# Open Reproducible Research

Concepts, challenges, and solutions

Markus Konkol, Research Software Engineer









## **Learning Goals**

Upon completion of this lecture, you will be able to

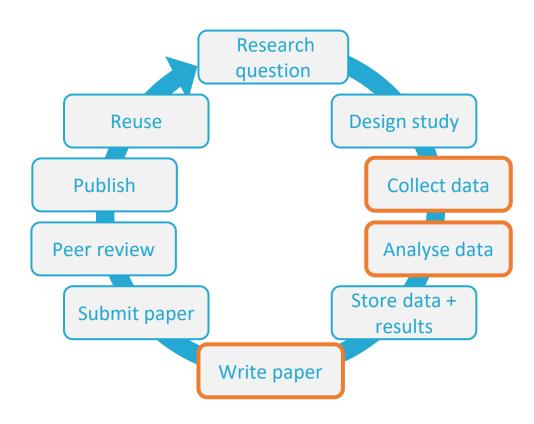
- Articulate what Open Reproducible Research is
- Understand which obstacles impede Open Reproducible Research
- Apply Open Reproducible Research principles to your own work
- Choose appropriate tools to publish Open Reproducible Research



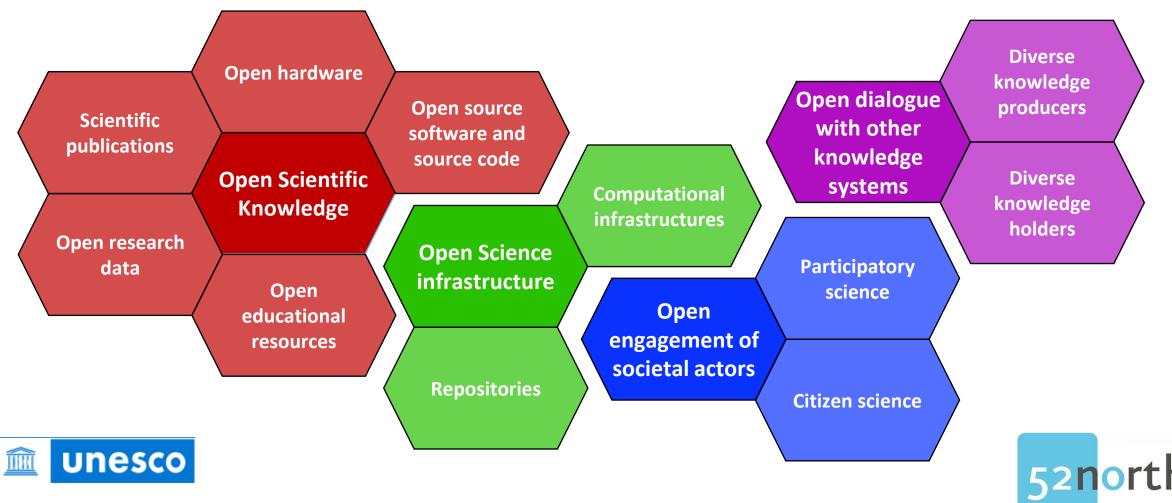
#### **Agenda**

- 1. Introduction to Open Reproducible Research
- 2. The reproducibility crisis
- 3. Obstacles impeding reproducibility
- 4. Five recommendations for ORR
- 5. Principles and best practices
- 6. Opportunities coming with ORR









"[..] an article about a computational result is advertising, not scholarship. The actual scholarship is the [...] complete set of instructions which generated the figures.."

(Claerbout's claim)

Further reading: Buckheit and Donoho (2010)

"The problem is that most modern science is so complicated, and most journal articles so brief, it's impossible for the article to include details of many important methods and decisions made by the researcher as he analyzed his data on his computer."

Further reading: Marwick (2015)

"From time to time over the past few years, I've politely refused requests to referee an article on the grounds that it lacks enough information for me to check the work."

Further reading: Stark (2018)



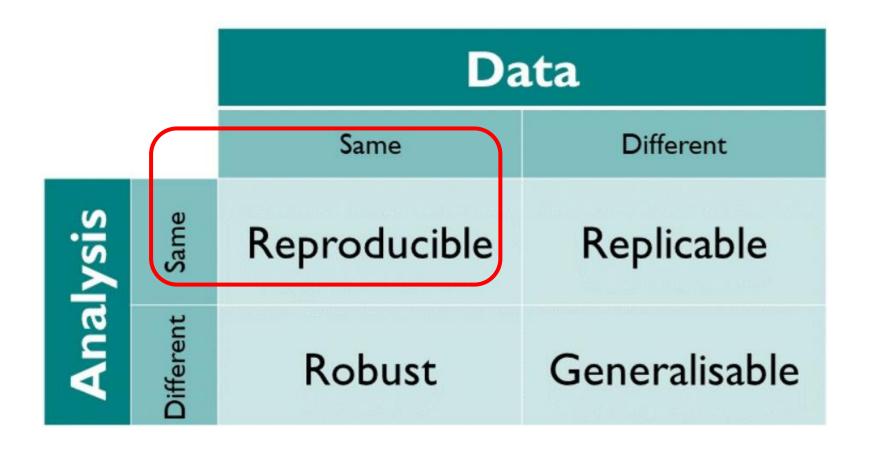
**Reproducible Research** refers to achieving the **same results** (e.g., tables, figures, numbers) as reported in the paper by using the **same source code and data**.

