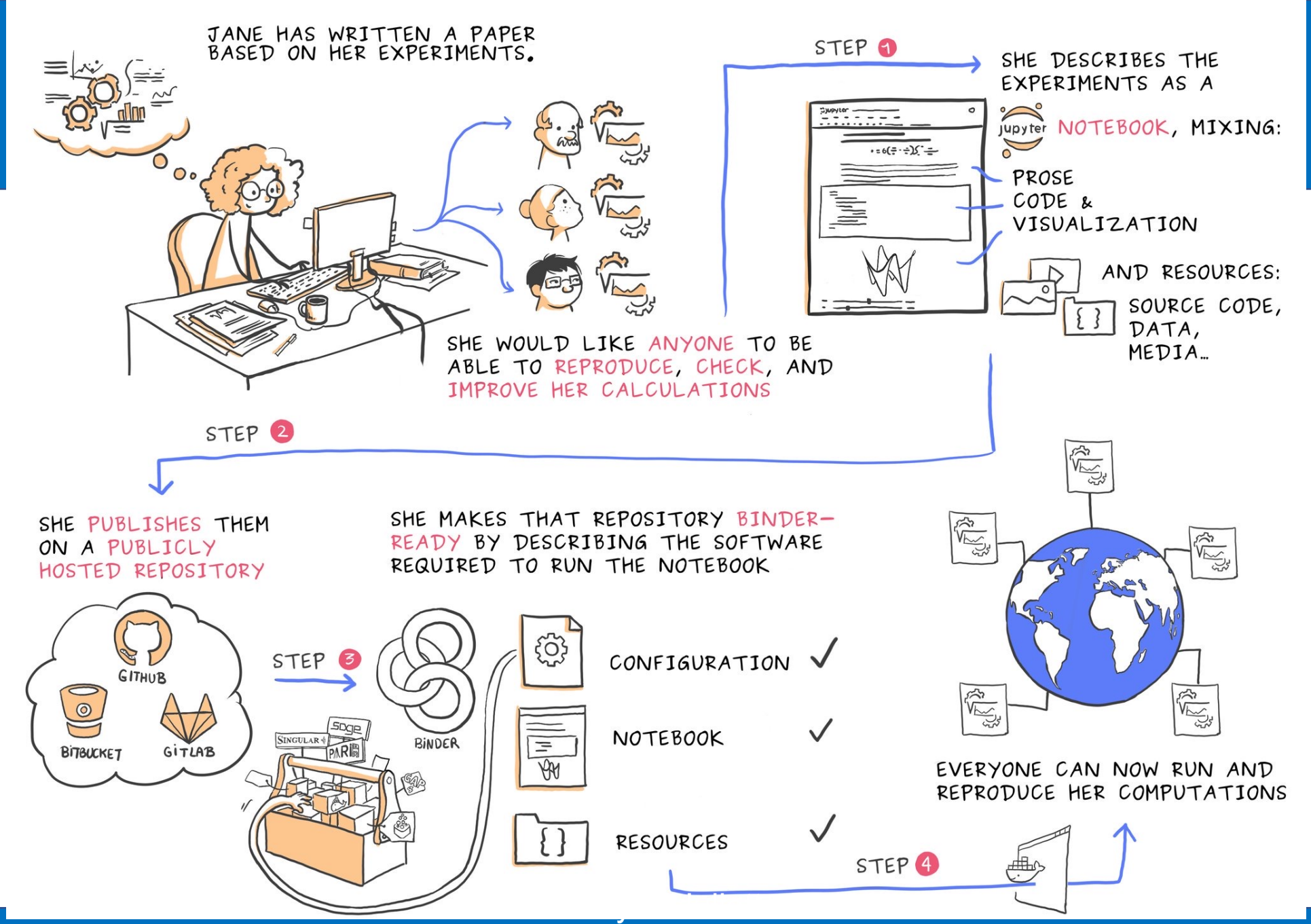
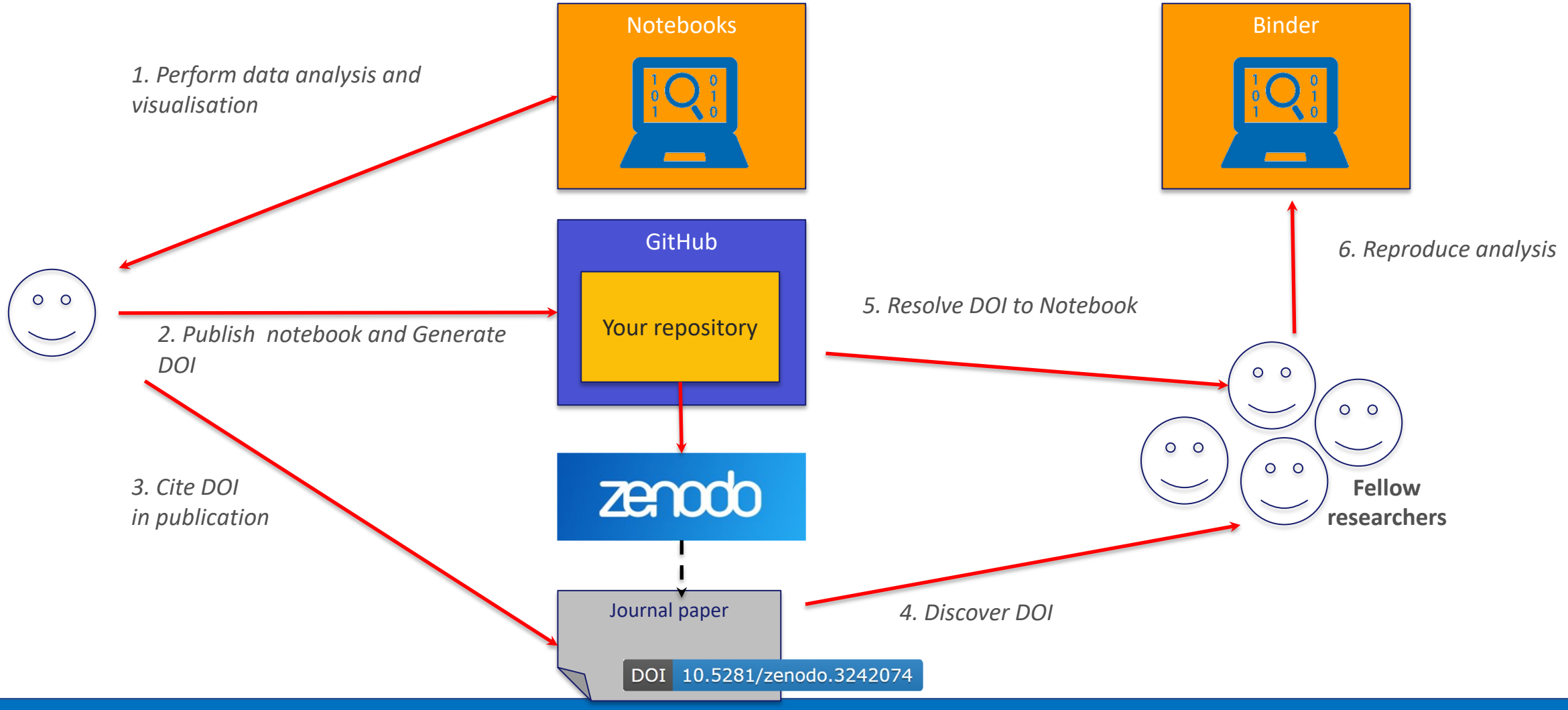
Reproducible Research and Data Analysis Exercise

