Code execution during peer review

with CODECHECK and at the AGILE conference

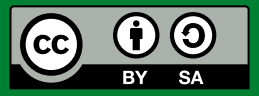
https://codecheck.org.uk/ | https://reproducible-agile.github.io/

Daniel Nüst @ Collaborations Workshop 2022 (CW22), 2022-04-04

Institute for Geoinformatics, University of Münster | http://nüst.de | @nordholmen

Slides: https://bit.ly/cw22-keynote-daniel

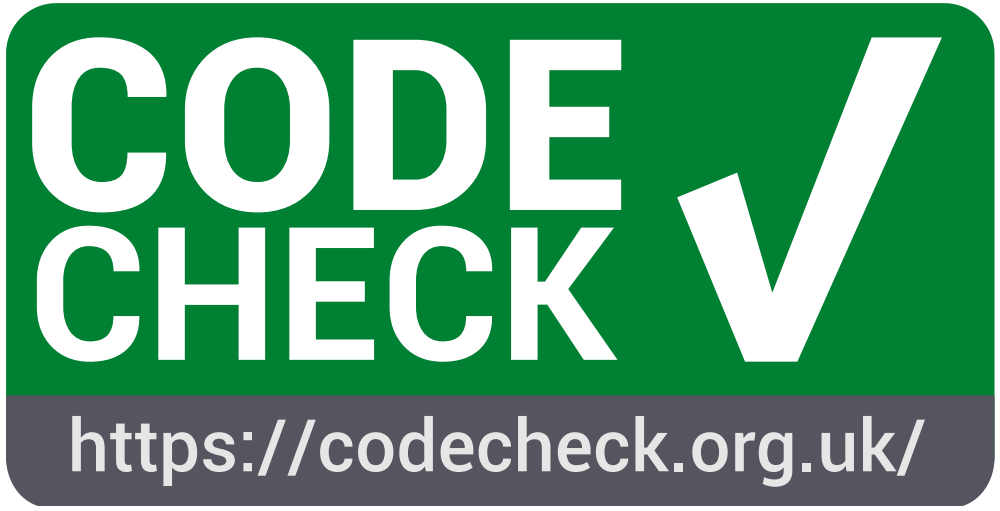
DOI:10.6084/m9.figshare.19487573



Agenda

HTML slides: https://bit.ly/cw22-keynote-daniel

PDF slides: https://doi.org/10.6084/m9.figshare.19487573



https://reproducible-agile.github.io

Declarations and acknowledgements

Declarations

Reproducibility Chair AGILE conference

CODECHECK paper: https://f1000research.com/articles/10-253/v2

Acknowledgements

CODECHECK: Mozilla mini science grant, UK SSI; editors @ *Gigascience*, *eLife*, *Scientific Data*

Reproducible AGILE received funding as an AGILE Initiative

All work was supported by the project Opening Reproducible Research (o2r) with funding by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) under project numbers PE 1632/10-1 and PE 1632/17-1.

CODECHECK: Evaluating the reproducibility of computational results reported in scientific journals

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https://codecheck.org.uk/

CODECHECK in one slide

Premise: paper submitted to peer review.

1. We take your paper, code and datasets.
1. We run your code on your data.
1. If our results match your results, go to step 5.
1. Else we talk to you to find out where code broke. If you fix your code or data, we return to step 2 and try again.
1. We write a report summarising that we could reproduce your outputs (document error messages, possibly mismatches we see)
1. We work with you to freely share your paper, code, data and our reproduction.

