
Why you need a reproducible computing environment (and how Binder can help)

The #TuringWay team
University of Manchester workshop, 1st March 2019



Neurohackweek 2016

Photo credit: Chris Gorgolewski

The science is the code

An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.

Buckheit and Donoho

(paraphrasing John Claerbout)

WaveLab and Reproducible Research, 1995

What does reproducible mean?

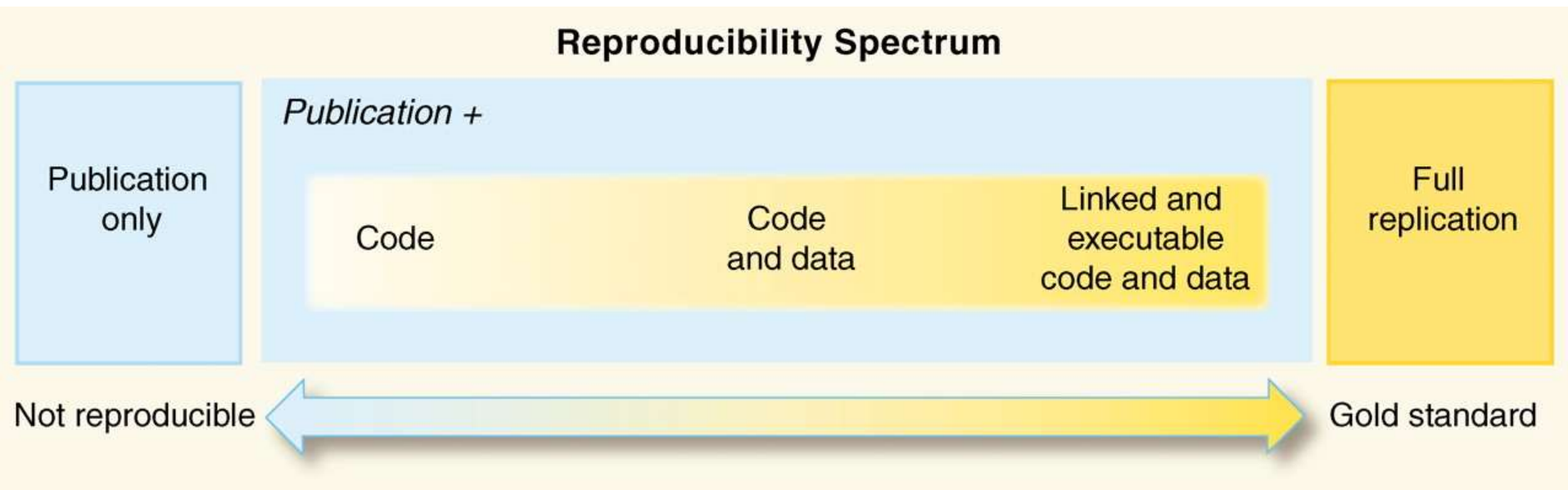
		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable

Upsetting take home message

*Sharing your code and
data isn't enough!*



You need the computational environment too



You need the computational environment too

Reproducibility Spectrum

Publication
only

Publication +

Code

Full

Not reproducible



You need the computational environment too

- Hardware (GPU, CPU)
- Operating system (mac, windows, linux)
- Software
 - Language version
 - Package versions

And all the interactions between the different layers



Capturing your local environment

PyPA » pip 19.0.3 documentation » Reference Guide »

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Previous topic

pip freeze

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- pip freeze
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Usage

```
pip freeze [options]
```

Description

Output installed packages in requirements format.
packages are listed in a case-insensitive sorted order.



https://pip.pypa.io/en/stable/reference/pip_freeze

Capturing your local environment

PyPA » pip 19.0.3 documentation » Reference Guide »

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pip freeze

Contents

- pip freeze
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Usage

```
pip freeze [options]
```

Examples

1. Generate output suitable for a requirements file.

```
$ pip freeze
docutils==0.11
 Jinja2==2.7.2
 MarkupSafe==0.19
 Pygments==1.6
 pytz==1.2.2
```

2. Generate a requirements file and then install from it in another environment.

```
$ env1/bin/pip freeze > requirements.txt
$ env2/bin/pip install -r requirements.txt
```



https://pip.pypa.io/en/stable/reference/pip_freeze

Requirements.txt

Branch: master ▾

[requirements](#) / requirements.txt

Find file

Copy path



yuvipanda Bump numpy pin

a73ba12 16 days ago

[2 contributors](#)



