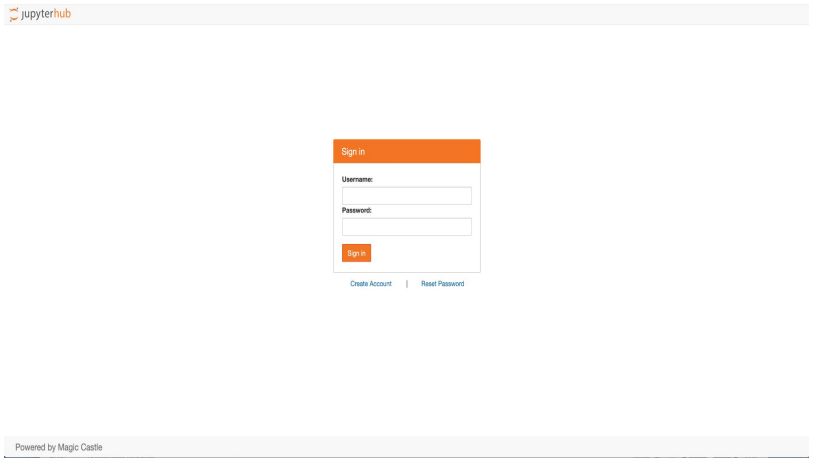
Provide instructions on install, including prerequisites. Explain how to navigate folder structure and files, how to run code.

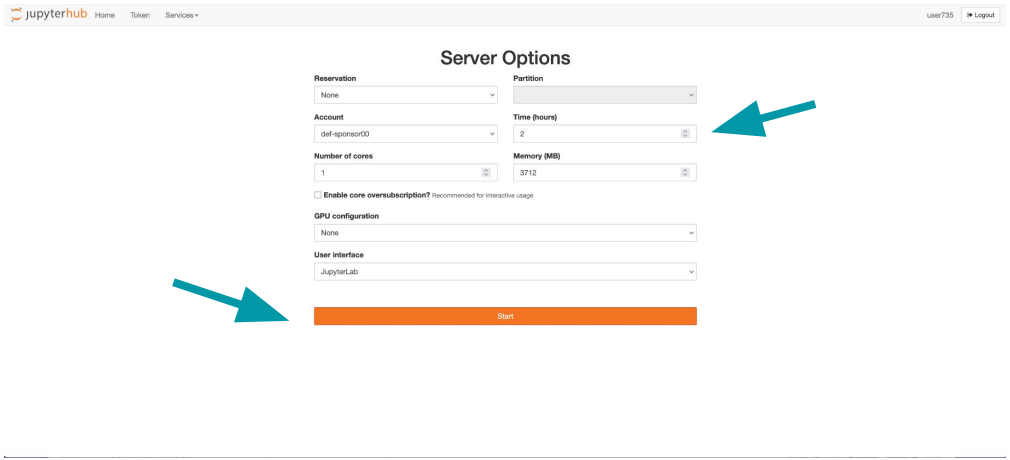
File-level Description

Describe files to ensure completeness of understanding - how many variables do they contain, define codes, specify units, etc.

Exercises- accessing the computing environment

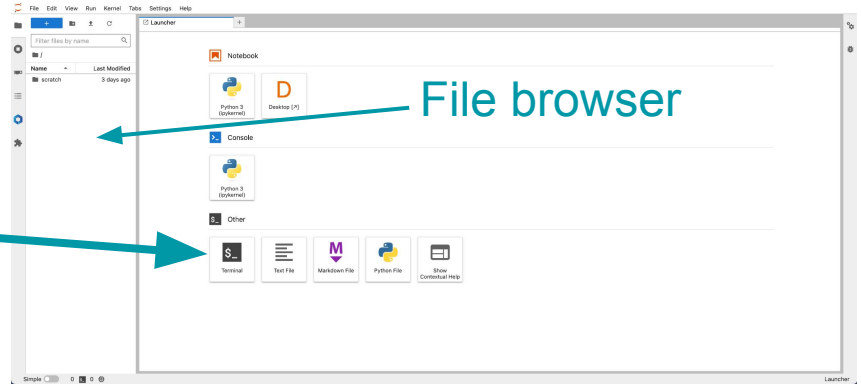
- Go to https://jupyter.coss2025b.c3.ca in your web browser
- Sign in using your provided username and password.
- Change “Time” to about 2.5 hours, and click Start
- Let us know if any questions!