Premise

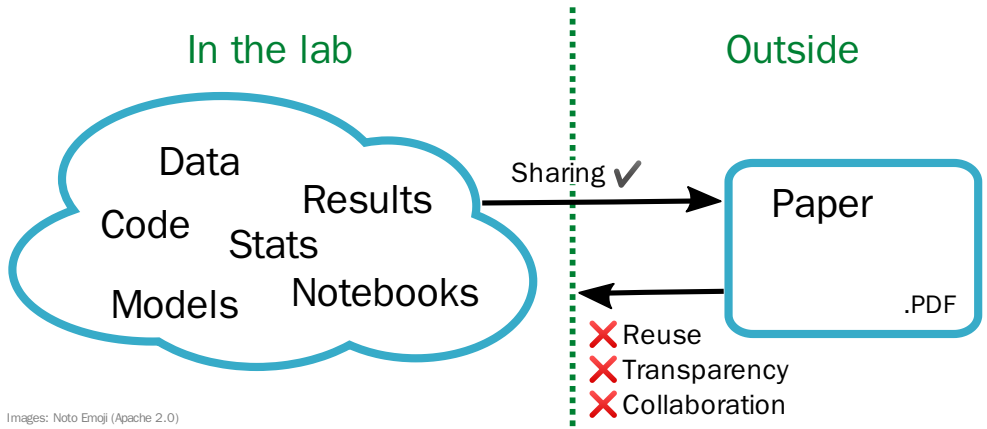


Figure 1 of https://doi.org/10.12688/f1000research.51738.2

We should be sharing material on the left, not the right.

"Paper as advert for Scholarship" (Buckheit & Donoho, 1995)

https://media0.giphy.com/media/mBpVZelPdn269zc07N/giphy.gif

Approaches to code sharing

- Barnes (2010): "Publish your computer code: it is good enough"
- Informal 'code buddy' system
- Community-led *research compedia* - https://research-compendium.science/
- Code Ocean (Nature trial)
- Certify reproducibility with confidential data (CASCAD) (Pérignon et al 2019)

The CODECHECK philosophy

- Systems like Code Ocean set the bar high by "making code reproducible *forever* for *everyone*"
- CODECHECK simply asks "was the code executable *once* for *someone* else?""
- We check the code runs and generates the expected number of output files
- The contents of those output files must not strictly be checked, though in practice until today they are; in any case outputs available for others (authors) to see
- The validity of the code is *not* checked; complement to scientific peer review

More details see paper and CODECHECK principles.

