IT Services

Reproducible Scientific Computing and Data Analysis

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Scientific IT Services, ETH Zurich

November 5, 2025

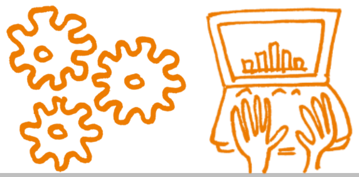
Slides & Materials: https://siscourses.ethz.ch/reproducible_computing/

BY NC SA

Overview of today's workshop

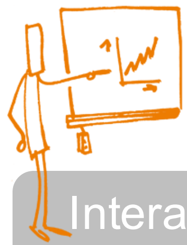
Setting the Scene

Managing your Source Code



Managing Dependencies & Computing Environments

Virtualizing Computing Environments



Interactive Computational Notebooks

Reproducible Computing Platforms

Image credit: Open Science Training Handbook

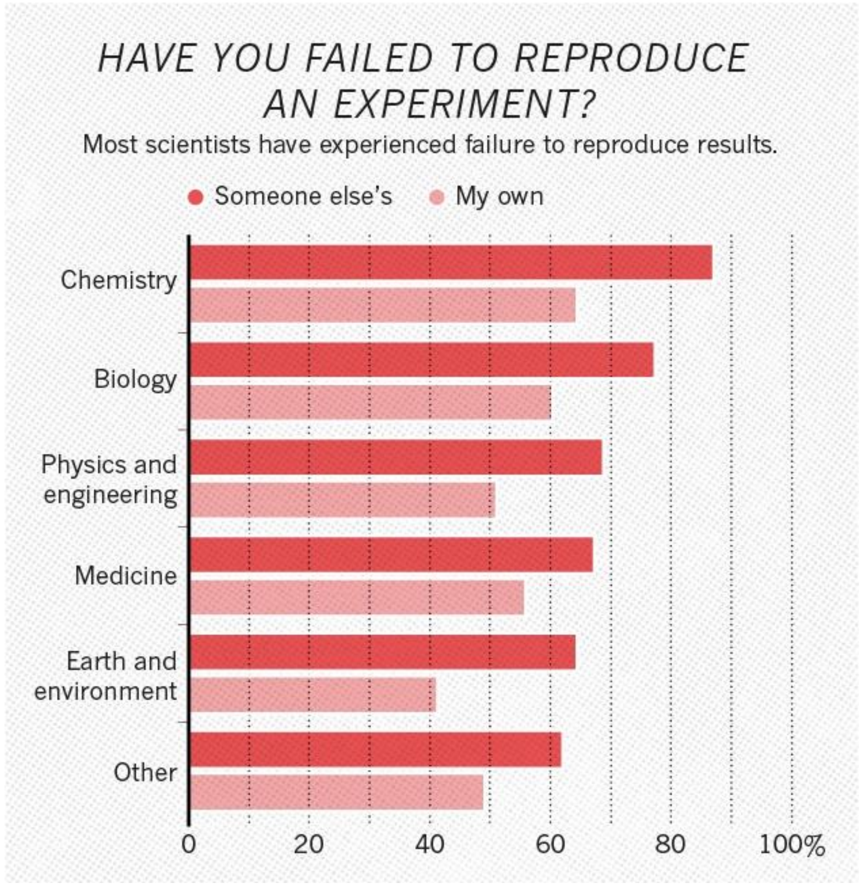
Setting the Scene

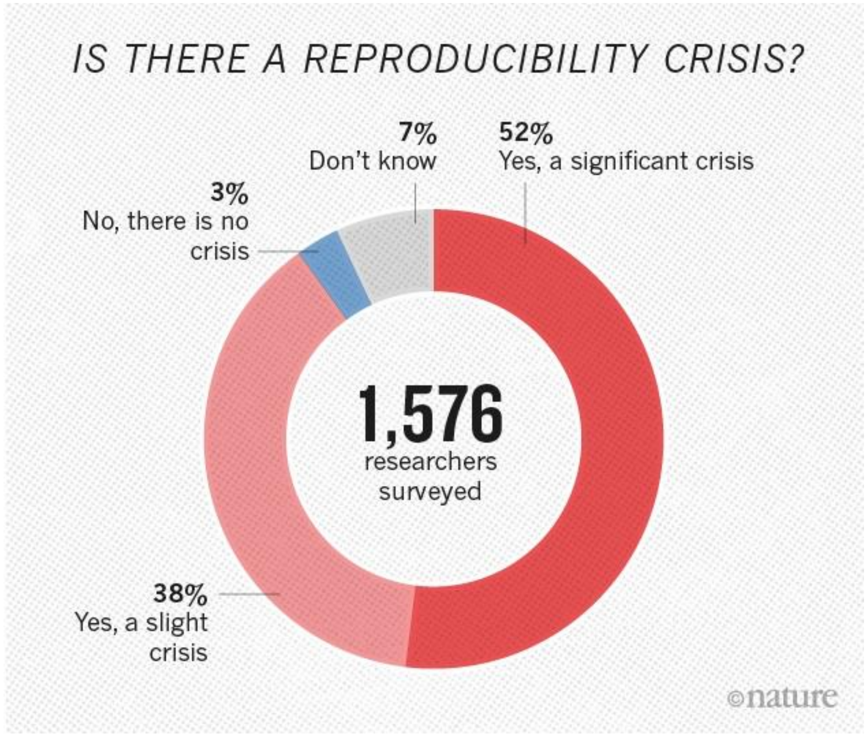
The Economist
Washington's lawyer surplus
How to do a nuclear deal with Iran
Investment tips from Nobel economists
Junk bonds are back
The meaning of Sachin Tendulkar
HOW SCIENCE GOES WRONG

The National Academies of SCIENCES · ENGINEERING · MEDICINE
CONSENSUS STUDY REPORT
Reproducibility and Replicability in Science

Reproducibility & Replicability in Science

Nature survey on reproducibility across all scientific domains





[Nature 533, 452–454 (26 May 2016) doi:10.1038/533452a](https://doi.org/10.1038/533452a)

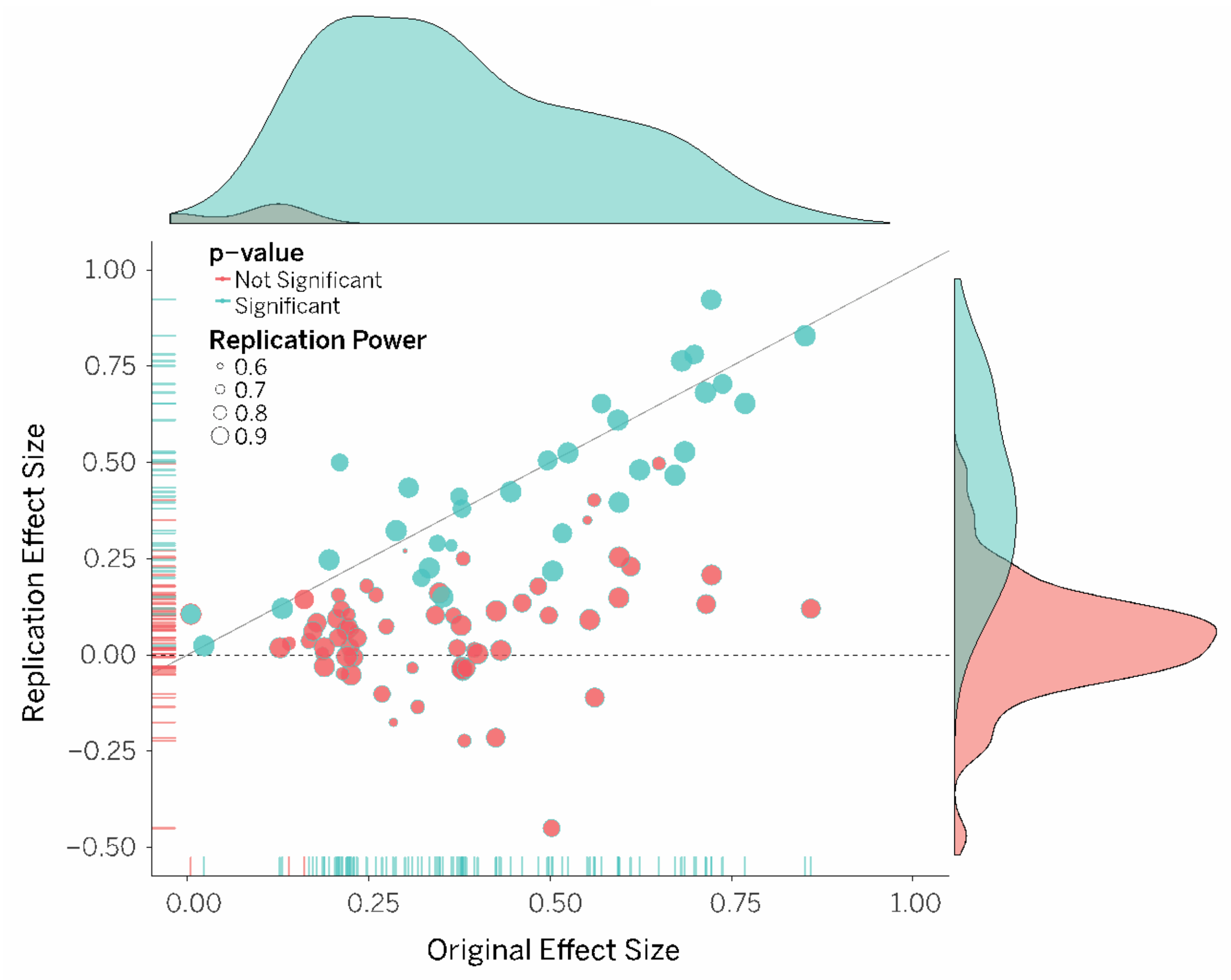
Reproducibility & Replicability in Science

RESEARCH ARTICLE

Estimating the reproducibility of psychological science

Open Science Collaboration*,†
+ See all authors and affiliations

Science 28 Aug 2015:
Vol. 349, Issue 6251, aac4716
DOI: 10.1126/science.aac4716



The *Reproducibility project*

- Replicate 100 experiments published in top psychology journals
- One-half to two-thirds of original findings could not be observed in the replication study

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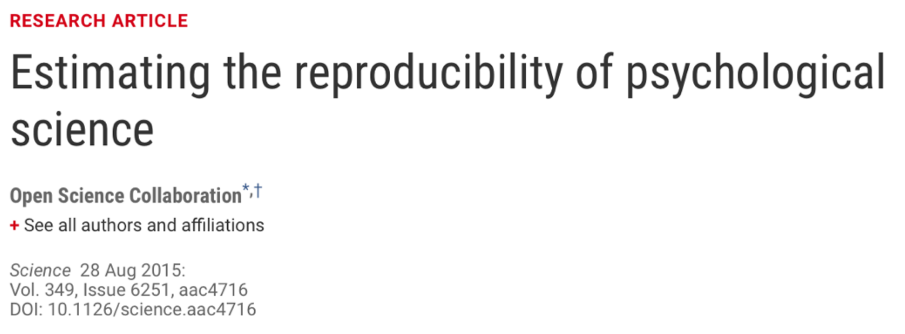

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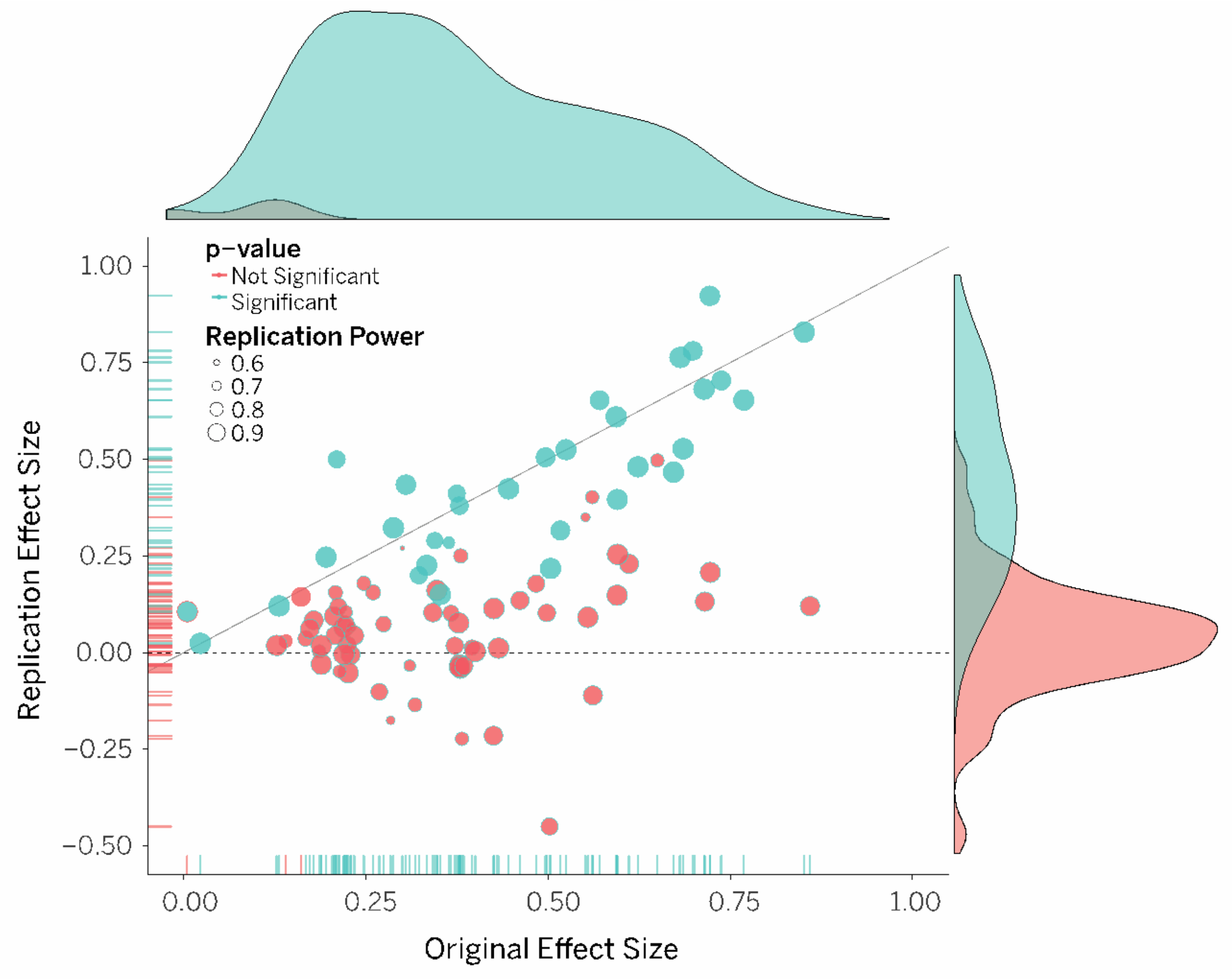
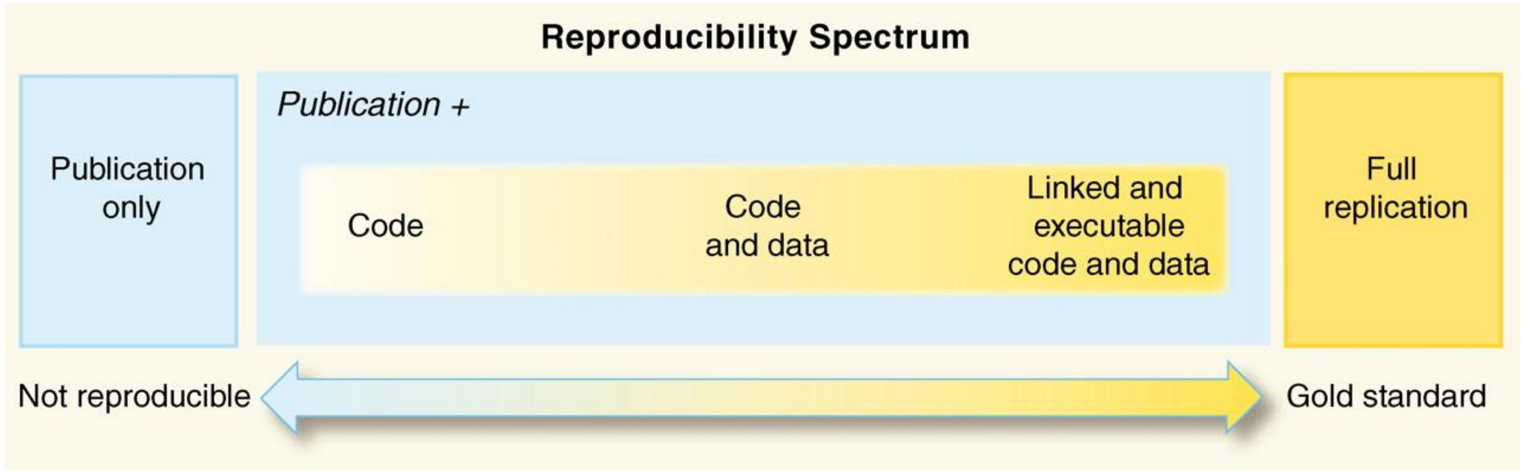


Reproducibility & Replicability in Science

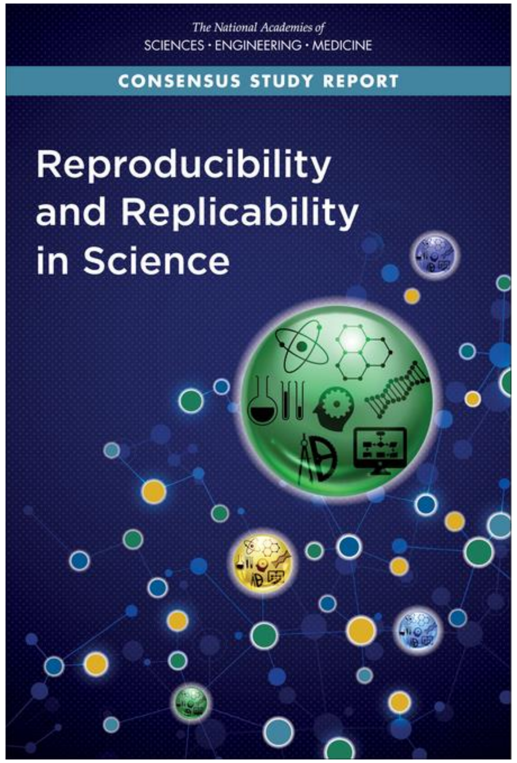
Replication:
new data and / or new method in independent study = same finding

Reproducible research:
same data + same method = same results



Peng (2011). doi:10.1126/science.1213847

Defining the Scope: Computational Reproducibility


The National Academies of SCIENCES · ENGINEERING · MEDICINE
CONSENSUS STUDY REPORT
Reproducibility and Replicability in Science

«**Reproducibility** is obtaining consistent results using the same input data, computational steps, methods, and code and conditions of analysis. The term is synonymous with *"computational reproducibility"*... »

«To help ensure the reproducibility of computational results, researchers should **convey clear, specific, and complete information about any computational methods and data products that support their published results in order to enable other researchers to repeat the analysis**, unless such information is restricted by non-public data policies. That information should include the data, study methods, and **computational environment**. »

National Academies of Sciences, Engineering, and Medicine (2019). https://doi.org/10.17226/25303

Reproducibility ≠ Correctness

Computational Reproducibility: What can go wrong?