In Open Reproducible Research, these materials are publicly accessible.

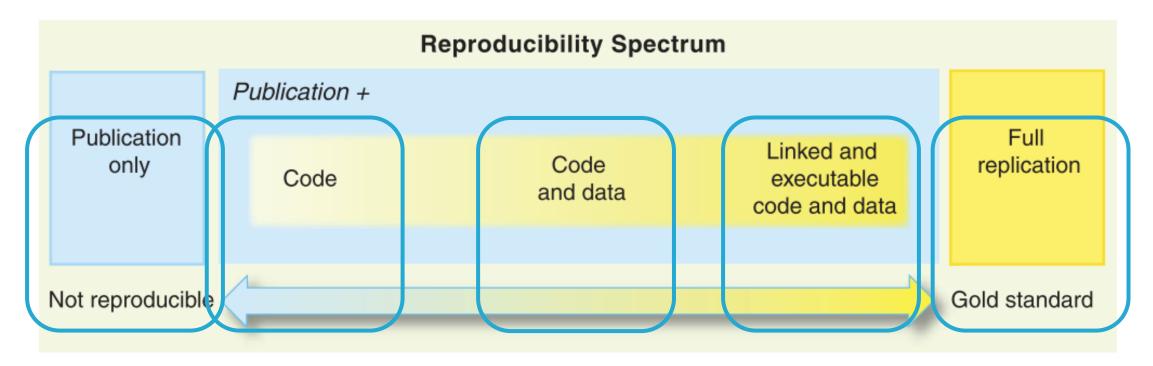
Replicable Research refers to coming to similar conclusions based on the same analysis, but newly collected data.

Reproducibility & Replicability are both essential for **transparent**, **verifiable**, and **reusable** scientific work.









**Fig. 1.** The spectrum of reproducibility.



#### Lessons learned:

- 1. Source code to run the analysis and research data are as important as the scientific article.
- 2. Open Reproducible Research: Same research data, same source code, same results.
- 3. Reproducibility is not necessarily a binary concept but rather a spectrum.
- 4. Reproducibility + replicability + robustness + generalisability describe different concepts.



## Why is unreproducible research a problem?

- The analysis is not fully transparent and easily understandable.
  - Difficult/impossible to describe analysis in pure text.
  - Access to source code can be a shortcut.
- The analysis is not verifiable.
  - Reviewers need to trust the results.
  - Investigating the analysis in any case a complex task.
- The analysis is not reusable.
  - Waste of time and money (duplication of efforts).
  - Waste of opportunities for collaborations and credit.









#### Five 'selfish' reasons to do reproducible research

Reason number 1: reproducibility helps to avoid disaster

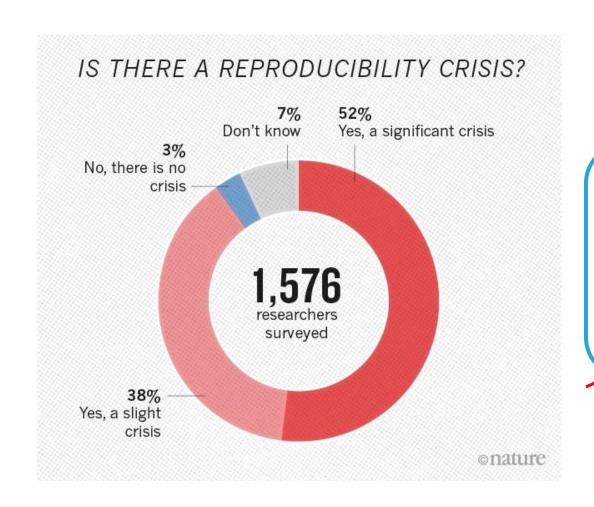
**Reason number 2:** reproducibility makes it easier to write papers

Reason number 3: reproducibility helps reviewers see it your way

Reason number 4: reproducibility enables continuity of your work

Reason number 5: reproducibility helps to build your reputation





Reproducible Research refers to achieving the same results (e.g., tables, figures, numbers) as reported in the paper by using the same source code and data. In Open Reproducible Research, these materials are publicly accessible.



#### COMPUTER SCIENCE

# Artificial intelligence faces reproducibility crisis

Unpublished code and sensitivity to training conditions make many claims hard to verify

#### **By Matthew Hutson**

ast year, computer scientists at the University of Montreal (U of M) in Canada were eager to show off a new speech recognition algorithm, and they wanted to compare it to a benchmark, an algorithm from a well-known scientist. The only problem: The benchmark's source code wasn't published. The researchers had to recreate it from the

(AAAI) in New Orleans, Louisiana, reproducibility was on the agenda, with some teams diagnosing the problem—and one laying out tools to mitigate it.