The CODECHECK example process implementation

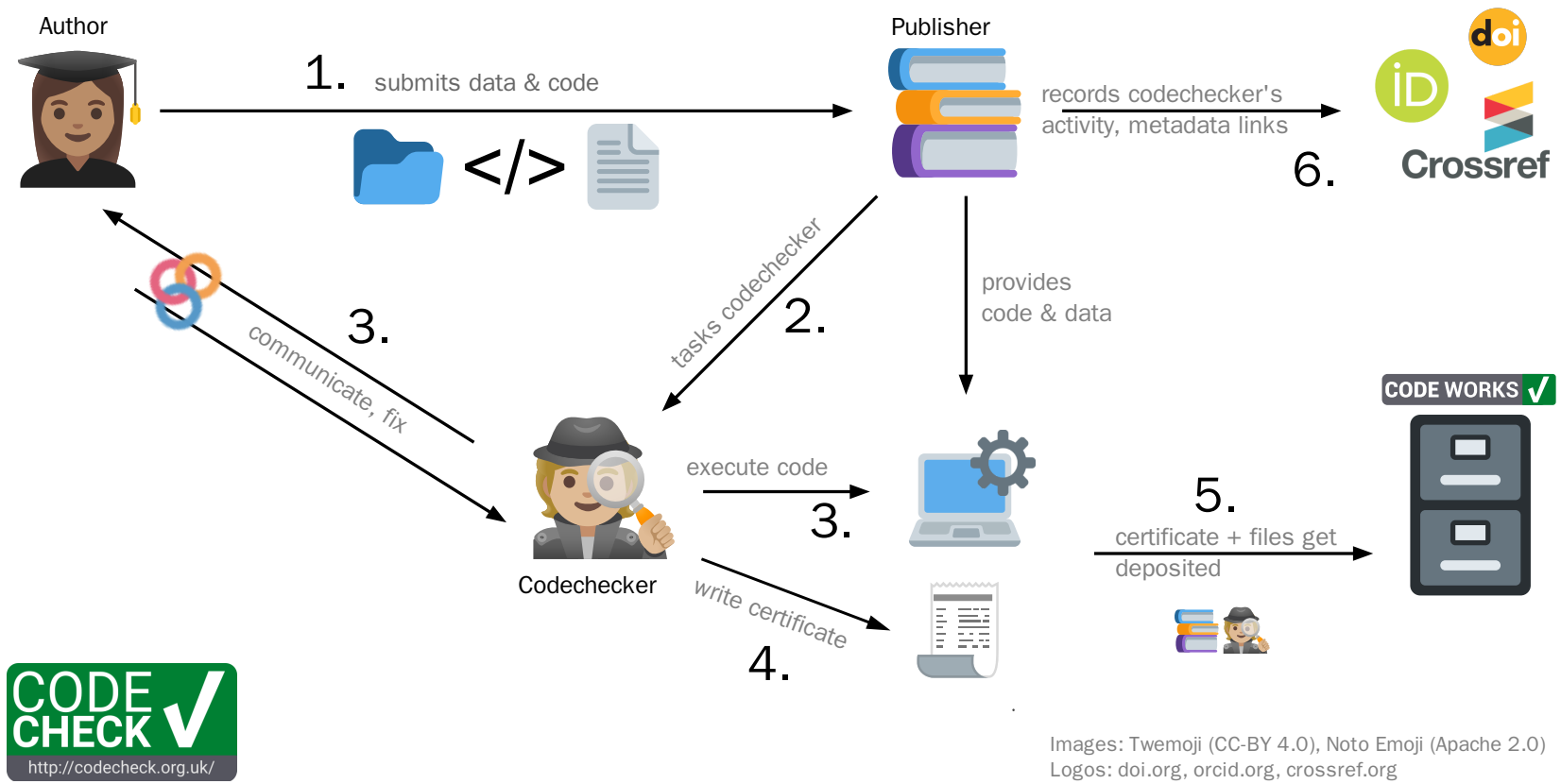


Figure 2 of https://doi.org/10.12688/f1000research.51738.2

Variations in a codecheck

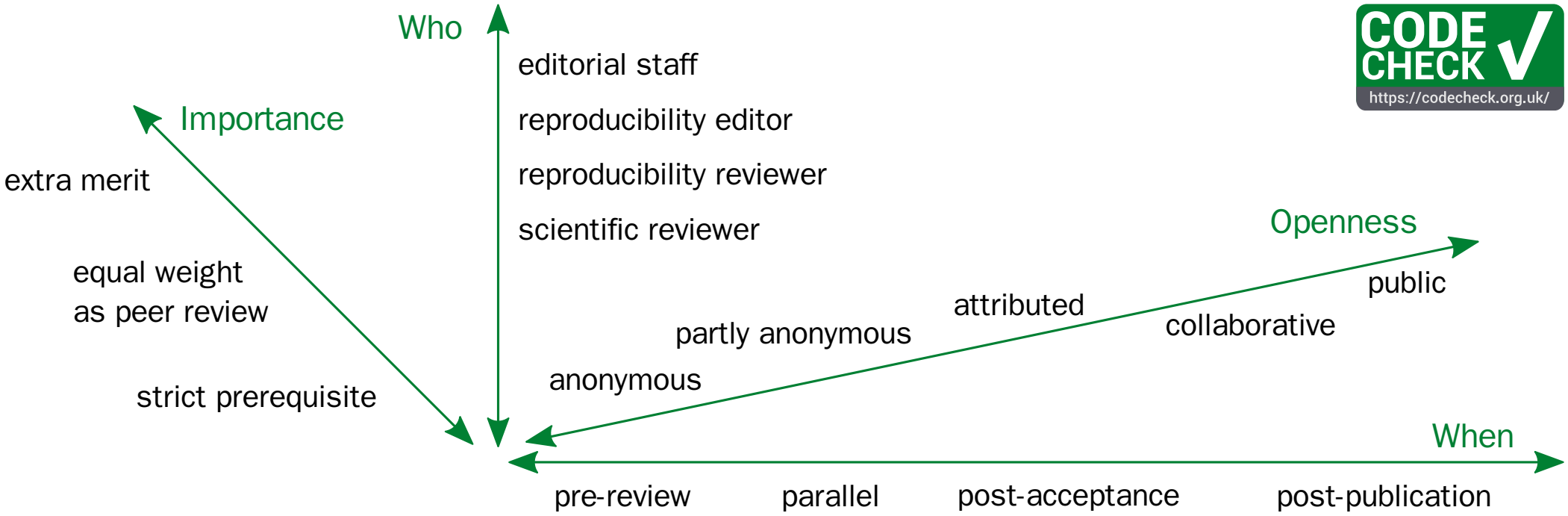


Figure 3 of https://doi.org/10.12688/f1000research.51738.2

Core principles

1. Codecheckers record but don't investigate or fix.
2. Communication between humans is key.
3. Credit is given to codecheckers.
4. Workflows must be auditable.
5. Open by default and transitional by disposition.

Who does the work?

1. AUTHOR provides code/data and instructions on how to run.
2. CODECHECKER runs code and writes certificate.