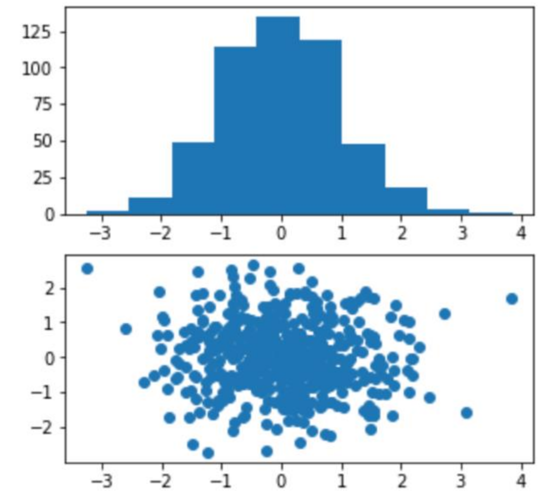
- Code only runs on specific **operating system**
  - Examples: Windows / Linux scripts, special programs (e.g. *SigmaPlot*)
- Code has specific **external dependencies**
  - Example: wget https://zenodo.org/record/1234567/files/dataset.zip
- Code has specific **internal dependencies** (libraries, modules etc.)

```python
import matplotlib.pyplot as plt
import numpy as np

np.random.seed(42)
data = np.random.randn(2, 500)

fig, axs = plt.subplots(2, 1, figsize=(5, 5))
axs[0].hist(data[0])
axs[1].scatter(data[0], data[1])

plt.show()
```



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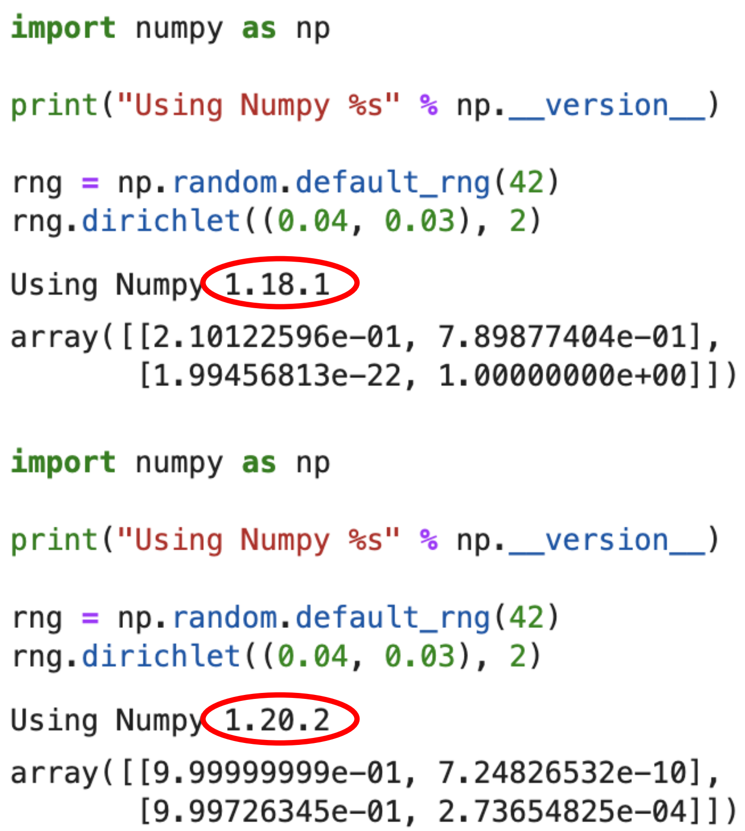
- Code has specific **version dependencies**
- Code may rely on availability of specific **software licenses**
  - Example: fastaread function in the MATLAB Bioinformatics Toolbox



```
import numpy as np

print("Using Numpy %s" % np.__version__)

rng = np.random.default_rng(42)
rng.dirichlet((0.04, 0.03), 2)

Using Numpy 1.18.1

array([[2.10122596e-01, 7.89877404e-01],
       [1.99456813e-22, 1.00000000e+00]])
```

```
import numpy as np

print("Using Numpy %s" % np.__version__)

rng = np.random.default_rng(42)
rng.dirichlet((0.04, 0.03), 2)

Using Numpy 1.20.2

array([[9.99999999e-01, 7.24826532e-10],
       [9.99726345e-01, 2.73654825e-04]])
```

See https://numpy.org/doc/stable/release/1.19.0-notes.html#changed-random-variate-stream-from-numpy-random-generator-dirichlet

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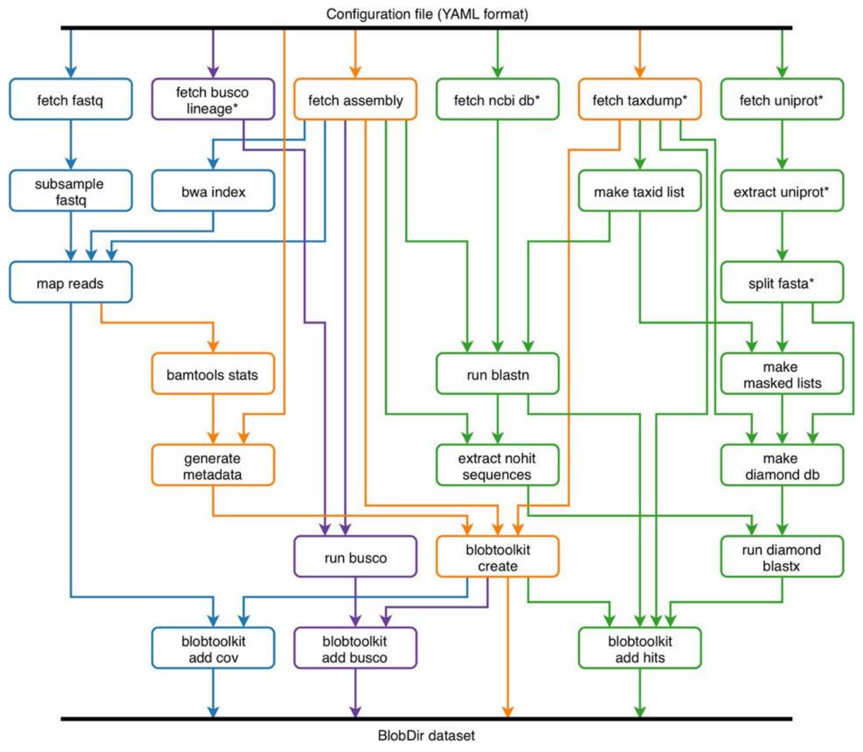

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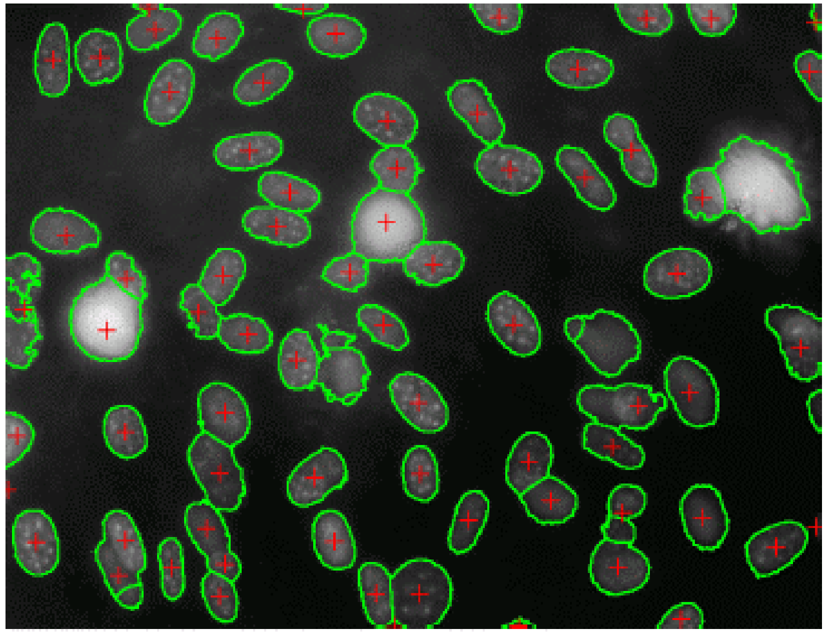
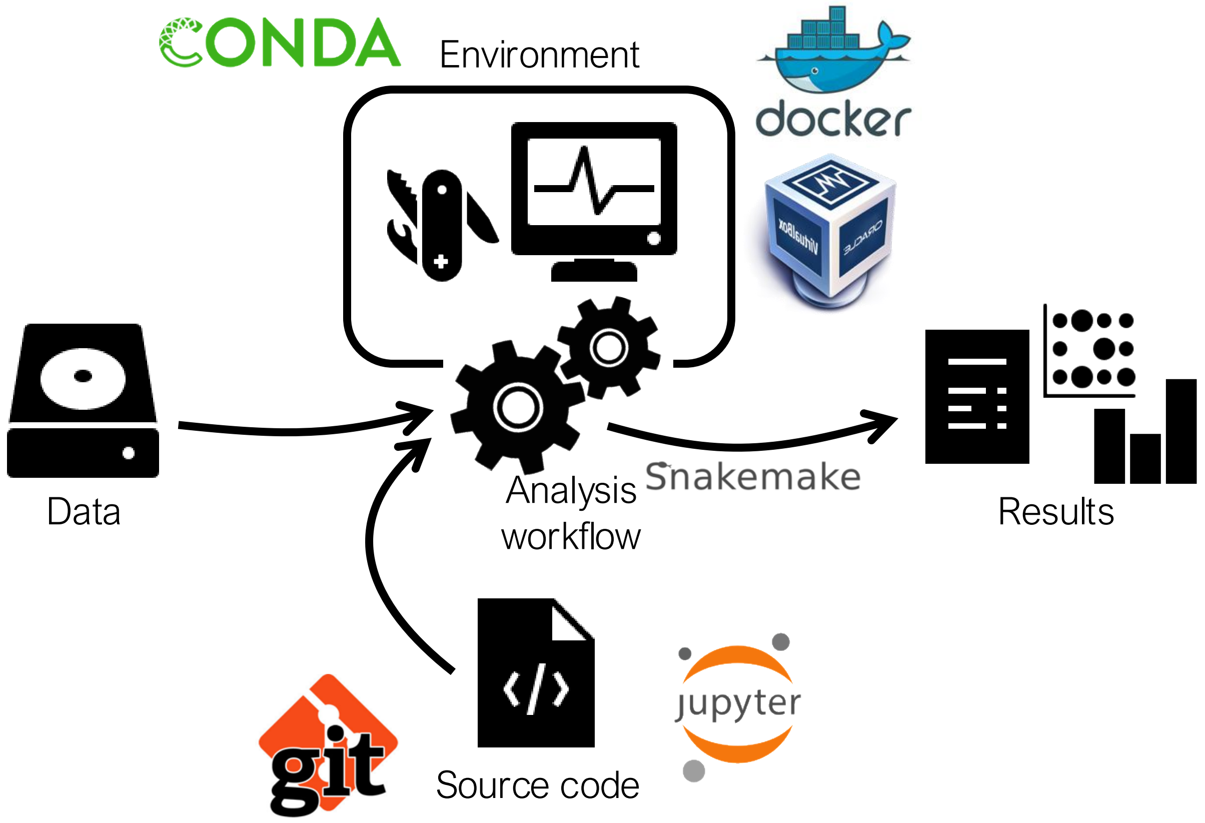
- Analysis workflow may rely on **manual steps**



Computational Reproducibility: Pieces of the Puzzle

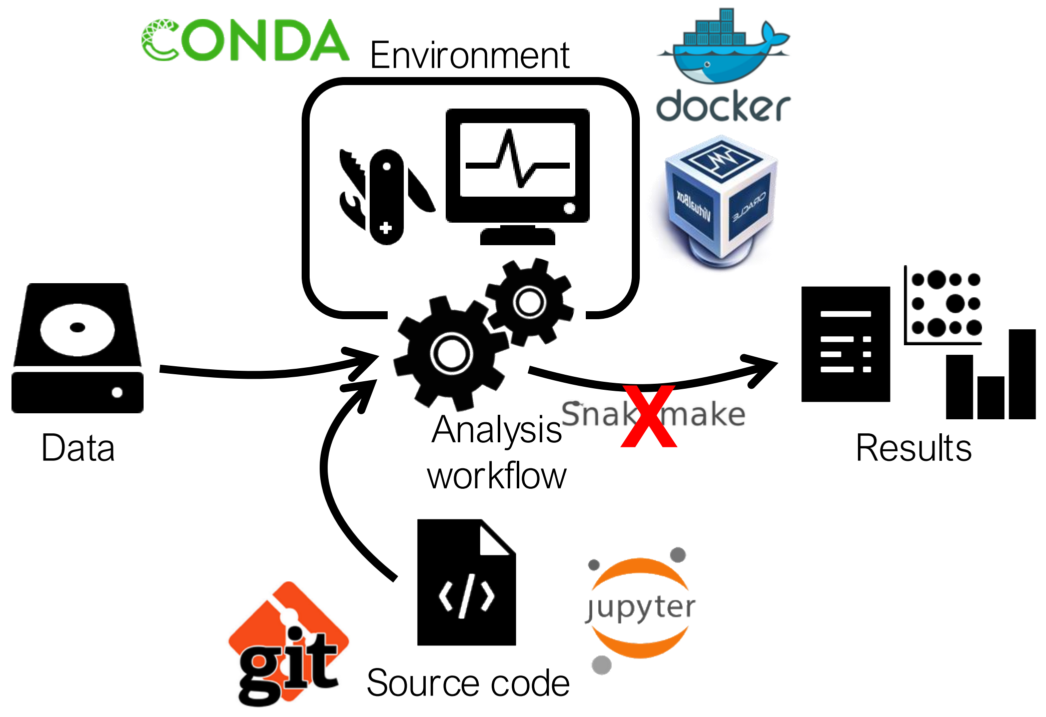
All parts of a computational analysis have to be reproducible!



Slide credit: L. Wigge, R. Ågren & J. Sundh (NBIS & SciLifeLab, Sweden)

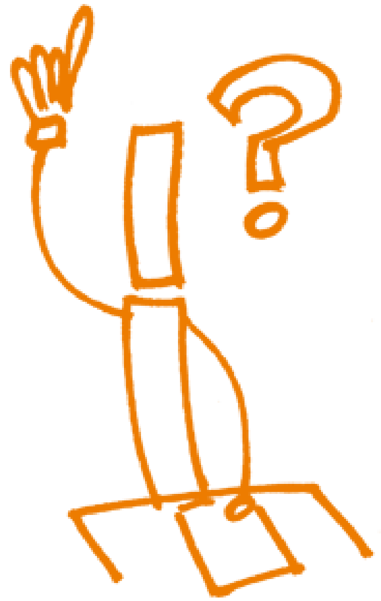
Computational Reproducibility: Pieces of the Puzzle

What is covered in today's workshop?



Part 1	**Version control** Track and backup your project history
Part 2	**Environment management** Setup and manage your project environment
Part 3	**Virtual machines / containers** Make your project self-contained and distributable
Part 4	**Notebooks** Document your exploratory analysis
Part 5	**Reproducible computing platforms** Out-of-the-box computational reproducibility

Computational Reproducibility: Questions?



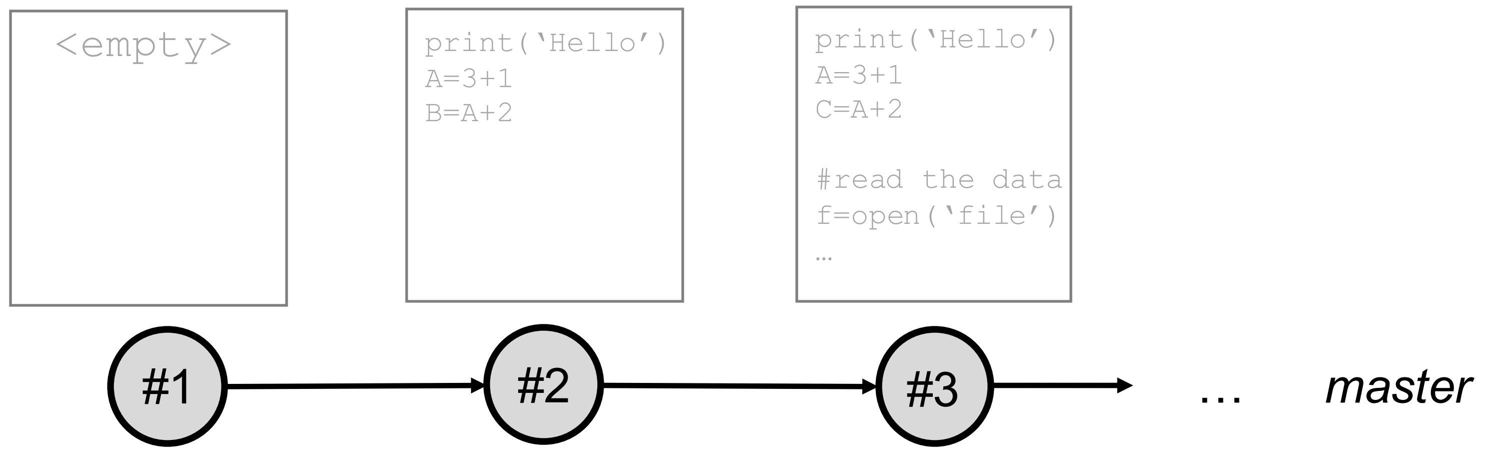
Tell us a bit about yourself

data
workflow
web
open
possible
guide
reproduction
tools
end
work
research
framework
web-based
example
study
reliability
analysis
ability
overall
used
science
free
reproducibility
need
include
bioinformatics
steps
results
researchers
workflows
cases
number
code
computational
automated
without
practices
process
five
reproducible
pillars
step
errors
patient
similar
software
findings
ensure
end-to
scripted

