



A Practical Introduction to Reproducible Computational Workflows

Make your code reproducible by
anyone, anywhere

Tools and Infrastructure



Computational Notebooks:
Jupyter Notebook
Jupyter Lab



Cloud environment to run
computational notebooks
(including RStudio)



Source package and
environment
management system



Source code
repository

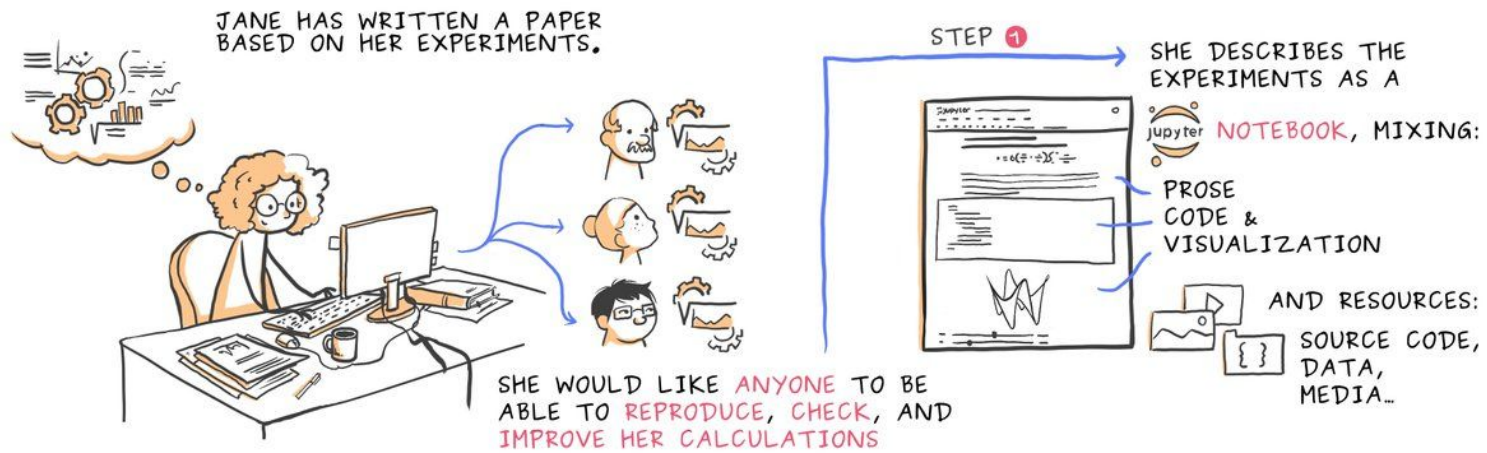
The binder Project