3. PUBLISHER oversees process, helps depositing artifacts, and persistently publishes certificate.

Who benefits?

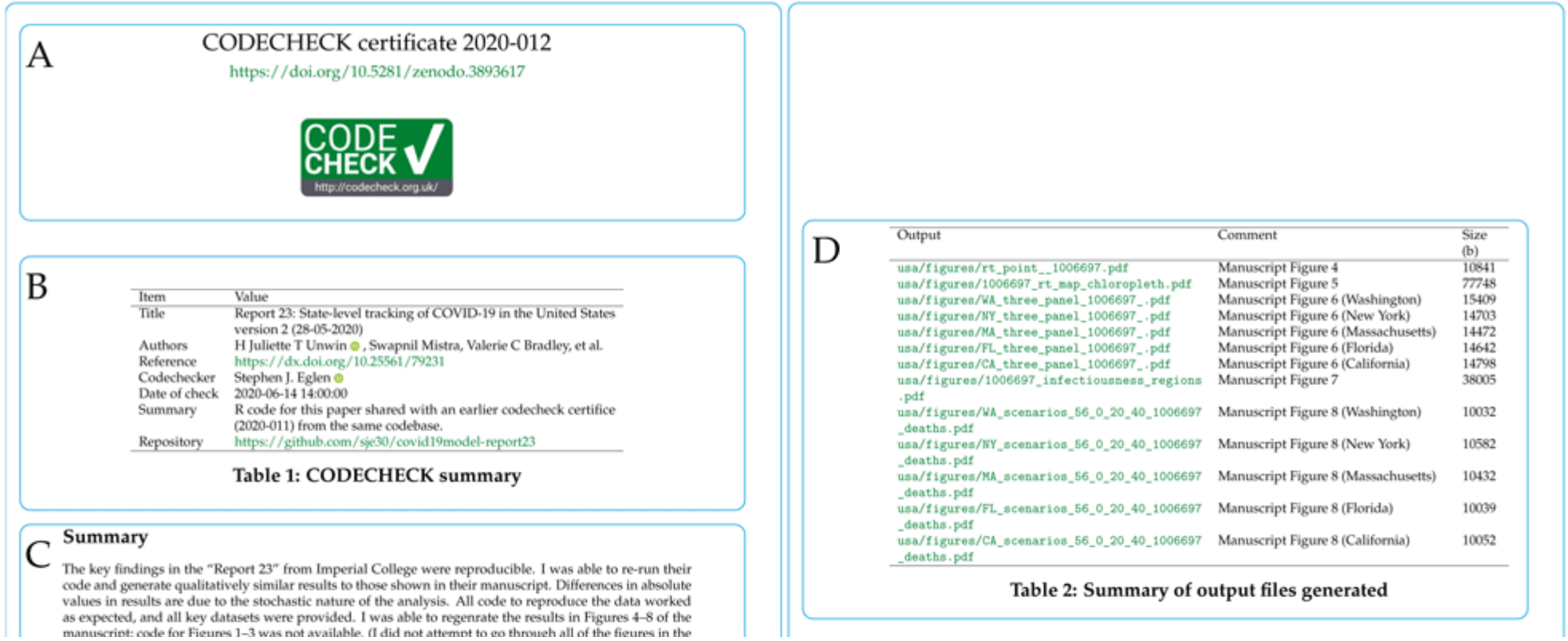
1. AUTHOR gets early check that "code works"; gets snapshot of code archived and increased trust in stability of results.
2. CODECHECKER gets insight in latest research and methods, credit from community, and citable object.
3. PUBLISHER Gets citable certificate with code/data bundle to share and increases reputation of published articles.
4. PEER REVIEWERS can see certificate rather than check code themselves.
5. READER Can check certificate and build upon work immediately.