Exercises- downloading the data

1. Open Terminal
   a. From Launcher
   b. Or under *File-> New -> Terminal*
2. From Terminal, enter the below command to download the data:




```
$ git clone https://github.com/saehuber/reproducibility-workshop-202
```

3. Navigate to “reproducibility-workshop-2025” folder in file browser (left)

Exercise 1

1. Import the dataset into Jupyter notebook

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```

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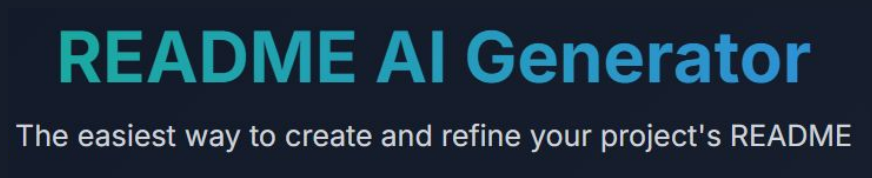
3. Draft a readme using this template

https://github.com/eli64s/readme-ai

- Automated readme generator for GitHub repositories
- Uses OpenAI, Google Gemini, and other LLM APIs to generate readme

HOW WELL DID IT WORK?

😠👎



https://www.gitdevtool.com/readme

template-based editor
better for software

McMaster University

README Generator

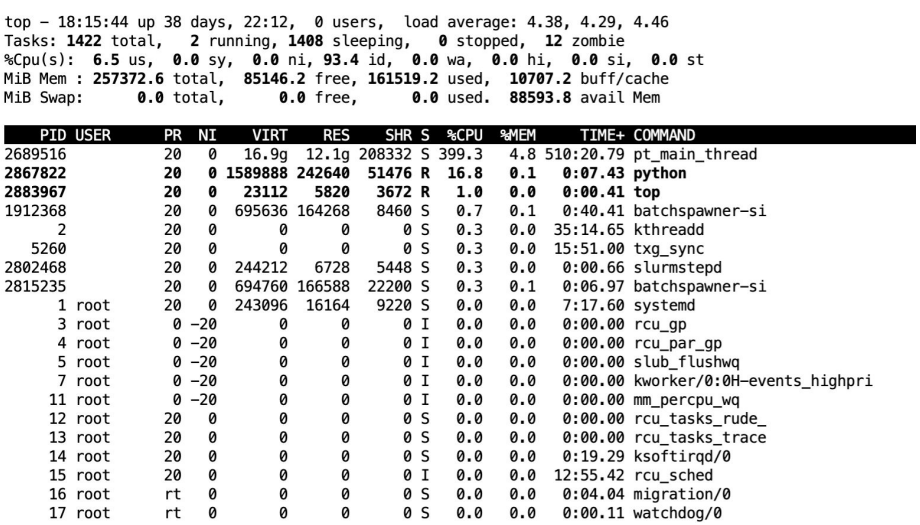
https://rdm.mcmaster.ca/readme

template-based editor
better for datasets

Automating your workflow with scripts

Common workflow styles

- GUI (graphical user interface)
- Command line interfaces
- Executable scripts



```
top - 18:15:44 up 38 days, 22:12,  0 users,  load average: 4.38, 4.29, 4.46
Tasks: 1422 total,   2 running, 1408 sleeping,   0 stopped,  12 zombie
%Cpu(s):  6.5 us,  0.0 sy,  0.0 ni, 93.4 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
MiB Mem : 257372.6 total,  85146.2 free, 161519.2 used,  10707.2 buff/cache
MiB Swap:      0.0 total,      0.0 free,      0.0 used.  88593.8 avail Mem

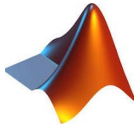
    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
2689516           20   0   16.9g  12.1g 208332 S 399.3   4.8 510:20.79 pt_main_thread
2867822           20   0 1589888 242640  51476 R  16.8   0.1   0:07.43 python
2883967           20   0   23112   5820   3672 R   1.0   0.0   0:00.41 top
1912368           20   0  695636 164268   8460 S   0.7   0.1   0:40.41 batchspawner-si
      2           20   0       0      0      0 S   0.3   0.0  35:14.65 kthreadd
   5260           20   0       0      0      0 S   0.3   0.0  15:51.00 txg_sync
2802468           20   0  244212   6728   5448 S   0.3   0.0   0:00.66 slurmstepd
2815235           20   0  694760 166588  22200 S   0.3   0.1   0:06.97 batchspawner-si
      1 root      20   0  243096  16164   9220 S   0.0   0.0   7:17.60 systemd
      3 root       0 -20       0      0      0 I   0.0   0.0   0:00.00 rcu_gp
      4 root       0 -20       0      0      0 I   0.0   0.0   0:00.00 rcu_par_gp
