



The Turing Way Workshop:

Reproducible, Open and
FAIR Research

Session 1

Emma Karoune, Eirini Zormpa & Anne Lee Steele

Pronouns: she/her/hers



Emma Karoune



Historic England

The
Alan Turing
Institute



- **Archaeobotanist/Palaeoecologist**

- FAIR Phytoliths project
- Open reference collections

- **Open Researcher & Community Manager**

- Tools, practices and systems programme
 - Turing Way
 - DECOVID/ Turing-RSS Lab
- SSI Fellow/ UK-Elixir FAIR data Fellow



Link to Emma's SSI Fellows page

Eirini

Community Manager Open Collaboration

- AI for Multiple Long-term Conditions Research Support Facility
- The Turing Way
- The Carpentries
- R Ladies

Background

- PhD in Psycholinguistics



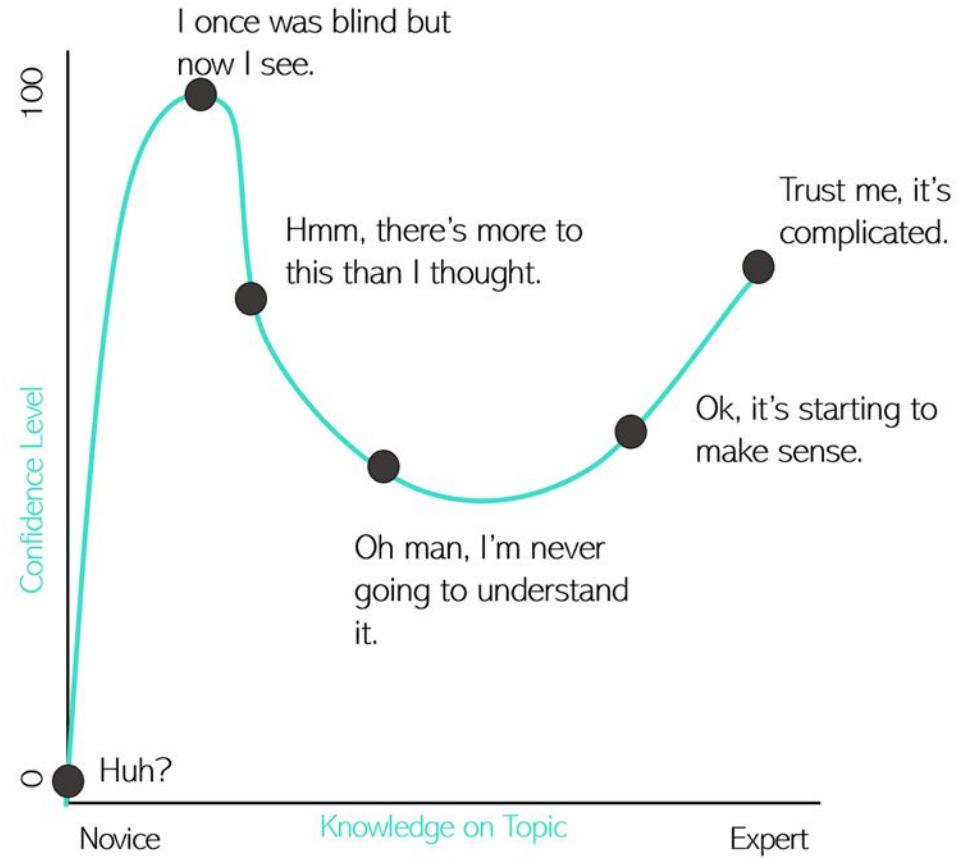
Learning Objectives

- **Problem**: Scientific errors have real world effect
- Define what **reproducible research** is
- Understand what **open science** practices are
- Identify **FAIR principles** for your research
- Differentiate between FAIR and open data/research
- Learn how to **implement a reproducible workflow**

Disclaimer:

You probably already know all about it!

Kaylee Somerville, The Hidden Power of Intellectual Humility - The Decision Lab. 2020.
<https://thedecisionlab.com/insights/society/the-hidden-power-of-intellectual-humility>



Adapted from: Squad. (2018, December 13). Dunning-Kruger Effect: Definition, Test, Examples & Quiz. Science Terms. <https://scienceterms.net/psychology/dunning-kruger-effect/>

Scientific errors have real world effects

Researchers have an obligation to consider the ethical standards (right actions) and their impact on society.



Scientific errors have real world effects

	B	C	I	J	K	L	M	
2				Real GDP growth Debt/GDP				
3				30 or less	30 to 60	60 to 90	90 or above	30 or less
4	Country	Coverage						
26				3.7	3.0	3.5	1.7	5.5
27	Minimum			1.6	0.3	1.3	-1.8	0.8
28	Maximum			5.4	4.9	10.2	3.6	13.3
29								
30	US	1946-2009	n.a.	3.4	3.3	-2.0	n.a.	
31	UK	1946-2009	n.a.	2.4	2.5	2.4	n.a.	
32	Sweden	1946-2009	3.6	2.9	2.7	n.a.	6.3	
33	Spain	1946-2009	1.5	3.4	4.2	n.a.	9.9	
34	Portugal	1952-2009	4.8	2.5	0.3	n.a.	7.9	
35	New Zealand	1948-2009	2.5	2.9	3.9	-7.9	2.6	
36	Netherlands	1956-2009	4.1	2.7	1.1	n.a.	6.4	
37	Norway	1947-2009	3.4	5.1	n.a.	n.a.	5.4	
38	Japan	1946-2009	7.0	4.0	1.0	0.7	7.0	
39	Italy	1951-2009	5.4	2.1	1.8	1.0	5.6	
40	Ireland	1948-2009	4.4	4.5	4.0	2.4	2.9	
41	Greece	1970-2009	4.0	0.3	2.7	2.9	13.3	
42	Germany	1946-2009	3.9	0.9	n.a.	n.a.	3.2	
43	France	1949-2009	4.9	2.7	3.0	n.a.	5.2	
44	Finland	1946-2009	3.8	2.4	5.5	n.a.	7.0	
45	Denmark	1950-2009	3.5	1.7	2.4	n.a.	5.6	
46	Canada	1951-2009	1.9	3.6	4.1	n.a.	2.2	
47	Belgium	1947-2009	n.a.	4.2	3.1	2.6	n.a.	
48	Austria	1948-2009	5.2	3.3	-3.8	n.a.	5.7	
49	Australia	1951-2009	3.2	4.9	4.0	n.a.	5.9	
50								
51				4.1	2.8	2.8	=AVERAGE(L30:L44)	

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Reinhart, Rogoff... and Herndon: The student who caught out the pros

By Ruth Alexander BBC News

© 20 April 2013

This week, economists have been astonished to find that a famous academic paper often used to make the case for austerity cuts contains major errors. Another surprise is that the mistakes, by two eminent Harvard professors, were spotted by a student doing his homework.

It's 4 January 2010, the Marriott Hotel in Atlanta. At the annual meeting of the American Economic Association, Professor Carmen Reinhart and the former chief economist of the International Monetary Fund, Ken Rogoff, are presenting a research paper called Growth in a Time of Debt



<https://statmodeling.stat.columbia.edu/2013/04/16/memo-to-reinhart-and-rogoff-i-think-its-best-to-admit-your-errors-and-go-on-from-there/>
<https://www.bbc.co.uk/news/magazine-22223190>

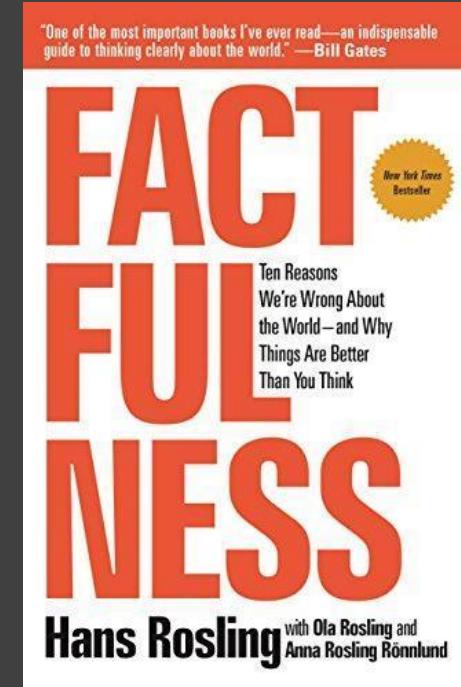
@turingway, CC-BY 4.0,
The Turing Way, DOI: 10.5281/zenodo.7684733

Scientific errors have real world effects

"We will redouble our efforts to avoid such errors in the future ..." - Authors

"mistaken way to examine (country specific) data provides an intellectual rationalisation for things that affect how people think about the world."

- Daniel Hamermesh



<https://www.gapminder.org/>, Rosling, H., Rönnlund, A. R., & Rosling, O. (2018). Factfulness: Ten Reasons We're Wrong About the World--and Why Things Are Better Than You Think. <https://www.bbc.co.uk/news/magazine-22223190>

@turingway, CC-BY 4.0,
The Turing Way, DOI: 10.5281/zenodo.7684733

Price of Popularity

Researchers in Australia used unreliable COVID-19 data and misreported that an anti-parasite drug could stop the virus from replicating in cells.



In a desperate attempt to save dying patients, doctors began justifying the drug's use against COVID-19 as the virus spread aggressively throughout Latin America.

Reardon, S. (2021). Flawed ivermectin preprint highlights challenges of COVID drug studies. *Nature*, 596, 173–174. doi: 10.1038/d41586-021-02081-w. Mega, E. R. (2020). Latin America's embrace of unproven COVID treatment hinders drug trials. *Nature*, 586, 481–482. doi: 10.1038/d41586-020-02958-2. Slides under DOI: 10.5281/zenodo.5568007

Post-publication Peer Review is Important, But ...

To consult the [experts] after an experiment is finished is often merely to ask to conduct a post mortem examination. [...] can perhaps say what the experiment died of. - Ronald Fisher



Avoid Errors Before the Harm Occurs

1. Mistaken research design or analysis processes
 - **Project design for open, FAIR & reproducible research**

Avoid Errors Before the Harm Occurs

1. Mistaken research design or analysis processes
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2. Wrong choices of tools and methods
 - **Data handling, data management, collaboration process**

Avoid Errors Before the Harm Occurs

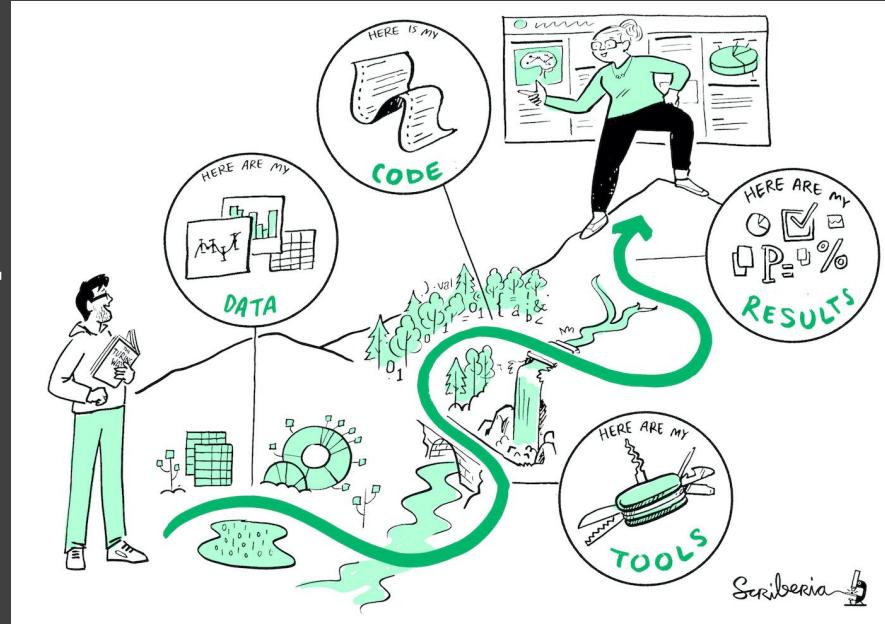
1. Mistaken research design or analysis processes
 - **Project design for open, FAIR & reproducible research**
2. Wrong choices of tools and methods
 - **Data handling, data management, collaboration process**
3. Inappropriate baseline comparison
 - **Lack of technical understanding (we won't discuss this!)**

Session 1 - Reproducible, Open and FAIR research

- What is reproducible research
- What is open research
- Concerns about opening up research
- Understanding FAIR data/research
- Making your research FAIR
- Setting up repositories and working collaboratively

Research Reproducibility

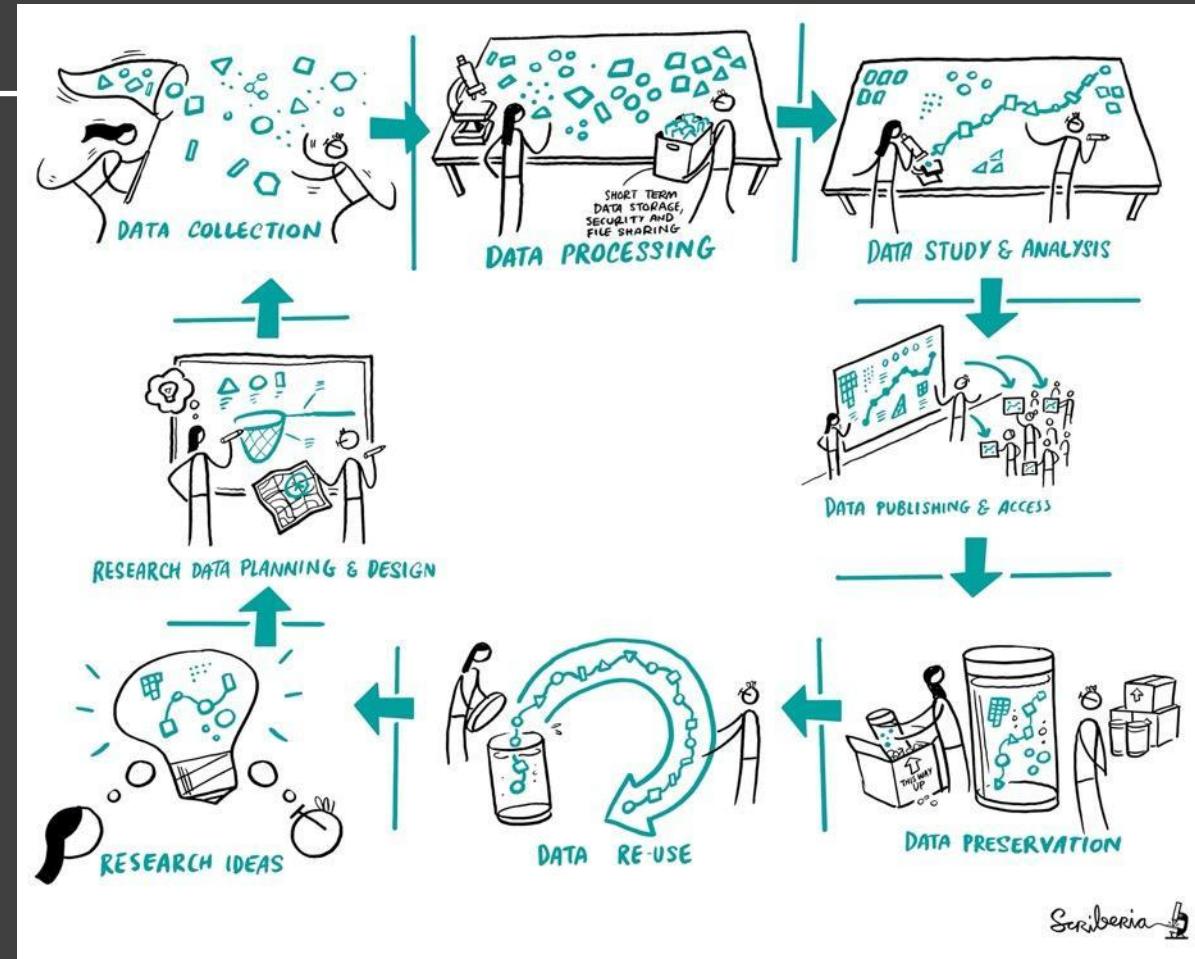
*Reproducible research saves
valuable time in verifying and
building upon existing solutions.*



		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable

Reproducible Research Workflows

		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable



Why do reproducible research?



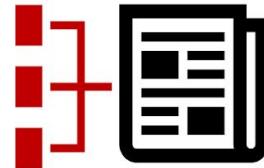
Track Project History



Collaborate & Review



Avoid Misinformation



Write Paper Efficiently



Get Credits Fairly



Ensure Continuity

Applying best practices in our research requires intention, resources, time and collaboration, which can be overwhelming.



Reflection exercise 1

What are some
barriers to
reproducibility?



Is not
considered for
promotion

Requires
additional
skills

Held to higher
standards than
others

Publication bias
towards novel
findings

Barriers to reproducible research

Support additional
users

Takes time

The Turing Way



An Open Source project that involves and supports its
diverse community to make data science **reproducible,**
ethical, collaborative and inclusive for everyone.

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

@turingway, CC-BY 4.0, The Turing Way, DOI: 10.5281/zenodo.7684733

Guide for Reproducible Research

Research

Overview

Open Research

Version Control

Licensing

Research Data Management

Reproducible Environments

BinderHub

Code quality

Code Testing

Code Reviewing Process

Continuous Integration

Reproducible Research with Make

Research Compendia

Credit for Reproducible Research

Risk Assessment

Case Studies

Guide for Reproducible Research

This guide covers topics related to skills, tools and best practices for research reproducibility.

The *Turing Way* defines reproducibility in data research as data and code being available to fully rerun the analysis.

There are several definitions of reproducibility in use, and we discuss these in more detail in the [Definitions of Reproducibility](#) section of this chapter. While it is absolutely fine for us each to use different words, it will be useful for you to know how *The Turing Way* defines *reproducibility* to avoid misunderstandings when reading the rest of the handbook.



A book: “Work in Progress”

The Turing Way

Search this book...