The most basic problem is that researchers often don't share their source code. At the AAAI meeting, Odd Erik Gundersen, a computer scientist at the Norwegian University of Science and Technology in Trondheim, reported the results of a survey of 400 algorithms presented in papers at two

- Checked 400 papers for reproducibility.
- 6% included source code of the algorithms.
- 30% included test data.
- 54% included a limited summary of the source code (a.k.a. pseudocode).
- Reasons for unavailable source code:
  - Source code is work in progress.
  - A company owned the source code.
  - Hidden to keep competitive advantage.
  - Stolen or lost.



#### PLOS BIOLOGY ⑥ OPEN ACCESS PERSPECTIVE Low availability of code in ecology: A call for urgent action Antica Culina , Ilona van den Berg, Simon Evans, Alfredo Sánchez-Tójar Published: July 28, 2020 • https://doi.org/10.1371/journal.pbio.3000763 Article Authors Metrics Comments Media Coverage Correction Abstract 9 Dec 2020: The PLOS Biology Staff (2020) Correction: Low availability of code in Introduction ecology: A call for urgent action. PLOS Biology 18(12): e3001048. https://doi.org Where are we now? /10.1371/iournal.pbio.3001048 | View correction

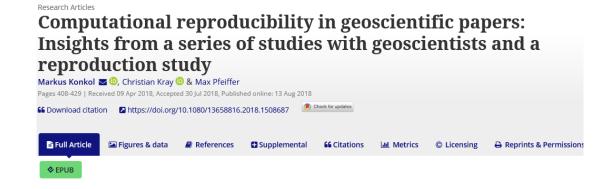
- Checked 346 papers for reproducibility.
- 27% had source code attached.
- 79% were accompanied by data.
- Is data more important than code?
  - NO! The analysis is the context of the data.
  - Paper, data, and analysis belong together.
  - Needed to achieve transparency, verifiability, and reusability



Abstract

Where do we go from

. . . . . . .



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Related rese

People also read

Practical Reprod

Daniel Nüst et al

teproducibility

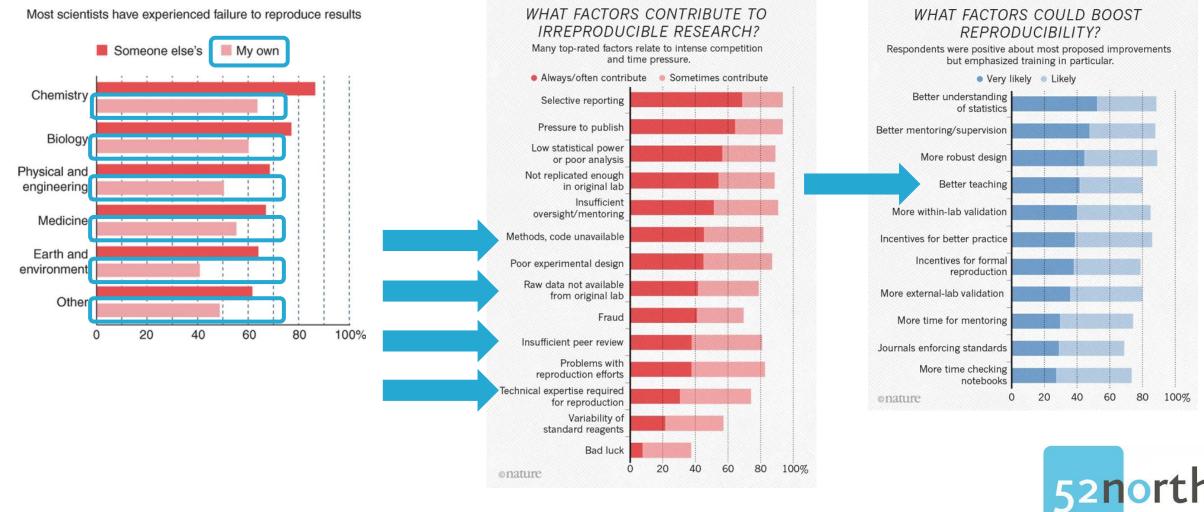
and challenges f

Reproducibility is a cornerstone of science and thus for geographic research as well. However, studies in other disciplines such as biology have shown that published work is rarely reproducible. To assess the state of reproducibility, specifically computational reproducibility (i.e. rerunning the analysis of a paper using the original code), in geographic research, we asked geoscientists about this topic using three methods: a survey (n = 146), interviews (n = 9), and a focus group (n = 5). We asked participants about their understanding of open reproducible research (ORR), how much it is practiced, and what obstacles hinder ORR. We found that participants had different understandings of ORR and that there are several obstacles for authors and readers (e.g. effort, lack of openness). Then, in order to complement the subjective feedback from the participants, we tried to reproduce the results of papers that use spatial statistics to address problems in the geosciences. We selected 41 open access papers from *Copernicus* and *Journal of* 

- Checked 41 papers that had code and data attached for executability and reproducibility.
- 2 out of 41 papers were executable + reproducible.
  - Several technical issues.
  - Several content-related differences.
  - More on that later...



ABSTRACT



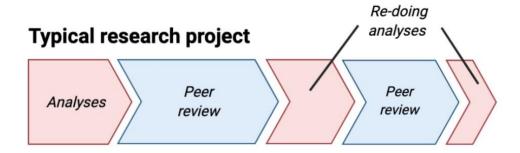
#### Lessons learned:

- 1. Reproducibility is needed to get <u>transparent</u>, <u>verifiable</u>, and <u>reusable</u> research results.
- 2. Reproducibility is beneficial for all + yourself ("Five 'selfish' reasons...").
- 3. Many research articles do not have the source code and data attached.
- 4. Access to source code and data does not necessarily mean that the results are reproducible.
- 5. Are unreproducible research results necessarily wrong? Unclear...