      5 root       0 -20       0      0      0 I   0.0   0.0   0:00.00 slub_flushwq
      7 root       0 -20       0      0      0 I   0.0   0.0   0:00.00 kworker/0:0H-events_highpri
     11 root       0 -20       0      0      0 I   0.0   0.0   0:00.00 mm_percpu_wq
     12 root      20   0       0      0      0 S   0.0   0.0   0:00.00 rcu_tasks_rude_
     13 root      20   0       0      0      0 S   0.0   0.0   0:00.00 rcu_tasks_trace
     14 root      20   0       0      0      0 S   0.0   0.0   0:19.29 ksoftirqd/0
     15 root      20   0       0      0      0 I   0.0   0.0  12:55.42 rcu_sched
     16 root      rt   0       0      0      0 S   0.0   0.0   0:04.04 migration/0
     17 root      rt   0       0      0      0 S   0.0   0.0   0:00.11 watchdog/0
```

Scripting languages

- Bash
  - awk/sed 

- Python

- R



- Matlab

- Perl

- Julia

Basic bash commands

```
$ ls      lists files and directories

$ pwd     print working directory

$ cd      change directory

$ mkdir   create new directory

$ touch   update/create new file

$ cp      copy files (add -R for copying folders)

$ mv      move files

$ rm      remove (add -R for deleting folders)
```

A first bash script

```
#!/bin/bash

echo “Hello world” #print out the text “Hello world”

cd src #move into to “src” directory

python my_python_script.py #Run using a python interpreter
```

Sample use cases for scripts

- Analyze output files in separate folders (or the same ones)
- Prepare input files for multiple jobs
- Compile a new software
- Set up a virtual environment

If you have to do it more than once, write a script.

If you want to remember how you did it, write a script.

Document your code

- Do everything with scripts/save commands
- Specify software environment version
- Specify all dependencies (& versions!)
- Use relative paths
- Annotate scripts explaining steps and decisions
- GenAI may be helpful for getting started (but is not entirely trustworthy!)

****Print out configuration****

- R: sessionInfo()
- Py: IPython.sys_info()
  pip freeze

Using loops

Bash

```
#!/bin/bash

# Loop through all subfolders

for dir in $(pwd)/*; do

    if [ -d "$dir" ]; then

        echo "$dir"

    fi

done
```

Python

```
import os

for item in os.listdir(os.getcwd()):

   item_path = os.path.join(os.getcwd(),item)

    if os.path.isdir(item_path):

        print(item_path)
```

Using variables

Bash

```
#!/bin/bash

current_directory=$(pwd)

# Loop through all subfolders

for dir in "$current_directory"/*; do

    if [ -d "$dir" ]; then

        echo "$dir"

    fi

done
```