Welcome

- Guide for Reproducible Research
- Guide for Project Design
- Guide for Communication
- Guide for Collaboration
- Guide for Ethical Research
- Community Handbook
- Afterword

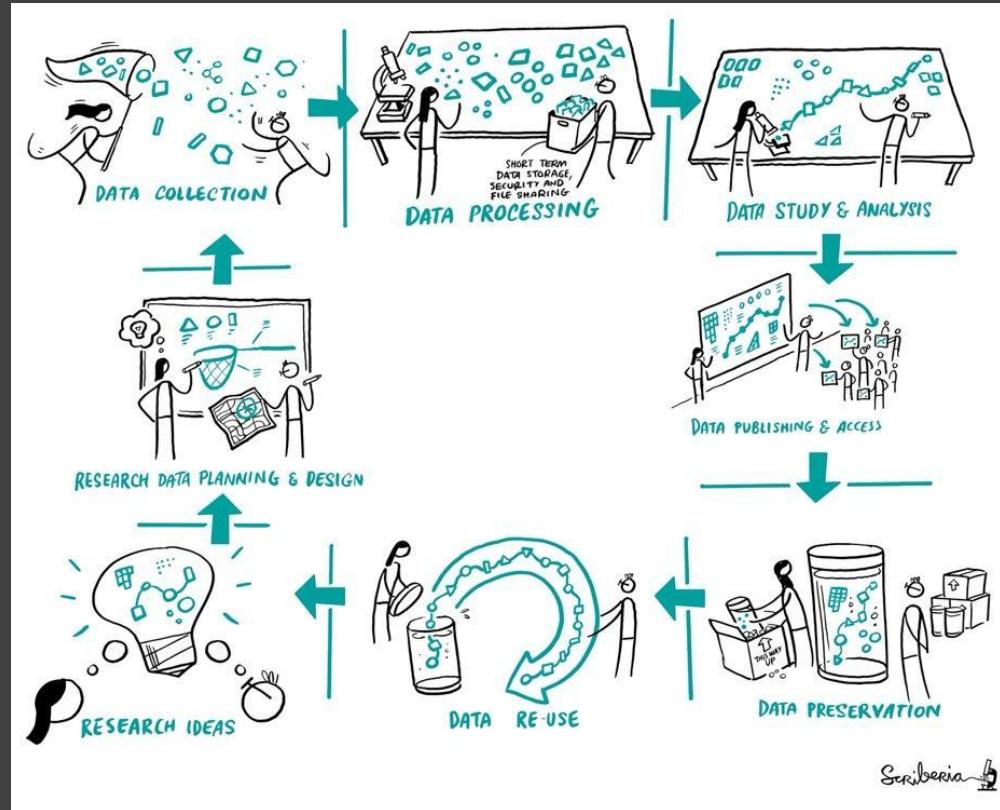
Visit our [GitHub Repository](#)

This book is powered by [Jupyter Book](#)



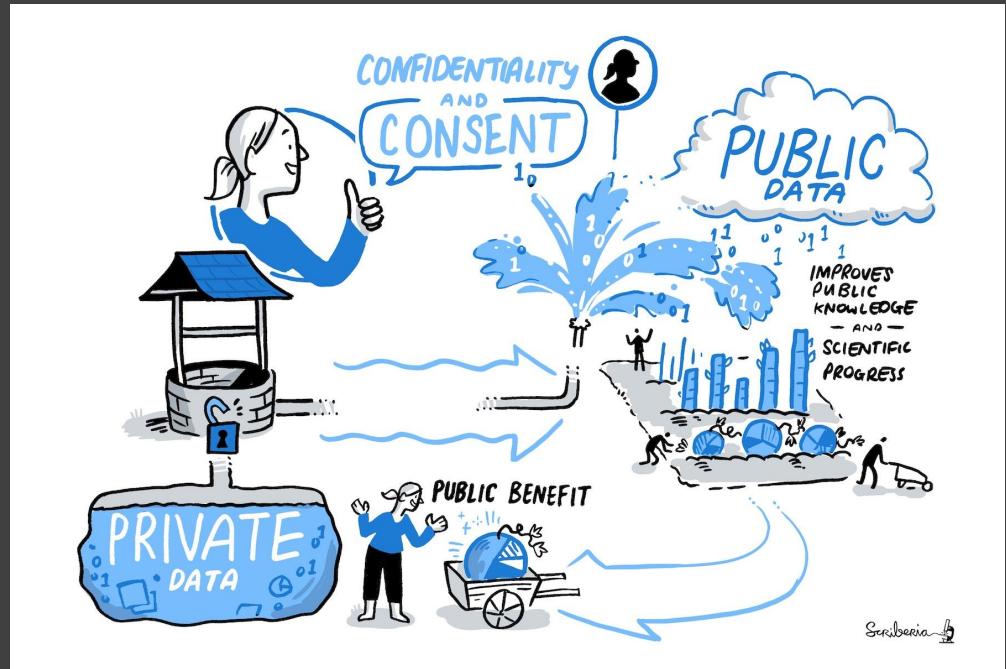
Reproducible workflows

- Applying reproducibility principles throughout the project's lifecycle
- Open source vs. "Inner" source



Privacy and sensitivity concerns

- Is the data too sensitive?
- Do I have permission to share openly?
- I don't want others to see all my work
- I don't know how to share my work



Reflection exercise 2

- What motivates you to share your work?
- What concerns you about sharing your work?



Breakout room: 10 minutes

What do you need to consider to ensure your work is reproducible?

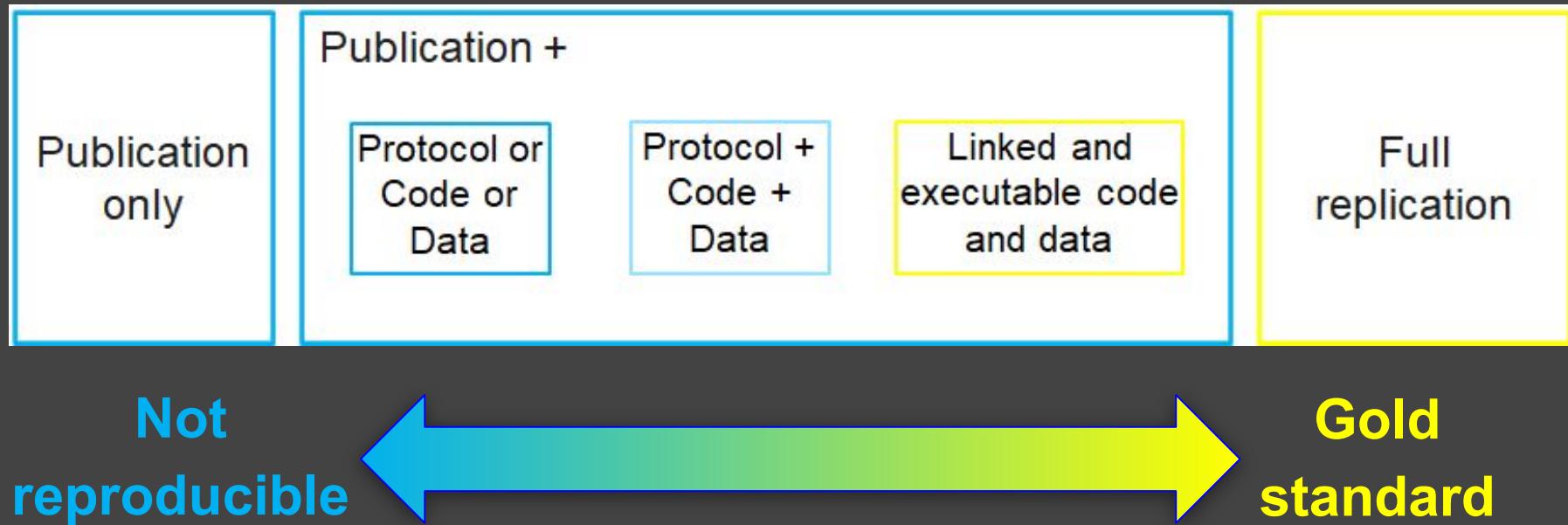
- Research object: (1) Data, (2) code, (3) workflow, (4) documentation
- Practices: Version control, licensing, data management, communication, collaboration, reusability, long-term archiving
- Instructions: (i) Each room is assigned a research object. (ii) Nominate a notetaker in your room. (iii) Select 1 or 2 practices. (iv) Discuss at what stages of research cycle these practices are applied. (v) Report!

Breakout Room: 15 Minutes

What do you need to consider to ensure your work is reproducible?

- **Research object:** (1) Data, (2) code, (3) workflow, (4) documentation
- **Practices:** Version control, licensing, data management, communication, collaboration, reusability, long-term archiving
- **Instructions:** (i) Each room is assigned a research object. (ii) Nominate a notetaker in your room. (iii) Select 1 or 2 practices. (iv) Discuss at what stages of research cycle these are practices applied. (v) Report!

Reproducible Research Spectrum



Adapted from Peng 2011

<https://www.science.org/doi/abs/10.1126/science.1213847>

Reproducibility: Where should we start?

Reproducible research workflow:

1. Collaboration

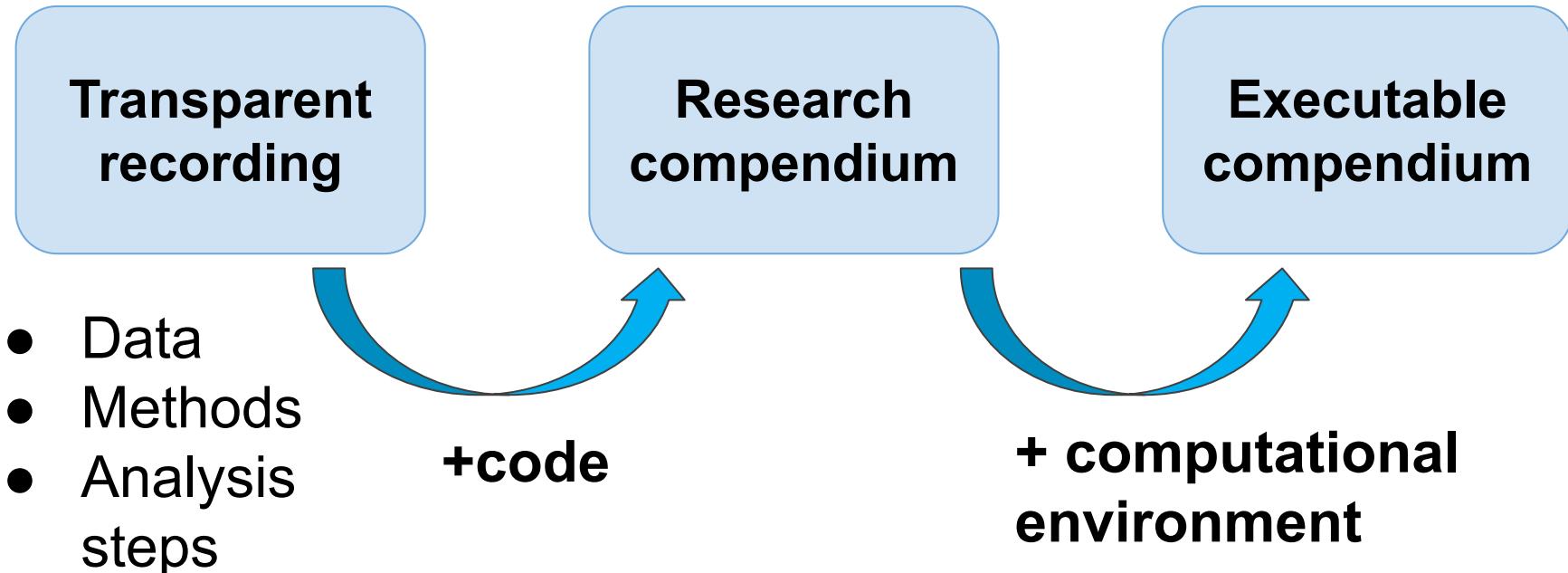
- Using collaborative, version controlled and **open ways** to work with others.

2. Transparency

- Clear documentation of methods, data, code - **openly shared** research compendium.

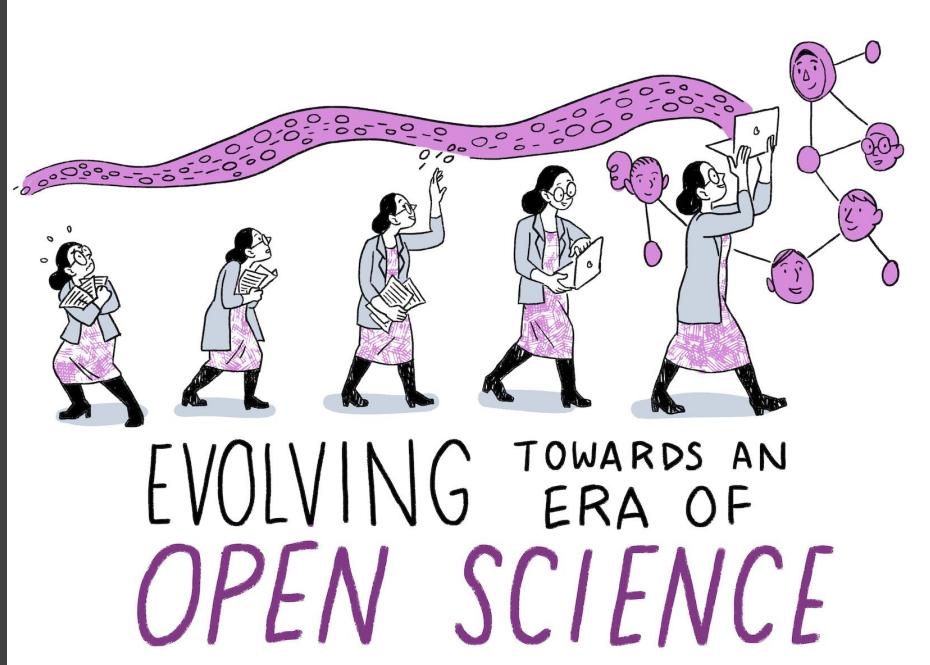


Three computational skill levels for reproducibility



Karoune, E., and Plomp, E.(2022) Removing Barriers to Reproducible Research in Archaeology. Zenodo, ver. 5 peer-reviewed and recommended by Peer Community in Archaeology.<https://doi.org/10.5281/zenodo.7320029>.

Open Science to enable Collaboration and Transparency



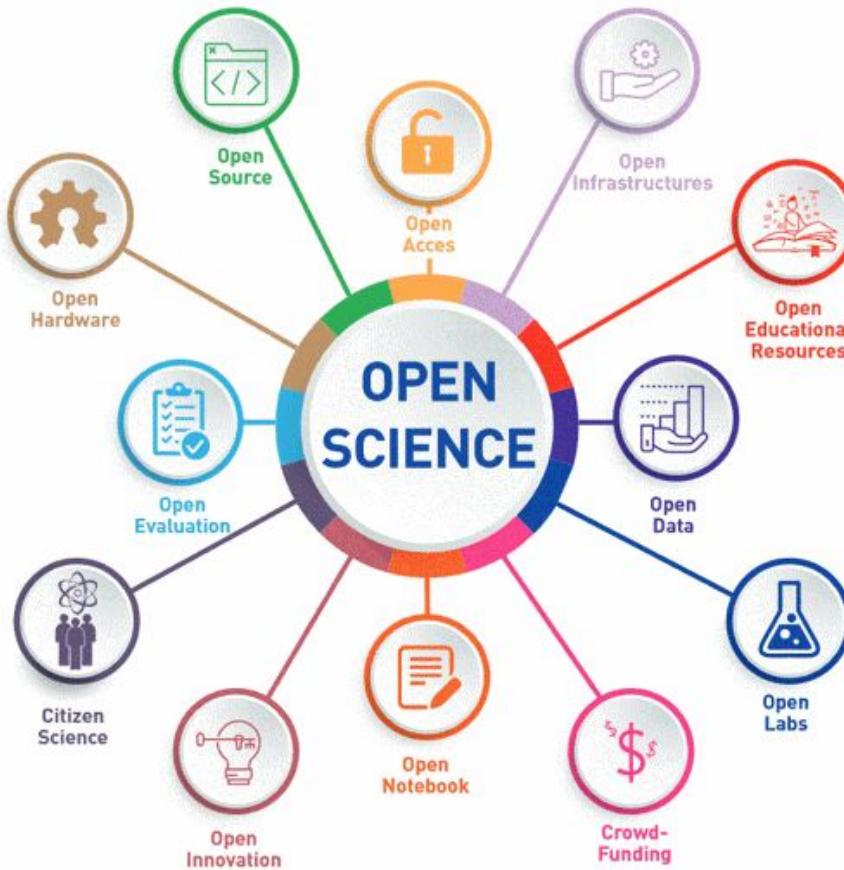
- Open Science practices **remove barriers** from sharing and using scientific resources **at all stages** of research.
- Make research findings **accessible to all** rather than keeping them locked away (for example, behind a paywall).

Open Science aims to transform research by making it more transparent → accessible → reliable → reproducible → reusable → collaborative → beneficial to society.