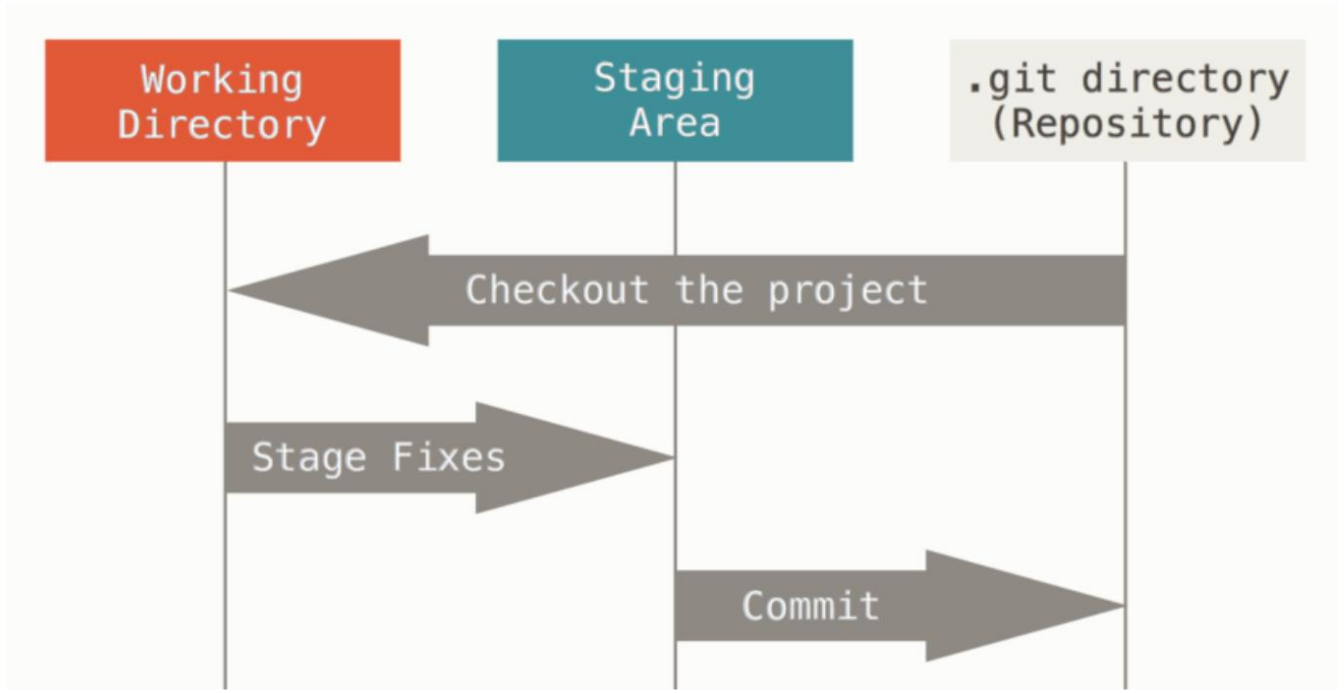
Managing your Source Code

Code Management

- Code management is the process of handling changes in source code
- Proper code management is essential to ensure **reproducible results**
- Professional code management relies on **Version Control Systems** (VCS)
  - Version control: tracking changes made to text files over time
- **Git** is by far the most popular version control system used world-wide in the software community



How do I track the changes in my code with git?



The basic Git workflow

- Modify files in your working directory
- Selectively stage the changes you want to be part of your next commit, adding `only` those changes to the staging area
- Make a commit, which takes the files as they are in the staging area and stores that snapshot permanently to your .git directory

[demo]

Test case : a program that takes in three files and print their content. Text_1.txt contains the string “one”, text_2.txt ”two”, etc

```
git_demo 13:58:33 >>ls
total 32
-rw-r-xr-x  1 nmarounina  staff  49 Mar  7 13:57 print_all.sh
-rw-r--r--  1 nmarounina  staff   4 Mar  7 13:54 text_1.txt
-rw-r--r--  1 nmarounina  staff   4 Mar  7 13:54 text_2.txt
-rw-r--r--  1 nmarounina  staff   6 Mar  7 13:54 text_3.txt
git_demo 13:59:00 >>./print_all.sh
one
two
three
git_demo 13:59:02 >>
```

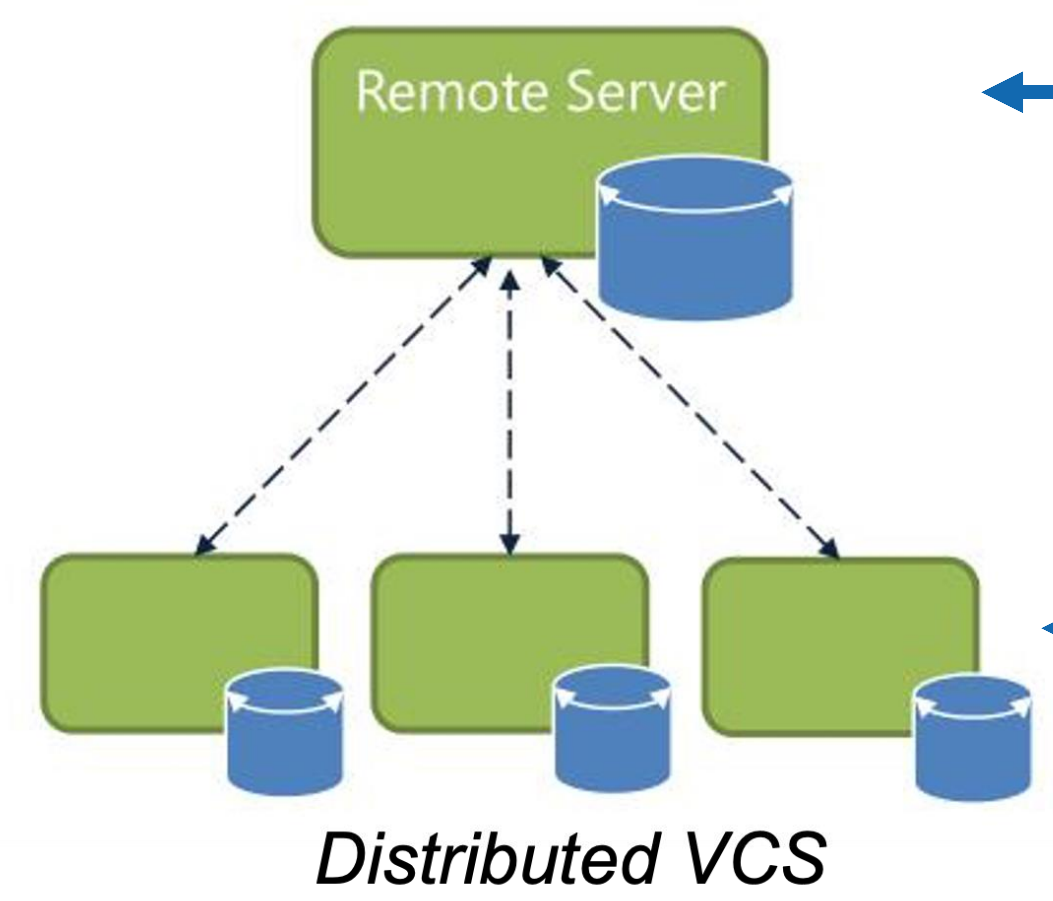
Start with git :

```
git_demo 13:59:20 >>git init #initialises git
Initialized empty Git repository in /Users/nmarounina/Desktop/git_demo/.git/
git_demo 13:59:24 >>
git_demo 13:59:34 >>git add * #adds all files to the staging
git_demo 13:59:40 >>git status #prints information about the current staging area
On branch main

No commits yet

Changes to be committed:
  (use "git rm --cached <file>..." to unstage)
        new file:   print_all.sh
        new file:   text_1.txt
        new file:   text_2.txt
        new file:   text_3.txt

git_demo 13:59:50 >>
```

First commit :

```
git_demo 13:59:52 >>git commit -m "Initial commit” #creating the first commit/snapshot
[main (root-commit) d5badf3] Initial commit
 4 files changed, 5 insertions(+)
 create mode 100755 print_all.sh
 create mode 100644 text_1.txt
 create mode 100644 text_2.txt
 create mode 100644 text_3.txt
git_demo 14:00:16 >>git log #lists all of the commits for this project
commit d5badf3593de0e511005eee061132d77cdde0823 (HEAD -> main)
Author: Nadia Marounina <nmarounina@ethz.ch>
Date:   Thu Mar 7 14:00:10 2024 +0100

    Initial commit
git_demo 14:00:20 >>
```

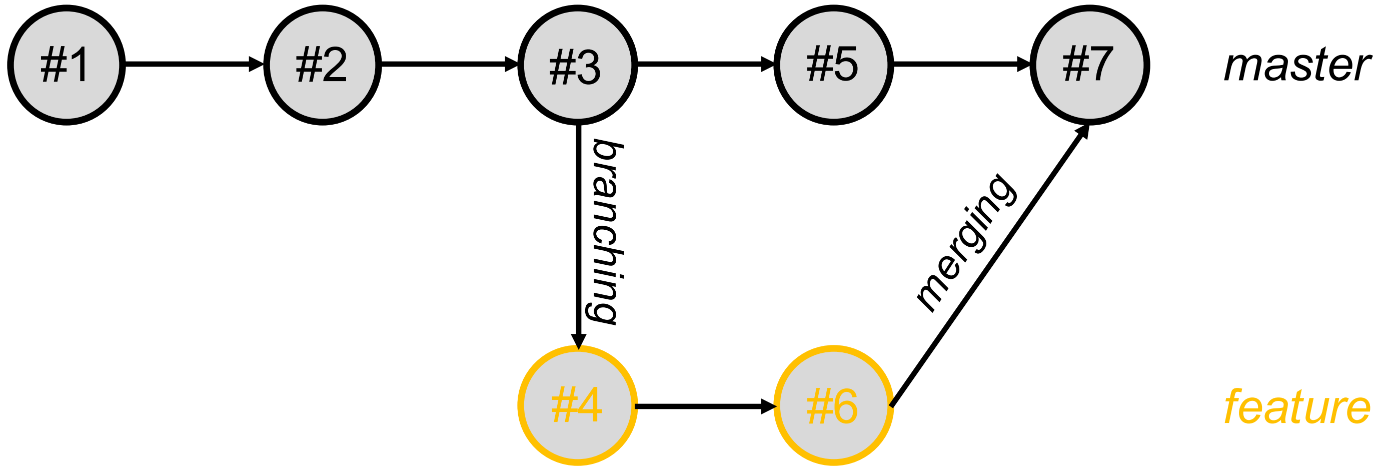
Git : How to share my code with others ?



GitHub, Gitlab, etc..

Personal workstations

Git branching & merging



Git branches & merges

- The initial / default branch is typically called *master* or *main*
- Git manages branches very efficiently
- When merging merging branches, conflicts must be resolved carefully

[demo]

Creating a new branch:

```
git_demo 14:03:15 >>git branch numbers #creates a new branch named "numbers"
git_demo 14:04:00 >>git status
On branch main
nothing to commit, working tree clean
git_demo 14:04:03 >>git branch #list all branches for the project
* main
  numbers
git_demo 14:04:35 >>git checkout numbers #switch to the new branch
Switched to branch 'numbers'
git_demo 14:04:53 >>
```

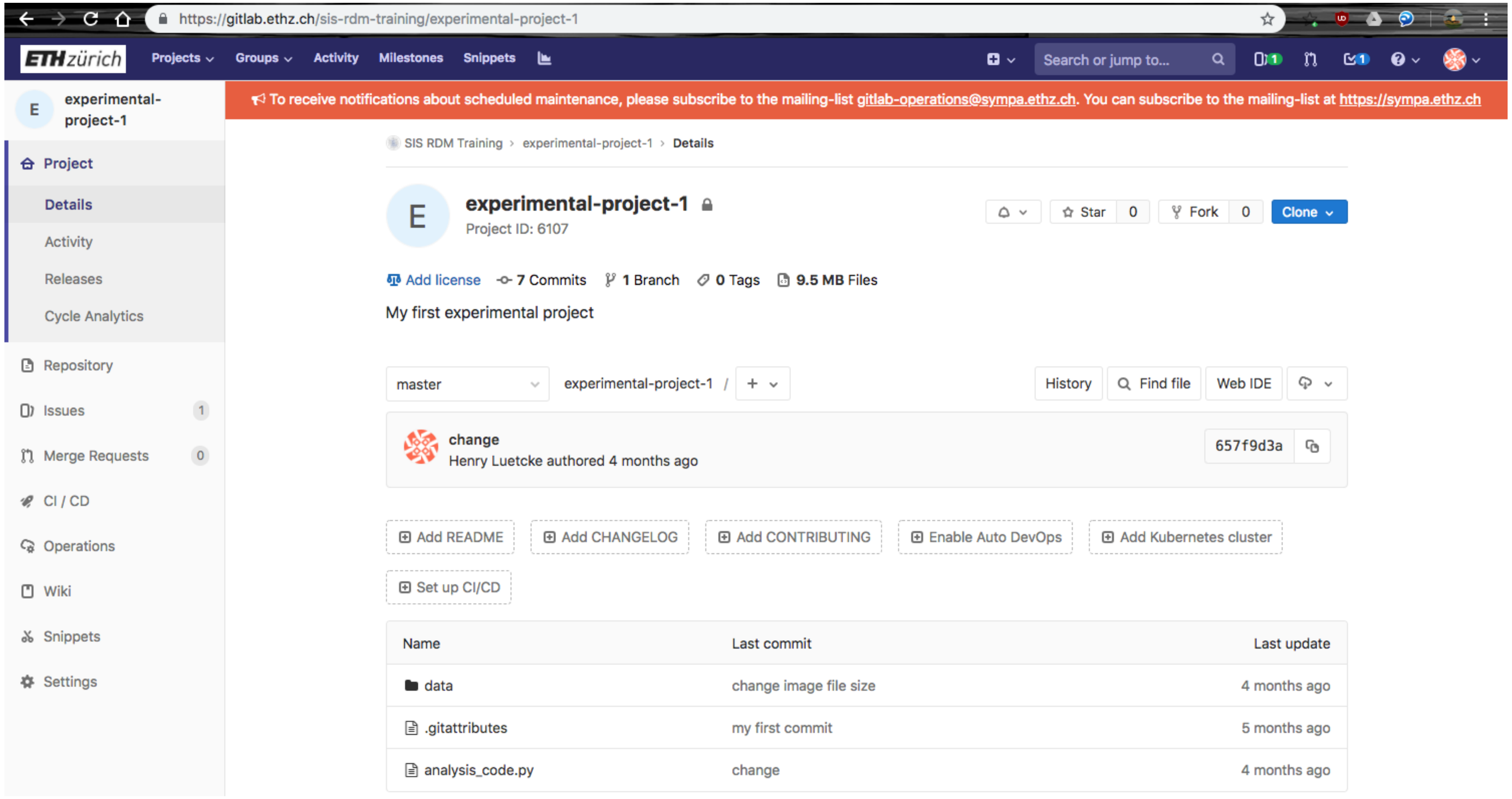
After changing the three text files in the new branch and commiting it again :

```
git_demo 14:04:56 >>vi text_1.txt #vi is a text editor. Here I change ‘one’ to ‘1’…
git_demo 14:05:07 >>vi text_2.txt #... ‘two’ to ‘2’
git_demo 14:05:16 >>vi text_3.txt  #... ‘three’ to ‘3’
git_demo 14:05:29 >>./print_all.sh
1
2
3
git_demo 14:05:37 >>git commit -m "Changed from text to number” #the change has been
committed
[… output excluded …]
git_demo 14:05:51 >>
```

By switching branches, you change your files in your folder:

```
git_demo 14:06:39 >>git checkout main
Switched to branch 'main'
git_demo 14:07:29 >>./print_all.sh
one
two
three
git_demo 14:07:40 >>git checkout numbers
Switched to branch 'numbers'
git_demo 14:07:45 >>./print_all.sh
1
2
3
git_demo 14:07:46 >>
```

ETH Zurich GitLab Service



https://gitlab.ethz.ch/sis-rdm-training/experimental-project-1
Projects Groups Activity Milestones Snippets
Search or jump to...

To receive notifications about scheduled maintenance, please subscribe to the mailing-list gitlab-operations@sympa.ethz.ch. You can subscribe to the mailing-list at https://sympa.ethz.ch

experimental-project-1

Project ID: 6107

My first experimental project

change

Henry Luetcke authored 4 months ago

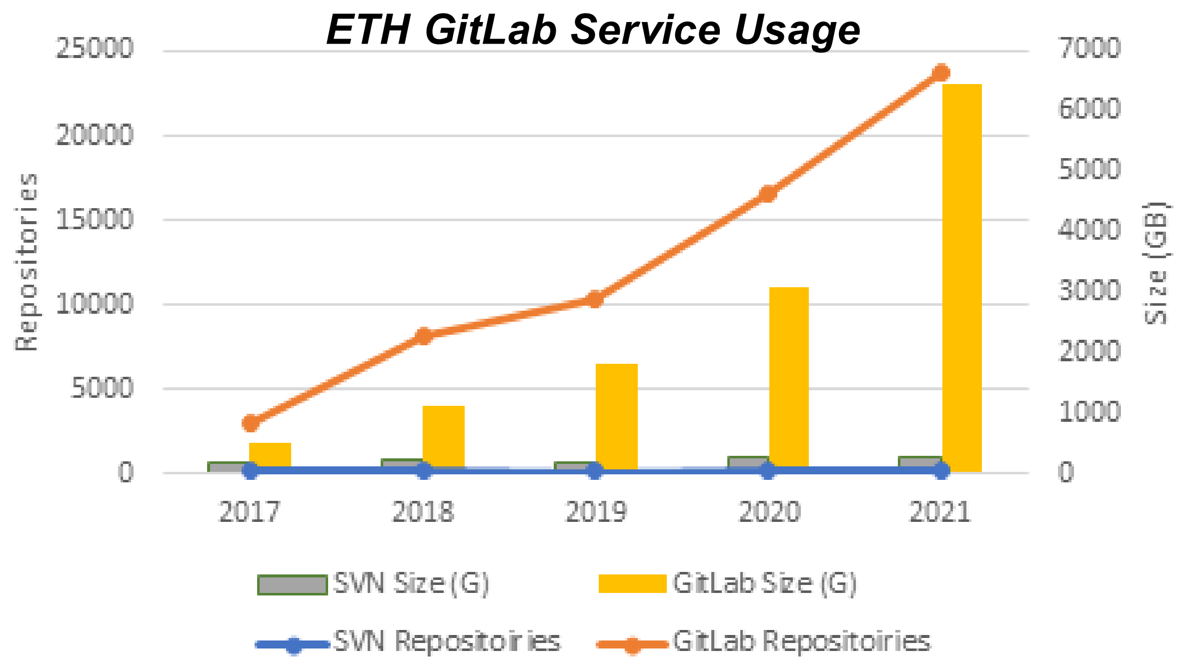
657f9d3a

Name	Last commit	Last update
data	change image file size	4 months ago
.gitattributes	my first commit	5 months ago
analysis_code.py	change	4 months ago

https://gitlab.ethz.ch

ETH Zurich GitLab Service

- Integrated file, task and documentation management for individuals and / or groups
- Private, group and public repositories
- Built-in light-weight Wiki (protocols, list of materials etc.)
- Free for small repositories (< 2GB), otherwise yearly price of 250 CHF / TB / year
- Local and remote copies (off-site backup)
- Data can be exported (e.g. to Github)
- Built-in Container registry