Python

```
import os

current_dir = os.getcwd()

for item in os.listdir(current_dir):

   item_path = os.path.join(current_dir, item)

    if os.path.isdir(item_path):

        print(item_path)
```

Using GenAI for creating scripts

Shell

```shell
#!/bin/bash

# Get the current working directory
BASE_FOLDER="$(pwd)"

# Loop through all subdirectories in the current folder
for dir in "$BASE_FOLDER"/*/; do
  if [ -d "$dir" ]; then
    echo "Processing directory: $dir"
    # Add your custom commands here
  fi
done

```

Usage:

1. Save this as `loop_current_subfolders.sh`.
2. Make it executable: `chmod +x loop_current_subfolders.sh`.
3. Run it from any directory: `./loop_current_subfolders.sh`.

Would you like this to include hidden folders or recurse into deeper subdirectories as well?

Using GenAI for creating scripts

Python

```python
import os

def loop_through_subfolders(base_folder):
    for root, dirs, files in os.walk(base_folder):
        for dir_name in dirs:
            subfolder_path = os.path.join(root, dir_name)
            print(f"Processing directory: {subfolder_path}")
            # Add your custom logic here

# Example usage
if __name__ == "__main__":
    folder_path = "/path/to/your/folder"  # Replace with your target folder
    loop_through_subfolders(folder_path)

```

Notes:

- This script uses `os.walk()` to recursively traverse all subdirectories.
- You can replace `"/path/to/your/folder"` with any directory path you want to process.

Would you like this script to perform any specific actions inside each subfolder (e.g., list files, copy files, analyze contents)?

Using GenAI for understanding a script

Copilot

This Bash script lists all **subdirectories** (not files) in the **current working directory**. Here's a breakdown of what each line does:

Shell

```
#!/bin/bash

```

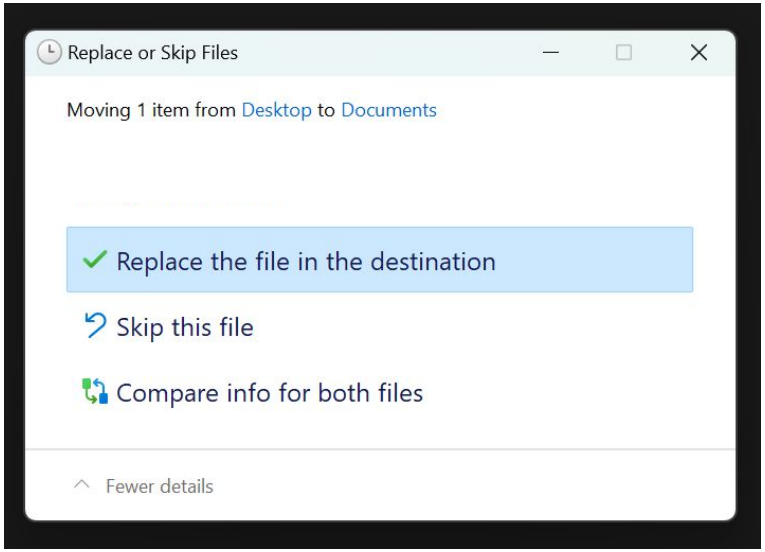
- This is the **shebang** line. It tells the system to use the Bash shell to interpret the script.