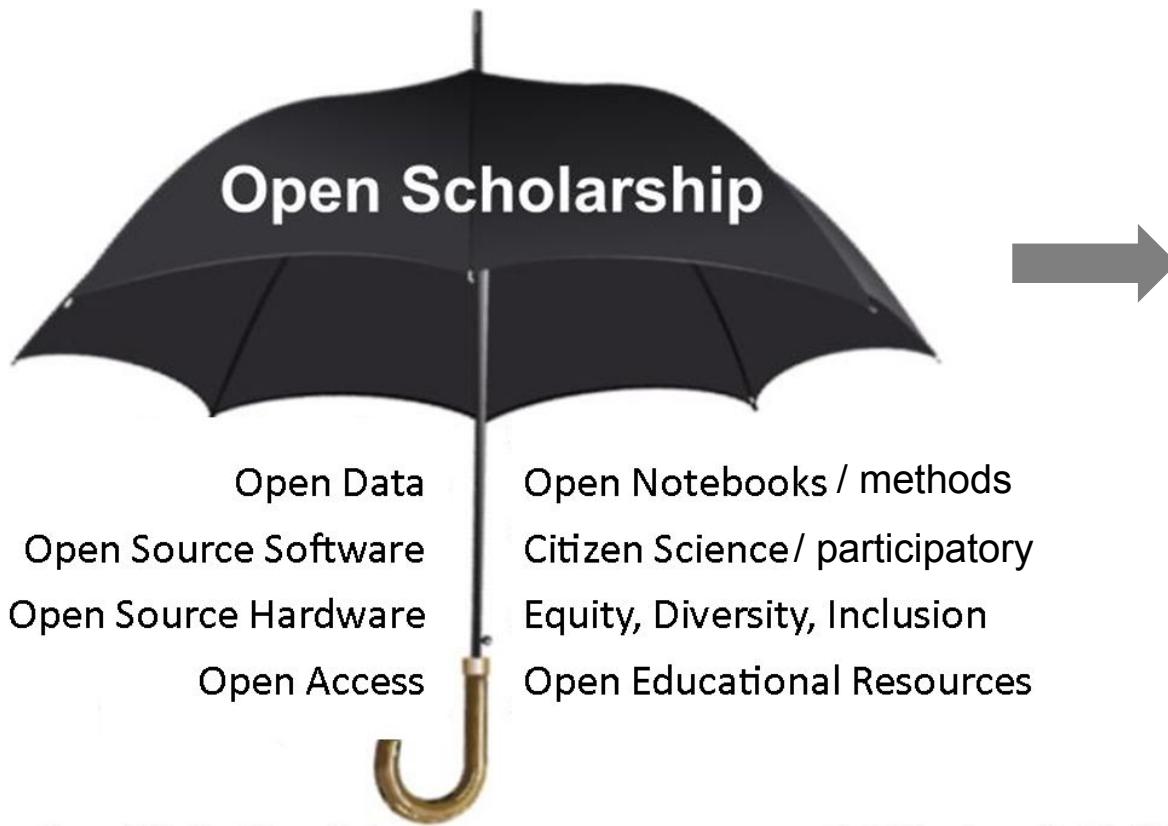
To achieve this openness in research, we need to make each element of the research process ...

- *publicly available,*
- *with permission to view, use, modify and distribute, and*
- *description for how one can collaborate.*

Open Science is an umbrella term for open research practices



What are some barriers we should work to remove?



Transparency →
Reproducibility →
Research Quality →
Sustainability



Collaboration →
Inclusive Research →
Equity and Diversity →
Global Accessibility

Open Science

Open Research

Open Scholarship



We are going to use these terms interchangeably today to cover important considerations for you!



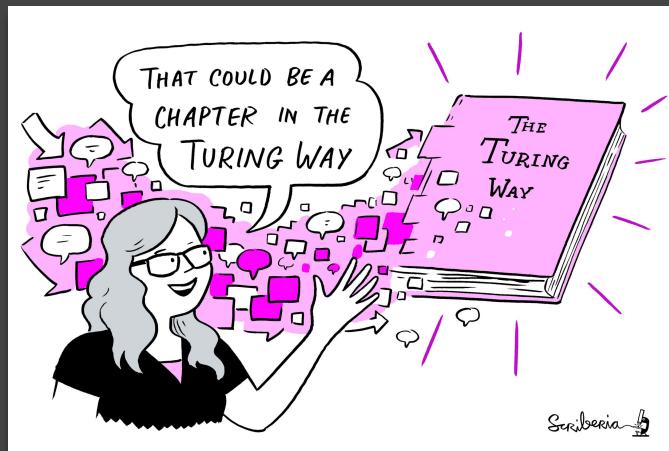
Book:
the-turing-way.netlify.app/

GitHub:
github.com/alan-turing-institute/the-turing-way

Twitter:
twitter.com/turingway

Email:
theturingway@gmail.com

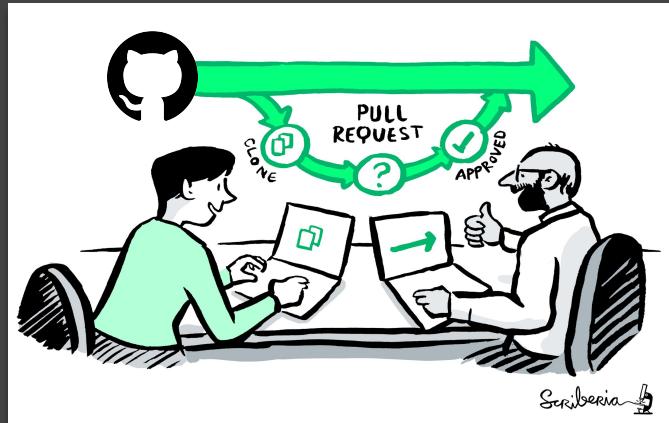
A Book



A Community



An Open Source Project

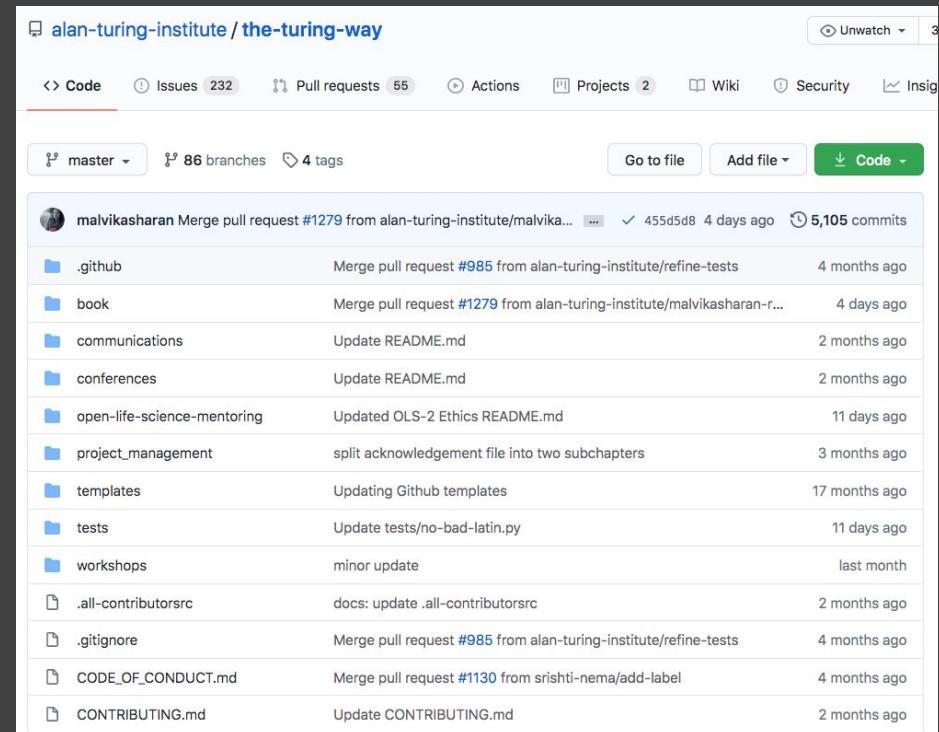


A Culture of Collaboration



A Collaborative, Version Controlled and Open Project

- Shared online
- Designed for open collaboration
- Hosted on GitHub with history and versions
- Described with open license
- Community oriented



📁 .github	Remove prettier configuration	
📁 book	minor update	
📁 communications	Fix typos	
📁 conferences	Add KW formatting pedantry	
📁 project_management	Update online-collaboration-cafe.md	
📁 templates	Updating Github templates	
📁 tests	Add "et cetera" as a deprecated Latinism	
📁 workshops	Remove mis-pasted text	
📄 .all-contributorsrc	Merge pull request #991 from alan-turing-institute/all-contributors/a...	5 days ago
📄 .gitignore	ignore pptx in workshop folder	9 months ago
📄 .travis.yml	add html-proof file again	last month
📄 CODE_OF_CONDUCT.md	her -> their	6 months ago
📄 CONTRIBUTING.md	Update CONTRIBUTING.md	2 months ago
📄 GOVERNANCE.md	Read through months later	5 months ago
📄 LICENSE.md	Fix typo in licence	2 months ago
📄 README.md	Merge pull request #991 from alan-turing-institute/all-contributors/a...	5 days ago
📄 book_skeleton.md	Update book_skeleton.md	13 months ago
📄 contributors.md	Add myself to contributors.md	11 months ago
📄 tips_and_tricks_survey.md	Update tips_and_tricks_survey.md	14 months ago
📄 ways_of_working.md	Adjust team contact section	5 months ago



Scriberia

An Open Science project

- everyone can freely read, reuse, distribute, modify and help develop
 - the project belongs to the research community (CC-BY license)
 - Builds in collaboration with other projects

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The Turing Way

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September 2, 2020 (v2) [Presentation](#) [Open Access](#)

Challenges in Assessing Contributions to Reproducible Research and Open Science

Sharan Malvika; Helen Sitar

DORA Panel Addressing Roadblocks in Research Assessment Reform Panel organiser and moderator: Helen Sitar
Speakers: Malvika Sharan (presentation in this Zenodo deposit) with Elena Simukovic, David Carr, Ulrich Drinagl, Anne Letho, Serhiu Nazarovets About the panel: Research evaluation

Uploaded on September 2, 2020

1 more version(s) exist for this record

View

August 11, 2020 (v1) [Presentation](#) [Open Access](#)

FSC2020 Lightning Talk: The Turing Way

Esther Plomp, Kirstie Whitaker;

Lightning talk presented by Esther Plomp on the 3rd of August 2020 for the Force11 Scholarly Communication Institute (FSC2020). Reproducible research is necessary to ensure that scientific work can be trusted. By sharing data, analysis code and the computational environment used to generate the r

Uploaded on August 11, 2020

View

August 6, 2020 (v1) [Journal article](#) [Open Access](#)

The Turing Way workshop on Boost your reproducibility with Binder

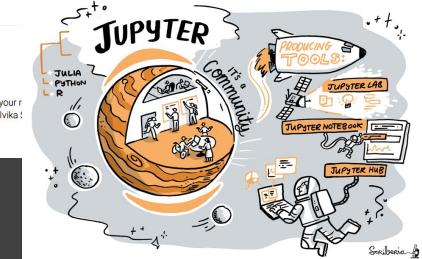
Sharan, Malvika;

This workshop was organized with the UKDRI team. Title: The Turing Way workshop on Boost your r Binder Date: 11 June, 2020 (13:00 - 17:00 GMT) Instructors: Kirstie Whitaker, Sarah Gibson, Malvika !

Unpublished by [AcademicZenodo](#)

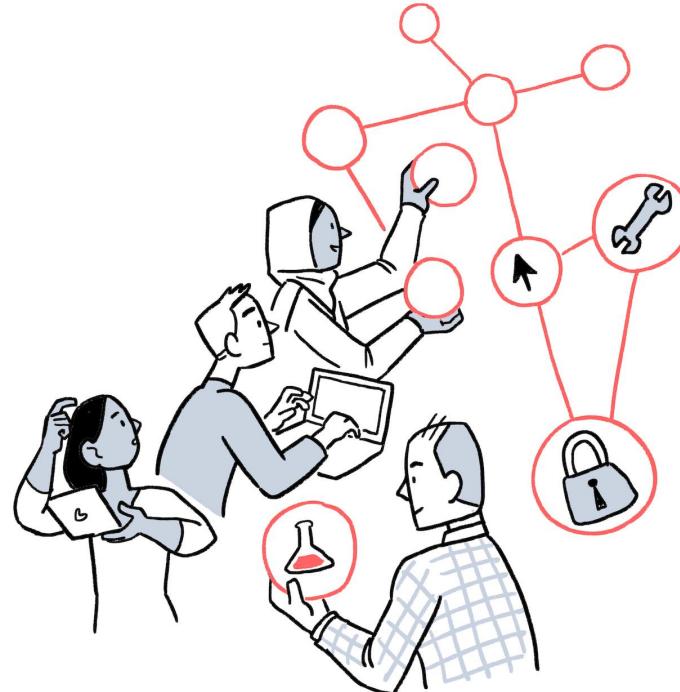
The Turing Way

Reproducible research is necessary to ensure that scientific work can be trusted. This means that others can understand and verify the results. Publishers are beginning to require that publications include access to the underlying data and the analysis code. The goal is to ensure that all results can be independently verified and built upon in future work. This is sometimes easier said than done. Sharing these research outputs means understanding data management, library sciences, software development, and continuous integration techniques that are not widely taught or expected of academic researchers and data scientists. The Turing Way is a framework to support students, teachers, and other users and editors in ensuring that reproducible data science is "too easy to do". It will include training material on version control, analysis testing, and open and transparent communication with future users, and build on Turing Institute case studies and



Open Science:

Where should we start?

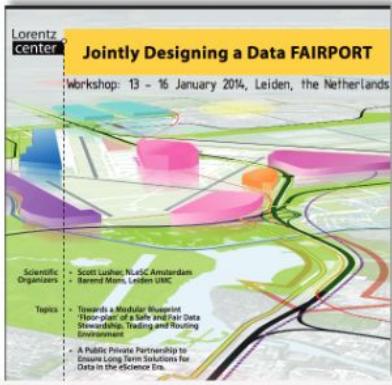


Scriberia

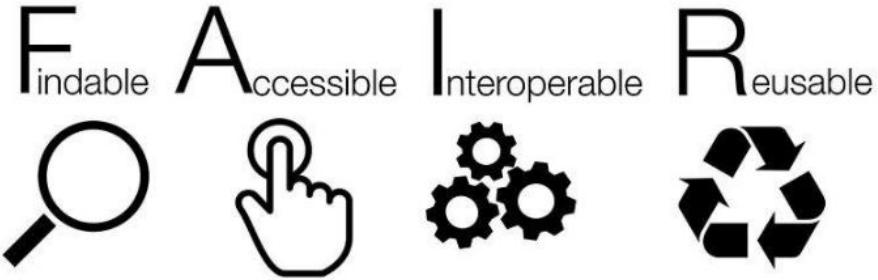
FAIR principles

- Findable,
- Accessible
- Interoperable
- Reusable





2014



SCIENTIFIC DATA
SPINGER NATURE

OPEN Comment: The FAIR Guiding Principles for scientific data management and stewardship

SUBJECT CATEGORIES

- » Publication characteristics

Mark D. Wilkinson, Michel Dumontier, IJssbrand Jan Aalbersberg, Gabrielle Appleton, Myles Axton, Arie Baak, Niklas Blomberg, Jan-Willem Boiten, Luiz Bonino da Silva Santos, Philip E Boume, Jildau Bouwman, Anthony J Brookes, Tim Clark, Mercé Crosas, Ingrid Dillo, Olivier Dumon, Scott Edmunds, Chris T Evelo, Richard Finkers, Alejandra Gonzalez-Beltran, Alasdair J G Gray, Paul Groth, Carole Goble, Jeffrey S. Grethe, Jaap Hemmenga, Peter A.C. 't Hoen, Rob Hooft, Tobias Kuhn, Ruben Kok, Joost Kok, Scott J. Lusher, Maryann E. Martone, Albert Mons, Abel L. Packer, Bengt Persson, Philippe Rocca-Serra, Marco Roos, Rene van Schaik, Susanna-Assunta Sansone, Erik Schultes, Thierry Sengstag, Ted Slater, George Strawn, Monica A. Swertz, Mark Thompson, Johan van der Lei, Erik van Mulligen, Jan Velterop, Andra Waagmeester, Peter Wittenburg, Katherine Wolstencroft, Jun Zhao, and Barend Mons

SCIENTIFIC DATA | 3:160018 | DOI: 10.1038/sdata.2016.18

A set of principles to enhance the value of all digital resources

Developed and endorsed by researchers,
service providers, publishers, funding
agencies and industry partners

FAIR principles from Wilkinson et al. (2016)
DOI: 10.1038/sdata.2016.18

FAIR data analogy



Annotation makes it easier to find important things

You would not buy food with no labels!

Labels make different foods easier to find and access in stores, combine with other foods (interoperable) and use in different ways.



Adapted from talk by Philippe Rocca-Serra (2020)

What is the meaning of FAIR data ?

F = Findable



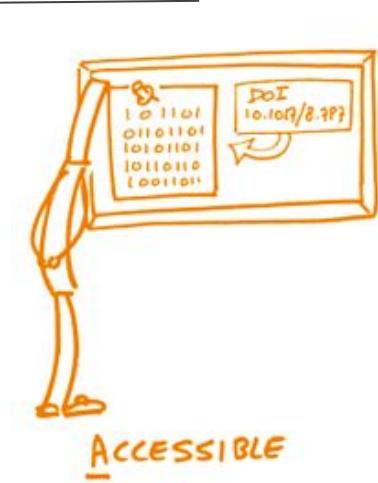
*in an **online** data catalogue / archive / portal*
findable by humans and by machines

- [ENA](#) for DNA sequences
- [GBif](#) and [OBIS](#) for biodiversity data
- [Biolimage Archive](#) for images of biological material
- [Zenodo](#) as a general-purpose open-access repository

Standardised and **rich** discovery **Metadata** explaining:

- Who:** is the **author / contact person** for questions
- How:** were the data created --> **procedures / protocols**
- How:** to **access** the data, consider **licenses**
- What:** **keywords** describe the data
- What:** **parameters** were measured, **species** & **geography** covered
- When:** were the **data** and **updates** created

What is the meaning of FAIR data ?



A = Accessible Data & Metadata

*from catalogue/archive/portal
via **machine to machine** and **human interfaces***

- **Web interfaces** for human searches & downloads
- **APIs** for searching & accessing
- Clear **instructions** for access (download, request access,..)
- **Keeping metadata** when data is deleted
- **Metadata update** when updating data / information
- **All data levels** should be archived: raw data is the most important and at a minimum must be provided

What is the meaning of FAIR data ?



I = Interoperable

readable & understandable by humans / code :

- Community-accepted** data formats & file types
 - **open** (non-proprietary)
 - **sustainable** (think in 10 years from now)
- Clear, controlled vocabulary** for data & metadata
 - **describing** all relevant terms/values/units
 - **specific** → data/metadata “dictionary”
- Your data should be **standalone**, packaged up with
 - all **necessary information and files** to allow the data to be understood by anyone at any time
- Readable** by code:
 - **machine readable** descriptions of data: files and format

What is the meaning of FAIR data ?