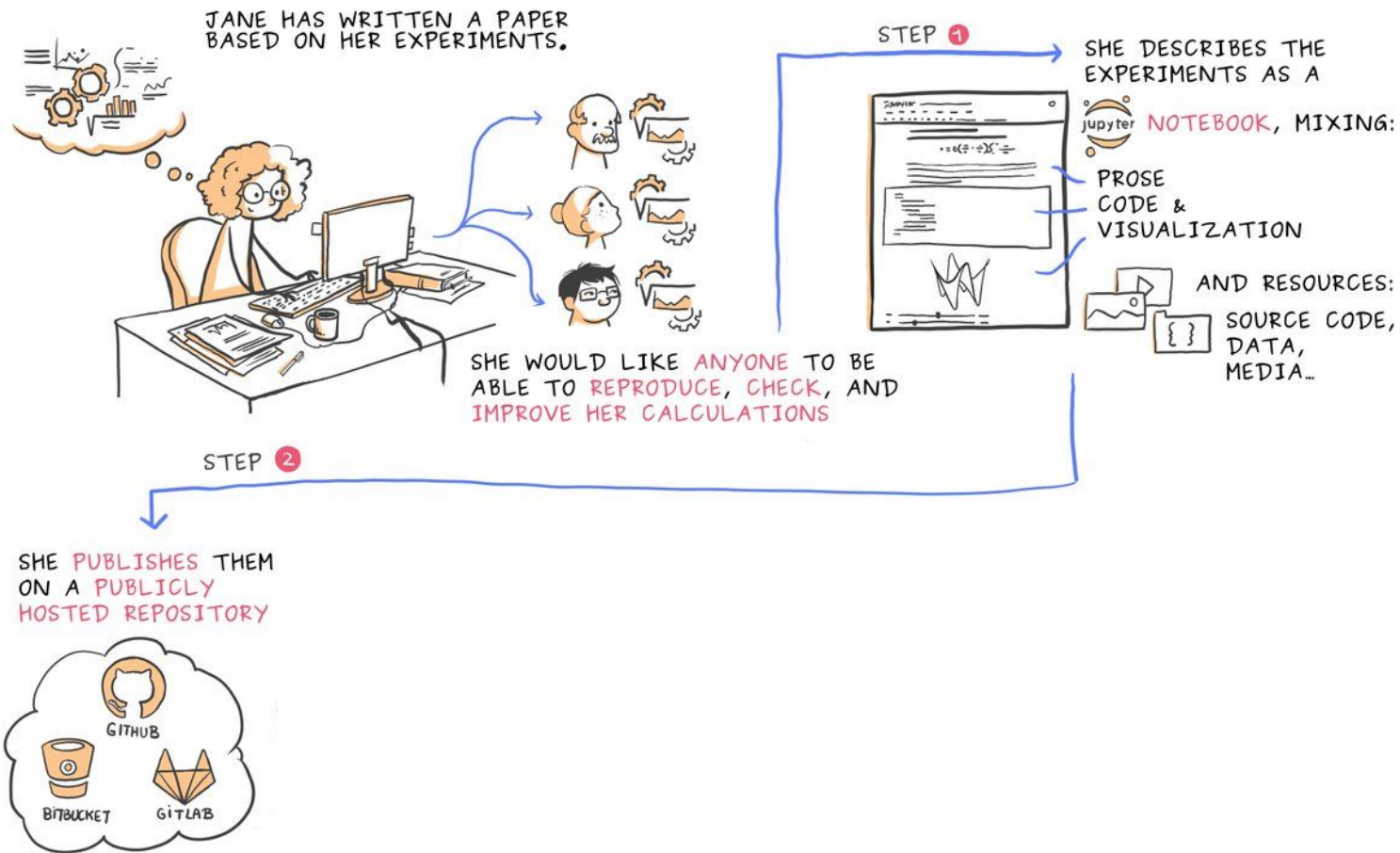
A community that builds **free and open-source** tools
for **reproducible, sharable scientific environments**
that are **workflow- and platform-agnostic**.

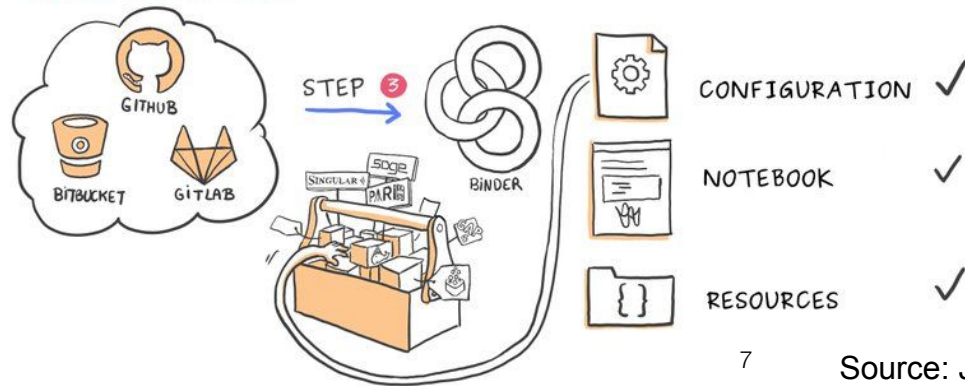
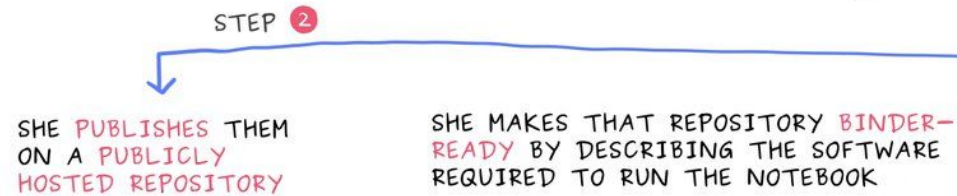


Source: Chris Holdgraf, bit.ly/2019-elifesc-holdgraf









JANE HAS WRITTEN A PAPER
BASED ON HER EXPERIMENTS.