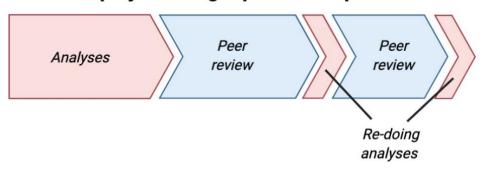


# **Obstacles impeding ORR**

"Working reproducibly costs too much time, I need to publish papers!"

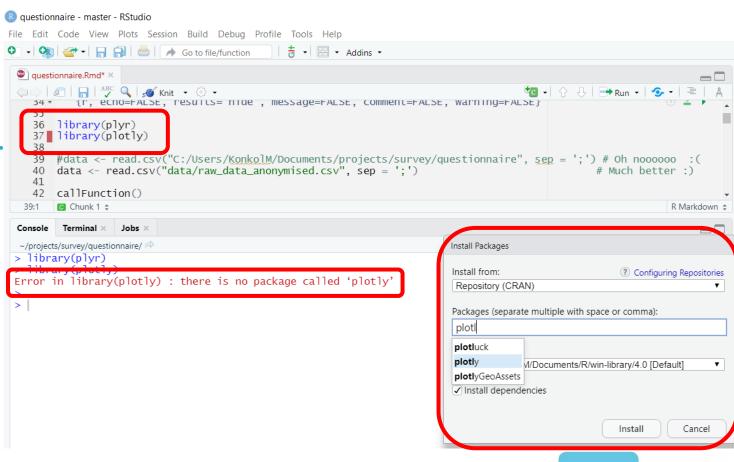


#### Research project using reproducible practices





- Three categories of technical issues.
- Minor issues rather easy to solve.
- Example error: Library not found but available in repository.



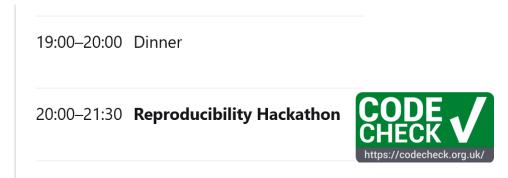
- Substantial issues require more effort.
- Example error: Wrong file directory.

Solution: Use relative instead of

absolute file paths.

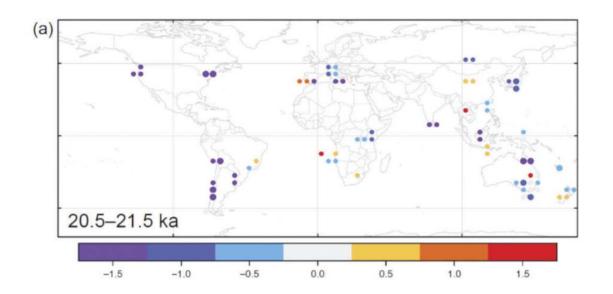


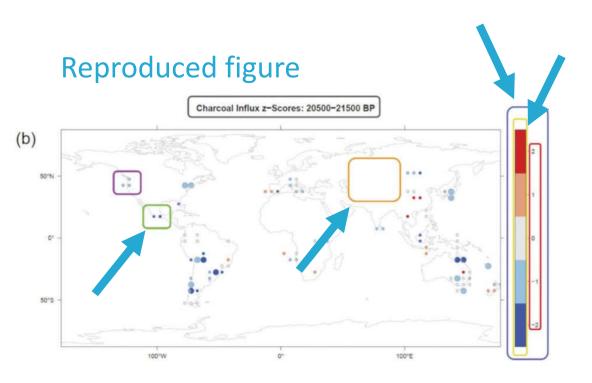
- <u>Severe</u> issues require time, knowledge about the programming language, and understanding of the source code.
- Example error: cannot open file dataABC.csv. No such file or directory.
  - Was the file available in the folder? No
  - Was the file created by the source code? No 😥
  - Contact author → get missing source code snippet that produced dataABC.csv.
- Solution: Ask a colleague to run your analysis.





#### Original figure





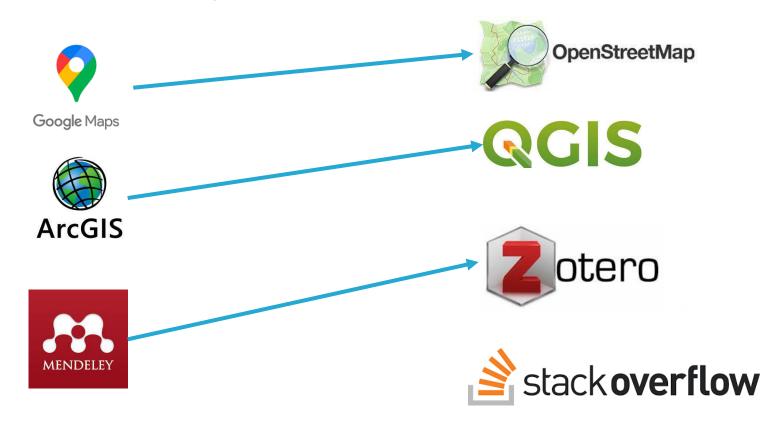


#### Lessons learned:

- Technical issues are of different complexity.
- Minor issues are easy to solve and require less time.
- Substantial issues require knowledge of the programming language.
- Severe issues require knowledge of the programming language and understanding of the source code.
- Reproduced figures can have differences related to the design + the numbers.