CODECHECK Register

Certificate	Repository	Type	Issue	Report	Check date
2020-001	codecheckers/Piccolo-2020	journal (GigaScience)	NA	http://doi.org/10.5281/zenodo.3674056	2019-02-14
2020-002	codecheckers/Reproduction-Hancock	community	2	http://doi.org/10.5281/zenodo.3750741	2020-04-13
2020-003	codecheckers/Hopfield-1982	community	1	https://doi.org/10.5281/zenodo.3741797	2020-04-06
2020-004	codecheckers/Barto-Sutton-Anderson-1983	community	4	https://doi.org/10.5281/zenodo.3827371	2020-05-14
2020-005	codecheckers/Larisch-reproduction	community	5	https://doi.org/10.5281/zenodo.3959175	2020-07-23
2020-006	codecheckers/Detorakis-reproduction	community	6	https://doi.org/10.5281/zenodo.3948353	2020-07-16
2020-008	codecheckers/covid-uk	community (preprint)	8	http://doi.org/10.5281/zenodo.3746024	2020-04-09
2020-009	codecheckers/2020-cov-tracing	community (preprint)	9	http://doi.org/10.5281/zenodo.3767060	2020-04-26
2020-010	codecheckers/covid-report9	community (preprint)	14	https://doi.org/10.5281/zenodo.3865491	2020-05-29
2020-011	codecheckers/covid19model-nature	community (in press)	18	https://doi.org/10.5281/zenodo.3893138	2020-06-13
2020-012	codecheckers/covid19model-report23	community (preprint)	19	https://doi.org/10.5281/zenodo.3893617	2020-06-14
2020-013	codecheckers/Spitschan2020_bioRxiv	community (preprint)	20	https://doi.org/10.5281/zenodo.3947959	2020-07-14
2020-014	codecheckers/Sadeh-and-Clopath	community	21	https://doi.org/10.5281/zenodo.3967326	2020-07-28
2020-015	codecheckers/Liou-and-Bateman	community	22	https://doi.org/10.5281/zenodo.3978402	2020-08-04
2020-016	codecheckers/OpeningPractice	journal (J Geogr Syst)	15	https://doi.org/10.5281/zenodo.3981253	2020-06-02
2020-017	codecheckers/JGSY-D-19-00087	journal (J Geogr Syst)	24	https://doi.org/10.5281/zenodo.4003848	2020-08-27

Example certificate

Figure 4 of https://doi.org/10.12688/f1000research.51738.2 (click image to scroll)



A

CODECHECK certificate 2020-012

https://doi.org/10.5281/zenodo.3893617

CODE CHECK ✓ http://codecheck.org.uk/

B

Item	Value
Title	Report 23: State-level tracking of COVID-19 in the United States version 2 (28-05-2020)
Authors	H Juliette T Unwin, Swapnil Mistra, Valerie C Bradley, et al.
Reference	https://dx.doi.org/10.25561/79231
Codechecker	Stephen J. Eglen
Date of check	2020-06-14 14:00:00
Summary	R code for this paper shared with an earlier codecheck certifice (2020-011) from the same codebase.
Repository	https://github.com/sje30/covid19model-report23