REUSABLE

R = Re-usable

Know *how I can trust, repeat, re-analyse, re-use* the data.

Necessary to provide:

- Data **usage licence** --> full terms & conditions
- Data **provenance** --> metadata and information on:
 - every data life-cycle stage
 - documentation / protocols / references
 - link to accompanying data and publications
 - instruments & software used
- Relationship** between the different levels of data you provide is documented:
raw--> quality controlled -->processed-->published

What is a data life-cycle? Data provenance

Data Life-Cycle:

- covers the entire period of time over which data exists
- encompasses all the stages: **first Capture** → **data re-use**

1. Sample acquisition → raw data:

sample preparation, experimental settings / parameters, raw data acquisition

2. Data **quality control**: checking and updating of collected data

documentation of QC procedures

3. Data **processing & analysis**: guided by scientific question

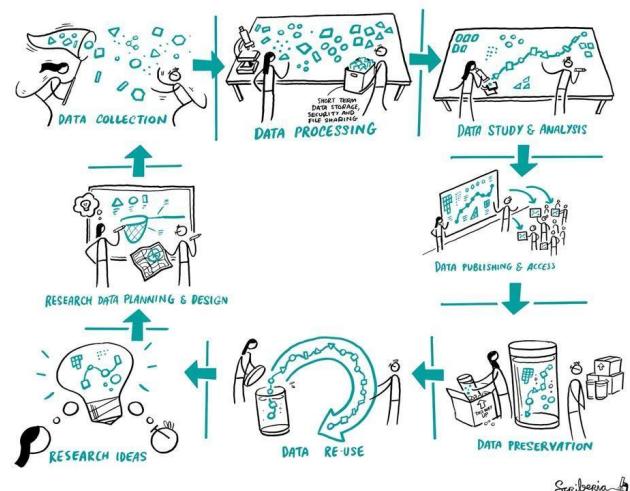
documentation of processing steps, analysis methodology

4. **Archiving & publication**: data are placed in an online catalogue

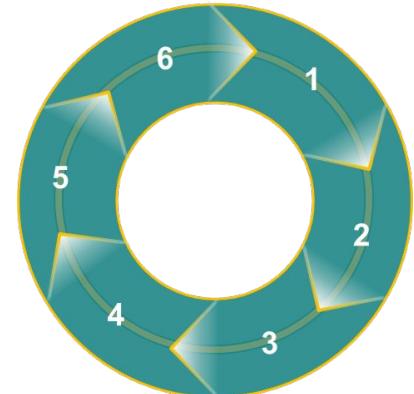
discovery metadata, provenance metadata, provenance files, references and links

5. Data **dissemination / integration**: adding data to well known portals, brokers

6. Data **reuse**: only possible with sufficient provenance information!



Sorberia

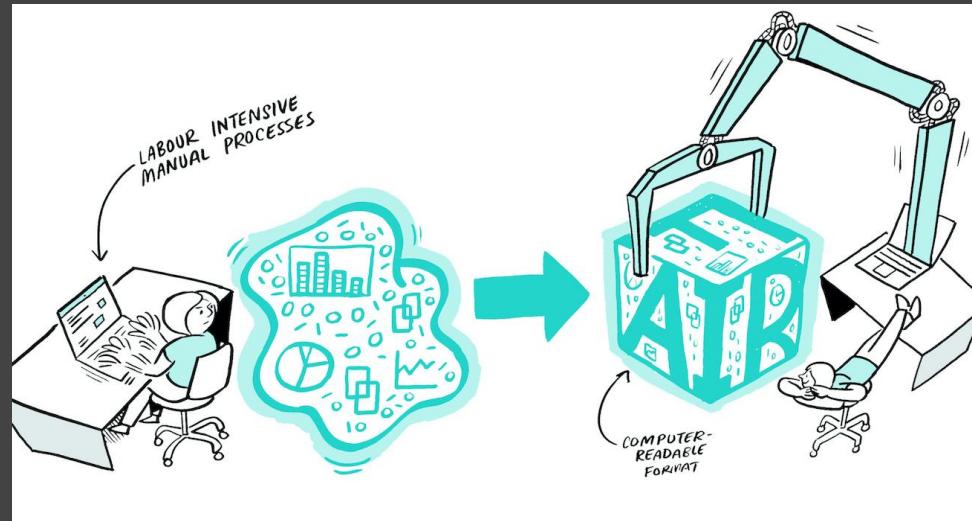


Breakout Room: FAIR Reflection

What part of your research lifecycle/outputs can be made open?

What you will have to do in your project to maintain "this" aspect of FAIR.

- Room 1: Findable
- Room 2: Accessible
- Room 3: Interoperable
- Room 4: Reusable



Reproducible research doesn't always mean open

- Reproducibility can be facilitated by open, but **open is a choice**
- Reproducibility needs to be considered at all stages
- As open as possible, **as closed as necessary**
 - Open principles should be applied when you can
 - NEVER for private, confidential or sensitive data
- Always apply FAIR (**F**indable, **A**ccessible, **I**nteroperable, **R**Reusable)

Reproducibility

- Is my code **correct**?
- Can others **read and test** it?
- Is my **workflow robust**?
- Have I provided **guidance**?
- Is my work **citable**?

Reproducibility should ensure higher scientific standards allowing others to test and reuse your work ...

Open Source

- Is my code **freely available**?
- Can others **modify and share** it?
- Is my **workflow reusable**?
- Have I provided **permission**?
- Is my work **open for collaboration**?

... and Open Source should allow anyone to reuse, report errors, fix issues, build on and collaborate

FAIR doesn't need to be open

- FAIR does not require data to be open
- FAIR requires open metadata
- Detailed information about research/data should be open
- FAIR applies open standards for interoperability

Box 2 | The FAIR Guiding Principles

To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
- A1.1 the protocol is open, free, and universally implementable
- A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

To be Reusable:

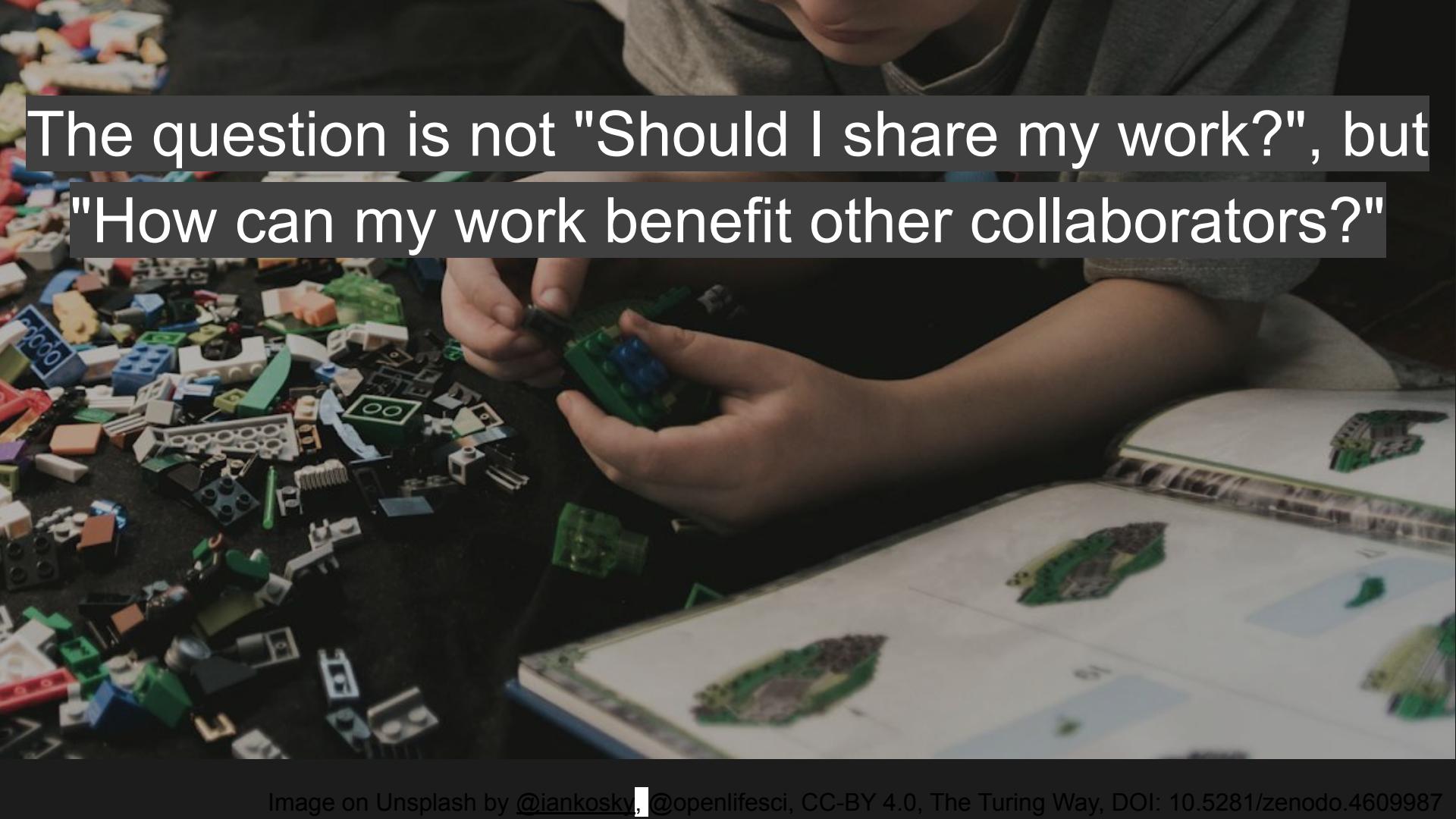
- R1. meta(data) are richly described with a plurality of accurate and relevant attributes
- R1.1. (meta)data are released with a clear and accessible data usage license
- R1.2. (meta)data are associated with detailed provenance
- R1.3. (meta)data meet domain-relevant community standards

Metadata: information about the “data descriptors” that facilitate cataloguing data and data discovery

Is this Reproducible, Open or FAIR?



- TARO is a PhD researcher in a health data science team
- Collaborates with people in their team of engineers and data scientists
- They have written Python code for a commonly used dataset
- Their supervisor suggested them to publish their work online
- Created a public repository to share their code, data and documentation
- Sent out an email to their team members to use their code



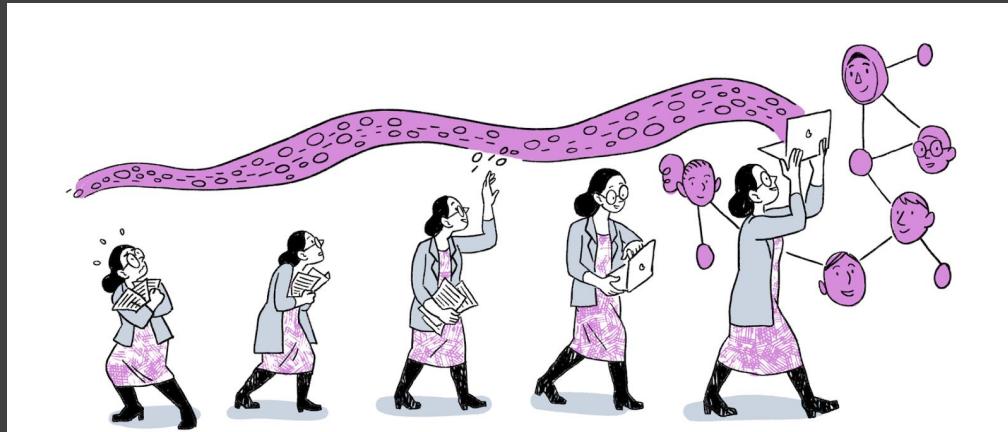
The question is not "Should I share my work?", but
"How can my work benefit other collaborators?"

You are your number one collaborator!

Good practices benefit (future) you!



Open Science path is self defined!



- Reproducibility is essential.
- Open Science involves many concepts - take the steps that are possible.
- FAIR provides guidance for actionable steps that make your work reproducible.
- *Ask for feedback and help whenever you can.*

Several ways to practice Open Science

- Develop sustainable tools/resources
- Make your research objects accessible to more people
- Create learning materials so others can learn
- Teach a skill so you can upskill yourself as well as others
- Contribute to collaborative projects, invite collaborations
- Publish pre-prints so you can share your work early on

All of these while you gain visibility and credit for your work

Reproducible & Open Science Projects



Online Repository



License/Permission



Documentation



Version Control



Dependencies
and data



Review & Verify



Report/Fix Bugs



Release & Cite

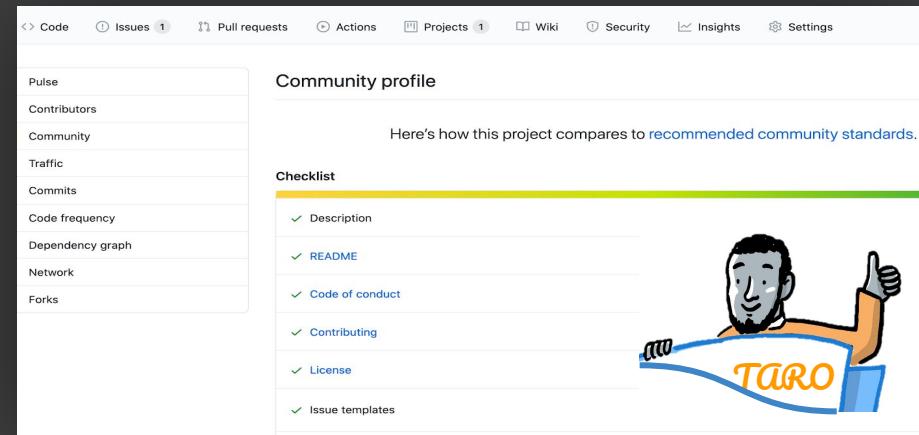
Is this Reproducible, Open or FAIR?



- TARO is a PhD researcher in a health data science team
- Collaborates with people in their team of engineers and data scientists
- They have written Python code for a commonly used dataset
- Their supervisor suggested them to publish their work online
- Created a public repository to share their code, data and documentation
- Sent out an email to their team members to use their code

Ensure Use and Reuse

- Create a [project repository](#)
- Create a [README file](#) with information on their scripts
- Add an [open license](#) in their repository for reuse
- Make it [easy to test](#)
- Add a [minimum guideline](#) for reporting errors
- Release [citable versions](#) of documentation/code/data



READMEs for Open and Collaborative Projects

Motivation:

Learn how to communicate your project effectively.

Method:

Write clear description of the project in README file.

Why READMEs?



WELCOME

What is a README file?

- A clear and accessible description of your project
- Found in the root directory of your repository
- First stop for your collaborators and potential users

Could also be: website landing page, wiki

What should a good README include?

In your README file, make sure to include:

- what you're doing, what your motivation is
- what makes your project special and exciting
- who your collaborators are and how each has contributed. It's also a good idea to tell people how they can contribute to your project!
- where the key resources are

README example

STEMM Role Models App

Inspire future generations by providing the most exciting and diverse speakers for your conference.

[chat on gitter](#)

Welcome!

First and foremost, Welcome! 🎉 Willkommen! 🎉 Bienvenue! 🎉🎈🎈

Thank you for visiting the STEMM Role Models app project repository.

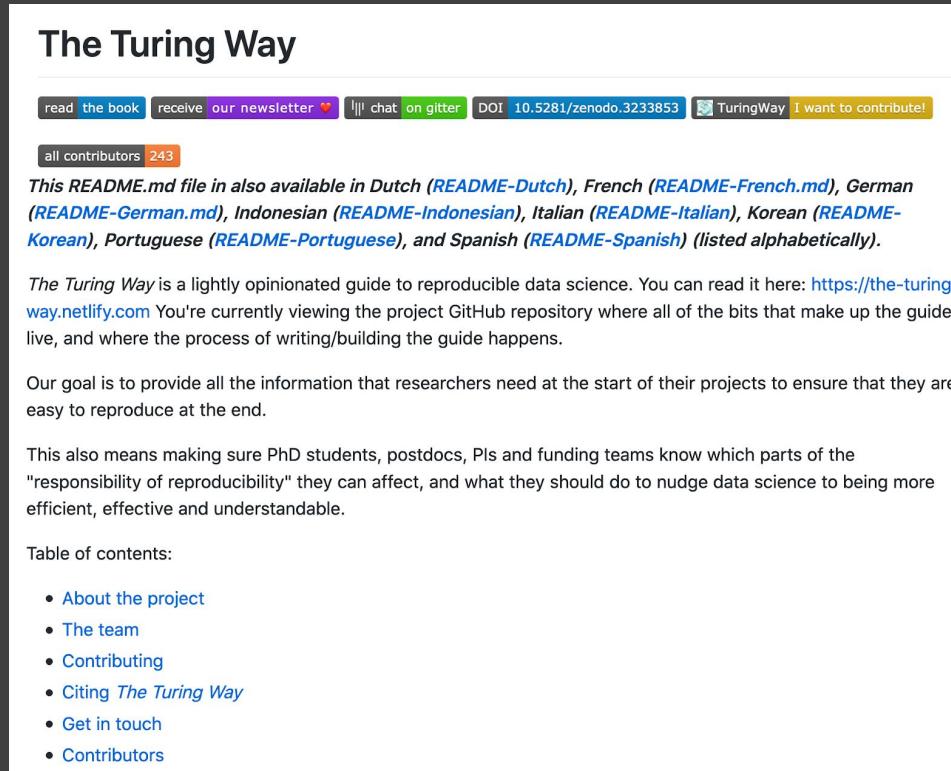
This document (the README file) is a hub to give you some information about the project. Jump straight sections below, or just scroll down to find out more.