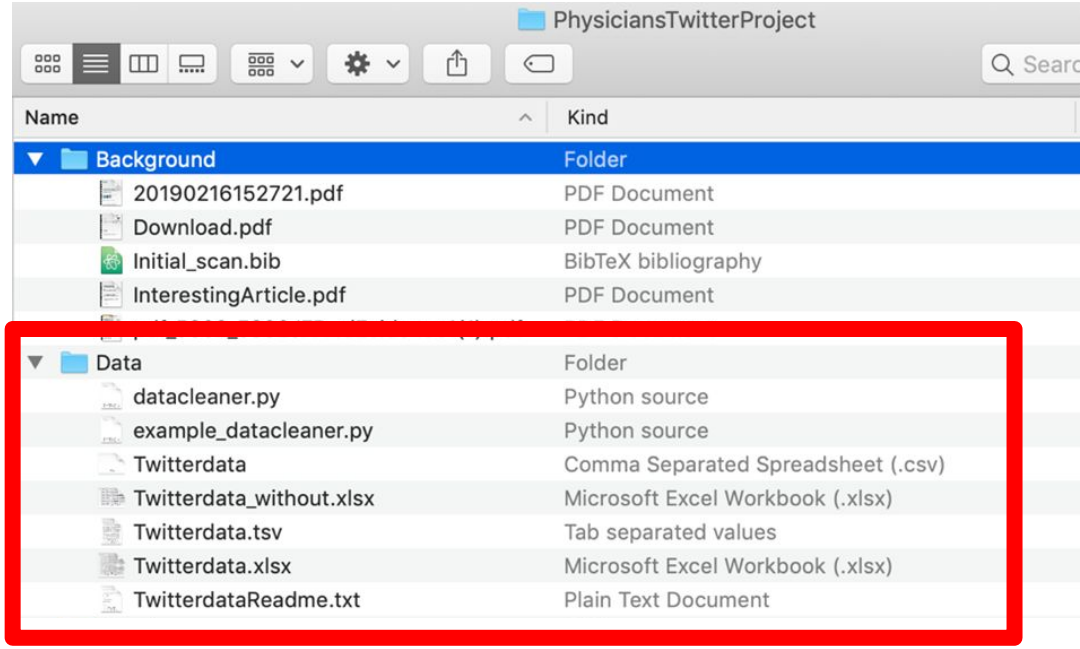
Shell

```
current_directory=$(pwd)

```

Version control

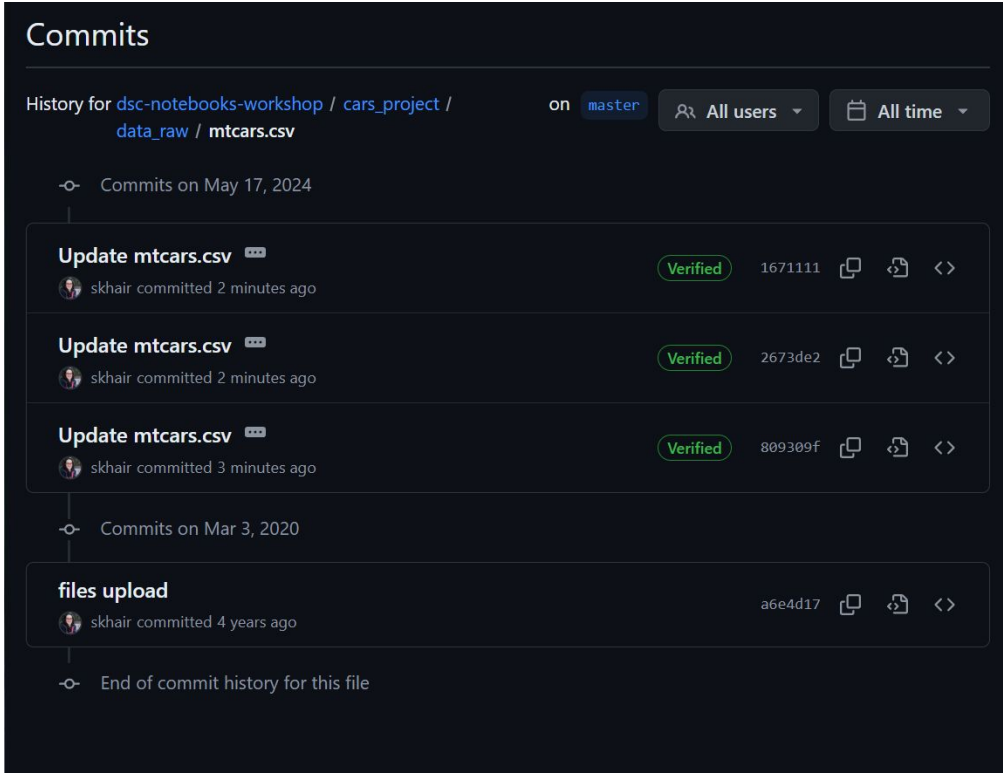




Don’t do this…

Version control

- **Audit** — see who made what changes and when.
- **Undo/redo work** — go back to a previous version as needed.