4 lines (3 sloc) | 45 Bytes

Raw

Blame

History




```
1 numpy==1.16.*
2 matplotlib==3.*
3 seaborn==0.8.1
```

<https://github.com/binder-examples/requirements>

Yet another markup language

Branch: master python-conda_pip / environment.yml Find file Copy path

 choldgraf adding a notebook 10ba338 on 23 Nov 2017

1 contributor

12 lines (11 sloc) | 165 Bytes Raw Blame History

```
1 name: example-environment
2 channels:
3   - conda-forge
4 dependencies:
5   - python
6   - numpy
7   - pip:
8     - nbgitpuller
9     - sphinx-gallery
10    - pandas
11    - matplotlib
```

https://github.com/binder-examples/python-conda_pip

Yet another markup language

Branch: master python-conda_pip / environment.yml Find file Copy path

choldgraf adding a notebook 10ba338 on 23 Nov 2017 1 contributor

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3   - conda-forge
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6   - numpy
7   - pip:
8     - nbgitpuller
9     - sphinx-gallery
10    - pandas
11    - matplotlib
```








(This is actually
a json file in the
background)




https://github.com/binder-examples/python-conda_pip

R and RStudio

Branch: master ▾ [r / install.R](#) Find file Copy path

 **betatim** Add example Shiny app 8c01f0d on 31 May 2018


4 contributors    

6 lines (5 sloc) | 148 Bytes Raw Blame History   

```
1  install.packages("tidyverse")
2  install.packages("rmarkdown")
3  install.packages("httr")
4  install.packages("shinydashboard")
5  install.packages('leaflet')
```

<https://github.com/binder-examples/r>

Pinning to a version on MRAN

 binder-examples / binder-r-description


Watch 1 Star 1 Fork 1

Code Issues 0 Pull requests 0 Projects 0 Wiki Insights

No description, website, or topics provided.

6 commits 1 branch 0 releases 1 contributor

Branch: master New pull request Create new file Upload files Find file Clone or download

 gedankenstuecke add readme & test notebook Latest commit d55e70d on 25 Sep 2018

R	first commit	5 months ago
DESCRIPTION	first commit	5 months ago
NAMESPACE	first commit	5 months ago
README.md	add readme & test notebook	5 months ago
test-library.ipynb	add readme & test notebook	5 months ago

<https://github.com/binder-examples/binder-r-description>

Pinning to a version on MRAN

binder-examp

<> Code ⓘ Is

No description, we

6 co

Branch: master

gedankenstuecke

R

DESCRIPTION

NAMESPACE

README.md

test-library.ipyn

README.md

Specifying an R environment by having a DESCRIPTION file

Jupyter+R: **launch** **binder**

RStudio: **launch** **binder**

Binder supports using R and RStudio, with libraries pinned to a specific snapshot on [MRAN](#).

If you specify a `runtime.txt` file that is formatted like:


```
r-<YYYY>-<MM>-<DD>
```

where YYYY-MM-DD it will use the MRAN snapshot of that day for setting up the R runtime.

Without specifying a `runtime.txt` it will use a 2-day old snapshot of MRAN.

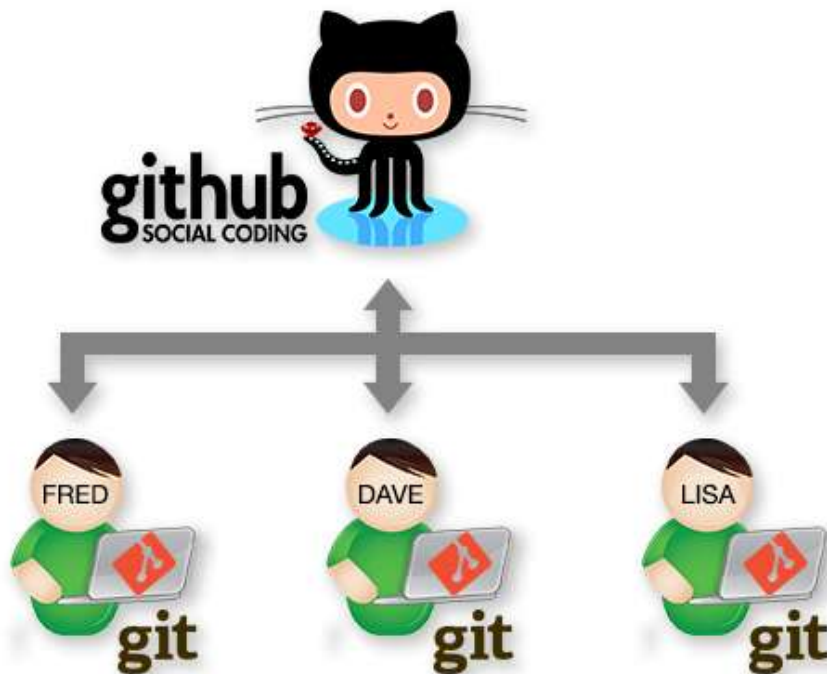
Both [RStudio](#) and [IRKernel](#) are installed by default, so you can use either the Jupyter notebook interface or the RStudio interface.

<https://github.com/binder-examples/binder-r-description>

A photograph of a bright blue sky filled with large, white, puffy cumulus clouds. The clouds are scattered across the frame, with some appearing closer and more detailed, while others are further away and softer. The overall scene is bright and airy.

*You could also share this
information in the cloud!*

Put your code in the cloud



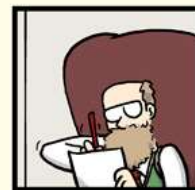
"FINAL".doc



FINAL.doc!



FINAL_rev.2.doc



FINAL_rev.6.COMMENTS.doc



FINAL_rev.8.comments5.
CORRECTIONS.doc



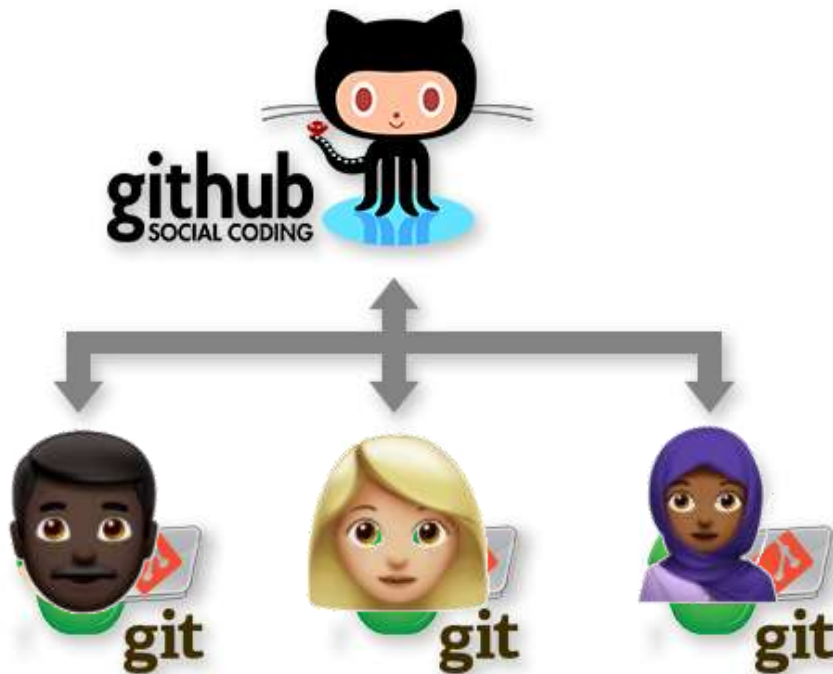
FINAL_rev.18.comments7.
corrections9.MORE.30.doc



FINAL_rev.22.comments49.
corrections.10.##\$%WHYDID
ICOMETOGRADSCHOOL?????.do



Put your code in the cloud



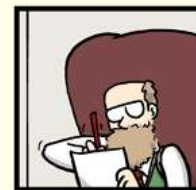
"FINAL".doc



FINAL.doc!



FINAL_rev.2.doc



FINAL_rev.6.COMMENTS.doc



FINAL_rev.8.comments5.
CORRECTIONS.doc



FINAL_rev.18.comments7.
corrections9.MORE.30.doc



FINAL_rev.22.comments49.
corrections.10.##\$%WHYDID
ICOMETOGRADSCHOOL?????.do

JORGE CHAN © 2012

A server is someone else's computer





Our Data Centers

AWS pioneered cloud computing in 2006, creating cloud infrastructure that allows you to securely build and innovate faster. We are continuously innovating the design and systems of our data centers to protect them from man-made and natural risks. Then we implement controls, build automated systems, and undergo third-party audits to confirm security and compliance. As a result, the most highly-regulated organizations in the world trust AWS every day. Take a virtual tour of one of our data centers to learn about our security approach to protect the data of millions of active monthly customers.