**Recommendation 1:** Use open source software instead of commercial software.





#### **Recommendation 2:** Learn a scripting language.





- Scripts describe every step of an analysis
- Human-readable description of what the code does
- Others can understand
  - What has been done
  - How it has been done







- Not reproducible
- No step-by-step description
- No control over the algorithms



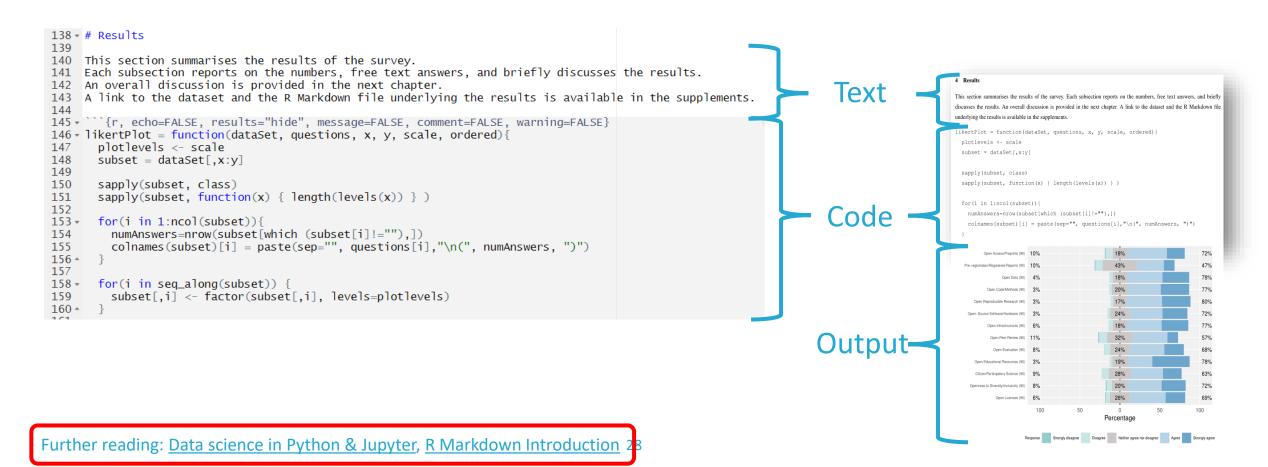
**Recommendation 3:** Learn a computational notebook format.



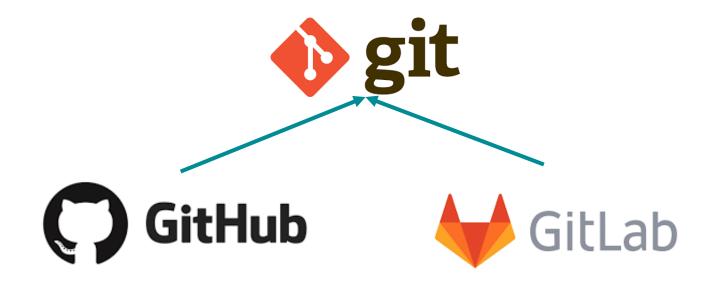




#### **Recommendation 3:** Learn a computational notebook format.



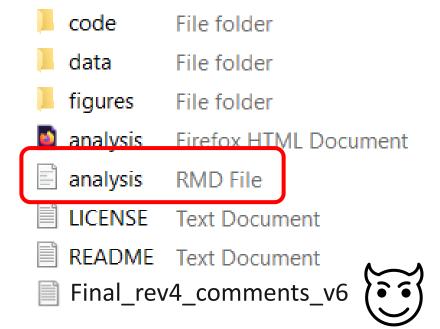
**Recommendation 4:** Learn a collaborative software development tool.





#### **Recommendation 5:** Document your source code.

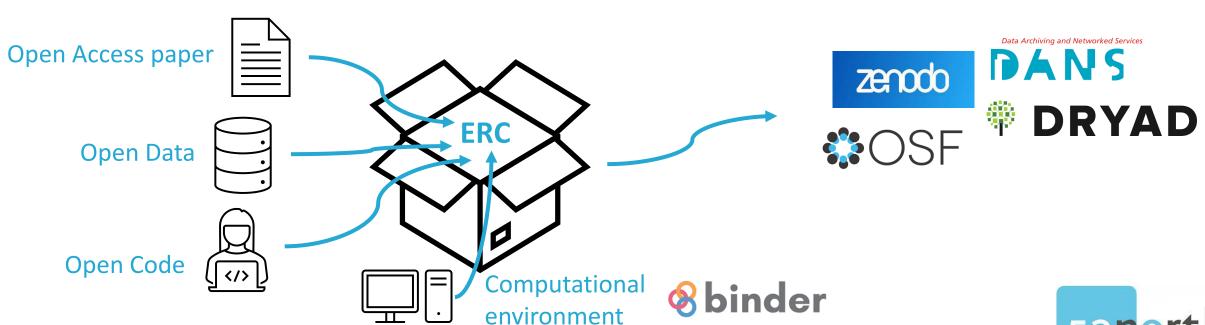
- Create a clean workspace with a hierarchical folder structure and name files properly.
- Include a README text file to explain the code.
  - What does the software?
  - How can I install it?
  - Are there any computational requirements (e.g., operating system)?
  - How can I use it?
  - How long does the analysis take?
- Add a LICENSE, e.g., MIT License, APACHE License, or GNU.