- [What are we doing? \(And why?\)](#)
- [Who are we?](#)
- [What do we need?](#)
- [How can you get involved?](#)
- [Get in touch](#)
- [Find out more](#)
- [Understand the jargon](#)

- Welcome message!
- Project description & vision
- How to:
 - Test and verify
 - Fix errors
 - Use (license)
 - Get involved
 - Report issues

Source: [STEMM Role Models App](#)

README example



The screenshot shows the README page for "The Turing Way". At the top, there's a navigation bar with links for "read the book", "receive our newsletter", "chat on glitter", "DOI 10.5281/zenodo.3233853", "TuringWay", and "I want to contribute!". Below this, a button says "all contributors 243". The main content area starts with a note that the README is available in multiple languages. It then describes the project as a lightly opinionated guide to reproducible data science, mentioning the GitHub repository where the guide is built live. The goal is to provide information for researchers to ensure their projects are easy to reproduce. This also involves educating PhD students, postdocs, PIs, and funding teams about reproducibility. A table of contents is provided at the bottom.

The Turing Way

read the book receive our newsletter ❤️ ||| chat on glitter DOI 10.5281/zenodo.3233853 TuringWay I want to contribute!

all contributors 243

This README.md file is also available in Dutch ([README-Dutch](#)), French ([README-French.md](#)), German ([README-German.md](#)), Indonesian ([README-Indonesian](#)), Italian ([README-Italian](#)), Korean ([README-Korean](#)), Portuguese ([README-Portuguese](#)), and Spanish ([README-Spanish](#)) (listed alphabetically).

The *Turing Way* is a lightly opinionated guide to reproducible data science. You can read it here: <https://the-turing-way.netlify.com> You're currently viewing the project GitHub repository where all of the bits that make up the guide live, and where the process of writing/building the guide happens.

Our goal is to provide all the information that researchers need at the start of their projects to ensure that they are easy to reproduce at the end.

This also means making sure PhD students, postdocs, PIs and funding teams know which parts of the "responsibility of reproducibility" they can affect, and what they should do to nudge data science to being more efficient, effective and understandable.

Table of contents:

- [About the project](#)
- [The team](#)
- [Contributing](#)
- [Citing *The Turing Way*](#)
- [Get in touch](#)
- [Contributors](#)

- project description
- list of authors & contributors
- contact information
- links to related material
- installation instructions
- tutorials and requirements
- how to run associated tests

Assignment: create a project repository

- Create a **GitHub repository** for your project
- Add a **README file** to communicate about your work
- *Optional:* try to add a usage licence to your repository.
 - This allows others to reuse, modify, and build upon your work
 - We will cover licences in the next session)

Use *The Turing Way* chapter on README files to guide your assignment:
<https://the-turing-way.netlify.app/project-design/project-repo/project-repo-readme.html>

Create a GitHub Repository with README file

Create a new repository

A repository contains all the files for your project, including the revision history.

Initialize this repository with:

Skip this step if you're importing an existing repository.

Add a README file

This is where you can write a long description for your project. [Learn more.](#)

Add .gitignore

Choose which files not to track from a list of templates. [Learn more.](#)



Note

Three lessons about README

- Know your users and what they need
- Get users doing powerful things quickly
- Watch out for jargon!

Source: Hao Ye. (2021, March). Collaborations Workshop 2021 Mini-Workshop: README tips to make your project more approachable (Version v1.0.0). Zenodo. <http://doi.org/10.5281/zenodo.4647391>

End of Part 1: Further Reading and Examples

- [The Turing Way README](#)
- [Open Life Science README](#)
- Purple Booth's [README Template](#)
- Thoughtbot's Blog on [How to Write a Good README](#)
- Matias Singer's curated [List of Awesome READMES](#)



The Turing Way Workshop: Reproducible, Open and FAIR Research

Session 2

Emma Karoune, Eirini Zormpa & Anne Lee Steele

Pronouns: she/her/hers



Anne



Community Manager, The Turing Way

- Fellow, Open Knowledge Foundation & Internet Society
- Maintainer, Open Source Social Science
- Resident, Wikimedia Unlock Program
- Ethnographer, OpenStreetMap
- Mentor, Open Life Science

Background

- Anthropologist/Sociologist by training
- Data journalism



Session 2 - Project communication, collaboration and sharing

- **Review Assignment 1**
- License to allow reuse of your research outputs in a way YOU want
- Make your work **citable**: Digital Object Identifiers, Zenodo
- Setting online repository for **collaboration**
 - CoC, Contributing guidelines, continuous integration
- **Reproducible environment** and sharing to aid reproducibility: **Binder**
- Revisiting how these contribute to implementing FAIR practices
- What more you can do.

Assignment: Create a project repository

Add top-level files: **README** and **LICENSE**

- Also try to add a License - to allow others to use, modify, build upon your work

Use The Turing Way chapter for README to guide your assignment

<https://the-turing-way.netlify.app/project-design/project-repo/project-repo-readme.html>

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Assignment: Create a project repository

Add top-level files: **README** and **LICENSE**

- Also try to add a License - to allow others to use, modify, build upon your work

Use The Turing Way chapter for README to guide your assignment

<https://the-turing-way.netlify.app/project-design/project-repo/project-repo-readme.html>

Owner *



malvikasharan

Repository name *

2022-03-project-example



Great repository names are short and memorable. Need inspiration? How about [automatic-funicular](#)?

Description (optional)



Public

Anyone on the internet can see this repository. You choose who can commit.



Private

You choose who can see and commit to this repository.

Initialize this repository with:

Skip this step if you're importing an existing repository.



Add a README file

This is where you can write a long description for your project. [Learn more](#).



Add .gitignore

Choose which files not to track from a list of templates. [Learn more](#).



Choose a license

A license tells others what they can and can't do with your code. [Learn more](#).

This will set `main` as the default branch. Change the default name in your [settings](#).

[Create repository](#)

A screenshot of a GitHub repository page. At the top, there are buttons for 'main' (with a dropdown arrow), '1 branch' (with a dropdown arrow), '0 tags', 'Go to file', 'Add file', and 'Code'. Below this, a commit from 'malvikasharan' is shown: 'Initial commit' at 407389b 10 seconds ago, with 1 commit. A file named 'README.md' is listed with the same details. In the main content area, there is a file named 'README.md' containing the text '2022-03-project-example'. To the right of this file, there is an edit icon (a pencil symbol inside a box) which is highlighted with a red border.

1. Copy Template:

https://raw.githubusercontent.com/ha0ye/CW21-README-tips/main/template_README.md

- Another example from The Turing:

<https://github.com/alan-turing-institute/reproducible-project-template>

2. Add your project information

Bonus: Badges and Additional Information

README.md

The Turing Way



Contributing

🚧 This repository is always a work in progress and **everyone** is encouraged to help us build something that is useful to the many. 🚧

Everyone is asked to follow our [code of conduct](#) and to checkout our [contributing guidelines](#) for more information on how to get started.

If you are not familiar or confident contributing on GitHub, you can also contribute a case study and your tips and tricks via our [Google submission form](#).

Citing *The Turing Way*

You can reference *The Turing Way* through the project's Zenodo archive using DOI: [10.5281/zenodo.3233853](https://doi.org/10.5281/zenodo.3233853). DOIs allow us to archive the repository and they are really valuable to ensure that the work is tracked in academic publications.

Custom Badges

The Shields service (at shields.io) provides a way to create custom badges for your projects. These are badges are very common and are frequently used to show status information about the project, or demonstrate tools that were used for the development of your project.

Example badge:

Powered by PostgreSQL

Static

Using dash "-" separator

`https://img.shields.io/badge/<LABEL>-<MESSAGE>-<COLOR>`

Dynamic

Session 2 - Project communication, collaboration and sharing

- Review Assignment 1
- License to allow reuse of your research outputs in a way YOU want
- Make your work citable: Digital Object Identifiers, Zenodo
- Setting online repository for collaboration
 - CoC, Contributing guidelines, continuous integration
- Reproducible environment and sharing to aid reproducibility: Binder
- Revisiting how these contribute to implementing FAIR practices
- What more you can do.

Open Licenses

Motivation: Allow others to use, remix and share your work.

Process: Add an open license for use, remixing and sharing.

References: [Licensing Chapter in The Turing Way](#)

Disclaimer: We are not lawyers - always consult your data officer.

Truly Open Licenses: common elements



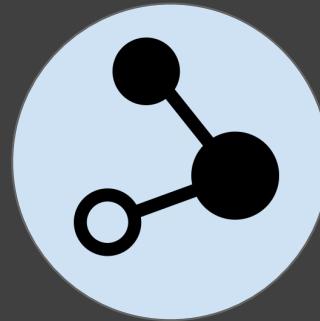
use

Anyone can use the work for any purpose



modify

Anyone can modify the work



share

Anyone can redistribute both the original and modified work

“Open source software is software that can be freely used, modified, and shared (in both modified and unmodified form) by anyone.“

- [GitHub Glossary, Open Source](#)

Attribution

Most open licenses require crediting the authors of the work.

Non-copyleft: Permissive, non-reciprocal - CC BY, MIT, BSD

- **do not require** derivative works to shared with the same license

Copyleft: Viral, reciprocal - CC BY-SA, GPLv3, MPL-2.0

- **require** derivative works to shared with the same license

Exception: CC0 (public domain, no copyright holder)

Licenses

							
Type	Permissive	Permissive	Permissive	Copyleft	Copyleft	Copyleft	
Provides copyright protection	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE
Can be used in commercial applications	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE	✓ TRUE
Provides an explicit patent license	✓ TRUE	✗ FALSE	✗ FALSE	✗ FALSE	✗ FALSE	✗ FALSE	✗ FALSE
Can be used in proprietary (closed source) projects	✓ TRUE	✓ TRUE	✓ TRUE	✗ FALSE	✗ FALSE partially	✗ FALSE for web	✗ FALSE
Popular open-source and free projects	Kubernetes Swift Firebase	Django React Flutter	Angular.js JQuery, .NET Core Laravel	Joomla Notepad++ MySQL	Qt SharpDevelop	SugarCRM Launchpad	

Licenses

Permission Overview

	Copyleft		Permissive	Proprietary
	Strong	Weak		
Use for anything	Yes	Yes	Yes	Sometimes
Private changes	Yes	Yes	Yes	Rarely
Distribute original	Same license, with source	Same license, with source	Same license, also binary-only ¹	Rarely
Distribute modified	Same license, with source	Same license, with source ²	Any license, also binary-only	Rarely
Distribute combined	Same license, with source	Any license, binary additions	Any license, also binary-only	Rarely

¹Under any license for the MIT license ²Relicensing LGPL to GPL is allowed

Permissive licenses grant the largest set of permissions to users. Copyleft licenses require redistribution of the original or modified source to use the same license, with weak copyleft licences allowing a different choice of license for the combined work. Proprietary licenses rarely provide any permissions beyond the right to use the software.

Licenses



Licenses

Permission Levels

The permission level provided by a Creative Commons data license can be understood from its name, which is a combination of two-letter “permission marks”. The only exception to this naming scheme is CC0, which will be introduced in the next section.

Permission Mark	What can I do with the data?
BY	Creator must be credited
SA	Derivatives or redistributions must have identical license
NC	Only non-commercial uses are allowed
ND	No derivatives are allowed

For example, the CC BY-ND license specifies that users must credit the creator of the data and cannot create any derivatives.

Licenses



Licenses

License	Domain	By	SA	Comments
Creative Commons CCZero (CC0)	Content, Data	N	N	Dedicate to the Public Domain (all rights waived)
Open Data Commons Public Domain Dedication and Licence (PDDL)	Data	N	N	Dedicate to the Public Domain (all rights waived)
Creative Commons Attribution 4.0 (CC-BY-4.0)	Content, Data	Y	N	
Open Data Commons Attribution License (ODC-BY)	Data	Y	N	Attribution for data(bases)
Creative Commons Attribution Share- Alike 4.0 (CC-BY-SA-4.0)	Content, Data	Y	Y	
Open Data Commons Open Database License (ODbL)	Data	Y	Y	Attribution-ShareAlike for data(bases)

<https://the-turing-way.netlify.app/reproducible-research/licensing/licensing-data.html>

Licenses

The screenshot shows a sidebar menu on the left and the main content area on the right.

Sidebar (Left):

- Welcome
- Guide for Reproducible Research**
 - Overview
 - Open Research
 - Version Control
- Licensing**
 - Software Licenses
 - Data Licenses
- Machine Learning Model Licenses**
 - Case Studies: Choosing an ML License

Main Content Area (Right):

Machine Learning Model Licenses

Like a software license, a Machine Learning (ML) model license governs the use, redistribution of the model and/or algorithm, and distribution of any derivatives of it. However, there are other components to an AI system, such as [data](#), [source code](#), or applications, which may have their own separate licenses. ML model licenses may restrict the use of the model for specific scenarios for which, due to the technical capabilities and limitations of the model informed by its model card, the licensor is not comfortable that the model is used.

While many ML models may utilise open software licensing (e.g. MIT, Apache 2.0), there are a number of ML model-specific licenses that may be developed for a specific model (e.g. [OPT-175B license](#), [BigScience BLOOM RAIL v1.0 License](#)), company (e.g. [Microsoft Data Use Agreement for Open AI Model Development](#)), or series of models (e.g. [BigScience OpenRAIL-M \(Responsible AI License\)](#)).

In summary, the growing list of ML licenses reflects the understanding that the ML model is distinct from the source code, and thus in need of new licensing options.

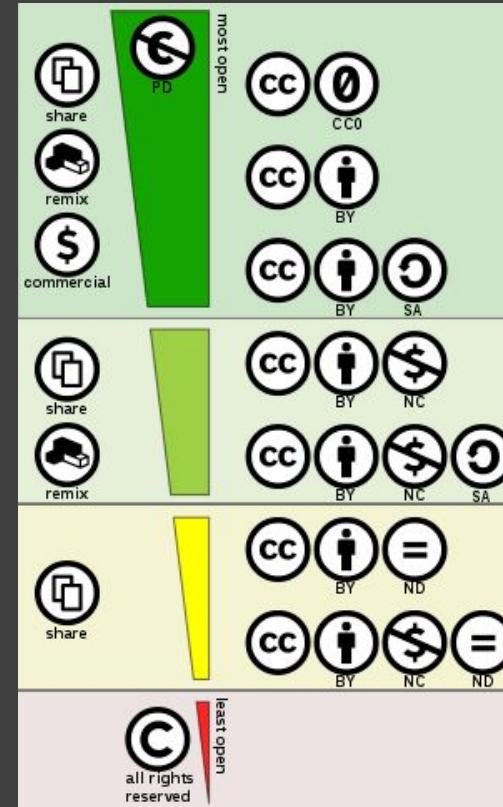
Reproduction and propagation of ML models

<https://the-turing-way.netlify.app/reproducible-research/licensing/licensing-ml.html>

Licenses are context-dependent

Use a **different license** for content, code and data. For example

- Writing/docs/images/metadata: **CC-BY**
- Code: **MIT License**
- Data will also have different license based on what you can/can't share!



Addressing Common Concerns

- Sharing something online does NOT automatically make it reusable.
- Sharing with a license does NOT give away your rights to publish, sell, etc.
- Work shared with an open license NOT to be used without attribution.
- *Not attributing to authors violates academic ethics.*

How to Apply License



yo yehudi stays away from humans! 🌈

@yoyehudi



Often when people want to make their research code open for others to re-use is applying a creative commons licence.

Awesome, you're off to a great start! 🚀 One hitch here is that [@creativecommons](#) licences aren't designed for code - see creativecommons.org/faq/#can-i-app... 1/2

Place the **full text of the license in a file named LICENSE** in the root directory.

Apply licenses to all components, **content: CC-BY, software: MIT, data: CC0**

Describe in README which license applies to which parts of your work.

GitHub can add a license for you

Create a new repository

A repository contains all the files for your project, including the revision history.

Initialize this repository with:

Skip this step if you're importing an existing repository.

Add a README file
This is where you can write a long description for your project. [Learn more](#).

Add .gitignore
Choose which files not to track from a list of templates. [Learn more](#).

Choose a license
A license tells others what they can and can't do with your code. [Learn more](#).

License: None ▾

This field is optional. You can change the default name in your [settings](#).

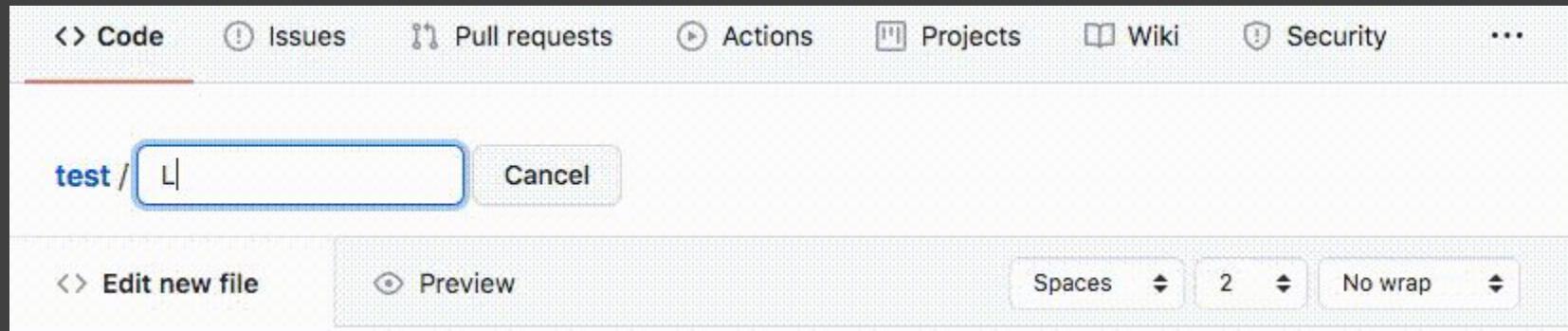
Filter licenses...

- ✓ None
- Apache License 2.0
- GNU General Public License v3.0
- MIT License
- BSD 2-Clause "Simplified" License
- BSD 3-Clause "New" or "Revised"

Contact GitHub Pricing

GitHub can add a license for you, Part 2

when adding a new file named LICENSE...