<https://aws.amazon.com/compliance/data-center/data-centers>



Our Data Centers

AWS pioneered cloud computing in 2006, creating cloud infrastructure that allows you to securely build and innovate faster. We are continuously innovating the design and systems of our data centers to protect them from man-



PERIMETER LAYER

AWS data center physical security begins at the Perimeter Layer. This layer includes a number of security features depending on the location, such as security guards, fencing, security fleets, intrusion detection technology, and other security measures.

EXPLORE »



DATA LAYER

The Data Layer is the most critical point of protection because it is the only area that holds customer data. Protection begins by restricting access and maintaining a separation of privilege for each layer. In addition, we deploy threat detector devices and system protocols, further safeguarding this layer.

EXPLORE »



INFRASTRUCTURE LAYER

The Infrastructure Layer is the data center building and the equipment and systems that keep it running. Components like back-up power equipment, the HVAC system, and fire suppression equipment are all part of the Infrastructure Layer.

EXPLORE »



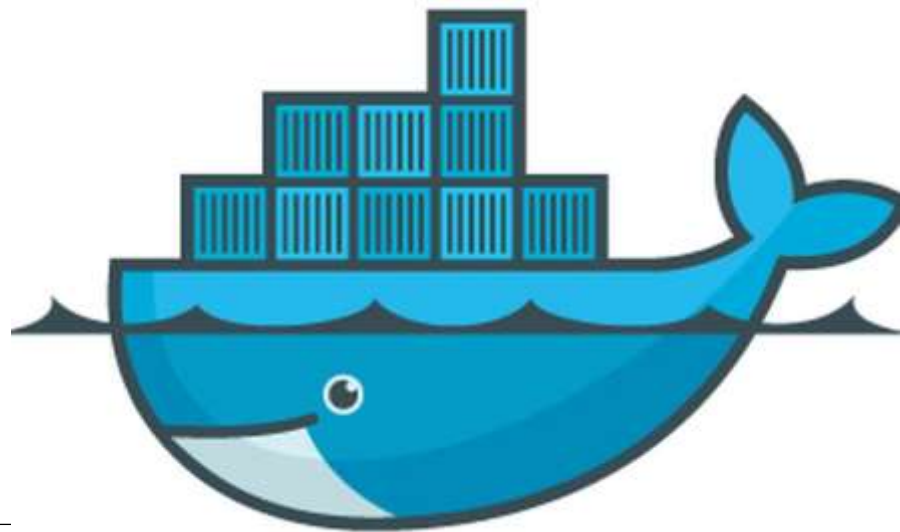
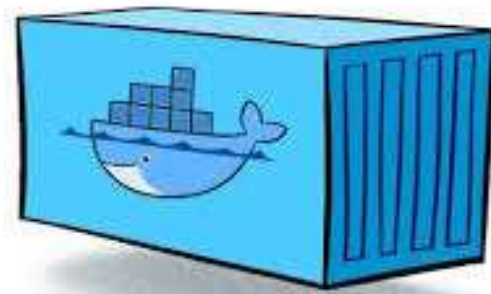
ENVIRONMENTAL LAYER

The Environmental Layer is dedicated to environmental considerations from site selection and construction to operations and sustainability. AWS carefully chooses our data center locations to mitigate environmental risk, such as flooding, extreme weather, and seismic activity.

EXPLORE »

These computers run software

- Docker is a container that bundles all the infrastructure and software together.
- You don't have to worry about all the different moving parts, just use the same set up and you'll be fine.

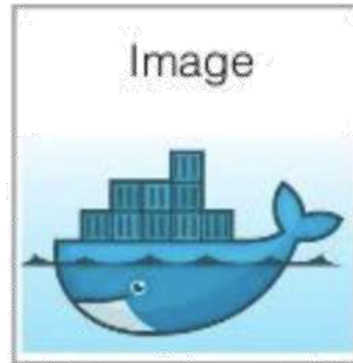


Human and machine readable files