Using version control

- Combines nicely with scripts and automation!
- Track changes
- Git example:

```
$ git diff
diff --git a/paper/manuscript.tex b/paper/manuscript.tex
index 3fe30be..7b6f0f1 100644
--- a/paper/manuscript.tex
+++ b/paper/manuscript.tex
@@ -20,7 +20,7 @@ This document was drafted with the assistance of Microsoft Copilot.

 \section{Introduction}
 The age of astronauts has been a topic of interest for many years.
-This paper presents a few simple statistical analysis of the age of astronauts.
+This paper presents a statistical analysis of the age of astronauts and some related analysis around age and spacewalk records.
```

Exercise 2:

1. Navigate to “exercise_2” folder in file browser
2. Review the different subfolders, files, and scripts.
    a. What are the input files, and what is produced?
    b. What does each script do?
3. You’ve received new data! Update the collection to use data from the aggregated file available for download from https://object-arbutus.cloud.computecanada.ca/RCSWorkshopMedia/2025-06-10-COSS-Reproducible-Research/astronauts_full.csv instead of the current input file

Capturing environment

Recap:

1. Documentation

- A “how-to” for reproducing your science. A great start! Everybody does this. (Right?)
- Small and portable
- Easy to archive and readable forever unless it’s saved in WordStar
- “Tell me what to do”
- “Tell me where to find the software tools I need”

BUT:

- The tools aren’t there anymore?
- The instructions are confusing/vague/incomplete

Recap:

2. Scriptage

- An automated playbook for reproducing your science. Awesome!
- Everybody can do this. (Right? Mostly. Lots of help available!)
- Still small and portable!
- Easy to archive and runnable forever unless it’s, uh, AmigaDOS
- “Show & tell me what to do”—can function as documentation!
- Encapsulates where to find the software tools needed

BUT:

- The tools aren’t there anymore? (404!)

So now what?

You could package up the necessary software and include that?

- Licensing - no way around that, probably, we'll have to set that aside for now, we'll have to assume open-source or freely distributable software.
- Do you package the binary, or the source?
- What about dependencies? Libraries, OS components

What if you could capture your software environment, and put that on a shelf or send it to someone?

Virtual machines

A virtual machine is a software representation of a computer, its operating system, software and configuration.

You can treat this like a regular computer, add whatever software and configure it however you like, and then make copies.

VMs are based on *images*. You take an image, create a VM from it, and add whatever you want, like installing your favourite language and libraries.

You can create your own images from a VM by taking a *snapshot.* This captures the entire configured state of the VM.

A VM instantiated from this snapshot will then be identical to the original.

Virtual machines, cont'd.

But.

- VM images can be huge and contain stuff you don't really need
- VM images can be tricky and/or tedious to create
- Multiple competing formats
- Portability is fantastic so long as where you want to run it supports that type of image
- VMs package up everything in case you need it.

Containers

Two ways to look at containers:

1. “VM Lite”
2. A mechanism for packaging software.

Containers encapsulate software and configuration but rely on the host machine’s kernel and hardware.

(Note we are talking about *application containers*, not *system containers*, which really are like “VM Lite” but have their own drawbacks, portability issues, etc.)

Containers, cont'd.

Yay!

- Smaller than VMs
- Only have what you need
- Easier to create–*we're going to make one in a few minutes!*
- More portable: two primary formats, each of which is runnable everywhere*

Boo.