Further Reading

Licensing Chapter in *The Turing Way*

- The Open Source Definition (10 Criteria) | opensource.org
- Legal Matters | producingoss.com
- Open Source Guide | opensource.guide
- Software: Choose an Open Source License | choosealicense.com
- Content: Choose a License | creativecommons.org

Contribution Guideline

Contributing to *The Turing Way*

🎉🍰 Welcome to *The Turing Way* repository! 🎉🍰

🌟💡 We're excited that you're here and want to contribute. 🌟💡

We want to ensure that every user and contributor feels welcome, included and supported to participate in *The Turing Way* community. We hope that the information provided in this document will make it as easy as possible for you to get involved.

We welcome all contributions to this project via GitHub issues and pull requests. Please follow these guidelines to make sure your contributions can be easily integrated into the projects. As you start contributing to *The Turing Way*, don't forget that your ideas are more important than perfect pull requests. ❤️

If you have any questions that aren't discussed below, please let us know through one of the many ways to [get in touch](#).

Table of contents

Been here before? Already know what you're looking for in this guide? Jump to the following sections:

- [Joining the community](#)
- [Inclusivity](#)
- [Get in touch](#)
- [Contributing through GitHub](#)
- [Writing in Markdown](#)
- [Where to start: issues](#)
 - [Issue labels](#)

CONTRIBUTING.md

- how to file a bug report
- how to suggest a feature
- how to contribute changes
- roadmap & project vision
- how contributors should ask for help and guidance

Code of Conduct

Code of Conduct

We value the participation of every member of our community and want to ensure that every contributor has an enjoyable and fulfilling experience. Accordingly, everyone who participates in the Turing Way project is expected to show respect and courtesy to other community members at all times.

Kirstie Whitaker, as PI of this project, and all project members, are dedicated to a *harassment-free experience for everyone*, regardless of gender, gender identity and expression, sexual orientation, disability, physical appearance, body size, race, age or religion. **We do not tolerate harassment by and/or of members of our community in any form.**

We are particularly motivated to support new and/or anxious collaborators, people who are looking to learn and develop their skills, and anyone who has experienced discrimination in the past.

To make clear what is expected, we ask all members of the community to conform to the following Code of Conduct.

- 1 Introduction
- 2 Code of Conduct
 - 2.1 Expected Behaviour
 - 2.2 Unacceptable Behaviour
 - 2.3 Consequences of Unacceptable Behaviour
 - 2.4 Feedback
- 3 Incident Reporting Guidelines
 - 3.1 Contact points

CODE_OF_CONDUCT.md

- What is expected of the contributors
- What culture do we want to promote
- What if something should be reported

Continuous Integration

The screenshot shows a GitHub pull request interface. At the top, there's a red 'Review required' badge with the text 'At least 1 approving review is required by reviewers with write access. [Learn more](#)'. To its right is a button to 'Add your review'. Below this, a green checkmark icon indicates 'All checks have passed' (7 successful and 2 neutral). A 'Hide all checks' link is available. A vertical scroll bar is visible on the right side of the list. The list includes several green checkmarks for CI jobs like 'CI / build-jb-and-check-links' and 'Check for Latin Phrases / latin-phrases', both successful. It also shows green checkmarks for 'Check for Lorem Ipsums / lorem-ipsums' and 'TestFileSizes / testfilesize' (both successful). There are two greyed-out items: 'Header rules' (Completed in 2m — No header rules processed) and 'Pages changed' (Completed in 2m — 160 new files uploaded). At the bottom, a red 'X' icon indicates 'Merging is blocked' with the note 'Merging can be performed automatically with 1 approving review.' A 'Merge pull request' button is at the bottom left, and a note says 'You can also [open this in GitHub Desktop](#) or view command line instructions.'

Practice of integrating changes to
a project made by individuals into a
main, shared version
-- frequently

Breakout

Make sure that you have done the following:

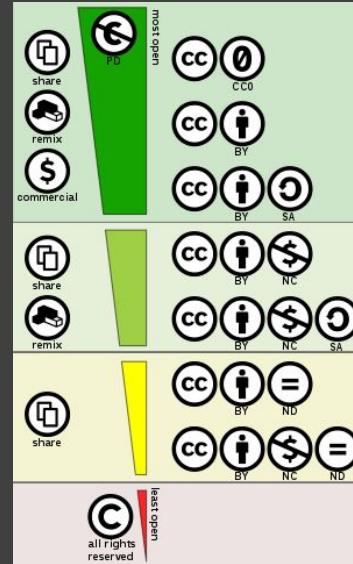
- Set up a project repository
 - Add a minimal README
 - Add a License
 - Add a License badge

You can use part of your project to use as example for this workshop!

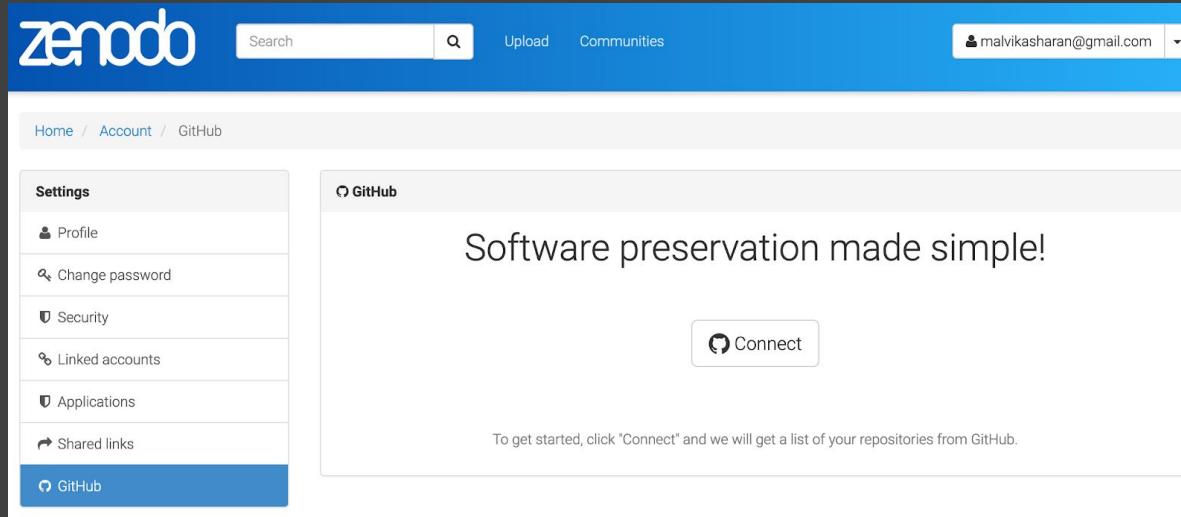
You can fork: <https://github.com/malvikasharan/2022-03-project-example>

If you have already done this, you could add:

- Contributing guide
 - Code of conduct



Making your work citable

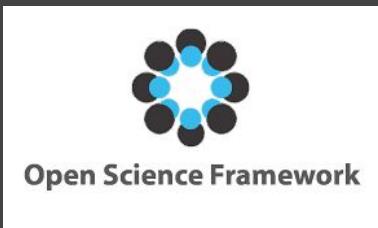


The screenshot shows the Zenodo account settings interface. The top navigation bar includes a search bar, upload and communities links, and a user profile dropdown. Below the navigation is a breadcrumb trail: Home / Account / GitHub. On the left, a sidebar titled 'Settings' lists options like Profile, Change password, Security, Linked accounts, Applications, Shared links, and GitHub, with 'GitHub' highlighted. The main content area features a 'GitHub' section with the heading 'Software preservation made simple!' and a 'Connect' button. A note below the button states: 'To get started, click "Connect" and we will get a list of your repositories from GitHub.'

A digital object identifier (DOI) is a persistent identifier used to identify research objects uniquely.

- Zenodo, Figshare
- Preprint servers
- Docker (env)
- ORCID (researchers)

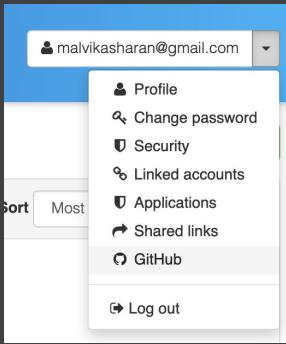
Upload to free openly accessible online repositories



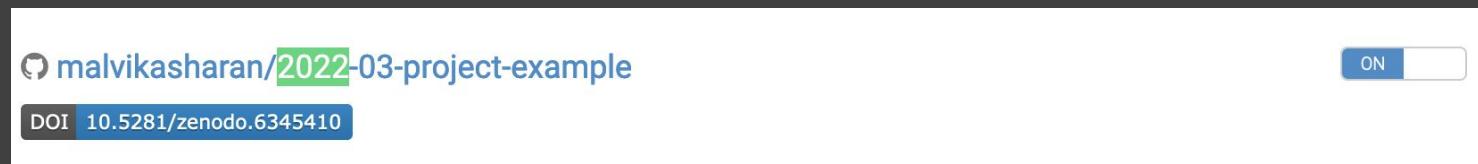
- Trustworthy digital repository (TDR)
- Allows to generate shareable DOI
- Digital Object Identifier

- Not a TDR
- cannot ensure long-term access

Zenodo

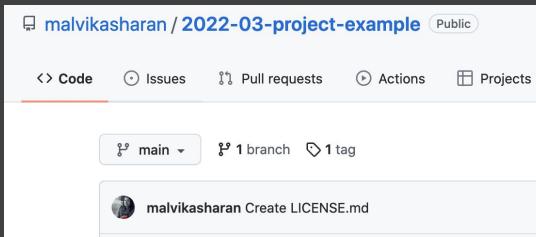


A screenshot of the Zenodo user profile sidebar. It shows a dropdown menu with the email address "malvikasharan@gmail.com". The menu includes options: Profile, Change password, Security, Linked accounts, Applications, Shared links, GitHub, and Log out. A "Sort" button and a "Most" dropdown are also visible.

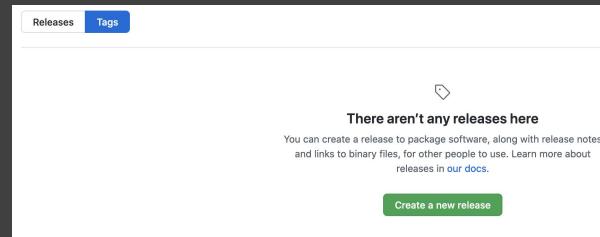


A screenshot of the Zenodo project page for "malvikasharan/2022-03-project-example". The page is public. A DOI badge indicates "DOI 10.5281/zenodo.6345410". A toggle switch labeled "ON" is present in the top right corner.

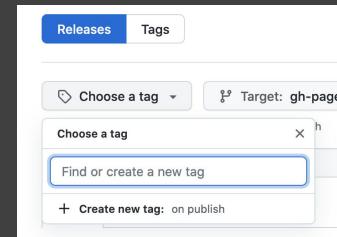
GitHub



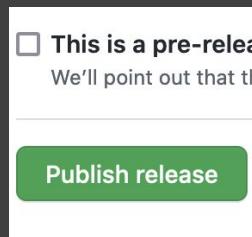
A screenshot of the GitHub repository "malvikasharan / 2022-03-project-example". The repository is public. It shows 1 branch and 1 tag. A file named "LICENSE.md" is listed.



A screenshot of the GitHub releases section. It displays a message: "There aren't any releases here". A button to "Create a new release" is shown.

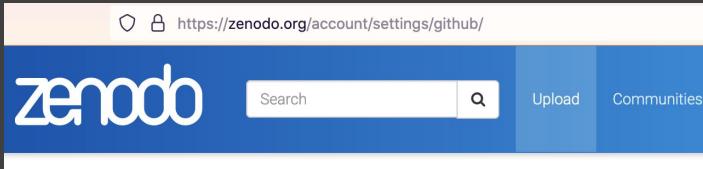


A screenshot of the GitHub tag creation dialog. It shows a search bar with "Find or create a new tag" and a button to "+ Create new tag: on publish".

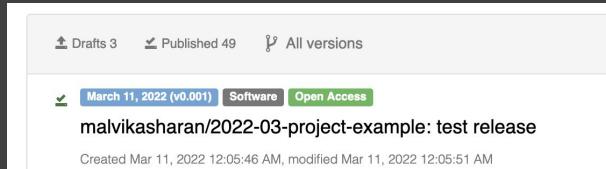


A screenshot of the GitHub release publish button. It features a green button labeled "Publish release". To its left is a checkbox with the text "This is a pre-release" and a note: "We'll point out that th".

Zenodo



A screenshot of the Zenodo account settings for GitHub. The URL is https://zenodo.org/account/settings/github/. The Zenodo logo is at the top. Below it is a search bar, an "Upload" button, and a "Communities" button.



A screenshot of the Zenodo project details page for "malvikasharan/2022-03-project-example: test release". It shows 3 drafts and 49 published versions. The release date is March 11, 2022 (v0.001), it's Software, and it's Open Access. The page also lists the DOI and related identifiers.

Publication date:
March 11, 2022

DOI:
DOI 10.5281/zenodo.6345410

Related identifiers:
Supplement to
<https://github.com/malvikasharan/2022-03-project-example/tree/v0.001>

License (for files):
[Other \(Open\)](#)

Citable DOI

All these aspects
enhance collaboration in
your project!

How to make your code
easy to test?



Reproducible computational environment

Reproducible research

same analysis steps on
the same dataset
produces same answer

		Data	
		Same	Different
Analysis	Same	(Reproducible)	Replicable
	Different	Robust	Generalisable

*“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.”*

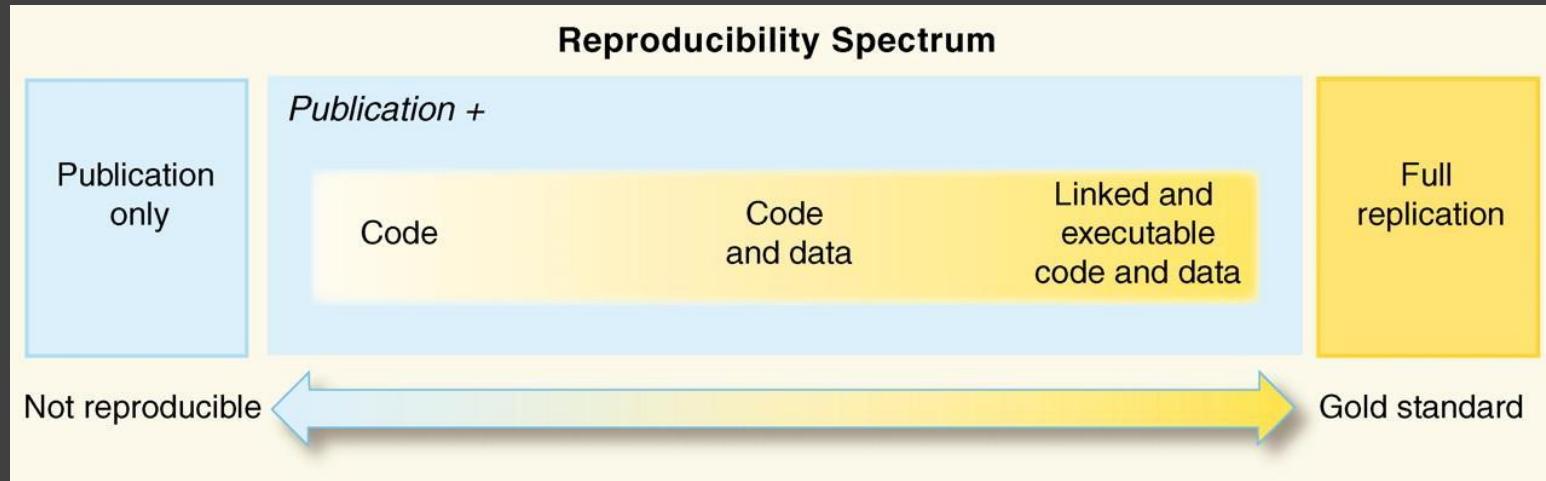
— Buckheit and Donoho (paraphrasing John Claerbout)
WaveLab and Reproducible Research, 1995

Take home message

sharing your code and
data isn't enough



You need the computational environment too



You need the computational environment too



What is a computational environment?

- hardware (e.g. CPU)
- software
 - operating system
 - programming languages
 - packages

What is a computational environment?

- hardware (e.g. CPU)
 - software
 - operating system
 - programming languages
 - packages
- 
- their versions
and their
configuration

What is a computational environment?

- hardware (e.g. CPU)

- software

- operating system
- programming languages
- packages

their versions
and their
configuration

and their
interaction

What is *Binder*?