```
FROM ubuntu:14.04
MAINTAINER John Doe <john.doe@example.com>
RUN apt-get update && apt-get install -y python-dev python-pip \
    && pip install Flask==0.10.1
EXPOSE 5000
CMD ["python", "app.py"]
```

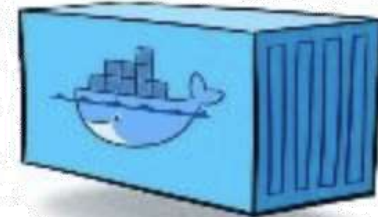
Dockerfile

build



Docker Image

run




Docker Container






<https://medium.com/platformer-blog/practical-guide-on-writing-a-dockerfile-for-your-application-89376f88b3b5>

Docker container

Branch: master ▾ [minimal-dockerfile](#) / Dockerfile Find file Copy path

 **minrk** use 3.7-slim 9402b58 on 20 Sep 2018

1 contributor

17 lines (14 sloc) | 357 Bytes Raw Blame History   

```
1 FROM python:3.7-slim
2 # install the notebook package
3 RUN pip install --no-cache --upgrade pip && \
4     pip install --no-cache notebook
5
6 # create user with a home directory
7 ARG NB_USER
8 ARG NB_UID
9 ENV USER ${NB_USER}
10 ENV HOME /home/${NB_USER}
11
12 RUN adduser --disabled-password \
13     --gecos "Default user" \
14     --uid ${NB_UID} \
15     ${NB_USER}
16 WORKDIR ${HOME}
```

<https://github.com/binder-examples/minimal-dockerfile>

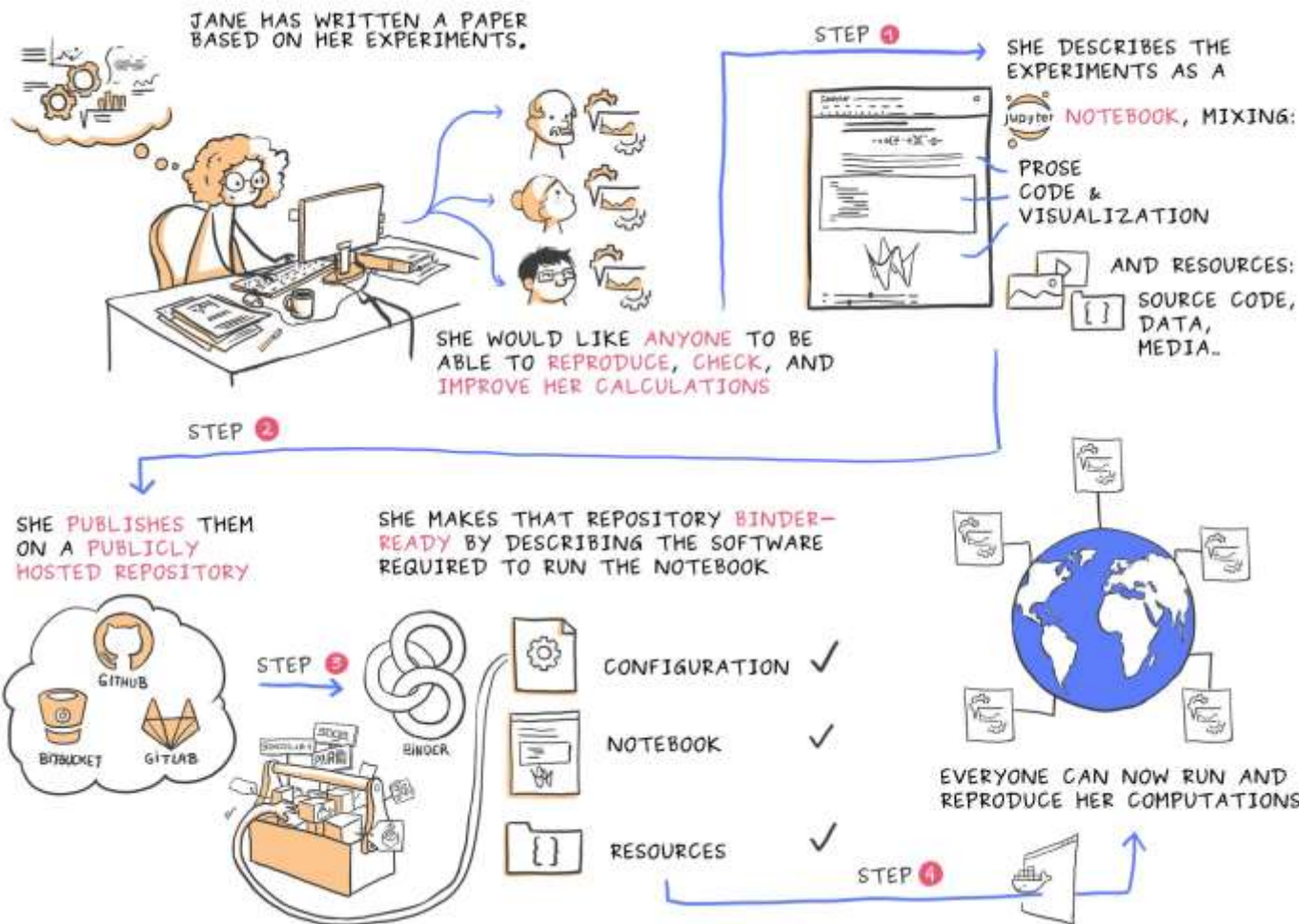
Small group exercise

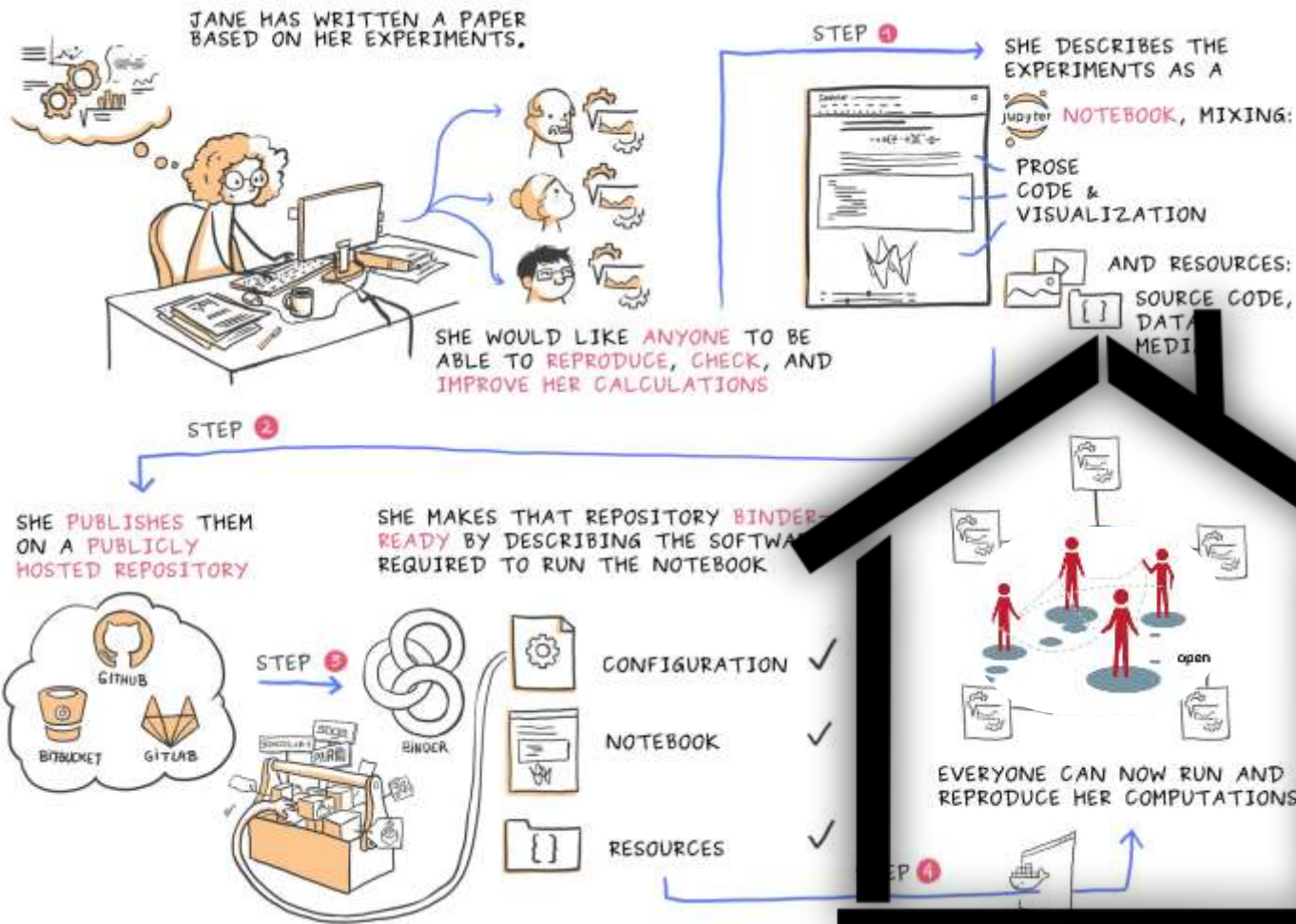
Please get into groups of 3-4 and explore the examples below.

Try to answer:

- *Are there differences between different branches?*
- *Does that give different results?*