Table 1: CODECHECK summary

C

Summary

The key findings in the "Report 23" from Imperial College were reproducible. I was able to re-run their code and generate qualitatively similar results to those shown in their manuscript. Differences in absolute values in results are due to the stochastic nature of the analysis. All code to reproduce the data worked as expected, and all key datasets were provided. I was able to regenrate the results in Figures 4–8 of the manuscript; code for Figures 1–3 was not available. (I did not attempt to go through all of the figures in the

D

Output	Comment	Size (b)
usa/figures/rt_point__1006697.pdf	Manuscript Figure 4	10841
usa/figures/1006697_rt_map_chloropleth.pdf	Manuscript Figure 5	77748
usa/figures/WA_three_panel_1006697_.pdf	Manuscript Figure 6 (Washington)	15409
usa/figures/NY_three_panel_1006697_.pdf	Manuscript Figure 6 (New York)	14703
usa/figures/MA_three_panel_1006697_.pdf	Manuscript Figure 6 (Massachusetts)	14472
usa/figures/FL_three_panel_1006697_.pdf	Manuscript Figure 6 (Florida)	14642
usa/figures/CA_three_panel_1006697_.pdf	Manuscript Figure 6 (California)	14798
usa/figures/1006697_infectiousness_regions.pdf	Manuscript Figure 7	38005
usa/figures/WA_scenarios_56_0_20_40_1006697_deaths.pdf	Manuscript Figure 8 (Washington)	10032
usa/figures/NY_scenarios_56_0_20_40_1006697_deaths.pdf	Manuscript Figure 8 (New York)	10582
usa/figures/MA_scenarios_56_0_20_40_1006697_deaths.pdf	Manuscript Figure 8 (Massachusetts)	10432
usa/figures/FL_scenarios_56_0_20_40_1006697_deaths.pdf	Manuscript Figure 8 (Florida)	10039
usa/figures/CA_scenarios_56_0_20_40_1006697_deaths.pdf	Manuscript Figure 8 (California)	10052

Table 2: Summary of output files generated

Limitations

1. CODECHECKER time is valuable, so needs credit.
2. Very easy to cheat the system, but who cares?
3. Authors' code/data must be freely available.
4. Deliberately low threshold for gaining a certificate.
5. High-performance compute is a resource drain.
6. Cannot (yet) support all thinkable/existing workflows and languages.

Next steps

1. Embedding into journals' workflows.
2. Training a community of codecheckers (❤️ ReproHack).
3. Funding for a codecheck editor.
4. Come and get involved

For more information please see: http://codecheck.org.uk and #CODECHECK


REPRODUCIBLE
AGILE

Reproducible AGILE

https://reproducible-agile.github.io/

2017, ‘18 & ‘19: Workshops on reproducibility

2019: Reproducible publications at AGILE conferences (initiative)

2020: AGILE Reproducible Paper Guidelines v1

2020: First AGILE reproducibility review; guidelines v2

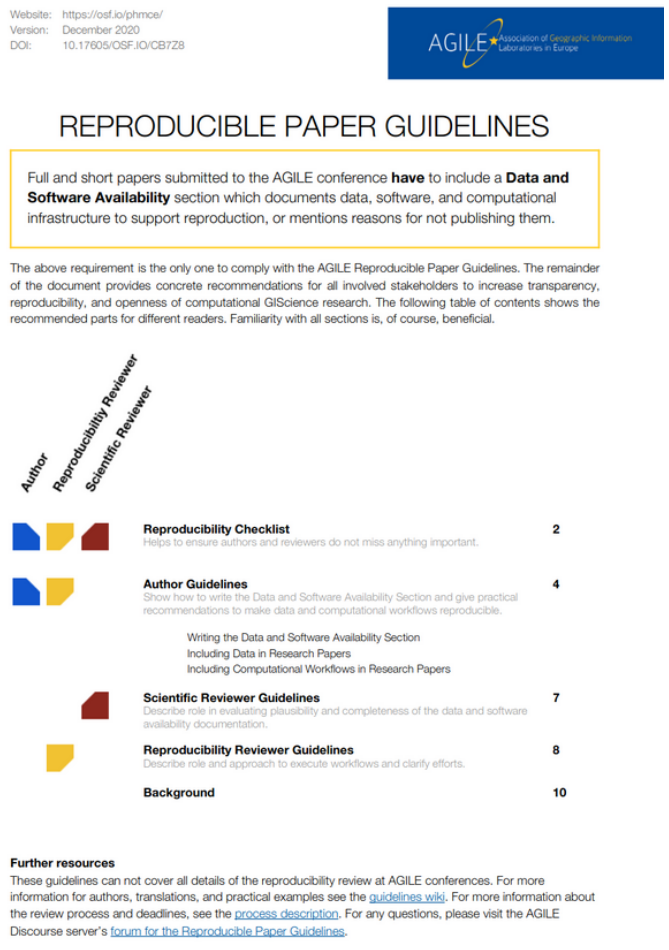
2021: Guidelines mandatory; repro reviews linked from papers: https://agile-giss.copernicus.org/articles/2/index.html