Share the <u>scientific paper</u>, <u>research data</u>, <u>source code</u>, and details of the <u>computational</u> <u>environment</u> that generate published findings in <u>open trusted repositories</u>.

• Such a package is also known as Executable Research Compendium (ERC).





Insert a persistent identifier (e.g., DOI) in the published article that links to the data and source code underlying the results

• Example: "Research data and source code supporting this publication is available on [name of the repository] and accessible via the following DOI: [doi to repository]"

If legitimate reasons to restrict access to the materials apply to your work, mention it.

• Example: "Research data and source code supporting this publication is not available due to [indicate reasons, e.g., licenses, data on human subjects, private or sensitive data etc.]

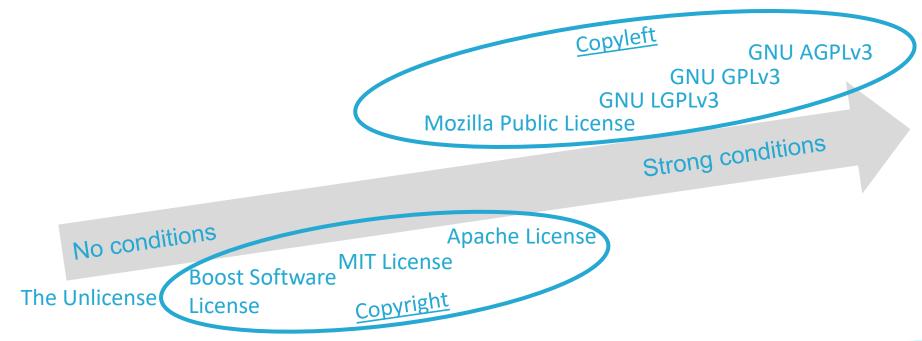


To enable credit for shared materials, citation should be standard practice.

• Example: Statistics were done using R 3.5.0 (R Core Team, 2018), the rstanarm (v2.13.1; Gabry & Goodrich, 2016) and the psycho (v0.3.4; Makowski, 2018) packages. The full reproducible code is available in Supplementary Materials.



Use open licensing when publishing source code.



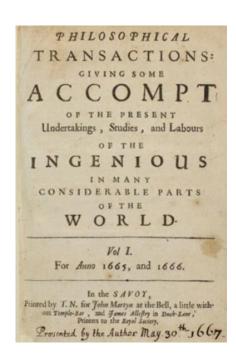


# Practical

#### Lessons learned:

- The Executable Research Compendium is a package including the paper, source code, data, and the computational environment.
- The scientific article should contain a persistent identifier that links to these materials.
- It is important to cite reused software, for example, packages.
- Source code should be released under an open license.















#### AGN as potential factories for eccentric black hole mergers

Received: 8 October 2020

Accepted: 10 December 2021

There is some weak evidence that the black hole merger named GW190521 had a non-zero eccentricity<sup>1,2</sup>. In addition, the masses of the component black holes exceeded the limit predicted by stellar evolution<sup>3</sup>. The large masses can be explained by successive mergers 4.5, which may be efficient in gas disks surrounding active galactic nuclei, but it is difficult to maintain an eccentric orbit all the way to the merger, as basic physics would argue for circularization. Here we show that active galactic nuclei disk environments can lead to an excess of eccentric mergers, if the interactions between single and binary black holes are frequent<sup>5</sup> and occur with mutual inclinations of less than a few degrees. We further illustrate that this eccentric population has a different distribution of the inclination between the spin vectors of the black holes and their orbital angular momentum at merger  $\!\!\!\!^7$  , referred to as the spin-orbit tilt, compared with the remaining circular mergers.

slack holes that eventually megin a citive galactic mode (AGO) disks.