- *Did you get what you'd expect?*

- https://github.com/annakrystalli/breaking_dplyr
- <https://github.com/binder-examples/matplotlib-versions>
- <https://github.com/sgibson91/CompEnv-PairedExample-1>
- <https://github.com/KirstieJane/CompEnv-PairedExample-2>





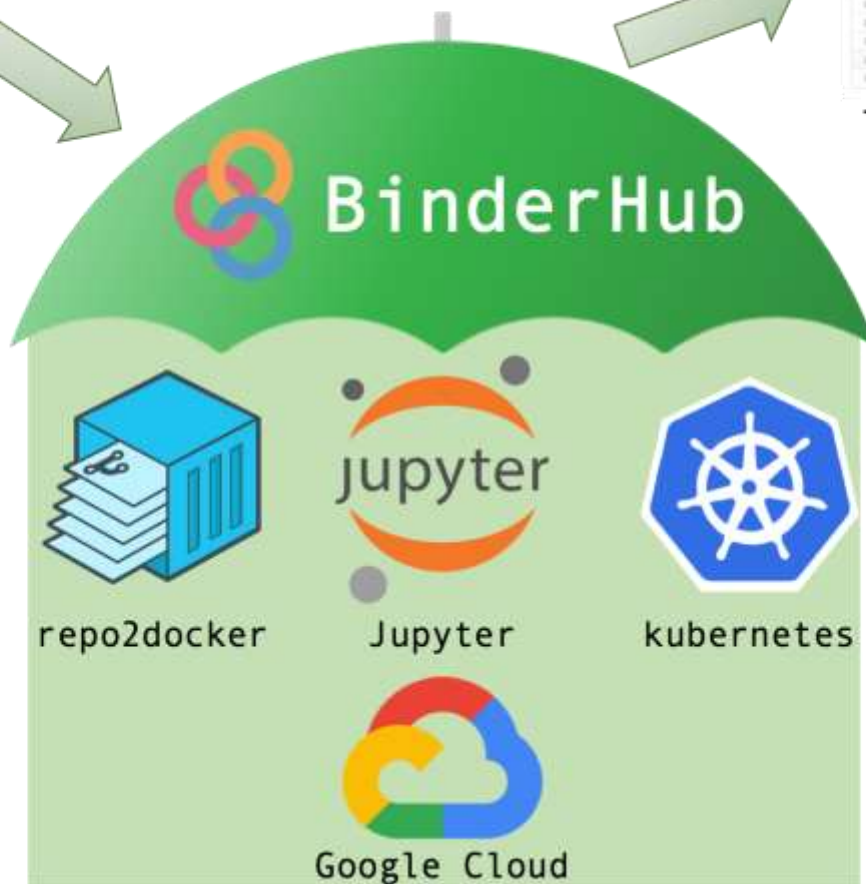
Courtesy of Juliette Belin: <https://twitter.com/JulietteTaka/status/1062735653929000960>

The public BinderHub instance

your GitHub repo



mybinder.org



interactive browser
with your code and
computational
environment



The Turing Way



#TuringWay



<https://github.com/alan-turing-institute/the-turing-way>



gitter.im/alan-turing-institute/the-turing-way