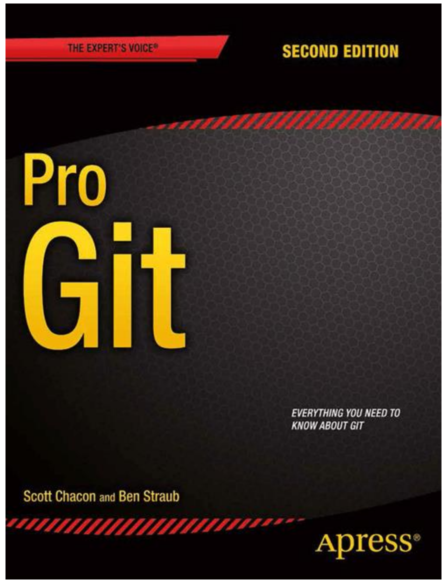
Git – General Recommendations & Resources

Recommendations for working with Git

- Commit early & often
- Provide short but meaningful commit messages
- Do not store large data files in Git repositories
  - e.g. images, movies, binary files
  - Use *.gitignore* file to exclude
  - Or consider tools such as git-lfs or git-annex
- Beware when resolving conflicts during *merge* or *pull* operations
  - A successful merge for Git may not be a successful merge for you

Resources for getting started with Git

- SIS can provide hands-on Git tutorials / workshops
- Pro Git book by S. Chacon & B. Straub
- Numerous tutorials available on the web / YouTube
  - W3Schools Git tutorial
  - Software Carpentry Git course
  - Git tutorial for scientists
- List of Git GUI clients


THE EXPERT'S VOICE®
SECOND EDITION
Pro
Git
EVERYTHING YOU NEED TO KNOW ABOUT GIT
Scott Chacon and Ben Straub
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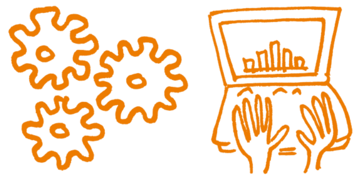
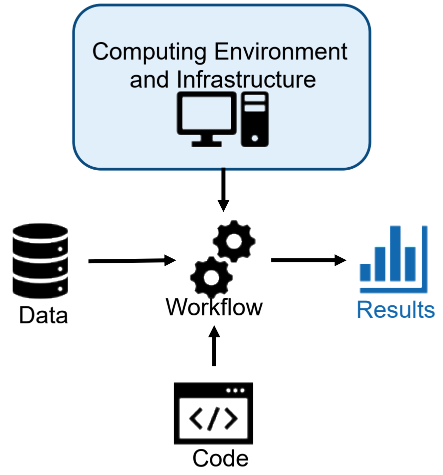
Management of source code: Questions?

Managing Dependencies & Computing Environments

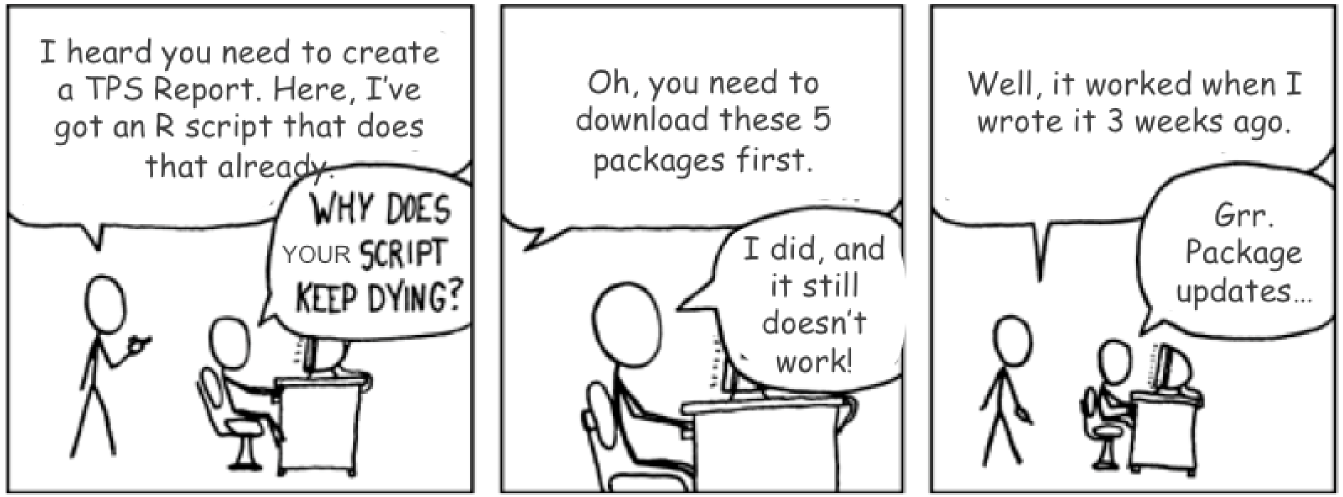


Reproducible Computing Environment

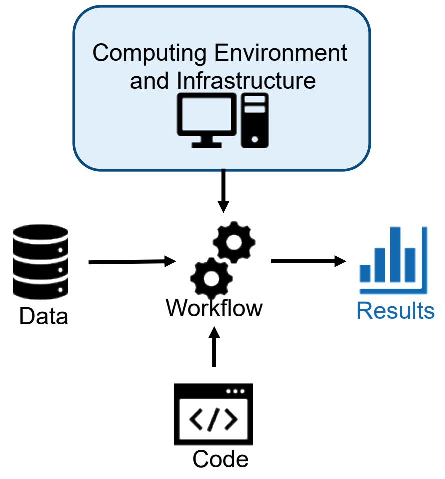


Problem:

Full reproducibility requires the possibility to recreate the system that was originally used to generate the results


I heard you need to create a TPS Report. Here, I've got an R script that does that already.
WHY DOES YOUR SCRIPT KEEP DYING?
Oh, you need to download these 5 packages first.
I did, and it still doesn't work!
Well, it worked when I wrote it 3 weeks ago.
Grr. Package updates...

Reproducible Computing Environment



Problem:

Full reproducibility requires the possibility to recreate the system that was originally used to generate the results

Solution:

Bundle your application and all dependencies

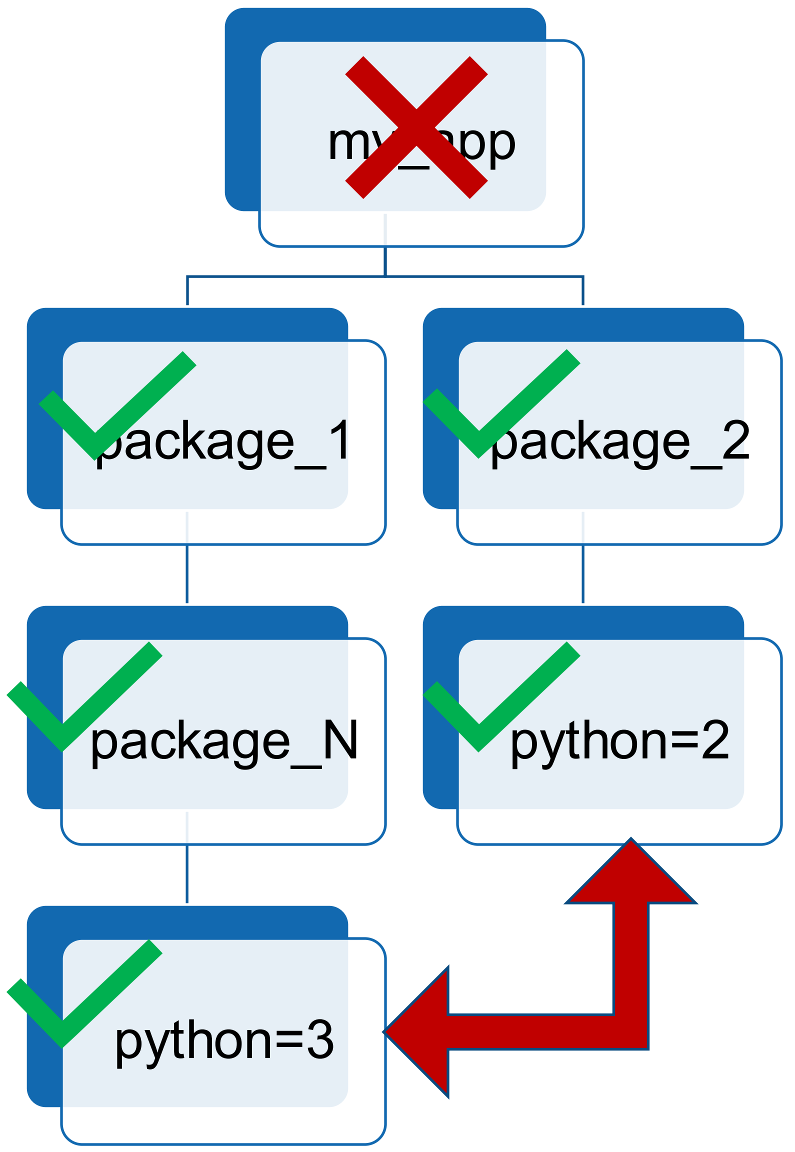
→ Environment Isolation & Dependency management

Tools:

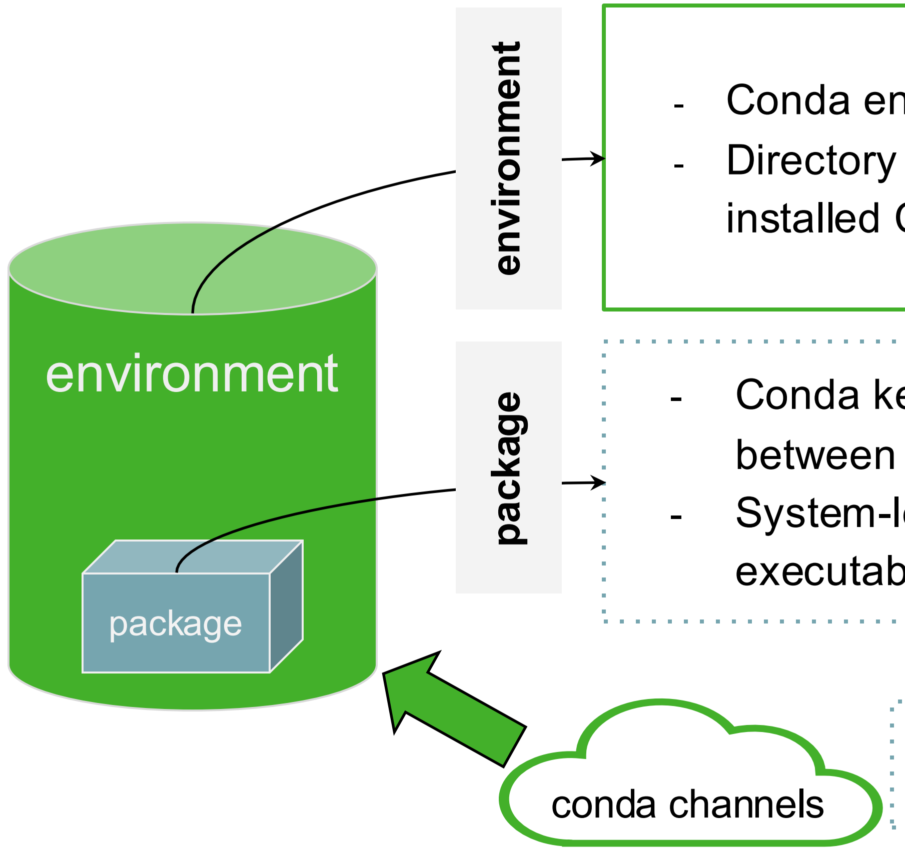
- Application / software level: Conda, pip, virtualenv, renv, Devbox
- Containerization: Docker
- Virtualization (Virtual Machine, VM): VirtualBox, Vmware, Parallels

Reproducible Environment for R and Python

- Open source: Anaconda, Miniconda, Miniforge
- Commercial support: Anaconda Enterprise
  - ***Note:*** *certain functionality requires a paid license outside education / academia*
- Multi-platform: Windows, macOS, Linux
- Environment Management System
  - Isolated computing environments on the same system
  - Documentation of the computing environment
- Package Management System
  - Supported programming Languages: Python, R, …
  - System libraries shipped in binary format
  - Resolve dependencies & conflicts between packages



Conda in a Nutshell



- Conda environments are isolated
- Directory containing specific collection of installed Conda packages

- Conda keeps track of the dependencies between packages
- System-level libraries, Python or other modules, executable programs, other components

- Remote directories with packages

environment.yml

```
channels:
- conda-forge

dependencies:
- python=3.8
- jupyterlab
```

Conda automatically creates an environment file with packages and dependencies

Slide credit: L. Wigge, R. Ågren & J. Sundh (NBIS & SciLifeLab, Sweden)

Environment and Package Management Systems

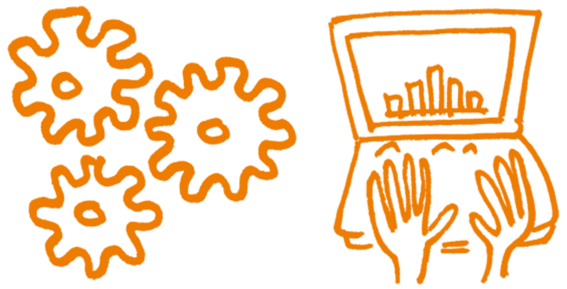
Language	**Environment Management**	**Package Management**	**Comments**
Python 2 (not supported)	virtualenv, conda	pip, conda	
Python 3	venv, virtualenv, pipenv poetry, uv, conda	pip, pipenv, poetry, uv, conda	Not all can install different Python versions
R	renv, conda	renv, conda	only conda can install different R versions
Julia	Pkg, conda	Pkg, conda	conda provides outdated Julia versions
Matlab	N/A	Add-on manager, Matlab Package Manager (unofficial)	Matlab search path determines dependencies

Alternatives to Conda are emerging!

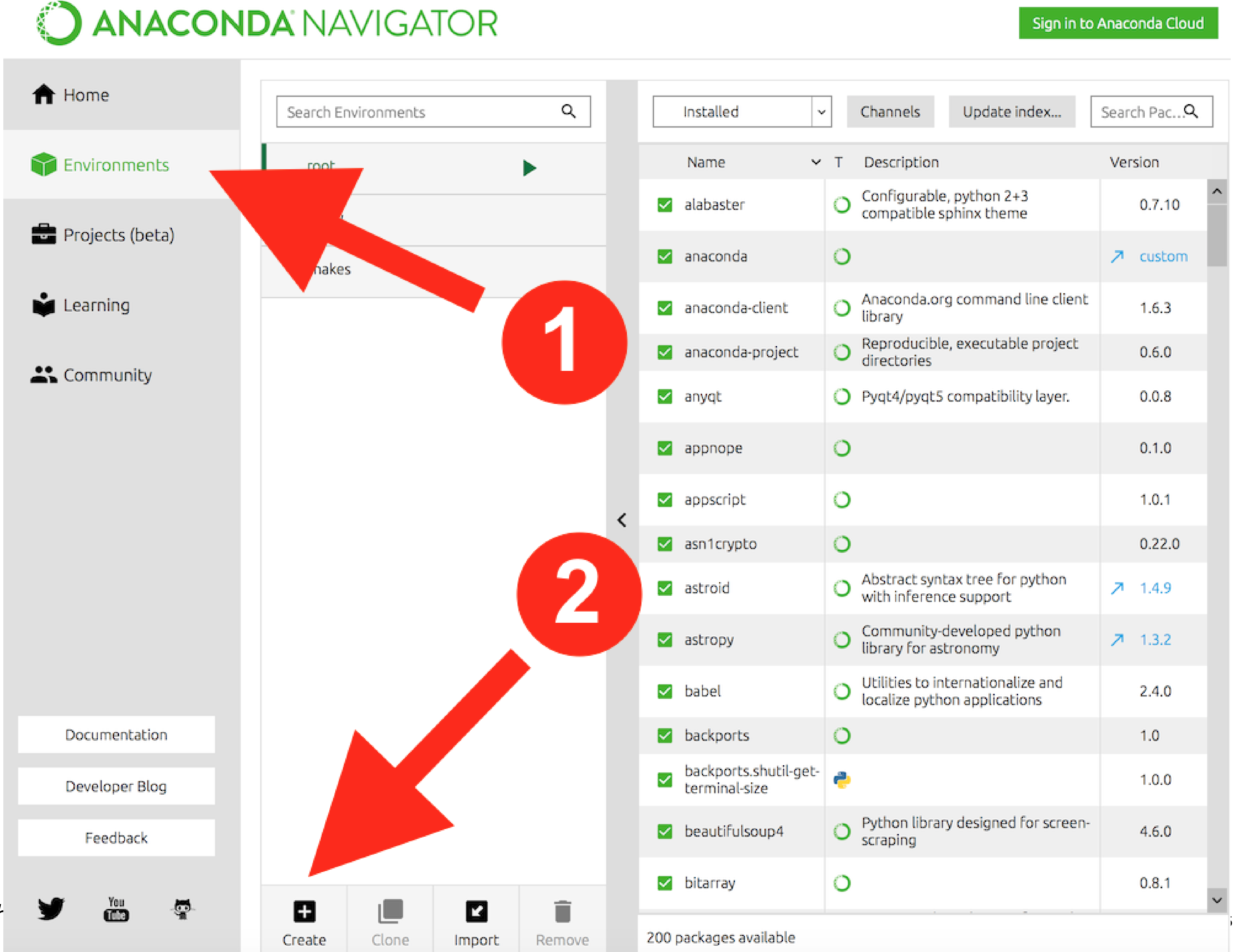
pixi

Devbox

Conda Hands-on Session



https://siscourses.ethz.ch/reproducible_computing/Conda.slidy.html



	Name	T	Description	Version
✓	alabaster	○	Configurable, python 2+3 compatible sphinx theme	0.7.10
✓	anaconda	○		↗ custom
✓	anaconda-client	○	Anaconda.org command line client library	1.6.3
✓	anaconda-project	○	Reproducible, executable project directories	0.6.0
✓	anyqt	○	Pyqt4/pyqt5 compatibility layer.	0.0.8
✓	appnope	○		0.1.0
✓	appscript	○		1.0.1
✓	asn1crypto	○		0.22.0
✓	astroid	○	Abstract syntax tree for python with inference support	↗ 1.4.9
✓	astropy	○	Community-developed python library for astronomy	↗ 1.3.2
✓	babel	○	Utilities to internationalize and localize python applications	2.4.0
✓	backports	○		1.0
✓	backports.shutil-get-terminal-size			1.0.0
✓	beautifulsoup4	○	Python library designed for screen-scraping	4.6.0
✓	bitarray	○		0.8.1

200 packages available

Conda - What can go wrong?