Interest of the control o interactions\*, the inclusion of gravitational wave emission during the interactions, which shockens show moto seems certain incoding many districts, such as the content of the parametric with note received in the parametric production of the parame

With this motivation, we explore how binary black holes merged through binary - model holds enterotements which she extracted by the property of the property

Black holes that eventually merge in active galactic nuclei (AGN) disks interacting black holes merge while they are all bound and interacting

interactions<sup>is</sup>, the inclusion of gravitational-wave emission during the is due to the difference in eccentricity distributions of the dynamically

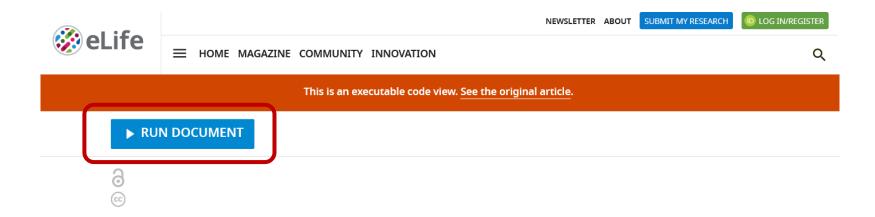
$$\frac{p_2^{(20)}}{p_2^{(00)}} = 10^1 \times \left[ \frac{m}{20M_{\odot}} \right]^{4/11} \frac{a}{1 \text{ AU}} \int_{0}^{4/11} \frac{t_{\text{NK}}}{10^5 \text{ years}} \int_{0}^{4/7} . \tag{1}$$

2022

1665







# Replication Study: Transcriptional amplification cells with elevated c-Myc



L Michelle Lewis, Meredith C Edwards, Zachary R Meyers, C Conover Talbot, Haiping Hao, David Blum, Reproducibility I Elizabeth Iorns, Rachel Tsui, Alexandria Denis, Nicole Perfito, Timothy M Errington University of Georgia, Bioexpression and Fermentation Facility, Georgia, United States; Johns Hopkins University, Deep Sec

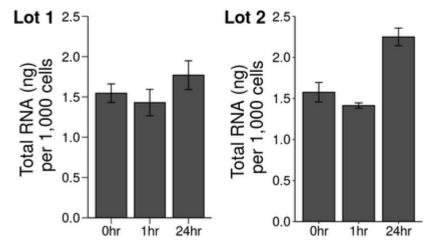




#### Induction of c-Myc in P493-6 cells and impact on total RNA levels.

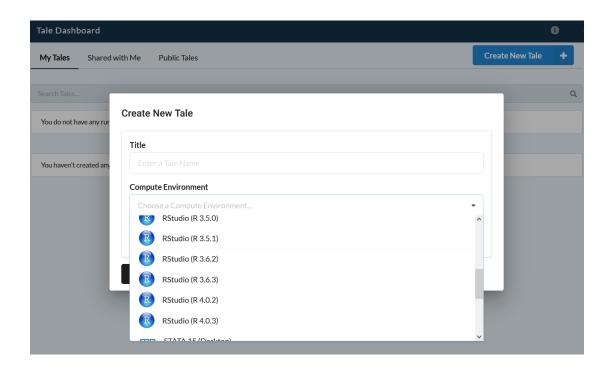
P493-6 cells were grown in the presence of tetracycline (Tet) for 72 hr and switched into Tet-free growth medium to induce c-Myc expression.

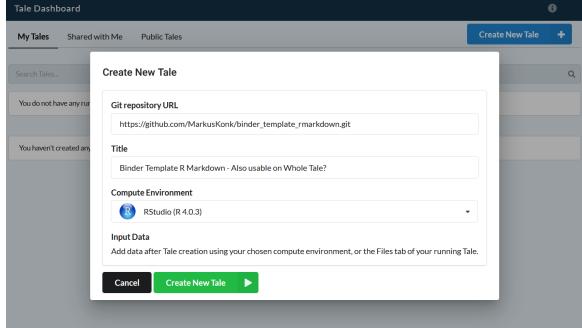
Cells were cultured in two separate lots of serum. (A) Representative Western blot using an anti-c-Myc antibody (top panels) or an anti-6-Myc antibody (bottom panel). Two exposures of the anti-c-Myc antibody are presented to facilitate detection of c-Myc.





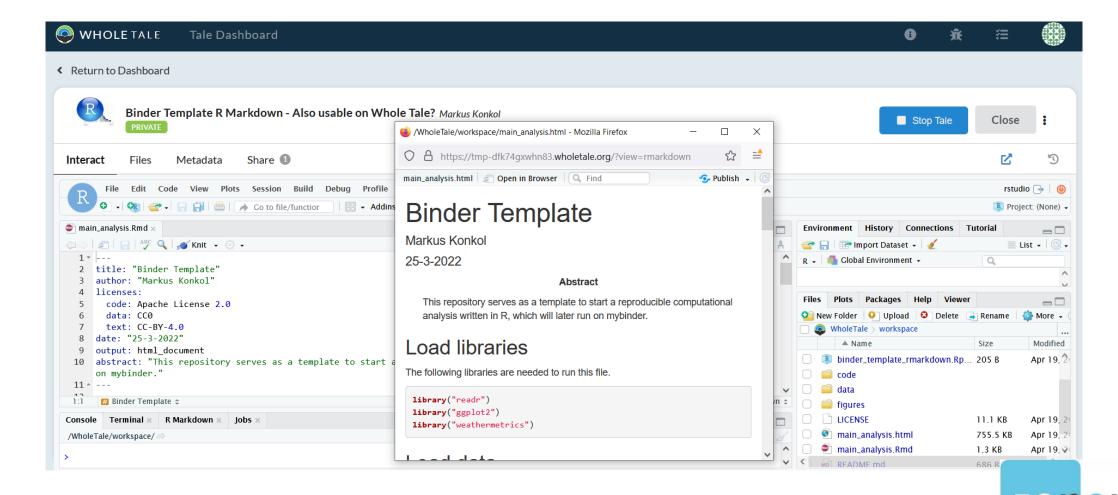








































#### Table 2 Overview of which application supports the corresponding criteria. (N/D = no data)

From: Publishing computational research - a review of infrastructures for reproducible and transparent scholarly communication