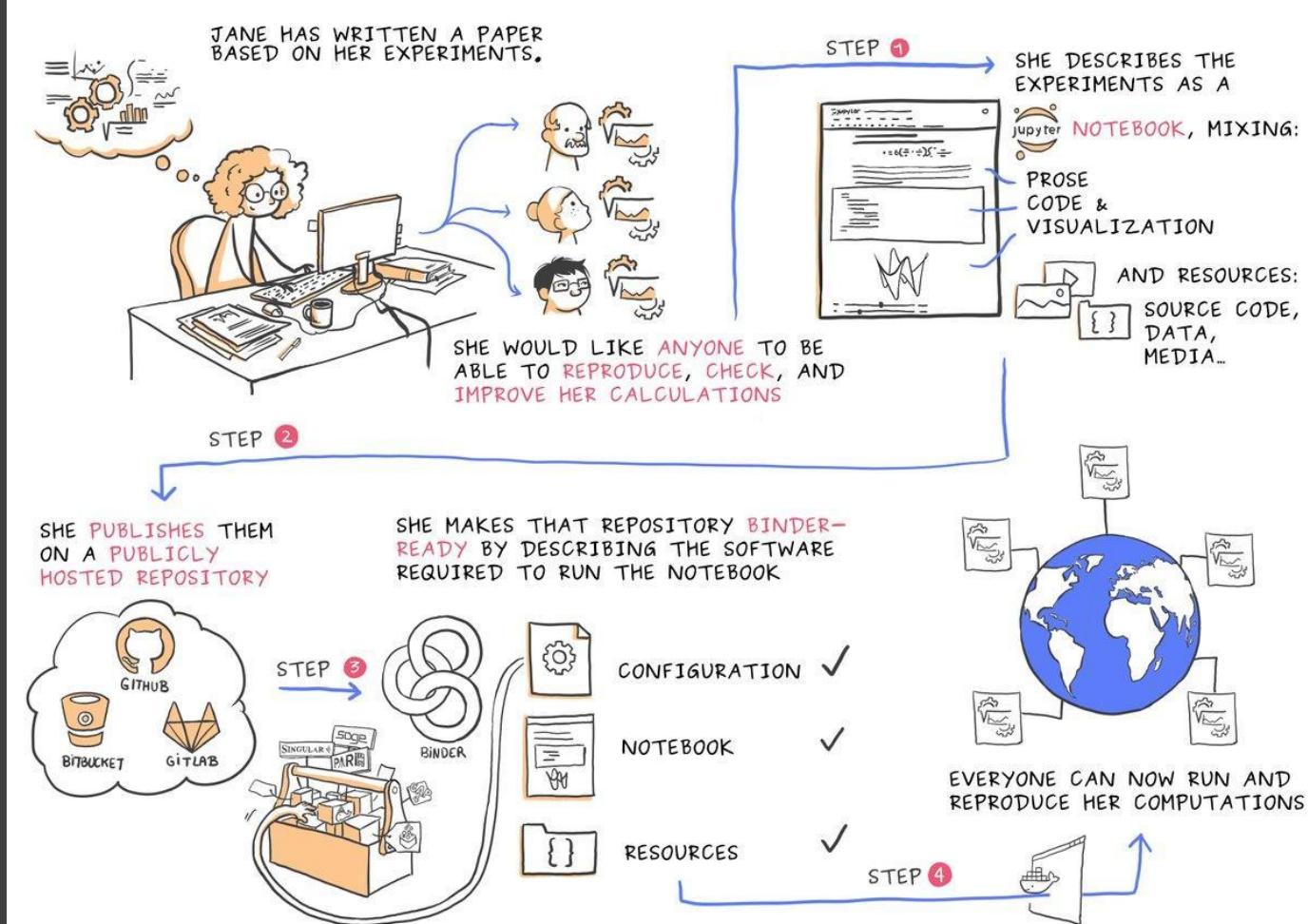
What is Binder?



choldgraf Distinguished Contributor

3 Nov '18

The Binder Project helps you create one-click, sharable, live code environments from public code repositories that runs entirely in the cloud.



Courtesy of Juliette Taka: [@turingway, CC-BY 4.0, The Turing Way, DOI: 10.5281/zenodo.7684733](https://twitter.com/mybinderteam/status/1082556317842264064)

Binder tutorial

Use the zero to binder workshop:

- Python -

<https://github.com/alan-turing-institute/the-turing-way/blob/main/workshops/bost-research-reproducibility-binder/workshop-presentations/zero-to-binder-python.md>

- R -

<https://github.com/alan-turing-institute/the-turing-way/blob/main/workshops/bost-research-reproducibility-binder/workshop-presentations/zero-to-binder-r.md>

What it looks like in GitHub

The screenshot shows a GitHub repository page for 'my-first-binder'. At the top, there's a navigation bar with links for Code, Issues, Pull requests, Actions, Projects, Wiki, Security, and Insights. Below the navigation bar, there's a file list showing several files updated by 'EKaroune' on Feb 21, 2021. The files include README.md, hello.R, install.R, postBuild, and runtime.txt. On the right side of the page, there's an 'About' section with a note that 'No description, website, or topics provided.' It also lists the Readme, 0 stars, 2 watching, and 0 forks. Below that is a 'Releases' section with a note that 'No releases published' and a link to 'Create a new release'. At the bottom of the page, there's a 'README.md' file preview and a 'my-first-binder' section. A red arrow points to a 'launch binder' button, which is highlighted with a pink border. To the right of the arrow, the text 'Press the launch button' is written in pink.

EKaroune / my-first-binder Public

Code Issues Pull requests Actions Projects Wiki Security Insights

main Go to file Add file Code About

EKaroune updated badge ... on Feb 21, 2021 8

File	Updated	Time Ago
README.md	updated badge	2 years ago
hello.R	create hello.R	2 years ago
install.R	update install R	2 years ago
postBuild	create postBuild file	2 years ago
runtime.txt	creat runtime txt file	2 years ago

README.md

my-first-binder

Press the launch button

To run code, you need:

- Hardware on which to run the code
- Software, including:
 - The code itself
 - The programming language (e.g. Python, R, Julia, and so on)
 - Relevant packages (e.g. pandas, matplotlib, tidyverse, ggplot)



Starting repository: EKaroune/my-first-binder/main

The Binder team has a site reliability guide that talks about what it is like to run a BinderHub.

Build logs

view raw hide

```
trying URL 'https://packagemanager.zetstudio.com/all/_linux/_bionic/2022-01-04+Y3JhbhiwyOjQ1MjYyMTU7Nz1BRkJEMsg/exo/contrib/sys_3.4.tar.gz'
Content type 'binary/octet-stream' length 53672 bytes (52 KB)
=====
downloaded 52 KB

trying URL 'https://packagemanager.zetstudio.com/all/_linux/_bionic/2022-01-04+Y3JhbhiwyOjQ1MjYyMTU7Nz1BRkJEMsg/exo/contrib/zip_2.2.0.tar.gz'
Content type 'binary/octet-stream' length 550921 bytes (508 KB)
=====
downloaded 538 KB

trying URL 'https://packagemanager.zetstudio.com/all/_linux/_bionic/2022-01-04+Y3JhbhiwyOjQ1MjYyMTU7Nz1BRkJEMsg/exo/contrib/gitoreads_0.1.1.tar.gz'
Content type 'binary/octet-stream' length 93297 bytes (91 KB)
=====
downloaded 91 KB

trying URL 'https://packagemanager.zetstudio.com/all/_linux/_bionic/2022-01-04+Y3JhbhiwyOjQ1MjYyMTU7Nz1BRkJEMsg/exo/contrib/ini_0.3.1.tar.gz'
```

Here's a non-interactive preview on nbviewer while we start a server for you. Your binder will open automatically when it is ready.



File Edit View Run Kernel Tabs Settings Help

+ C

Filter files by name

/

Name	Last Modified
gapminder....	a minute ago
R hello.R	6 minutes ago
R install.R	6 minutes ago
postBuild	6 minutes ago
README.md	6 minutes ago
runtime.txt	6 minutes ago

Launcher x +

hello.R

Notebook

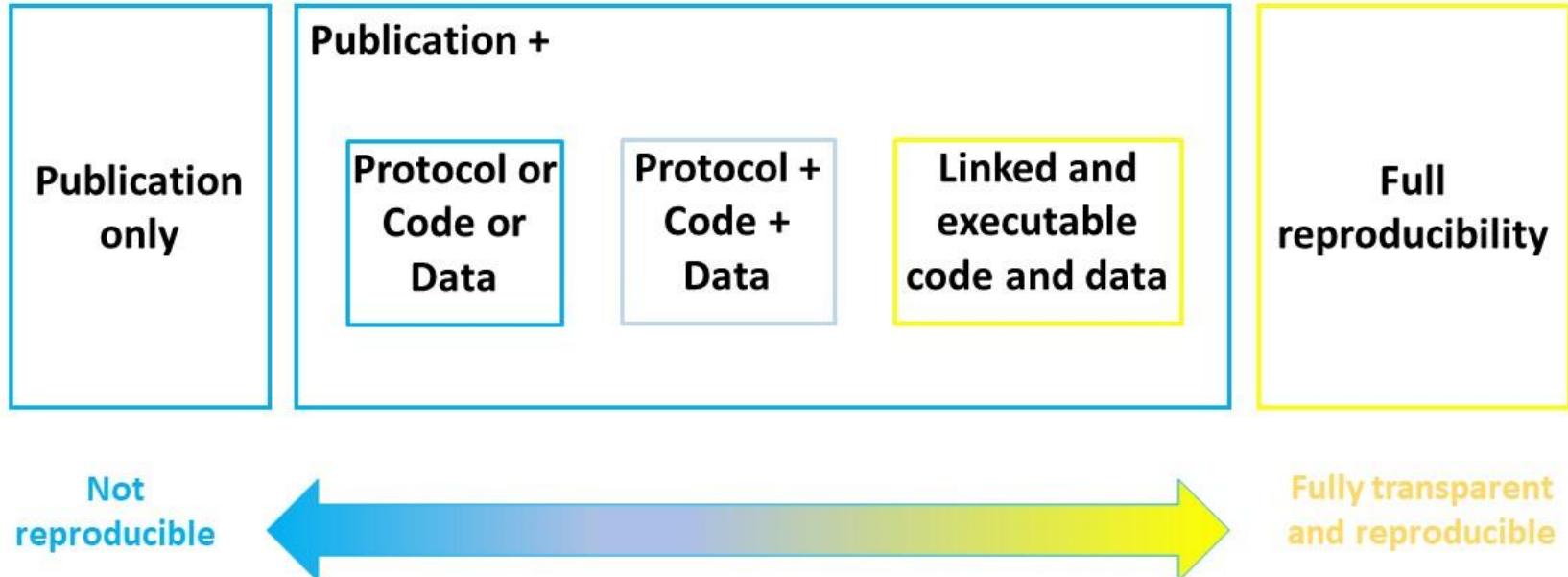
Python 3 (ipykernel) R RStudio [+] Shiny

Console

Python 3 (ipykernel) R

Other

Terminal Text File Markdown File Python File R File Show Contextual Help



An adapted reproducible spectrum (Peng 2011) with the addition of protocols.

Karoune, E., and Plomp, E.(2022) Removing Barriers to Reproducible Research in Archaeology. Zenodo, ver. 5 peer-reviewed and recommended by Peer Community in Archaeology.<https://doi.org/10.5281/zenodo.7320029>.

Other things you can do to make your work more FAIR and reproducible?

- Data and code in a repository with DOI
- Write a clear data and code availability statement
- Write a data paper/article
- Cite your data and code in your article
- Write a clear method/protocol
 - Use protocols.io

What is a data paper?

- Describes a dataset
- Does not include analysis or findings
- Data usually in an open repository
- Use a template to write it
- Data journals



FAIR in action

- **Dataset** archived in [IsoArcH](#)
- **Detailed description** of the dataset ([data article](#))
- **Scripts** of the figures in the data article on [GitHub/Zenodo](#)

Data Article

Neodymium isotopes in modern human dental enamel: An exploratory dataset for human provenancing

Esther Plomp  

Show more ▾

+ Add to Mendeley  Share  Cite

<https://doi.org/10.1016/j.dib.2021.107375> [Get rights and content](#)

Under a Creative Commons license 

Refers to E. Plomp, I.C.C. von Holstein, J.M. Koornneef, R.J. Smeets, J.A. Baart, T. Forouzanfar, G.R. Davies
Evaluation of neodymium isotope analysis of human dental enamel as a provenance indicator ...
Science & Justice, Volume 59, Issue 3, May 2019, Pages 322-331

 [Download PDF](#)

Data	Repository: IsoArcH [1]
accessibility	Data identification number: 10.48530/isoarch.2021.011 Direct URL: 10.48530/isoarch.2021.011 Software availability: https://doi.org/10.5281/ZENODO.5150520 [6]
	Data is available under the Creative Commons BY-NC-SA 4.0 license.

FAIR in action

Data article cites data and software

- [5] E. Plomp
Neodymium isotopes in modern human dental enamel: an exploratory dataset
IsoArcH (2021), [10.48530/ISOARCH.2021.011](https://doi.org/10.48530/ISOARCH.2021.011)
[View PDF](#) [Google Scholar](#)
- [6] E. Plomp, J.C. Peterson, [software] EstherPlomp/figures-Nd-data, Zenodo, 2021.
[doi:10.5281/ZENODO.5150520](https://doi.org/10.5281/ZENODO.5150520).
[Google Scholar](#)
- [7] C. Stantis, [software] stantis/IsoDataVis: first (Official) release, Zenodo, 2021.
[doi:10.5281/ZENODO.4743734](https://doi.org/10.5281/ZENODO.4743734).
[Google Scholar](#)

Don't forget your methods!

- Include a full method
 - Summaries aren't good enough
 - Use one reference if you followed that method exactly or state how you modified it.
- Put your method
 - Supplementary files are not good enough
 - In a repository with data and code
 - Protocols.io

Using protocols.io

Versions

 VERSION 2 ▾
SEP 30, 2022
[!\[\]\(23dbc135327d471eb8cfe6be3d58db18_img.jpg\) SHARE](#)
[!\[\]\(f9a1e904458281b18134c41d8e5309e6_img.jpg\) WORKS FOR ME 1](#)

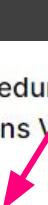
Phytolith extraction and counting procedure for modern plant material rich in silica skeletons V.2

DOI
dx.doi.org/10.17504/protocols.io.q26g74mb8gwz/v2

Francesca D'Agostini^{1,2}, Javier Ruiz-Pérez¹, Marco Madella^{1,3,4},
Vincent Vadez^{2,5}, Carla Lancelotti^{1,3}

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²DIADE Unit, IRD, University of Montpellier. Av. Agropolis 911, Montpellier 34394, France;
³ICREA-Catalan Institution for Research and Advanced Studies. Pg. Lluís Companys 23, Barcelona 08010, Spain;
⁴Department of Geography, Archaeology and Environmental Studies, University of Witwatersrand. 1 Jan Smuts Avenue, Braamfontein, Johannesburg 2000, South Africa;
⁵Crop Physiology Laboratory, ICRISAT. Patancheru 502324, Telangana, India

 fra.dagostini F D'Agostini
Universitat Pompeu Fabra, Université de Montpellier 

Gives a DOI 

COMMENTS 1
BOOKMARK
RUN
COPY / FORK
MORE ▾

Using protocols.io

STEPS WARNINGS MATERIALS METADATA METRICS

The protocol takes up to 10 days to complete, from when plant tissues are collected from the plant to when samples can be observed at the microscope and depending on the plant material and humidity conditions. Skipping the first drying steps (tips 1-2) allows for faster extractions. The number of samples that can be processed at one time depends on the laboratory space (mostly the furnace cabinet space and the centrifuge) and the experience of the practitioner.

Drying plant material

1 Note

The first steps (points 1 and 2) aim to obtain very clean and dry samples to evaluate biomass production before the extraction and to store plant tissues for future use. If biomass evaluation or storage are not needed, start directly from point 3.

Collect the tissues of interest from the whole plant. Store each sample in a separate paper bag and put the paper bags in a dryer. Paper bags prevent the formation of fungi and bacterial infection, allowing the evaporation of tissues' humidity. Collect the tissues of interest from the whole plant. Store each sample in a separate paper bag and put the paper bags in a dryer. Paper bags prevent the formation of fungi and bacterial infection, allowing the evaporation of tissues' humidity.

2 Leave the plant tissues to dry at 60-70°C in a dryer (we use a IWC125 Leec drying cabinet). Check the bags once a day to be sure they do not develop any fungi infection because of the heat. Weigh the samples until no weight loss is observed to be sure to have obtained completely dry tissues. Our dried samples weigh on average 45% less of the fresh biomass. Considering that each species/treatment and tissue has its own level of humidity, we suggest testing the tissues for their consistency to make sure they are dry; they will be completely dry when they become brittle (try to crush the leaves with your hands to check their consistency).

3 Wash samples in an ultrasound bath (we used a Ultasonic Proclean 3.0) at room temperature for 00:05:00 to remove extraneous debris (such as soil particles). To wash many samples simultaneously, use small glass beakers; put each sample in a labeled beaker and cover it with distilled water. Put all the beakers in the ultrasound bath and fill the container with water while paying attention not to overflow in the beakers. Cut the samples into pieces to fit into the beakers. 100 ml beakers are large enough to contain samples of grasses. Calibrate beaker and sample sizes based on the species under analysis.



Wet procedure

8 Note

These steps are fundamental to digest carbonates and oxidize organic material left from the ashing procedure and any form of organic material that was not removed.

Remove the ashes from the crucible with a spatula and place them in an Eppendorf tube of 5 ml. Use a clean spatula for each sample so not to contaminate between samples.



Ceramic crucibles containing the samples, covered with a lid. a) shows the plant tissue before ashing and b) shows the white ashes obtained after 12 hours in the oven.

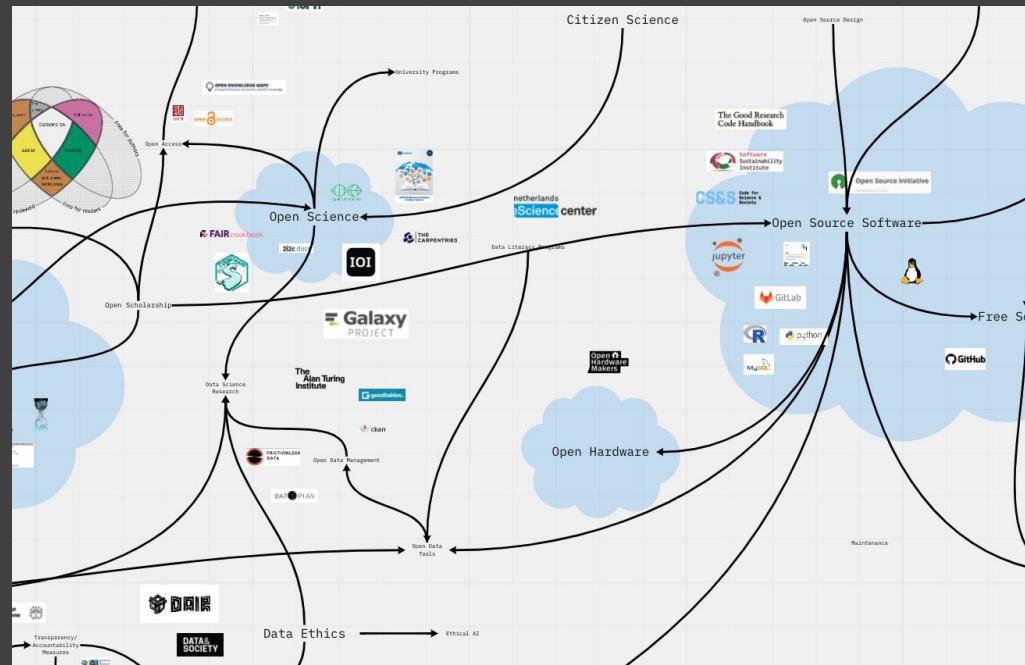
9 Add 900 µL of 10% v/v HCl and vortex the tube to stir the solution (we use an ES714R Maxi Mixer). Leave the HCl to react for 05:00:00 (or till the reaction stops) with the cap of the tube open. Do not let the sample dry by adding more HCl solution if necessary.