- The package metadata (dependency list) is updated (not very likely)
- The package is deleted by the owner
- The package is not available under another platform
- There is no conda package for what you are looking for
- Complex dependencies may fail or take a long time to resolve

Virtualizing Computing Environments

Conda - What can go wrong?

- The package metadata (dependency list) is updated (not very likely)
- **The package is deleted by the owner**
- **The package is not available under another platform**
- **There is no conda package for what you are looking for**
- Complex dependencies may fail or take a long time to resolve

Reproducible Environment

Problem:

Full reproducibility requires the possibility to recreate the system that was originally used to generate the results

Solution:

Bundle your application and all dependencies

→ Environment Isolation & Dependency management

Tools:

- Application / software level: Conda, pip, virtualenv, renv
- Containerization: Docker
- Virtualization (Virtual Machine, VM): VirtualBox, Vmware, Parallels

Reproducible Environment – Virtual Machines

- A virtual machine (VM) is an operating system (“guest”) that runs inside another computing environment (“host”).

- **Advantages:**
  - Allows multiple OS environments on a single physical computer
  - VMs are widely available and are easy to manage, maintain and distribute
  - Offers application provisioning and disaster recovery options

- **Drawbacks:**
  - They are not as efficient as a physical computer because the hardware resources are distributed in an indirect way.
  - Multiple VMs running on a single physical machine can deliver unstable performance

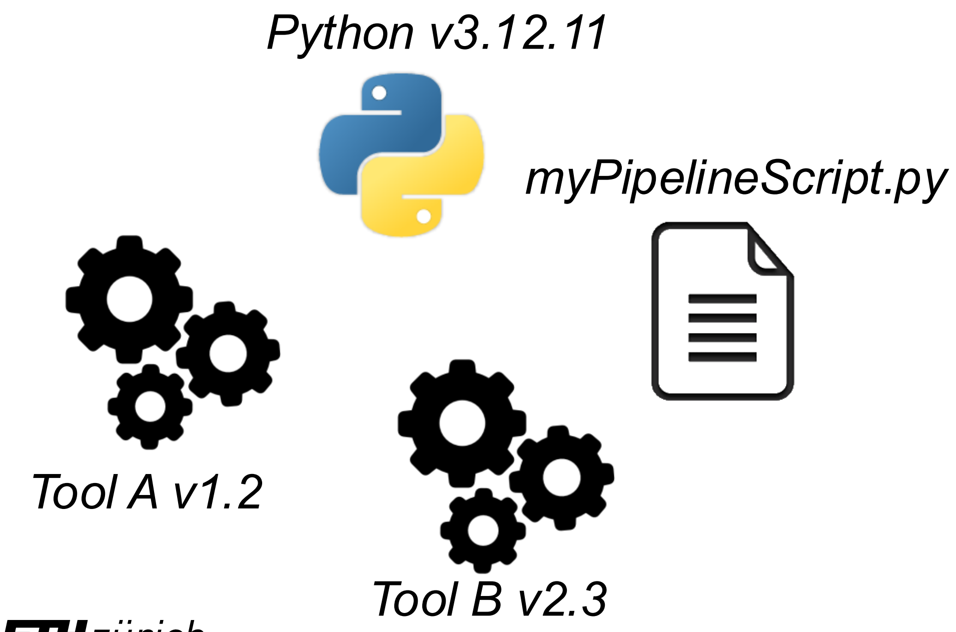
Source: https://searchservervirtualization.techtarget.com/definition/virtual-machine

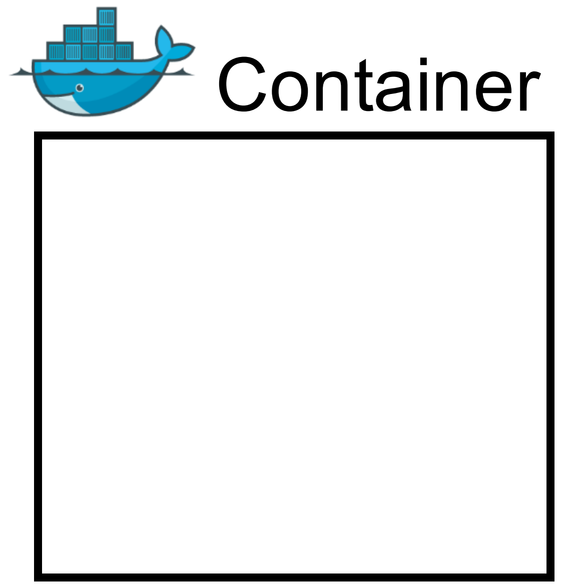
Reproducible Environment – Containerization

- ***Container****:* Operating system level **virtualization method** for running software without launching an entire virtual machine
- In simpler words: containers allow you to **package** your software / pipeline with the **dependencies** inside a **reproducible**, easy to **share**, **runnable** file

Reproducible Environment – Containerization

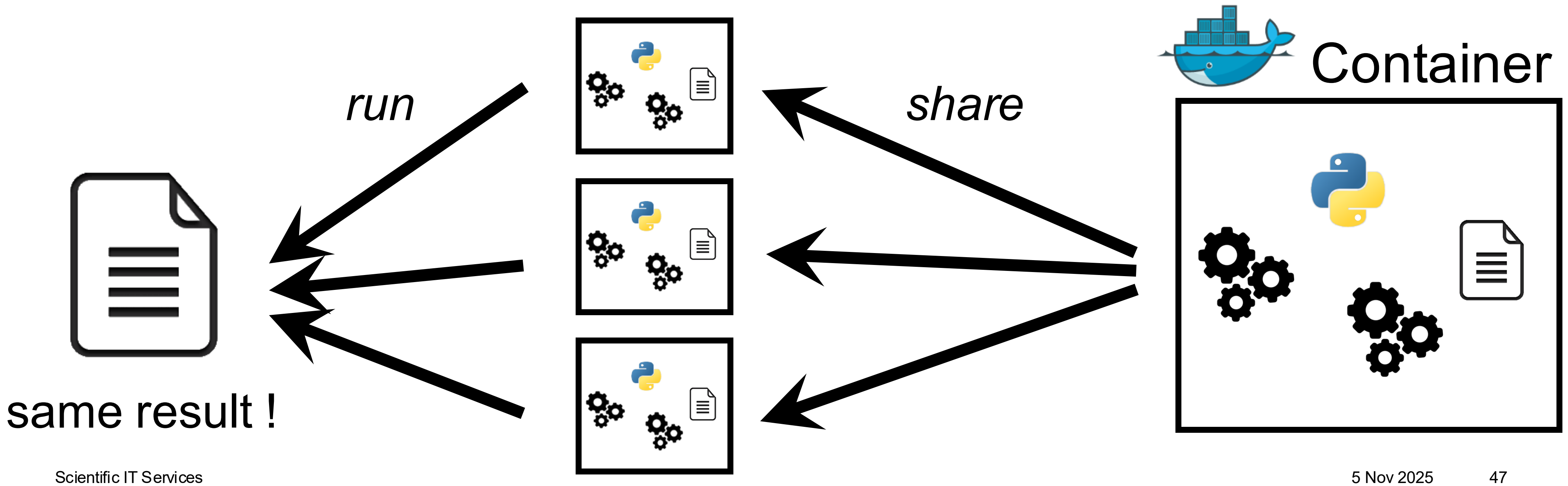
- ***Container**:* Operating system level **virtualization method** for running software without launching an entire virtual machine
- In simpler words: containers allow you to **package** your software / pipeline with the **dependencies** inside a **reproducible**, easy to **share**, **runnable** file
- Example: **Docker containers**



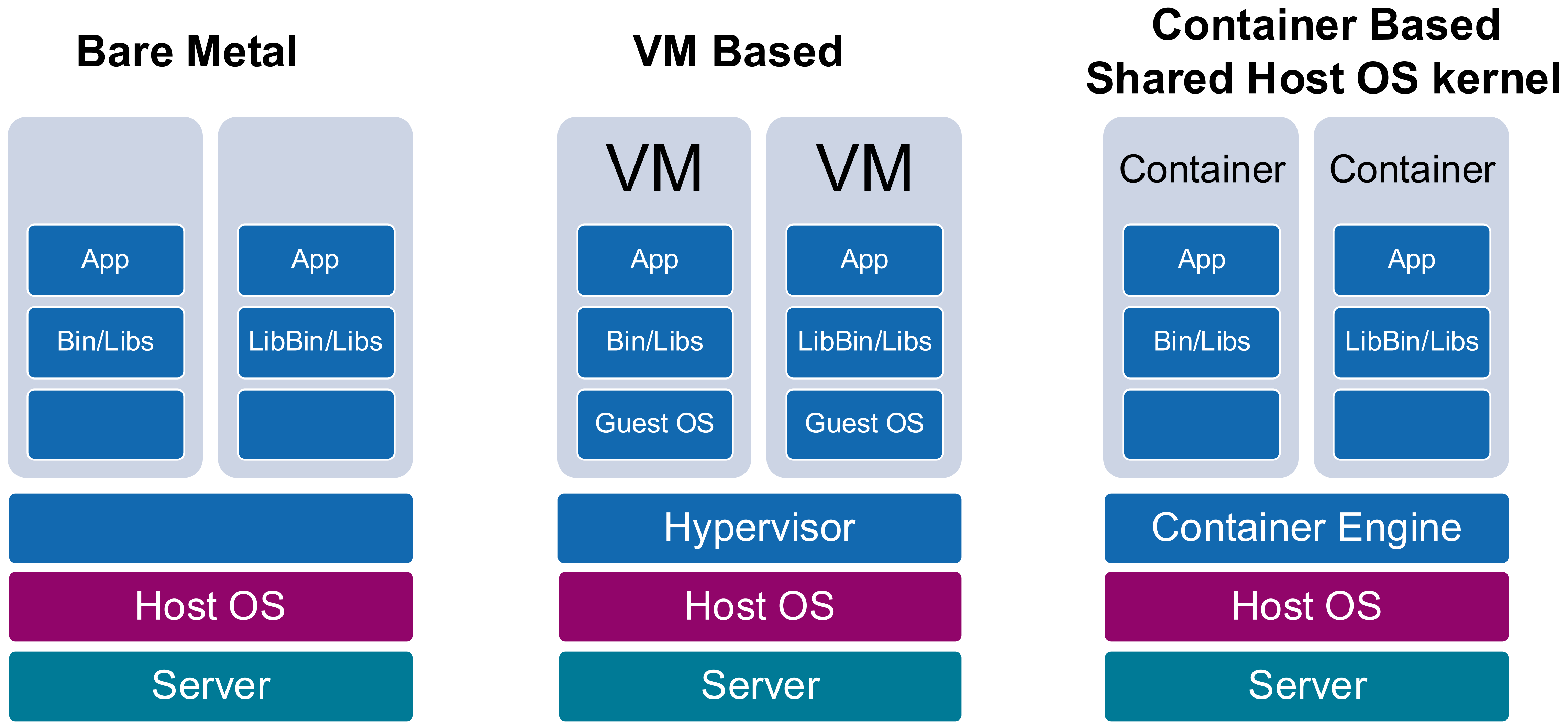


Reproducible Environment – Containerization

- ***Container**:* Operating system level **virtualization method** for running software without launching an entire virtual machine
- In simpler words: containers allow you to **package** your software / pipeline with the **dependencies** inside a **reproducible**, easy to **share**, **runnable** file
- Example: **Docker containers**



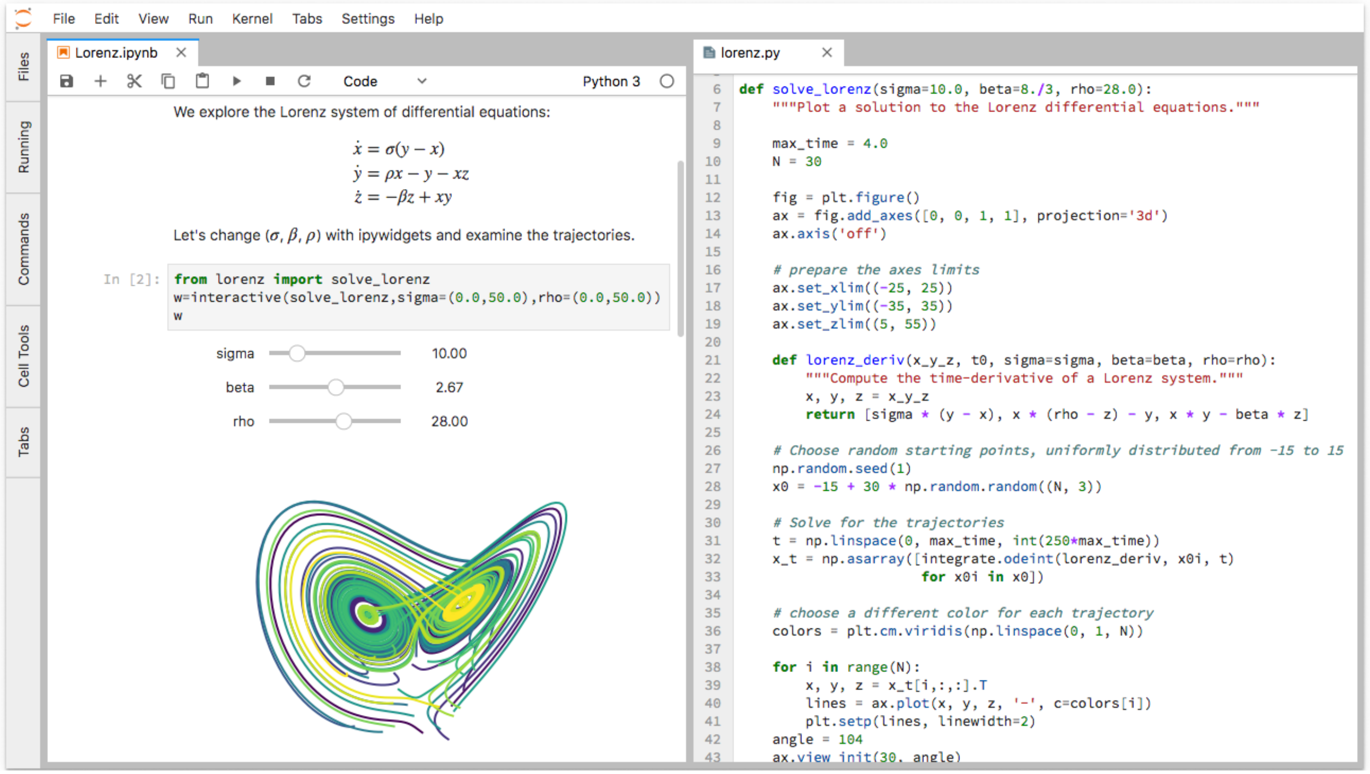
Bare Metal, Virtual Machine (VM) and Container (Docker)



Virtual Machines vs Containers

	VMs (Virtual Box)	Containers (Docker)
Use case	Complex Apps (GUI, …)	Data Analysis Scripts, Simple Apps, Microservices, Continuous Integration
Virtualization	Hardware-level	OS-level
Size	GB	MB
Startup time	Minutes	Seconds
Guest OS	Windows, macOS, Linux	Primarily Linux-based
Host OS	Windows, macOS, Linux	Linux, Windows 10 / macOS with hypervisor
Overhead (RAM, CPU)	High - reduced performance	Low - close to native performance
Security	Better (fully isolated)	Poorer (shared kernel)
How to use	Easy if you know to install OS	New things to learn
Getting started	www.virtualbox.org/manual/ch01.html	https://docs.docker.com/get-started/

Reproducible computational environment: Questions?



We explore the Lorenz system of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

Let's change (σ, β, ρ) with ipywidgets and examine the trajectories.

```
In [2]: from lorenz import solve_lorenz
        w=interactive(solve_lorenz,sigma=(0.0,50.0),rho=(0.0,50.0))
        w
```

```
sigma  10.00
beta    2.67
rho    28.00
```

```python
def solve_lorenz(sigma=10.0, beta=8./3, rho=28.0):
    """Plot a solution to the Lorenz differential equations."""

    max_time = 4.0
    N = 30

    fig = plt.figure()
    ax = fig.add_axes([0, 0, 1, 1], projection='3d')
    ax.axis('off')

    # prepare the axes limits
    ax.set_xlim((-25, 25))
    ax.set_ylim((-35, 35))
    ax.set_zlim((5, 55))

    def lorenz_deriv(x_y_z, t0, sigma=sigma, beta=beta, rho=rho):
        """Compute the time-derivative of a Lorenz system."""
        x, y, z = x_y_z
        return [sigma * (y - x), x * (rho - z) - y, x * y - beta * z]

    # Choose random starting points, uniformly distributed from -15 to 15
    np.random.seed(1)
    x0 = -15 + 30 * np.random.random((N, 3))

    # Solve for the trajectories
    t = np.linspace(0, max_time, int(250*max_time))
    x_t = np.asarray([integrate.odeint(lorenz_deriv, x0i, t)
                      for x0i in x0])

    # choose a different color for each trajectory
    colors = plt.cm.viridis(np.linspace(0, 1, N))

    for i in range(N):
        x, y, z = x_t[i,:,:].T
        lines = ax.plot(x, y, z, '-', c=colors[i])
        plt.setp(lines, linewidth=2)
    angle = 104
    ax.view_init(30, angle)
```

jupyter

R Studio®

MATLAB Live Editor

WolframAlpha NOTEBOOK EDITION™

Interactive Computational Notebooks

Interactive Notebooks

- Applications that combine documentation, code, input and output generated by the code, e.g. graphs, plots (*Nature 515, 151–152*)
- Useful for exploratory data analysis, sharing and reproducibility

RStudio

- Open source + commercial edition
- Mainly for development in R but other languages supported

jupyter

- Open source
- > 40 languages supported (Python, R, Julia, Matlab, IDL, etc.)