SHE WOULD LIKE **ANYONE** TO BE
ABLE TO **REPRODUCE, CHECK, AND**
IMPROVE HER CALCULATIONS

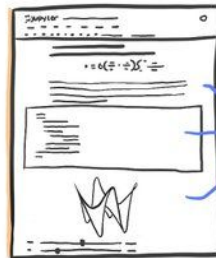
STEP 1

SHE DESCRIBES THE
EXPERIMENTS AS A

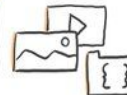


NOTEBOOK, MIXING:

PROSE
CODE &
VISUALIZATION



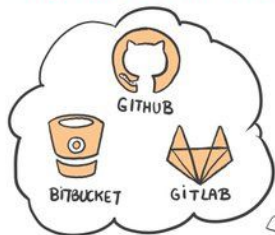
AND RESOURCES:



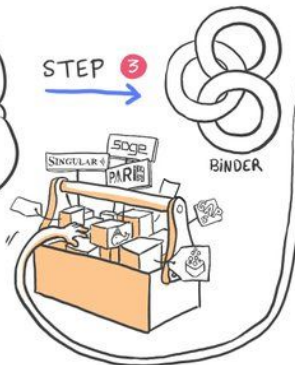
SOURCE CODE,
DATA,
MEDIA...

STEP 2

SHE **PUBLISHES** THEM
ON A **PUBLICLY**
HOSTED REPOSITORY



STEP 3



SHE MAKES THAT REPOSITORY **BINDER-**
READY BY DESCRIBING THE SOFTWARE
REQUIRED TO RUN THE NOTEBOOK

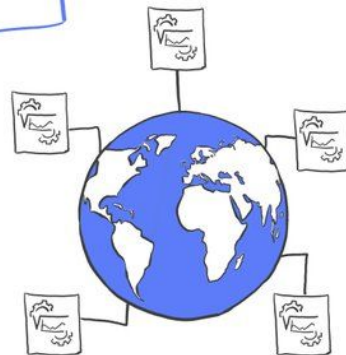
CONFIGURATION ✓

NOTEBOOK ✓

RESOURCES ✓



EVERYONE CAN NOW RUN AND
REPRODUCE HER COMPUTATIONS



STEP 4




How to configure a Repository for Binder?

“Binderize a repository”



Mybinder.org uses the files in **/binder** folder to create a conda environment.

The software dependencies are specified in **environment.yml**.

Branch: master ▾ [reproducible-computational-workflows](#) / **binder** /

 **pwrose** added postBuild file for py3Dmol

..

 environment.yml	added binder and environment.yml
 postBuild	added postBuild file for py3Dmol

environment.yml

```
name: ismb2019
channels:
  - conda-forge
  - rmg
dependencies:
  - python=3.7
  - numpy=1.16.4
  - pandas=0.24.2
  - matplotlib=3.1.0
  - seaborn=0.9.0
  - scikit-learn=0.21.2
  - ipywidgets=7.5.0
  - nodejs=11.14.0
  - jupyter=1.0.0
  - jupyterlab=1.0.2
  - nb_conda_kernels=2.2.2
  - py3dmol=0.8.0
```

Documentation: <https://mybinder.readthedocs.io>

Jupyter Lab Plugins

- Some interactive packages require a Jupyter Lab plugin
 - These plugins are specified in the **postBuild** file, e.g., [pywidgets](#)

```
#!/bin/bash
jupyter labextension install @jupyter-widgets/jupyterlab-manager@1.0
```

Branch: master ▾

[reproducible-computational-workflows](#) / binder /



pwrose added postBuild file for py3Dmol

..



[environment.yml](#)

added binder and environment.yml



[postBuild](#)

added postBuild file for py3Dmol

How to Launch Repo on <https://mybinder.org>?