Safety information

Work in a fume cupboard. Wear a lab coat and gloves when dealing with Hydrochloric acid.

Case Studies & Resources

There are lots of resources to check out in the open ecosystem... Explore these projects and find out what might work best for you!



Environmental Data Science Book

Mission

Support the publication of data, research and open-source tools for collaborative, reproducible and transparent Environmental Science

Features

- **Community-based model** for improving software practices in Environmental science
- Collaborative publication of executable and reproducible jupyter notebooks
- Promoting scalable tools in *python* (current), R & Julia (future) using cloud-optimized resources

Learnings from *The Turing Way*

Community & translation of Open Science concepts



the-environmental-ds-book.netlify.app

2i2c

Mission

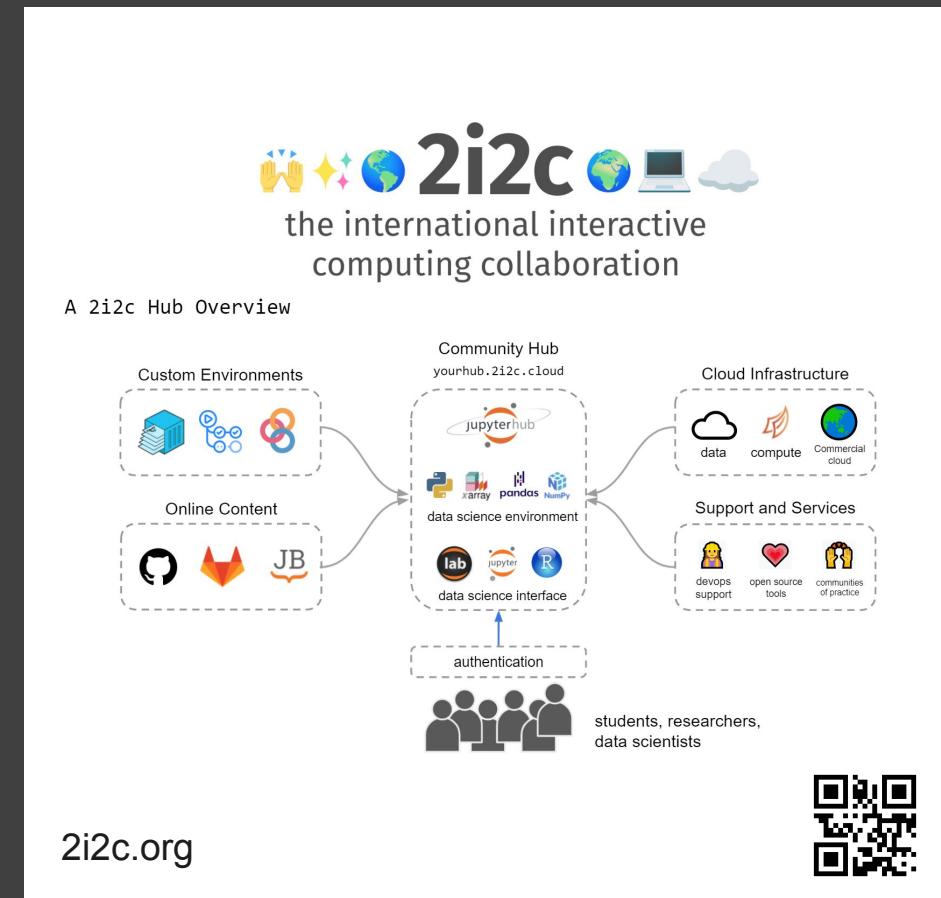
Make interactive computing more impactful through community-centered open infrastructure services

Features

- **Non-profit based model** for increasing openness and reproducibility in research
- Open source operations/dev-ops as a service
- Working with the tech industry (cloud providers) to democratise interoperable interactive computing

Learnings from *The Turing Way*

Emerging (engineers, product manager, community) roles & transparent communication (all documents)



2i2c.org

FAIR Cookbook

Mission

An *online, open and live resource for the Life Sciences with recipes that help you to make and keep data Findable, Accessible, Interoperable and Reusable;*

Features

- **Recipes** for working with data in a FAIR and open way
- Open platform for contribution

Learnings from *The Turing Way*

Open contribution methods, Github repository format, Scriberia images for demonstrating process of using FAIR principles



<https://faircookbook.elixir-europe.org/content/home.html>

Lab Handbooks & Reports

Our Handbook

Search this book...

What is Our Handbook?

USER GUIDE

- How to use this template
- Contributing to this template
- Code of conduct

TEMPLATE

- Welcome
- Research Interests
- Our Team
- Our Projects
- Research Environment
- Resources
- Glossary

Handbook created using Our Handbook. Powered by Jupyter Book.

Note

Here as part of the Bristol Data Week Research Group Handbook Sprint? [Read the workshop information](#)

What is Our Handbook?

We are working with researchers to build [Our Handbook](#): a research group staff handbook template materials to help you use it. We hope research group leaders and members will work together using these resources to:

- build a healthy, inclusive, enjoyable research culture in their group
- produce the most ethical and rigorous research possible

We welcome [contributions](#) in order to create a richer resource for others.

Why are we making this template handbook?

We think research culture could be better:

- researchers often feel stressed, unsupported, and/or isolated
- a lack of guidance in how to do research can contribute to unreliable research outputs

A lot of this can come down to the research culture within a group: the (unspoken) processes which impact both how it feels to work there and the quality of research outputs. There is little support for group leaders who wish to improve the research culture in their groups. We want to change that and make it easy.

We hope that, by reducing the barriers for groups to consider their research culture, we will:

- support group leaders in taking responsibility for it: to help them set standards for the quality

<https://very-good-science.github.io/our-handbook/guide/what-is-our-handbook.html>

Open Source in Environmental Sustainability

Preserving climate and natural resources with openness

Tobias Augspurger, Eirini Malliaraki and Josh Hopkins
Report 2023



Open Source in Environmental Sustainability

Search this book...

INTRODUCTION

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- Methodology
- Principles

INSIGHTS

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- Age
- Growth
- Ranking
- Programming Languages
- Licences
- Community
- Users and Usage
- Ecosystem Collaborations
- Funding Models
- Data Wishlist

RECOMMENDATIONS

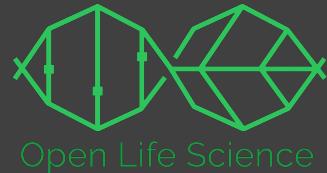
- Overall
- Technology
- Collaboration
- Funding

"The struggle to understand and steer the interaction between the bitsphere and the biosphere is the struggle for community in the broadest ecological context."
Ursula M. Franklin, The Real World of Technology (1989)

Executive Summary

Open source is everywhere. Its culture of transparent and collaborative innovation has transformed modern society, with over 97% of critical digital infrastructure and services depending on it. The role of open source has become increasingly important in addressing environmental challenges. Mathematical models, data and measurement tools, accumulated and shared over decades, have empowered communities worldwide with the understanding needed to preserve Earth's vital resources – fresh water, fertile soil, clean air, and a stable climate. Open cultural and technical approaches are essential for supporting traceable decision-making, building capacity for localisation and customisation, providing new opportunities for participation, and preventing greenwashing by ensuring transparency and trust. Yet, despite the transformative impact of open source, its potential within environmental sustainability is not well understood. This has resulted in a systemic lack of investment, ultimately limiting our collective capacity in addressing society's most pressing challenges. There is a clear need to accelerate open source

<https://report.opensustain.tech/chapters/index.html>



OLS program ▾ OLS-7 ▾ Policies ▾ About ▾ Stories



OLS

A mentoring & training program for Open Science ambassadors

Bérénice Batur (CC)

The **OLS** program is for people interested in **applying open principles** in their work and **becoming Open Science ambassadors** in their communities.

About

This is a **16-week long personal mentorship and cohort-based training**, where participants (organisers, hosts, mentors and project leads/mentees) of this program will:

- **share** their expertise and gain knowledge essential to create, lead, and sustain an Open Science project
- **connect** with members across different projects, communities, backgrounds, and identities
- **empower** each other to become effective Open Science ambassadors in their communities

Participants join this program with a **project** that they either are already working on or want to develop during this program **individually or in teams**.

Frictionless Data



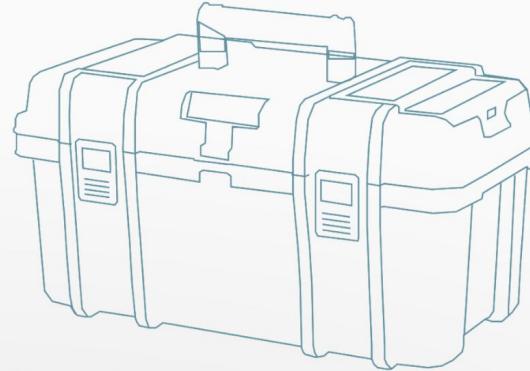
FRIC^{TIONLESS}
DATA

Data software and standards

Frictionless is an open-source toolkit that brings simplicity to the data experience - whether you're wrangling a CSV or engineering complex pipelines.

[Why Frictionless Data?](#)

[Get Started](#)



<https://frictionlessdata.io/>

AutSPACES



alan-turing-institute / AutSPACES Public

Code Issues Pull requests Discussions Actions Projects Wiki Security Insights

main 38 branches 0 tags Go to file Add file <> Code

File	Description	Last Commit
.github/ISSUE_TEMPLATE	rename general issue w/ real name	3 weeks ago
00-project-documentation	Merge pull request #429 from gedankenstuecke/moderation	last week
config	fix: Add missing value to env.template	2 years ago
docker	feat: Add postgresql package to docker	2 years ago
docs	Merge pull request #114 from alan-turing-institute/anoushka_code_...	2 years ago
locale	chore: Add django boilerplate platform	3 years ago
server	Merge branch 'main' into template_restructure	5 days ago
static	fix heading colors	5 days ago
tests	chore: Add django boilerplate platform	3 years ago
.all-contributorsrc	docs: update .all-contributorsrc [skip ci]	2 months ago
.dockerrcignore	fix: Remove unnecessary directory	2 years ago
.editorconfig	fix: Remove unnecessary directory	2 years ago
.gitignore	css files	2 years ago
.gitlab-ci.yml	fix: Remove unnecessary directory	2 years ago
Citscicartoon.png	Add files via upload	3 years ago
LICENSE	Initial commit	3 years ago
README.md	fix contributor link	3 weeks ago
code-of-conduct.md	Update code-of-conduct.md	3 weeks ago
contributing-guidelines.md	Update contributing-guidelines.md	3 years ago
dev_readme.md	Update dev_readme.md	3 weeks ago

About

Code repository for AutSPACES: the Autistica/Turing citizen science platform

accessibility psychology autism
mental-health citizen-science
environments open-research
consent-management accessible-design
participatory-science social-data-science
sensory-processing data-agency
the-alan-turing-institute autistica

Readme MIT license Code of conduct
23 stars 10 watching 15 forks

Releases No releases published

Packages No packages published

Contributors 15

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

Computational Communities



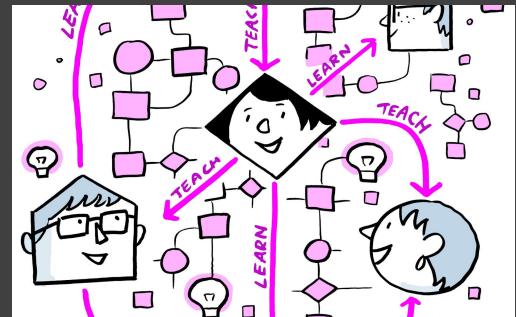
The Turing Way Guides



Reproducibility



Project design



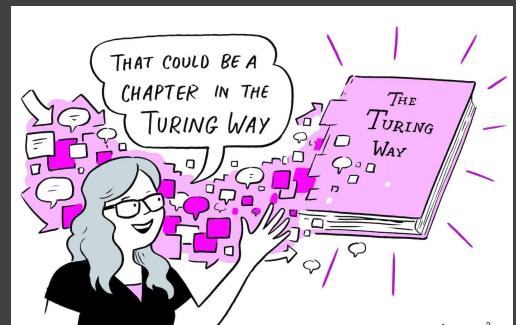
Communication



Collaboration



Ethical research

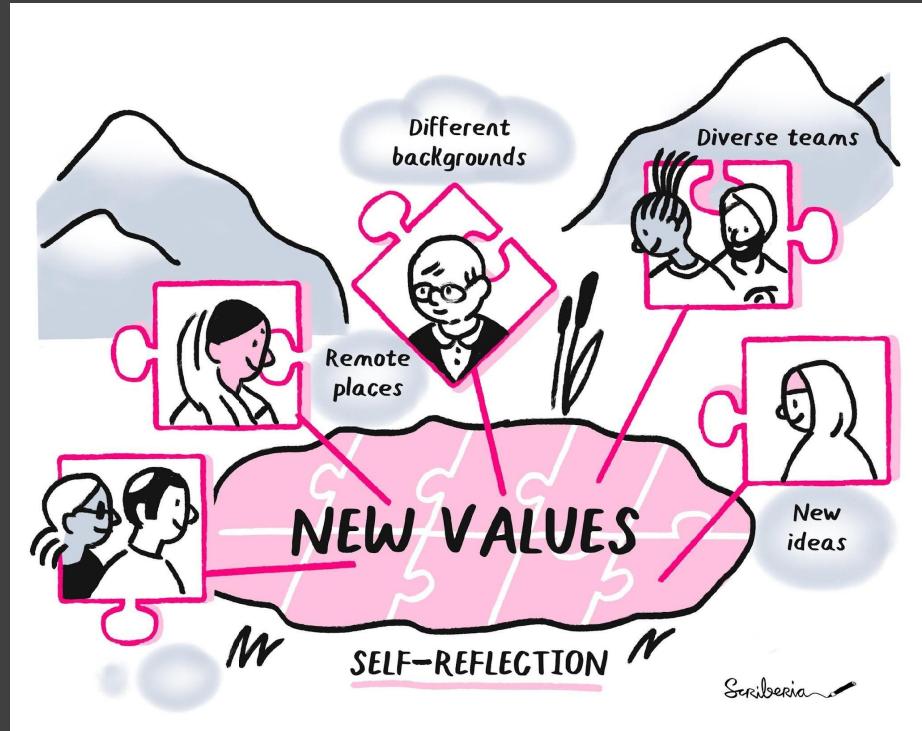


Community handbook

The Turing Way Events

- *Collaboration Cafes*
 - 1st & 3rd Wednesdays (14:00 UTC)
- *Coworking Calls*
 - Mondays (10:00 UTC)
- *Fireside Chats*
 - Monthly on Friday
- *More ways to connect*

bit.ly/turingway



Fireside Chat: Bi-monthly Informal Events

Coming soon:
Community care and
maintenance

3 March 2023
4pm BST

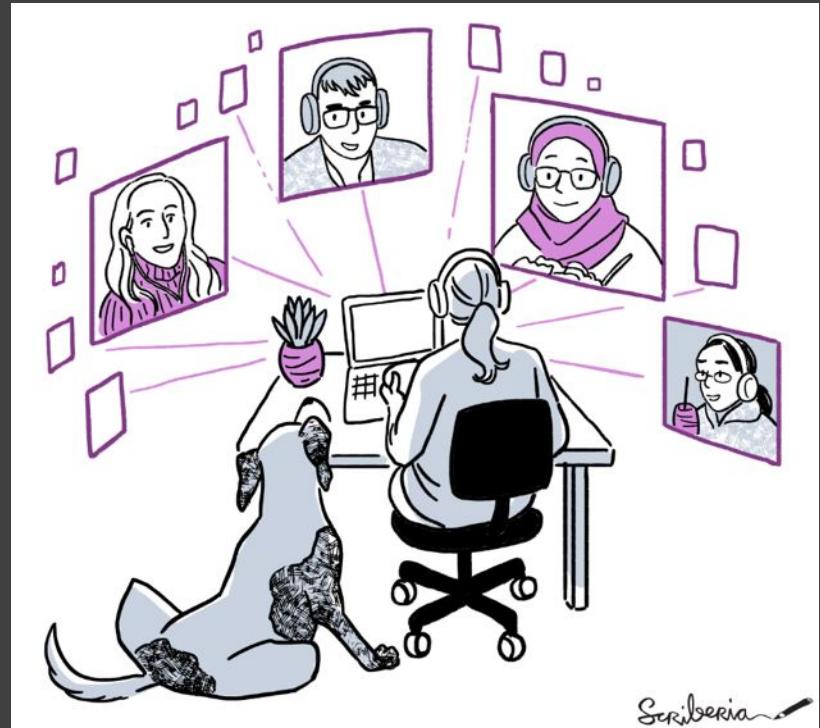
bit.ly/turingway



Attend a Book Dash

*Virtual week-long
Hackathon-like event to work
with others on *The Turing Way*:*

22 - 26 May 2023



Open Discussion / Reflection Questions

- Any questions on what we have covered?
- What have you found most useful or valuable for your own work or research?
- What would you like to learn more about?
- Do you need more help with your repository?
- Any other questions about Reproducible, Open and FAIR research?

Acknowledgements:

- *The Turing Way* team, Kirstie Whitaker, Malvika Sharan
 - *The Turing Way* community, contributors & collaborators
-
- Book: the-turing-way.netlify.com
 - Twitter: twitter.com/turingway
 - Fosstodon: fosstodon.org/@turingway
 - Newsletter: tinyletter.com/TuringWay
 - Slack: theturingway.slack.com/
 - GitHub: github.com/alan-turing-institute/the-turing-way
 - Original artwork by Scriberia: <https://doi.org/10.5281/zenodo.3332807>