University POLITEHNICA of Bucharest



https://twitter.com/JulietteTaka/status/1082735653929000960

Implement Open Science



1. Code storage and versioning

Git, GitHub, Sourcetree

Git

- A **free and open source** distributed **version control system** designed to handle everything from small to very large projects with speed and efficiency

- Is easy to learn and has a tiny footprint with lightning fast performance

- Has features like:
  - cheap local branching
  - convenient staging areas
  - multiple workflows

- https://git-scm.com

Git


Branching and Merging
Small and Fast
Distributed
Data Assurance
Staging Area
Free and Open Source

Git development platforms

- **Social networks for software development**
  - Git repository hosting services + extra features
  - web-based interfaces on top of Git
    - collaboration features: access control, wikis, issues, projects, etc.

- Examples:
  - GitHub
  - GitLab
  - Bitbucket
  - Perforce
  - Beanstalk
  - Codebase
  - etc.

2. Reproducible environments

Binder, Jupyter Notebooks

*This tutorial is based on https://the-turing-way.netlify.app/communication/binder/zero-to-binder.html

Binderize your repo

- Create a new repo on GitHub
- Make sure the repository is public, not private!
- Create a file called *hello.py* containing `print("Hello from Binder!")`
- Go to https://mybinder.org
- Type the URL of your repo into the “GitHub repo or URL” box
- As you type, the webpage generates a link in the “Copy the URL below…” box
- Open a new browser tab and visit that URL

Binderize your repo

- While you wait, BinderHub is:
  - fetching your repo from GitHub
  - analysing the contents
  - building a Docker image based on your repo
  - launching that Docker image in the cloud
  - connecting you to it via your browser

- How to run your script:
  - from the launch panel, select “Terminal”
  - in the new terminal window, type `python hello.py` and press Enter

Add dependencies

- Create a file called *requirements.txt* in your repo
- Add a line that says `numpy==1.14.5`
- Visit your Binder repo again
- Check the environment:
  - from the launch panel, select “Python 3” from the Notebook section to open a new notebook
  - type the following into a new cell:

```
import numpy
print(numpy.__version__)
numpy.random.randn()
```

- **!Changes made inside the Binder are not propagated in the repo!**
- You can also add the Binder badge to your repo launch binder

Access external data

- Small public files
  - add them directly into your GitHub repository
- Medium public files
  - from a few 10s MB up to a few hundred MB
  - add a file called *postBuild* to your repo → a shell script executed as part of the image construction (only once when a new image is built)
- Large public files
  - it is not practical to place large files in your GitHub repo or include them directly in the image
  - the best option is to use a library specific to the data format to stream the data as you're using it or to download it on demand as part of your code
- Private files
  - there is no way to access files which are not public

Access external data

- Go to your GitHub repo and create a file called *postBuild*
- Add this line: `wget -q -O gapminder.csv http://bit.ly/2uh4s3g`
- Update the *requirements.txt* file by adding `pandas` and `matplotlib`
- Relaunch your Binder
- Visualise the data by creating a new notebook and running the following:

```
%matplotlib inline

import pandas

data = pandas.read_csv("gapminder.csv", index_col="country")

years = data.columns.str.strip("gdpPercap_")  # Extract year from last 4 characters of each column name
data.columns = years.astype(int)              # Convert year values to integers, saving results back to dataframe

data.loc["Australia"].plot()
```

Sample Binder repos

- https://github.com/raduciobanu/trainrdm-example
- https://mybinder.readthedocs.io/en/latest/examples/sample_repos.html

3. Archiving code and software

Zenodo

Publish GitHub repo in Zenodo

Exercise

zenodo | Search | Upload | Communities | ciprian.dobre@cs.pub.ro

Home / Account / GitHub

Settings

- Profile
- Change password
- Security
- Linked accounts
- Applications
- Shared links
- GitHub

GitHub Repositories (updated 2 minutes ago) Sync now ...

Get started

1 Flip the switch

Select the repository you want to preserve, and toggle the switch below to turn on automatic preservation of your software.

ON

2 Create a release

Go to GitHub and create a release. Zenodo will automatically download a .zip-ball of each new release and register a DOI.

3 Get the badge

After your first release, a DOI badge that you can include in GitHub README will appear next to your repository below.

DOI 10.5281/zenodo.8475

(example)

Repositories

4. Reproducible research after data analysis

Overleaf, Gnuplot

Performing reproducible research

- **!Reminder from Monday!**

- After data analysis
  - **generate figures and tables directly from code**
  - **automate data pre-processing, analysis and manuscript generation as “one-button” processes**
  - increase access to publications by posting preprints
  - use data and code repositories for sharing (instead of personal websites)
  - create research compendiums → archives of data, code, software and products from a research project
  - in the published manuscript, offer explicit instructions regarding where to locate data, metadata and code

Performing reproducible research

- Overleaf
  - collaborative cloud-based LaTeX editor used for writing, editing and publishing scientific documents
  - https://www.overleaf.com
- Gnuplot
  - portable command-line driven graphing utility
  - http://www.gnuplot.info
- Directly generate Gnuplot charts in Overleaf using the *gnuplottex* package

THANK YOU!

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