- Relies on host system support, host system kernel

** sort of (sssh!)*

Containers, cont’d redux.

Two main types:

- Docker: microservices, Kubernetes, …
  - Composed of layers
  - Hugely popular, used by all major cloud providers
  - Sort of open source!
- Apptainer (né Singularity): for *science*. Can run on HPC.
  - Single image file
  - Built for research reproducibility!
  - Open source!

So, Apptainer

- Designed for HPC
- Designed for research
- Designed for reproducibility
- Support HPC usage profiles (MPI, InfiniBand, …)

The Bad News

Not magic.
Our national HPC environments use common software builds across heterogeneous environments so within the Alliance your analysis codes can run anywhere. Beluga down? Try a few cycles on Cedar.

This software stack is amazing and does what it sets out to do very well. But it does not lend itself to containerization.

I don’t have a solution for you on this. At least not a magic one.

Real-world example: containerizing Exercise 2

I set out to take Sarah's scripted analysis and make that into a portable container and ran into some problems.

- Uses lmod (`module load this-n-that`) - no easy way to reproduce this inside the container
- Had to *reproduce* as best I could, instead of *capture*, the environment
- Had to figure out the important parts of `module load scipy-stack/2023b`
- Adjusted the scripts to not depend on being in specific directories

Takes 15 minutes to build on a dedicated VM. Not great for a class exercise.

Definition file, etc. in repo under `exercise_3_pt1`.

Finished image under `/home/user0063/share/analysis2.sif`.

Exercise 3: Creating the definition file

A definition file for an Apptainer image is a text file with a simple format, traditionally with the extension “`.def`”.

Log in to the course computing environment using the supplied credentials, and use your favourite editor to start editing a file “`figgy.def`”.

If you’re interested after the course:
- https://apptainer.org/docs/user/latest/quick_start.html
- https://apptainer.org/docs/user/latest/definition_files.html

Exercise 3: The header section

In the header section we define the base for our image. Generally we build on other images.

- Using a Docker image
- We specify image and tag
- Apptainer supports *multi-stage builds* which we are not using here, but it's shown here to plant a seed.

```
Bootstrap: docker
From: python:3.11.5
Stage: build
```

Reference:

- https://apptainer.org/docs/user/latest/definition_files.html#header

Exercise 3: The `%files` section

We don’t need this for our exercise. I’m just telling you about it because it’s often important (see `exercise_3_pt1` for a practical example).

The **`%files`** section allows you to copy files from the host system into your container image.

(Remember, don’t actually add this to your definition!)

```
%files
  source/ /analysis
```

Reference:
- https://apptainer.org/docs/user/latest/definition_files.html#files

Exercise 3: The `%post` section

In the **`%post`** section we define a script that installs and configures software inside our image.

Text in this section defines a script which is run in building the image. Make sure it's indented properly so Apptainer knows when the script is done.

```
%post
  pip install pyfiglet==1.0.2
```

Reference:
- https://apptainer.org/docs/user/latest/definition_files.html#post

Exercise 3: The `%runscript` section

The **`%runscript`** section defines the script (indented like `%post`) that will execute when the container is run.

In our example, we run the pyfiglet tool that we installed in the `%post` section, but we could have a longer script with additional commands.

Note the `` `"$@"` ``: this allows us to pass arguments to the script when running our container.

```
%runscript
  pyfiglet "$@"
```

Reference:
- https://apptainer.org/docs/user/latest/definition_files.html#runscript

Exercise 3: The `%test` section

An optional **`%test`** section allows us to verify some aspect of our image during the build. If the script defined here exits with a non-zero status, the build fails. It can also be invoked afterwards with `apptainer test`.