WolframAlpha NOTEBOOK EDITION™

- Commercial
- Used in mathematical fields

MATLAB

- Commercial
- Used in scientific, engineering, mathematical fields

Interactive Notebooks: Jupyter

- **Jupyter notebook:** web-based interactive computational environment

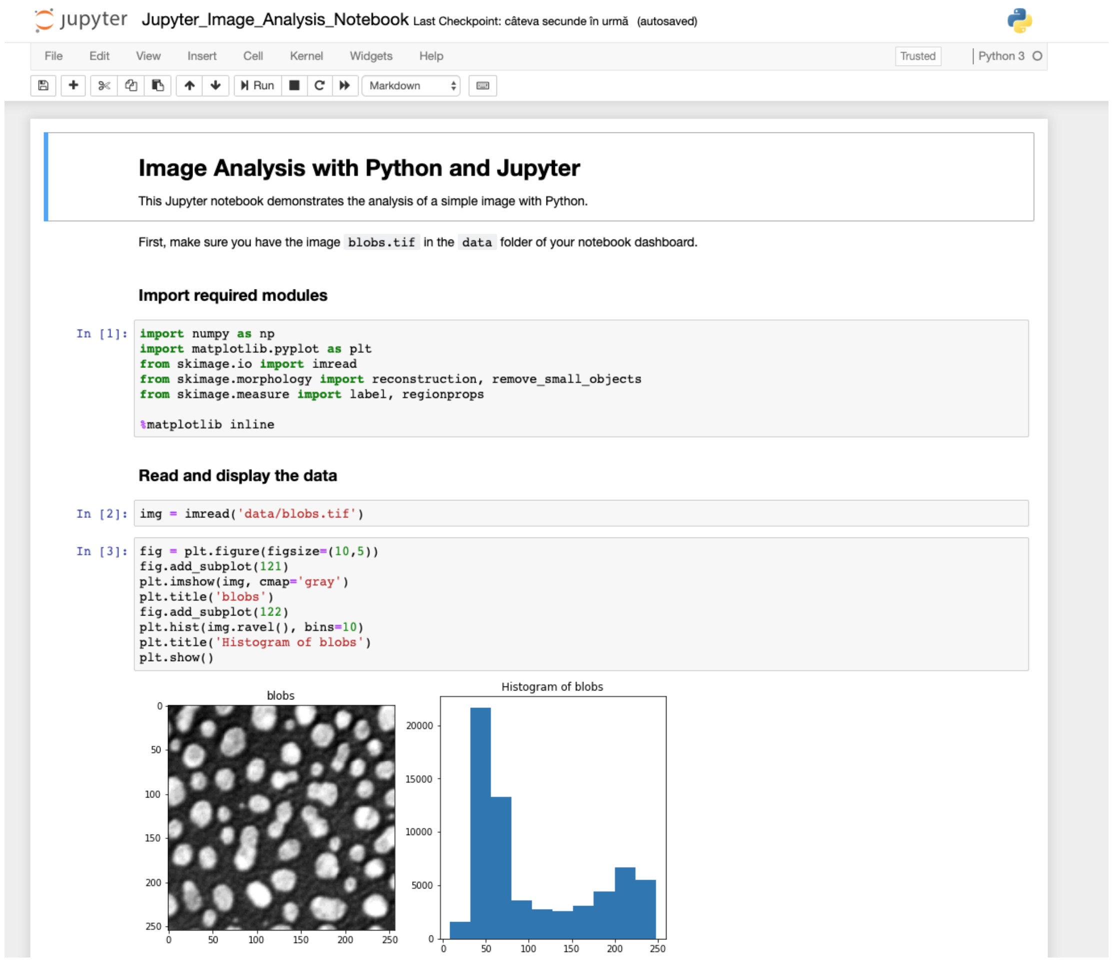

jupyter
Jupyter_Image_Analysis_Notebook Last Checkpoint: câteva secunde în urmă (autosaved)
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Trusted
Python 3
Run
Markdown

Image Analysis with Python and Jupyter

This Jupyter notebook demonstrates the analysis of a simple image with Python.

First, make sure you have the image `blobs.tif` in the `data` folder of your notebook dashboard.

Import required modules

```
In [1]: import numpy as np
        import matplotlib.pyplot as plt
        from skimage.io import imread
        from skimage.morphology import reconstruction, remove_small_objects
        from skimage.measure import label, regionprops

        %matplotlib inline
```

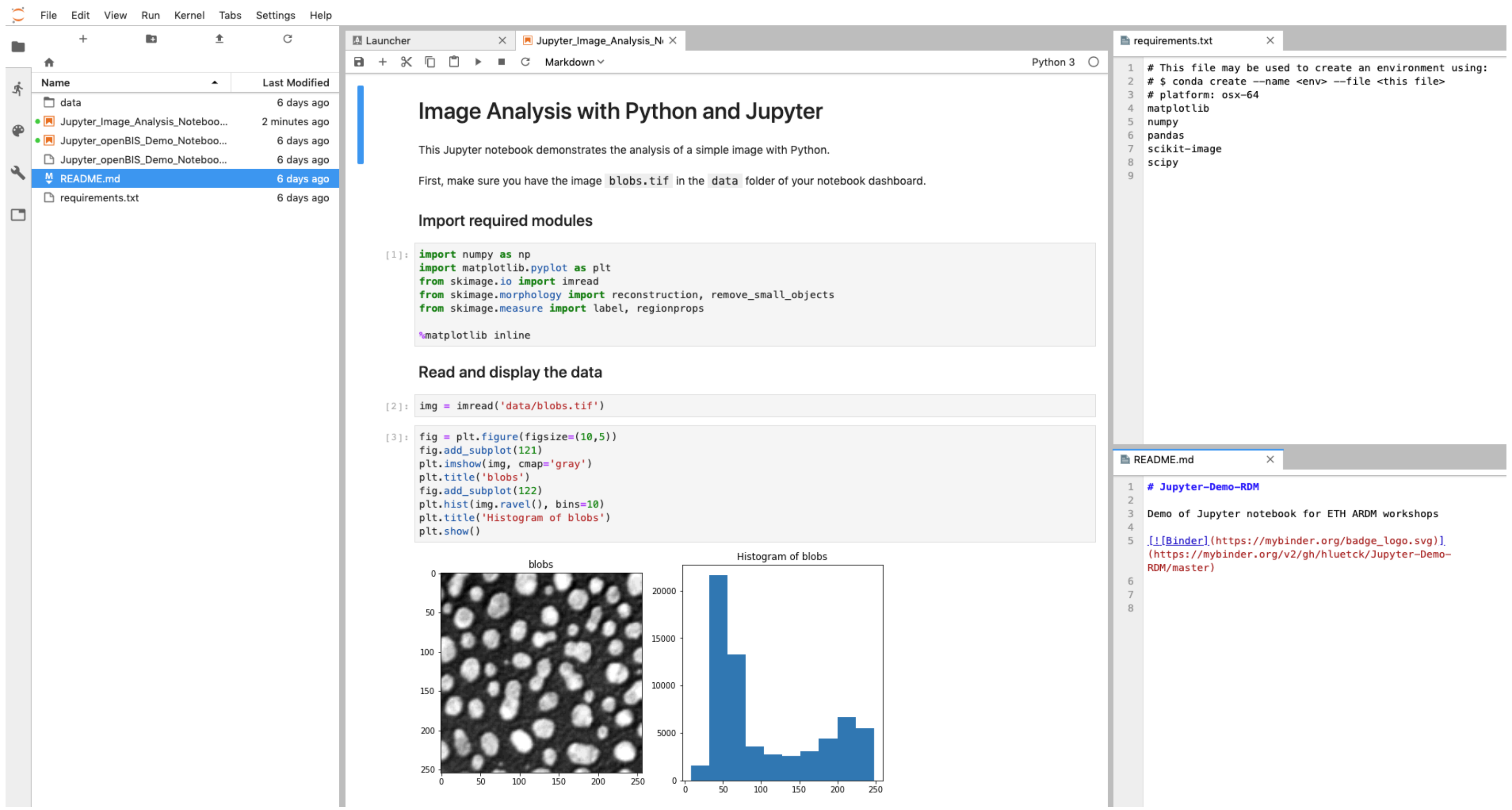
Read and display the data

```
In [2]: img = imread('data/blobs.tif')
```

```
In [3]: fig = plt.figure(figsize=(10,5))
        fig.add_subplot(121)
        plt.imshow(img, cmap='gray')
        plt.title('blobs')
        fig.add_subplot(122)
        plt.hist(img.ravel(), bins=10)
        plt.title('Histogram of blobs')
        plt.show()
```

Interactive Notebooks: Jupyter

- **Jupyter notebook:** web-based interactive computational environment
- **JupyterLab:** web-based interactive development environment for notebooks, code, and data



Name	Last Modified
data	6 days ago
Jupyter_Image_Analysis_Noteboo...	2 minutes ago
Jupyter_openBIS_Demo_Noteboo...	6 days ago
Jupyter_openBIS_Demo_Noteboo...	6 days ago
README.md	6 days ago
requirements.txt	6 days ago

Image Analysis with Python and Jupyter

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     plt.title('Histogram of blobs')
     plt.show()
```

```
# This file may be used to create an environment using:
# $ conda create --name <env> --file <this file>
# platform: osx-64
matplotlib
numpy
pandas
scikit-image
scipy
```

```
# Jupyter-Demo-RDM

Demo of Jupyter notebook for ETH ARDM workshops

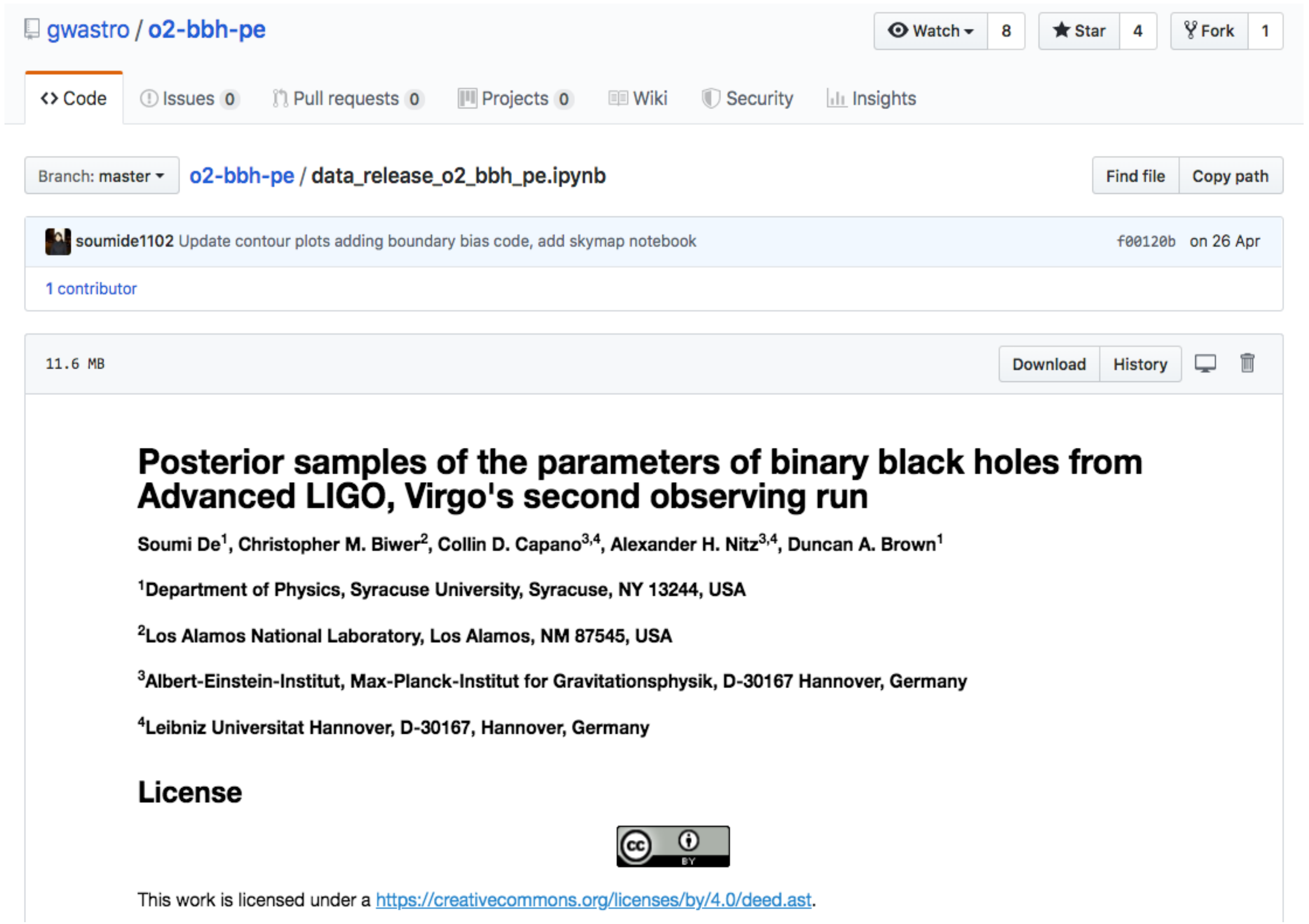
[![Binder](https://mybinder.org/badge_logo.svg)](https://mybinder.org/v2/gh/hluetck/Jupyter-Demo-RDM/master)
```

Interactive Notebooks: Jupyter

- **Jupyter notebook:** web-based interactive computational environment
- **JupyterLab:** web-based interactive development environment for notebooks, code, and data
- Dozens of programming languages supported (core: Julia, Python, R)
- Extensions to build simple user interfaces (sliders, buttons etc.)
- Notebook export in various formats (HTML, PDF, Python …)
- Integration with ETH scientific computing infrastructure
  (see https://jupyter.euler.hpc.ethz.ch/hub/)
- **JupyterHub:** multi-user version of the notebook for research labs

Interactive Notebooks: Jupyter [demo]

Gravitational wave physics



gwastro / o2-bbh-pe

Watch 8 | Star 4 | Fork 1

Code | Issues 0 | Pull requests 0 | Projects 0 | Wiki | Security | Insights

Branch: master | o2-bbh-pe / data_release_o2_bbh_pe.ipynb | Find file | Copy path

soumide1102 Update contour plots adding boundary bias code, add skymap notebook f00120b on 26 Apr

1 contributor

11.6 MB | Download | History

Posterior samples of the parameters of binary black holes from Advanced LIGO, Virgo's second observing run

Soumi De[1], Christopher M. Biwer[2], Collin D. Capano[3,4], Alexander H. Nitz[3,4], Duncan A. Brown[1]

[1]Department of Physics, Syracuse University, Syracuse, NY 13244, USA

[2]Los Alamos National Laboratory, Los Alamos, NM 87545, USA

[3]Albert-Einstein-Institut, Max-Planck-Institut for Gravitationsphysik, D-30167 Hannover, Germany

[4]Leibniz Universitat Hannover, D-30167, Hannover, Germany

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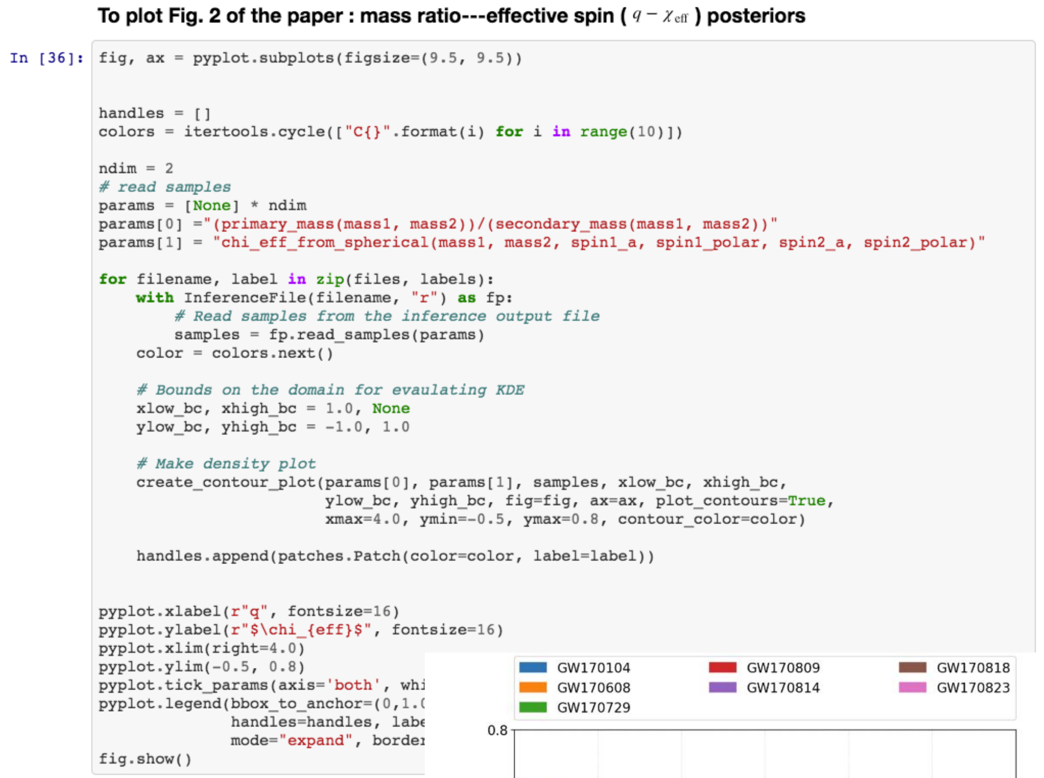


To plot Fig. 2 of the paper : mass ratio---effective spin ($q - \chi_{\rm eff}$) posteriors

```
In [36]: fig, ax = pyplot.subplots(figsize=(9.5, 9.5))


         handles = []
         colors = itertools.cycle(["C{}".format(i) for i in range(10)])

         ndim = 2
         # read samples
         params = [None] * ndim
         params[0] ="(primary_mass(mass1, mass2))/(secondary_mass(mass1, mass2))"
         params[1] = "chi_eff_from_spherical(mass1, mass2, spin1_a, spin1_polar, spin2_a, spin2_polar)"

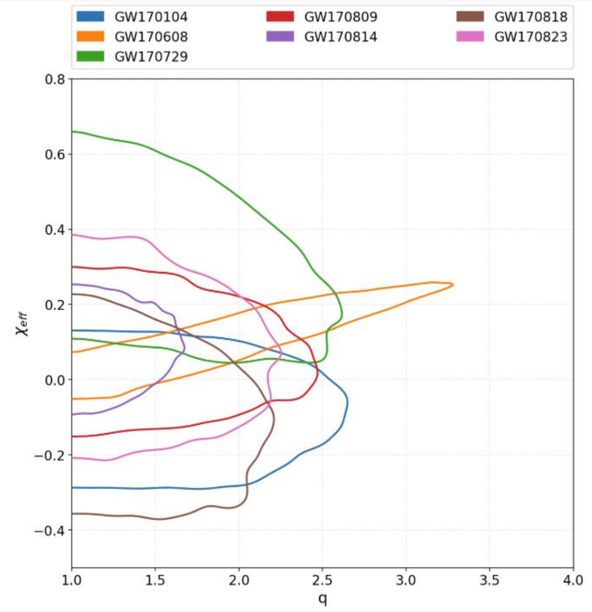
         for filename, label in zip(files, labels):
             with InferenceFile(filename, "r") as fp:
                 # Read samples from the inference output file
                 samples = fp.read_samples(params)
             color = colors.next()

             # Bounds on the domain for evaulating KDE
             xlow_bc, xhigh_bc = 1.0, None
             ylow_bc, yhigh_bc = -1.0, 1.0