<https://github.com/ISMB-ECCB-2019-Tutorial-AM4/reproducible-computational-workflows>

Build and launch a repository

GitHub repository name or URL

<https://github.com/ISMB-ECCB-2019-Tutorial-AM4/reproducible-computational-workflows>

GitHub ▾

Git branch, tag, or commit

Git branch, tag, or commit



Path to a notebook file (optional)

Path to a notebook file (optional)

File ▾

launch

Copy the URL below and share your Binder with others:

<https://mybinder.org/v2/gh/ISMB-ECCB-2019-Tutorial-AM4/reproducible-computational-workflows/master>



Copy the text below, then paste into your README to show a binder badge:

 launch binder



Make your code reproducible by anyone, anywhere

Share a link with your collaborators

Copy the URL below and share your Binder with others:

`https://mybinder.org/v2/gh/pwrose/reproducible-computational-workflows/master`



Add a Jupyter Notebook launch button to your repository README.md file

Copy the text below, then paste into your README to show a binder badge:



`\[\[Binder\]\(https://mybinder.org/badge_logo.svg\)\]\(https://mybinder.org/v2/gh/pwrose/reproducible-co`



Launch Link for a Specific Notebook

Build and launch a repository

GitHub repository name or URL

GitHub ▼

Git branch, tag, or commit



Path to a notebook file (optional)

File ▼

launch

Copy the URL below and share your Binder with others:



<https://mybinder.org/v2/gh/pwrose/reproducible-computational-workflows/master?filepath=3-jupyter%2Fjupyter-test.ipynb>

How to create a Launch Link for Jupyter Lab?

By default binder links to Jupyter Notebook

Copy the URL below and share your Binder with others:

```
https://mybinder.org/v2/gh/pwrose/reproducible-computational-workflows/master
```



To launch Jupyter Lab append **?urlpath=lab** to the launch link:

<https://mybinder.org/v2/gh/pwrose/reproducible-computational-workflows/master?urlpath=lab>

To launch a specific notebook in Jupyter Lab append

?urlpath=lab/tree/path-to-notebook/notebook.ipynb to the launch link:

<https://mybinder.org/v2/gh/pwrose/reproducible-computational-workflows/master?urlpath=lab/tree=3-jupyter/Jupyter-test.ipynb>

Hands-on Session

Binderize your Repository

<https://github.com/ISMB-ECCB-2019-Tutorial-AM4/reproducible-computational-workflows/5-binder/README.md>

Other Options to Share Jupyter Notebooks

- CyVerse VICE (Visual Interactive Computing Environment)
 - <http://learning.cyverse.org/projects/vice/en/latest/index.html>
 - **Free**, account sign-up required
 - More CPUs, memory and persistent storage (default 100GB)
 - Run notebooks for up to 48 hours
 - Suitable for production and compute intensive tasks
 - Supports Jupyter Lab, RStudio, Shiny applications
 - Funded by the US National Science Foundation
- Demo
 - <https://github.com/sbl-sdsc/mmtf-genomics>
- **CyVerse presentation by Jason Williams, Wednesday, July 24, 2 pm**
 - <https://www.iscb.org/ismbeccb2019-program/special-sessions#sst02>

Other Options to Share Jupyter Notebooks

- Commercial
 - Suited for ad hoc sharing of single Notebooks, not reproducible research
 - Google Collaboratory (uses Google Drive to share single Notebooks)
 - <https://colab.research.google.com>
 - Pros: more CPU, RAM and GPUs
 - Cons: limited options to customise execution environment
 - Microsoft Azure Notebooks
 - <https://notebooks.azure.com/>

A round of Applause for the Jupyter/Binder Team

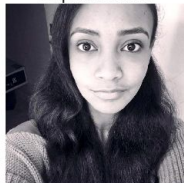
andrewosh



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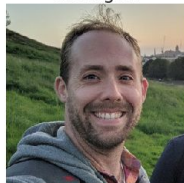
captainsafia



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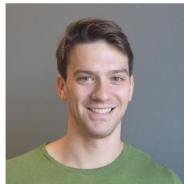
fperez



freeman-lab



henhc



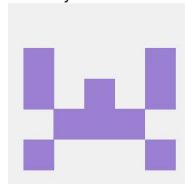
JamiesHQ



jhamrick



jzf2101



lheagy



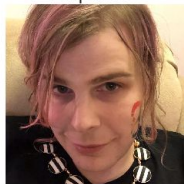
mbmilligan



minrk



mpacer



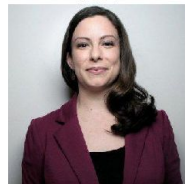
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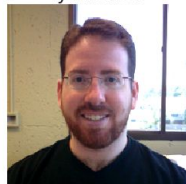
rgbkrk



Ruv7



ryanlovett



sgibson91



takluyver



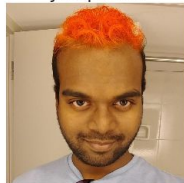
tgeorgeux



willingc



yuvipanda



Zsailer



you???