Our test here is pretty trivial, but it verifies that the program was installed and runs. A longer example is available in the definition file provided.

```
%test
  pyfiglet --version
```

Reference:
- https://apptainer.org/docs/user/latest/definition_files.html#test

Exercise 3: The `%help` section

The **`%help`** section is also optional and makes information available to the user if they invoke the `` `apptainer run-help` `` command on the container.

```
%help
  This container runs a Python Figlet script that prints
  a banner to the console from the text given on the
  command line.
```

Reference:

- https://apptainer.org/docs/user/latest/definition_files.html#help

Exercise 3: The `%labels` section

The **`%labels`** section, also optional, allows the specification of metadata in the container image. These are arbitrary, simple key-value pairs.

```
%labels
  Maintainer Drew Leske
  Version 0.0.1
```

Reference:
- https://apptainer.org/docs/user/latest/definition_files.html#labels

Exercise 3: Other sections

There are other sections we don’t need for our example and haven’t included but sometimes very useful:

- `%arguments` allows for customizing the image on build through the command line
- `%setup`: for preparation on the build host before %post (careful!)
- `%environment`: for setting env. variables for the container runtime

Maybe less useful:

- `%app`: advanced topic, left as an exercise to the reader
- `%startscript`: used when operating the container as an instance

Exercise 3: Building the container

That’s it! Save and close, and you now have a definition file. 🥳 Shall we try building it?

HOLD ON THOUGH

Exercise 3: Building the container on the cluster

Building containers can consume a non-trivial amount of resources, and for our trivial container, the building is more intensive than the running. The login node is not the place to do this as it will impact others. We'll submit this to the cluster as a job.

```
#!/bin/bash
#SBATCH --mem=1G

module load apptainer
unset APPTAINER_BIND
apptainer build -F figgy.sif figgy.def
```

I've provided a job file for this in the `exercise_3_pt2` directory: `make-figgy.job`. Copy this into the same directory as your figgy.def file, and then run:

```
$ sbatch make-figgy.job
Submitted batch job 114
```

Exercise 3: Building the container on the cluster

Watch for the build job to finish:

```
$ watch squeue
```

You should see your job. When it disappears hit `Ctrl-C` and you should have a job output file (ex. `slurm-114.out`) and if the build was successful, a new image file (`figgy.sif`).

No image file?
- Have look at the output file and see if you can figure out what the issue was, and try again.
- If all else fails, grab mine: `` `cp ~user0063/share/figgy.sif .` ``

Exercise 3: Try out your container

To use your container in this environment, you'll need to make the runtime available with `module load apptainer`. Then explore some of the things you can do:

```
$ module load apptainer
$ apptainer inspect figgy.sif     # look at the metadata
$ apptainer run-help figgy.sif    # get help running the container
$ apptainer run figgy.sif hi      # run the container with parameter "hi"
$ ./figgy.sif hi hello hooray     # also run the container
```

Exercise 3: Next steps

- Copy your container off the MC and run it somewhere else, like another Linux distro (so long as the apptainer runtime is there)

- Read up on Apptainer: https://apptainer.org/docs/user/latest/introduction.html

- Explore the Alliance's documentation on Apptainer: https://docs.alliancecan.ca/wiki/Apptainer

Afterparty!

TL;DR on Reproducibility

- Develop an organized filesystem
- Use clear file names
- Document your dataset with a readme
  - Authors and source info
  - Variable codes, units, etc.
  - Software version and dependencies
  - License
- Automate your workflow with scripts
- Annotate your code
- Implement version control practices
- Use containers to capture your computer environment

Git repository with our teaching materials:
https://github.com/saehuber/reproducibility-workshop-2025

Additional Resources:

Content in today's workshop was repurposed from an earlier 2019 workshop for data curators:

- Khair & Sawchuk. (2019). "Curating Data Sets for Reproducibility", GitHub repository. https://research-reuse.github.io/

Suggested readings on reproducibility:

- Broman, K. (n.d.) Initial steps toward reproducible research. Accessed May 2024 from https://kbroman.org/steps2rr/
- The practice of reproducible research: Case studies and lessons from the data-intensive sciences. Kitzes, J., Turek D., & Deniz, F. (Eds.). (2018). Oakland, CA: University of California Press. https://www.practicereproducibleresearch.org