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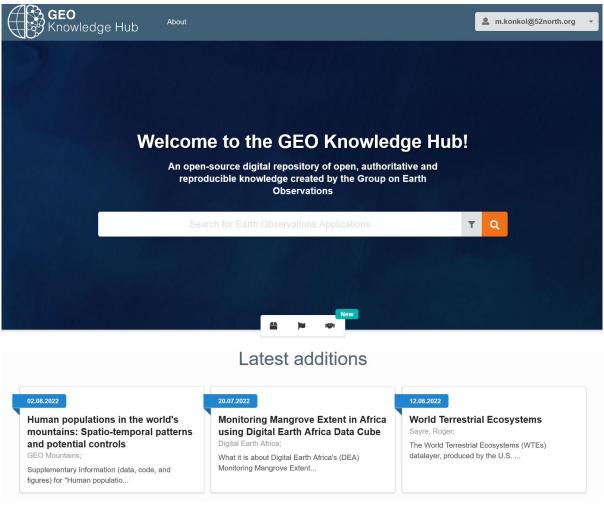
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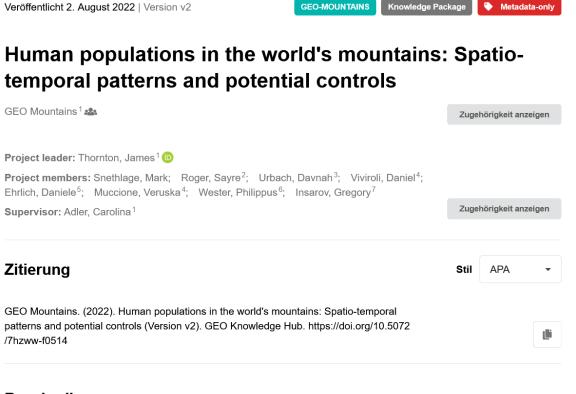
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### **GEO Knowledge Hub**





#### **GEO Knowledge Hub**



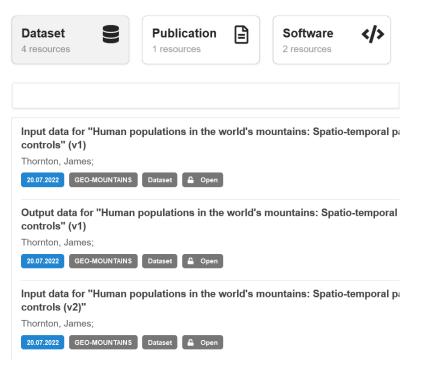
#### Beschreibung

Supplementary Information (data, code, and figures) for "Human populations in the world's mountains: Spatio-temporal patterns and potential controls (Thornton et al. 2022; https://doi.org/10.1371/journal.pone.0271466). The project involved collaboration between GEO Mountains, GEO Human Planet, and other organisations. The code provided enables the results of the study to be replicated, and the workflow transferred or extended to other applications.

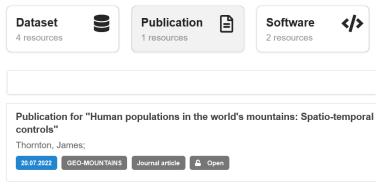


#### **GEO Knowledge Hub**

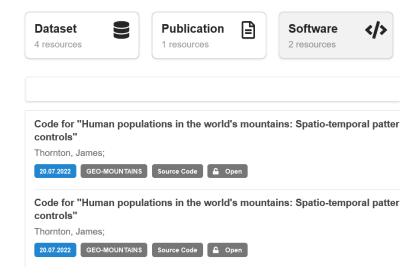
#### **Elements of the Knowledge Package**



#### **Elements of the Knowledge Package**



#### **Elements of the Knowledge Package**





#### Things to discuss and consider

Reproducing results can also mean reproducing errors.

Others might become discouraged to collect data for replication.

Is ORR the ultimate goal or just the basis?

Reproducible research is not necessarily of high quality.



#### Wrap up

- Reproducible Research refers to achieving the same results (e.g., tables, figures, numbers) as reported in the paper by using the same publicly available source code and data.
- Despite a number of ("selfish") reasons to do reproducible research, it is not common practice (due to missing time & skills).
- Accessible code and data is not necessarily reproducible (technical issues, design-related differences, deviating results).
- Reproducibility principles (e.g., Executable Research Compendium) and tools (Computational notebooks, Binder) can help to avoid issues.

19:00-20:00 Dinner







# THANK YOU!

"Openness is not all-or-nothing [...] Fully open research is a long-term goal, not a switch we should expect to flip overnight."

MCKIERNAN et al. (2016)

Last access of all URLs: 11th April 2021.

Alston, J. & Rick, J. (2020). A Beginner's Guide to Conducting Reproducible Research. <a href="http://dx.doi.org/10.32942/osf.io/h5r6n">http://dx.doi.org/10.32942/osf.io/h5r6n</a>

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