AGILE Reproducible Paper Guidelines

https://doi.org/10.17605/OSF.IO/CB7Z8

- Promotion, not exclusion
- Data and software availability section
- Author & reviewer guidelines
- Reproducibility checklist

14 successful reproductions in 2020 & '21



Website: https://osf.io/phmce/
Version: December 2020
DOI: 10.17605/OSF.IO/CB7Z8

AGILE Association of Geographic Information Laboratories in Europe

REPRODUCIBLE PAPER GUIDELINES

Full and short papers submitted to the AGILE conference **have** to include a **Data and Software Availability** section which documents data, software, and computational infrastructure to support reproduction, or mentions reasons for not publishing them.

The above requirement is the only one to comply with the AGILE Reproducible Paper Guidelines. The remainder of the document provides concrete recommendations for all involved stakeholders to increase transparency, reproducibility, and openness of computational GIScience research. The following table of contents shows the recommended parts for different readers. Familiarity with all sections is, of course, beneficial.

Author
Reproducibility Reviewer
Scientific Reviewer

Further resources
These guidelines can not cover all details of the reproducibility review at AGILE conferences. For more information for authors, translations, and practical examples see the guidelines wiki. For more information about the review process and deadlines, see the process description. For any questions, please visit the AGILE Discourse server's forum for the Reproducible Paper Guidelines.