             # Make density plot
             create_contour_plot(params[0], params[1], samples, xlow_bc, xhigh_bc,
                                 ylow_bc, yhigh_bc, fig=fig, ax=ax, plot_contours=True,
                                 xmax=4.0, ymin=-0.5, ymax=0.8, contour_color=color)

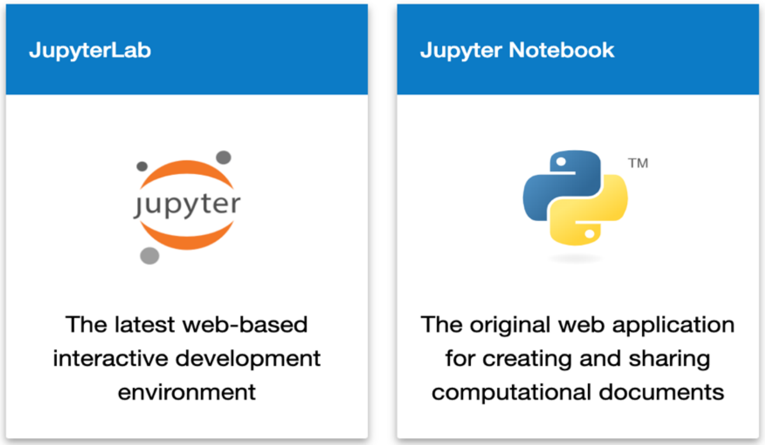
             handles.append(patches.Patch(color=color, label=label))


         pyplot.xlabel(r"q", fontsize=16)
         pyplot.ylabel(r"$\chi_{eff}$", fontsize=16)
         pyplot.xlim(right=4.0)
         pyplot.ylim(-0.5, 0.8)
         pyplot.tick_params(axis='both', whi
         pyplot.legend(bbox_to_anchor=(0,1.0
                    handles=handles, labe
                    mode="expand", borde
         fig.show()
```



Options for running Jupyter

- Local installation on your computer
- Dedicated JupyterHub server (e.g. running on virtual machine in the cloud or on Euler)
- Public cloud-based offerings
  - Renku: https://renkulab.io/
  - MyBinder: https://mybinder.org/
  - Google cloud: https://colab.research.google.com/notebooks
- To get started
  - https://jupyter.org/try



JupyterLab

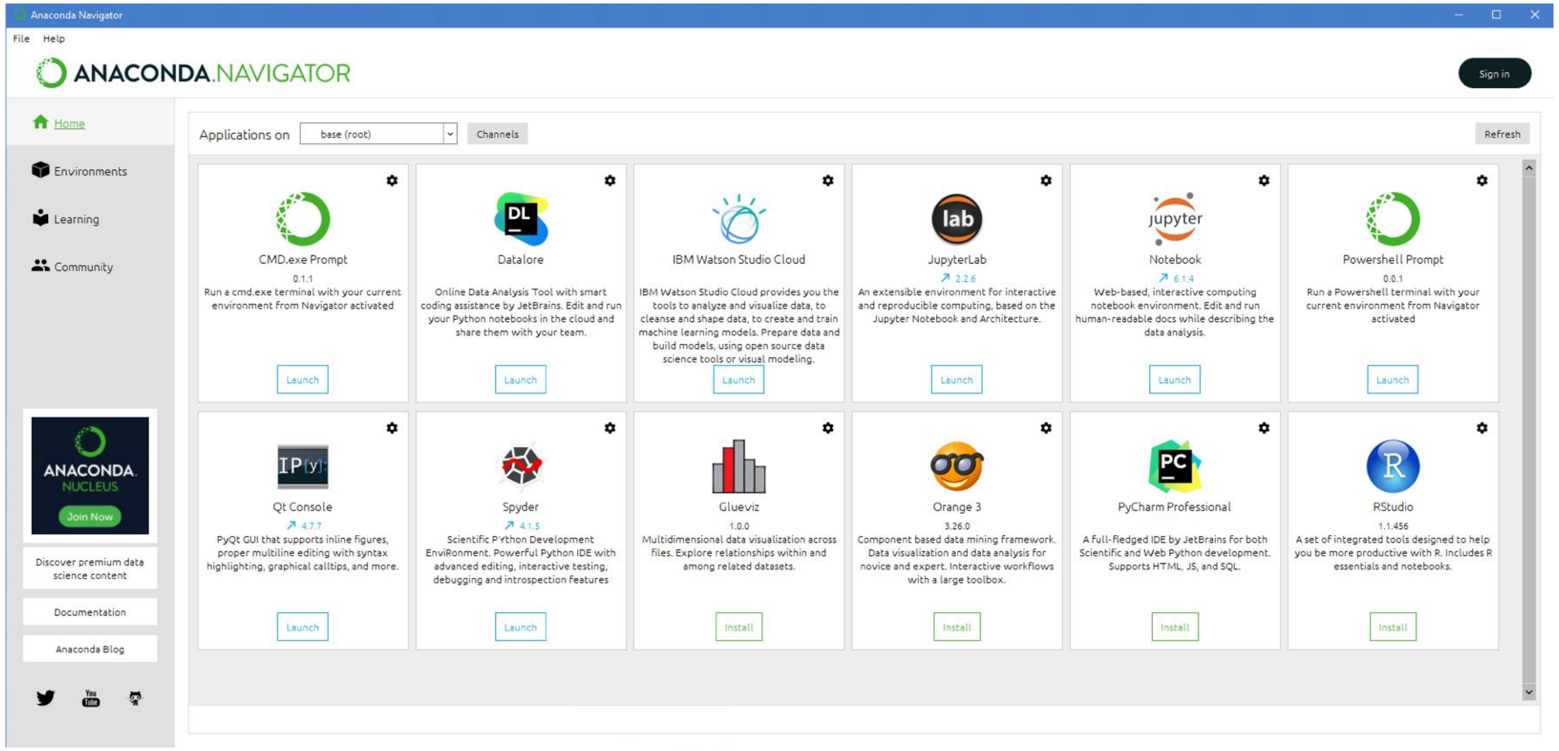
The latest web-based interactive development environment

Jupyter Notebook

The original web application for creating and sharing computational documents

Local installation of Jupyter

- **Option 1: Anaconda**
  - Installs Jupyter, Python, R and many other packages
  - Start JupyterLab or Notebook from Anaconda Navigator



CMD.exe Prompt
0.1.1
Run a cmd.exe terminal with your current environment from Navigator activated

Datalore
Online Data Analysis Tool with smart coding assistance by JetBrains. Edit and run your Python notebooks in the cloud and share them with your team.

IBM Watson Studio Cloud
IBM Watson Studio Cloud provides you the tools to analyze and visualize data, to cleanse and shape data, to create and train machine learning models. Prepare data and build models, using open source data science tools or visual modeling.

JupyterLab
↗ 2.2.6
An extensible environment for interactive and reproducible computing, based on the Jupyter Notebook and Architecture.

Notebook
↗ 6.1.4
Web-based, interactive computing notebook environment. Edit and run human-readable docs while describing the data analysis.

Powershell Prompt
0.0.1
Run a Powershell terminal with your current environment from Navigator activated

Qt Console
↗ 4.7.7
PyQt GUI that supports inline figures, proper multiline editing with syntax highlighting, graphical calltips, and more.

Spyder
↗ 4.1.5
Scientific PYthon Development EnviRonment. Powerful Python IDE with advanced editing, interactive testing, debugging and introspection features

Glueviz
1.0.0
Multidimensional data visualization across files. Explore relationships within and among related datasets.

Orange 3
3.26.0
Component based data mining framework. Data visualization and data analysis for novice and expert. Interactive workflows with a large toolbox.

PyCharm Professional
A full-fledged IDE by JetBrains for both Scientific and Web Python development. Supports HTML, JS, and SQL.

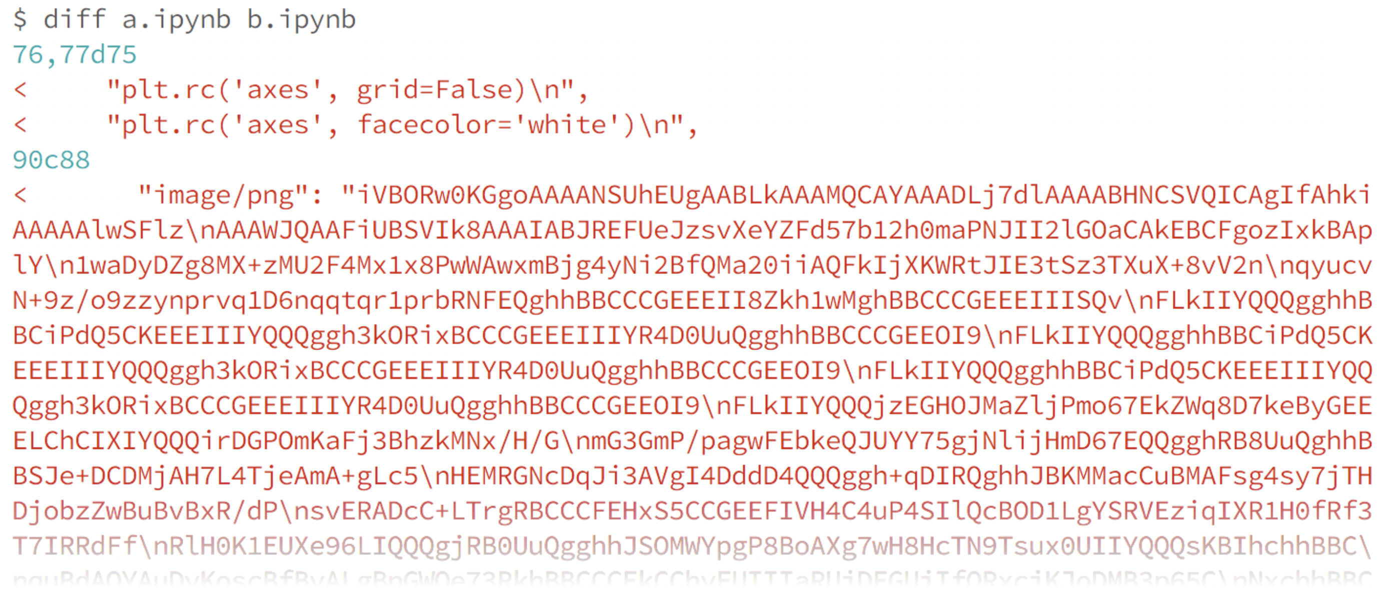
RStudio
1.1.456
A set of integrated tools designed to help you be more productive with R. Includes R essentials and notebooks.

Local installation of Jupyter

- **Option 1: Anaconda**
  - Installs Jupyter, Python, R and many other packages
  - Start JupyterLab or Notebook from Anaconda Navigator
- **Option 2: Miniconda**
  - conda install -c conda-forge jupyterlab
  - Start JupyterLab: jupyter-lab
  - Start Notebook: jupyter-nbclassic
- **Option 3: Python only**
  - pip install --upgrade pip wheel
  - pip install --upgrade jupyterlab
  - Start Lab / Notebook: jupyter-lab / jupyter-nbclassic

Interactive Notebooks – what can go wrong?

- **Versioning**
  - Version control of even moderately complex NBs is challenging
  - Tracking NB history is harder than for traditional source code
  - Some tools may help (e.g. *nbdime*, *Jupytext*)



```
$ diff a.ipynb b.ipynb
76,77d75
<     "plt.rc('axes', grid=False)\n",
<     "plt.rc('axes', facecolor='white')\n",
90c88
<       "image/png": "iVBORw0KGgoAAAANSUhEUgAABLkAAAMQCAYAAADLj7dlAAAABHNCSVQICAgIfAhki
AAAAAlwSFlz\nAAAWJQAAFiUBSVIk8AAAIABJREFUeJzsvXeYZFd57b12h0maPNJII2lGOaCAkEBCFgozIxkBAp
lY\n1waDyDZg8MX+zMU2F4Mx1x8PwWAwxmBjg4yNi2BfQMa20iiAQFkIjXKWRtJIE3tSz3TXuX+8vV2n\nqyucv
N+9z/o9zzynprvq1D6nqqtqr1prbRNFEQghhBBCCCGEEEII8Zkh1wMghBBCCCGEEEIIISQv\nFLkIIYQQQgghB
BCiPdQ5CKEEEIIIYQQQggh3kORixBCCCGEEEIIIYR4D0UuQgghBBCCCGEEOI9\nFLkIIYQQQgghBBCiPdQ5CK
EEEIIIYQQQggh3kORixBCCCGEEEIIIYR4D0UuQgghBBCCCGEEOI9\nFLkIIYQQQgghBBCiPdQ5CKEEEIIIYQQ
Qggh3kORixBCCCGEEEIIIYR4D0UuQgghBBCCCGEEOI9\nFLkIIYQQQjzEGHOJMaZljPmo67EkZWq8D7keByGEE
ELChCIXIYQQQirDGPOmKaFj3BhzkMNx/H/G\nmG3GmP/pagwFEbkeQJUYY75gjNlijHmD67EQQgghRB8UuQghhB
BSJe+DCDMjAH7L4TjeAmA+gLc5\nHEMRGNcDqJi3AVgI4DddD4QQQgh+qDIRQghhJBKMMacuBMAFsg4sy7jTH
DjobzZwBuBvBxR/dP\nsvERADcC+LTrgRBCCCFEHxS5CCGEEFIVH4C4uP4SIlQcBOD1LgYSRVEziqIXR1H0fRf3
T7IRRdFf\nRlH0K1EUXe96LIQQQgjRB0UuQgghhJSOMWYpgP8BoAXg7wH8HHcTN9Tsux0UIIYQQQsKBIhchhBBC\
nquBdAOYAuDyKoscBfByALgBnGWOe73RkhBBCCCFkCChyFUTTTaRUiDFGUiTfORxciKJoDMB3n65C\nNxchhBBC
```

Chattopadhyay et al. *(2020). What's Wrong with Computational Notebooks?*
doi:10.1145/3313831.3376729

Interactive Notebooks – what can go wrong?

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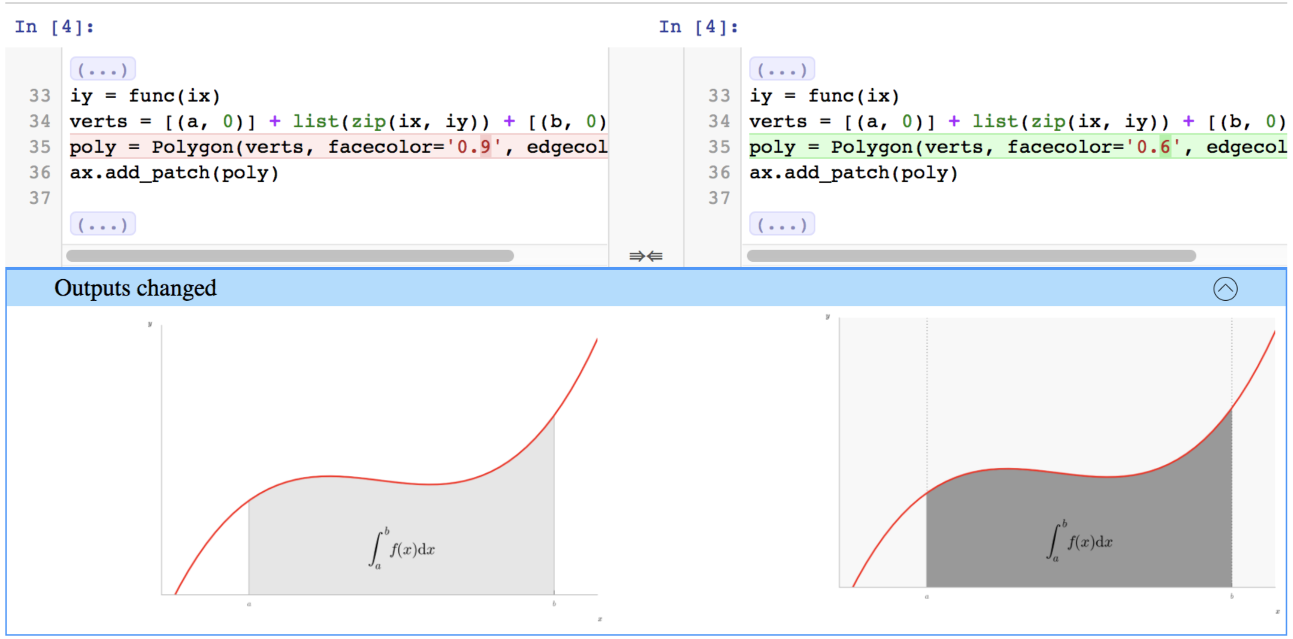
  - Tracking NB history is harder than for traditional source code
  - Some tools may help (e.g. *nbdime*, *Jupytext*)



```
In [4]:
(...)
iy = func(ix)
verts = [(a, 0)] + list(zip(ix, iy)) + [(b, 0)
poly = Polygon(verts, facecolor='0.9', edgecol
ax.add_patch(poly)

(...)
```

```
In [4]:
(...)
iy = func(ix)
verts = [(a, 0)] + list(zip(ix, iy)) + [(b, 0)
poly = Polygon(verts, facecolor='0.6', edgecol
ax.add_patch(poly)

(...)
```

Outputs changed

Chattopadhyay et al. *(2020). What's Wrong with Computational Notebooks?* *doi:10.1145/3313831.3376729*

Interactive Notebooks – what can go wrong?

- **Versioning**
  - Version control of even moderately complex NBs is challenging
  - Tracking NB history is harder than for traditional source code, especially with "classical" git
  - Some jupyter-targeted tools may help (e.g. *nbdime*)
- **Reproducibility**
  - Interactive working mode can result in hard-to-reproduce notebooks
  - Discipline is needed! Regular pruning & refactoring; *"Restart kernel & Run all"* is your friend
- **Collaboration**
  - Collaborative editing : has not been possible until recently. Must be done in JupyterHub or cloud.
- **Security**
  - Data confidentiality & access controls may be problematic

Chattopadhyay et al. *(2020). What's Wrong with Computational Notebooks?*
doi:10.1145/3313831.3376729

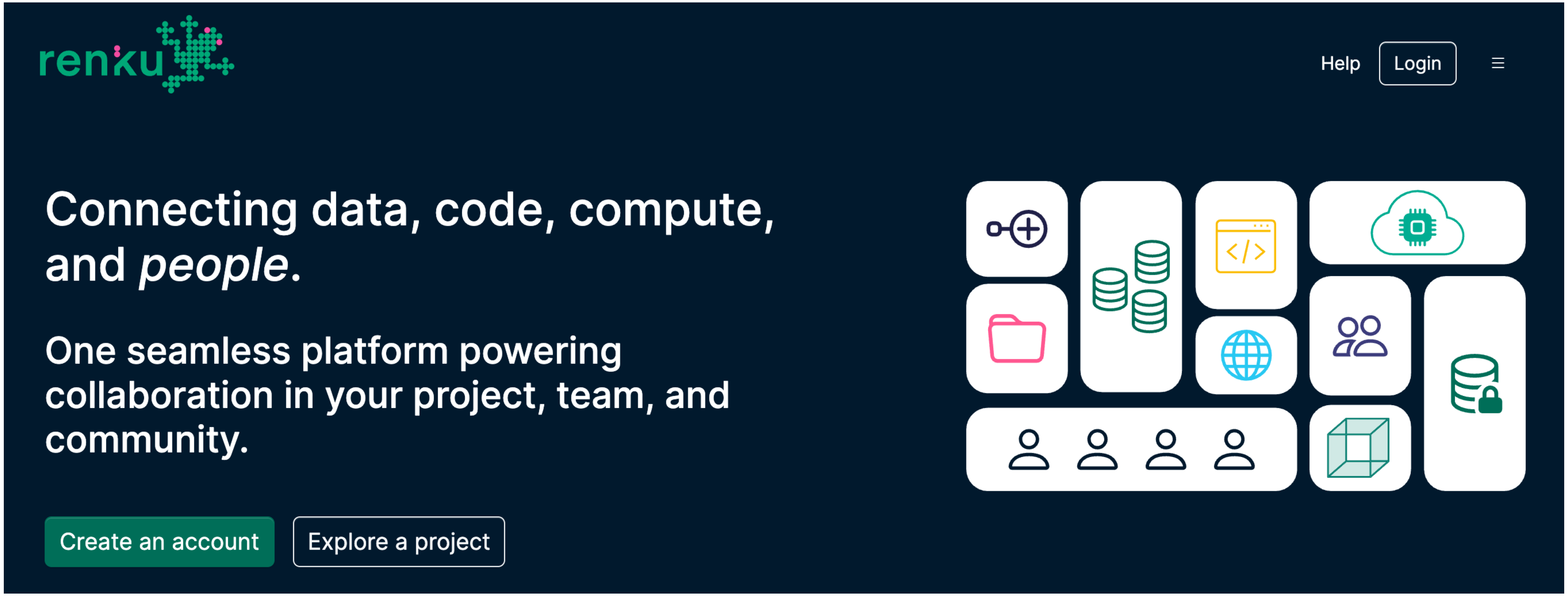
Reproducible Computing Platforms

Reproducible Computing Platforms

- Integrated, **web-based** solutions for **reproducible** and **collaborative** data analysis and **computing**
- Usually built upon **proven open-source technologies** (Git, Conda, Docker etc.)
- Technical **complexity hidden** from user (or made easily accessible)
- Platforms provide **low entry barrier** access to fully reproducible computing
- **Commercial platforms**
  - Examples: Code Ocean, Google Colaboratory, …
  - Costs are incurred by usage of underlying cloud infrastructure (storage, compute, data transfer!)
  - Beware of data ownership, licensing issues and general T&Cs
- **Community platforms**
  - Examples: mybinder, Renkulab.io
  - Usually free of charge but resources are limited

Reproducible Computing Platforms: *renkulab.io*

- Renkulab is a **platform for collaborative data science** from the Swiss Data Science Center (SDSC)



renku

Help Login

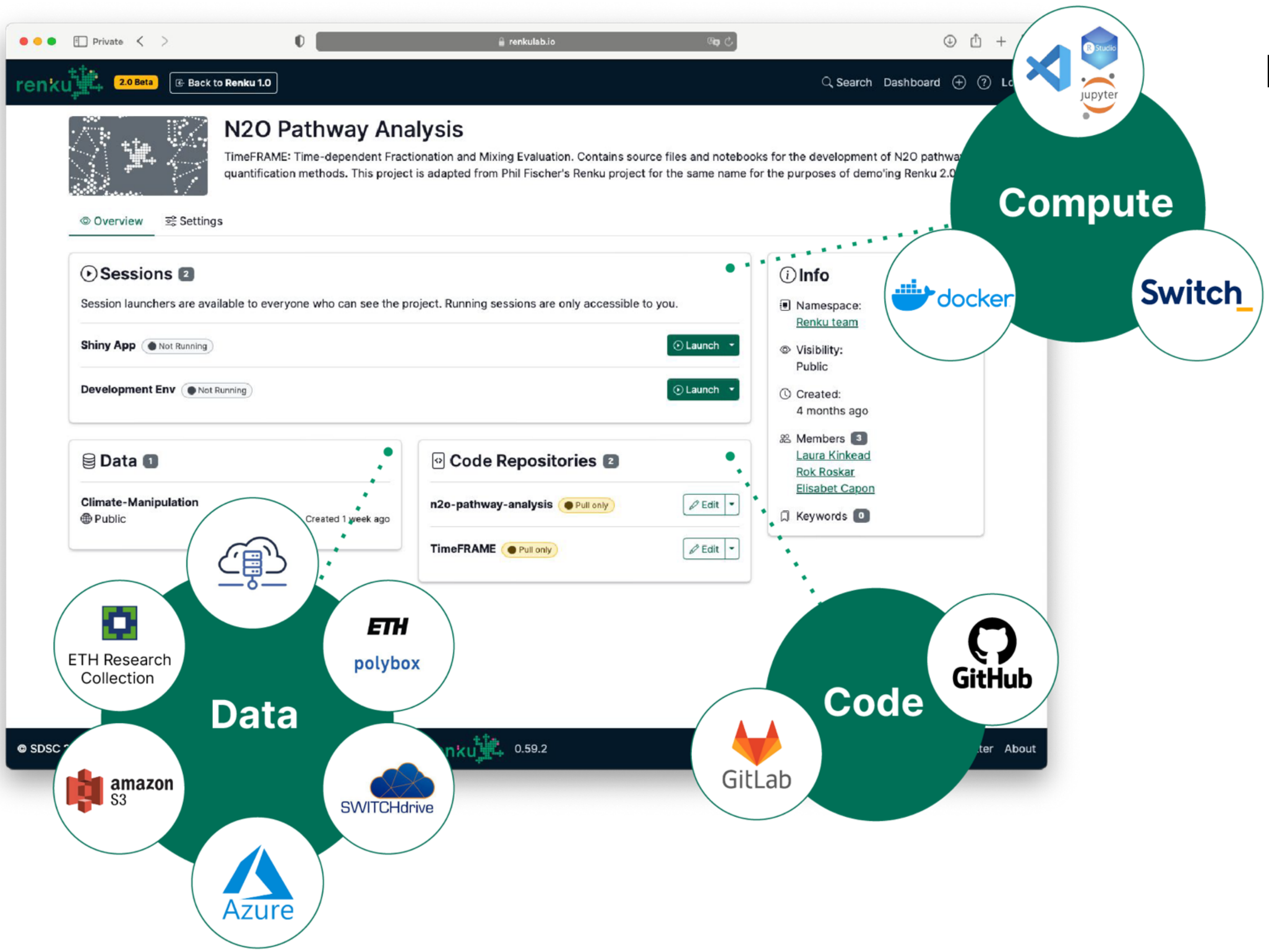
Connecting data, code, compute, and *people*.

One seamless platform powering collaboration in your project, team, and community.

Create an account Explore a project

Reproducible Computing Platforms: *renkulab.io*

- Renkulab is a **platform for collaborative data science** from the Swiss Data Science Center (SDSC)



N2O Pathway Analysis

TimeFRAME: Time-dependent Fractionation and Mixing Evaluation. Contains source files and notebooks for the development of N2O pathway quantification methods. This project is adapted from Phil Fischer's Renku project for the same name for the purposes of demo'ing Renku 2.0

Sessions 2

Session launchers are available to everyone who can see the project. Running sessions are only accessible to you.

Shiny App	Not Running	Launch
Development Env	Not Running	Launch

Info

Namespace: Renku team

Visibility: Public

Created: 4 months ago

Members 3: Laura Kinkead, Rok Roskar, Elisabet Capon

Keywords 0

Data 1

Climate-Manipulation, Public, Created 1 week ago

Code Repositories 2

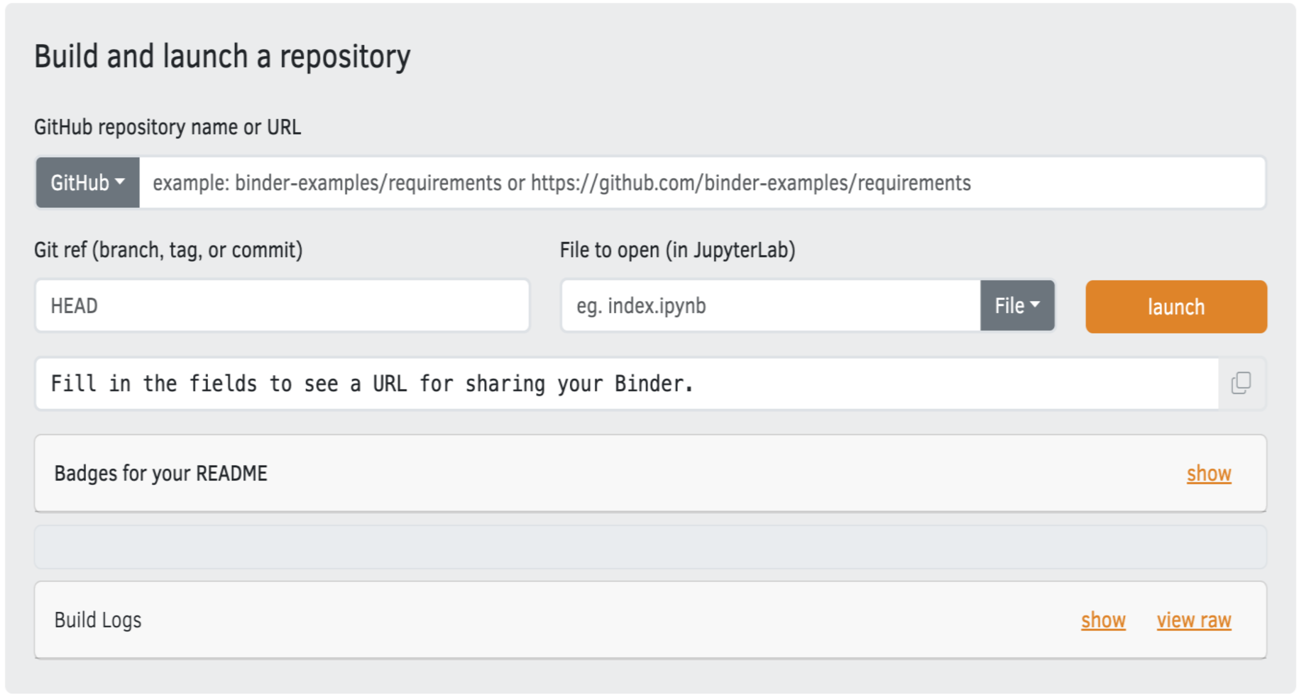
n2o-pathway-analysis	Pull only	Edit
TimeFRAME	Pull only	Edit

Learning more about Renkulab

- Login with your Switch edu-ID (or create a new account)
- Getting Started Tutorial
- More Renku Tutorials
- Renku How-To Guides

Reproducible Computing Platforms: *mybinder.org*

- Binder converts a Git repository into a collection of interactive notebooks
- Notebooks open in an executable environment → code becomes reproducible by anybody, anywhere


Build and launch a repository
GitHub repository name or URL
GitHub
example: binder-examples/requirements or https://github.com/binder-examples/requirements
Git ref (branch, tag, or commit)
File to open (in JupyterLab)
HEAD
eg. index.ipynb
File
launch
Badges for your README
show
Build Logs
show
view raw

```
Fill in the fields to see a URL for sharing your Binder.
```

How it works

1 **Enter your repository information**

Provide in the above form a URL or a GitHub repository that contains Jupyter notebooks, as well as a branch, tag, or commit hash. Launch will build your Binder repository. If you specify a path to a notebook file, the notebook will be opened in your browser after building.

2 **We build a Docker image of your repository**

Binder will search for a dependency file, such as requirements.txt or environment.yml, in the repository's root directory (more details on more complex dependencies in documentation). The dependency files will be used to build a Docker image. If an image has already been built for the given repository, it will not be rebuilt. If a new commit has been made, the image will automatically be rebuilt.

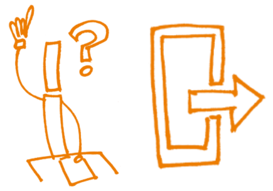
3 **Interact with your notebooks in a live environment!**

A JupyterHub server will host your repository's contents. We offer you a reusable link and badge to your live repository that you can easily share with others.

- Live example: https://github.com/hluetck/mybinder-demo-project

QUIZ TIME ...

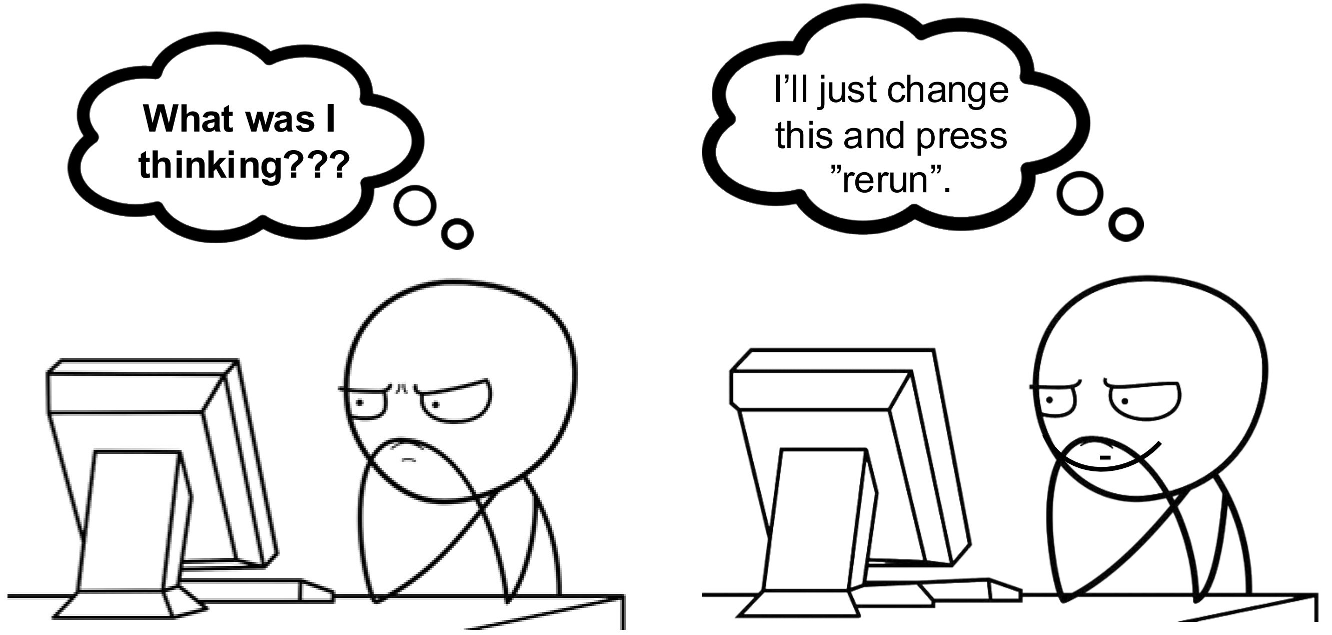
Wrap-up & Discussion



What’s in it for me?

One year in submission loop and reviewer comments are finally back…

Before workshop After workshop (and some effort) ☺



At the start of the project

- Forced to think about scope and limitations
- Improved structure and organization

During the project

- Easier to rerun experiments and analysis
- Closer interaction between collaborators
- Much of the manuscript "writes itself"

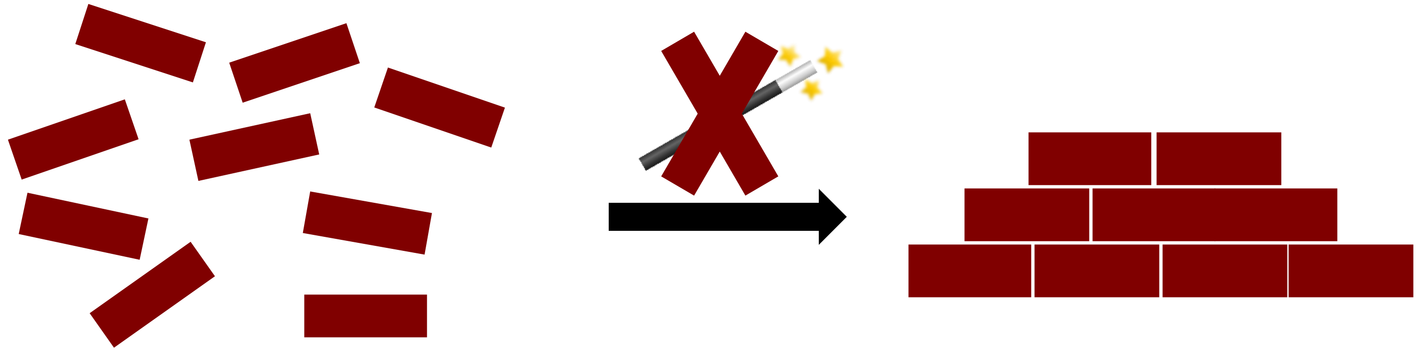
After the end of the project

- Faster resumption of research by others (or your future self), thereby increasing the impact of your work
- Increased visibility in the scientific community

Slide credit: L. Wigge, R. Ågren & J. Sundh (NBIS & SciLifeLab, Sweden)

What’s in it for me?

- Aim for improvement, not perfection!
- RDM requires **WORK** & **TIME**, but the time spent on this is an **investment** for the future!



Contact us for consultations / trainings on data management, version control, reproducible computational workflows or data science support

sis.helpdesk@ethz.ch

Contacts

https://siscourses.ethz.ch/reproducible_computing/

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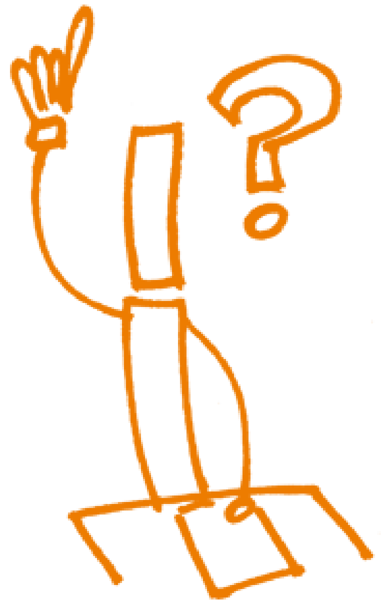
https://sis.id.ethz.ch/

Feedback: https://www.umfrageonline.ch/c/scientificcomputing

Any final questions on what we have discussed this morning?

https://siscourses.ethz.ch/reproducible_computing/



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