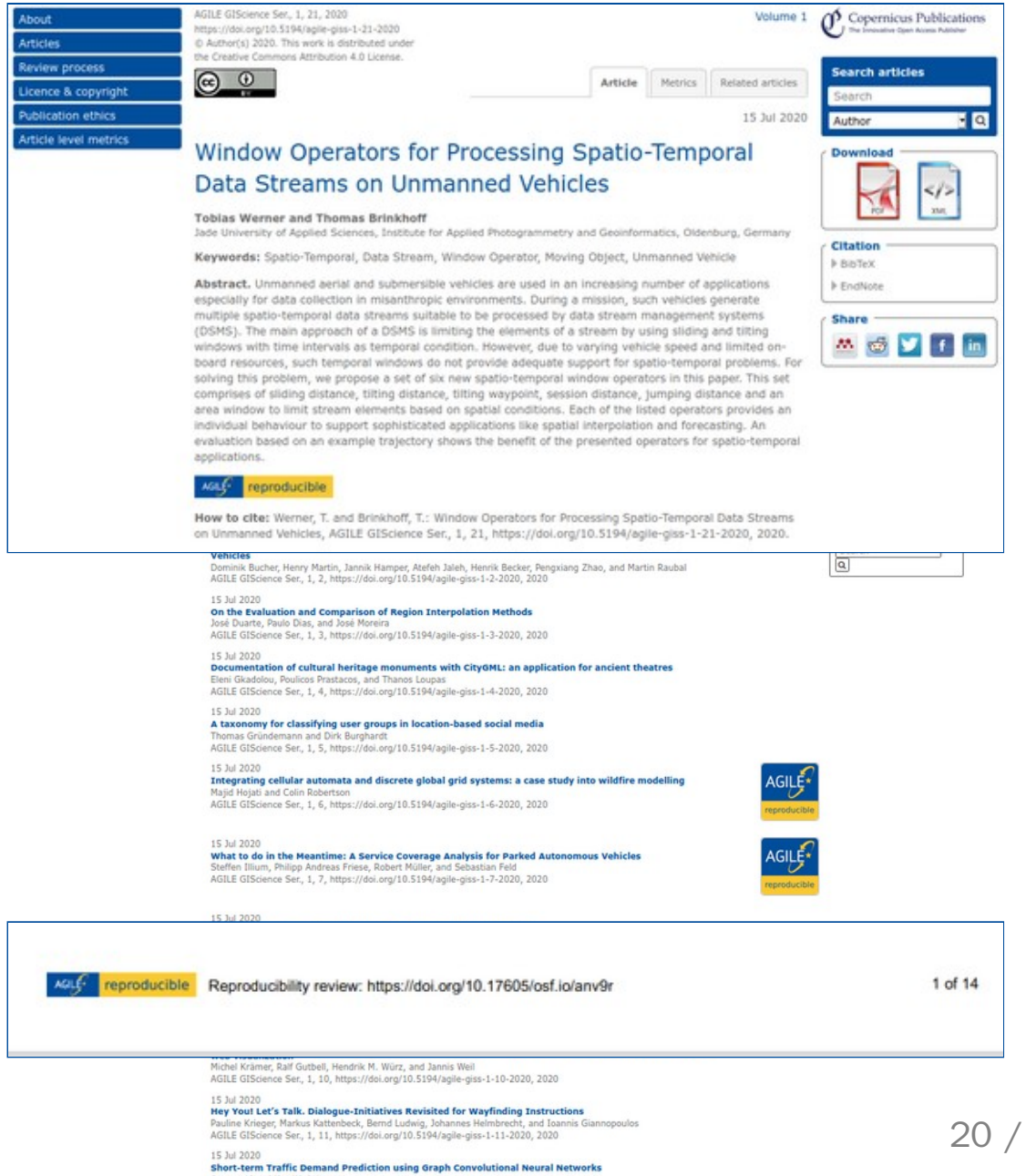
Review process

Reproducibility review after accept/reject decisions

Reproducibility review & communication

Community conference & volunteers

Badges on proceedings website, article website with link, and first article page (💖 Copernicus!)



How to put your community on a path towards more reproducibility in 5 ~~easy~~ hard steps

1️⃣ Build a team of enthusiasts (workshop, social events) 💪🧠

2️⃣ Assess the current state and raise awareness (workshop, paper) 🔬

3️⃣ Institutional support (🙏 AGILE Council 🙏 + committee chairs)

4️⃣ Positive encouragement (no reproduction != bad science) ✨

5️⃣ Keep at it! 🤗

(Next) steps

Reproducibility reviews 2022+

Grow reproducibility reviewer team

Continue community discourse

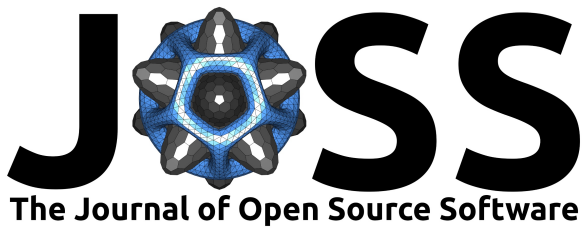
Re-assess new papers > impact?

Towards open scholarship: Open review if tenured?
Format-free first submission? CRediT?

What is RSE(ng) about this?

T ➡️ π

Code review != reproducibility review



Code Review Community working group

Code Review During Development session tomorrow!

https://tenor.com/view/ready-to-help-gif-18701931


Cultural Change
BBC
AMER
RICA

One thing on more reproducible research publications:

Have a README: all else is details.

(Inspired by Greg Wilson's Teching Tech Together (http://teachtogether.tech/en/index.html) Rule 1.)

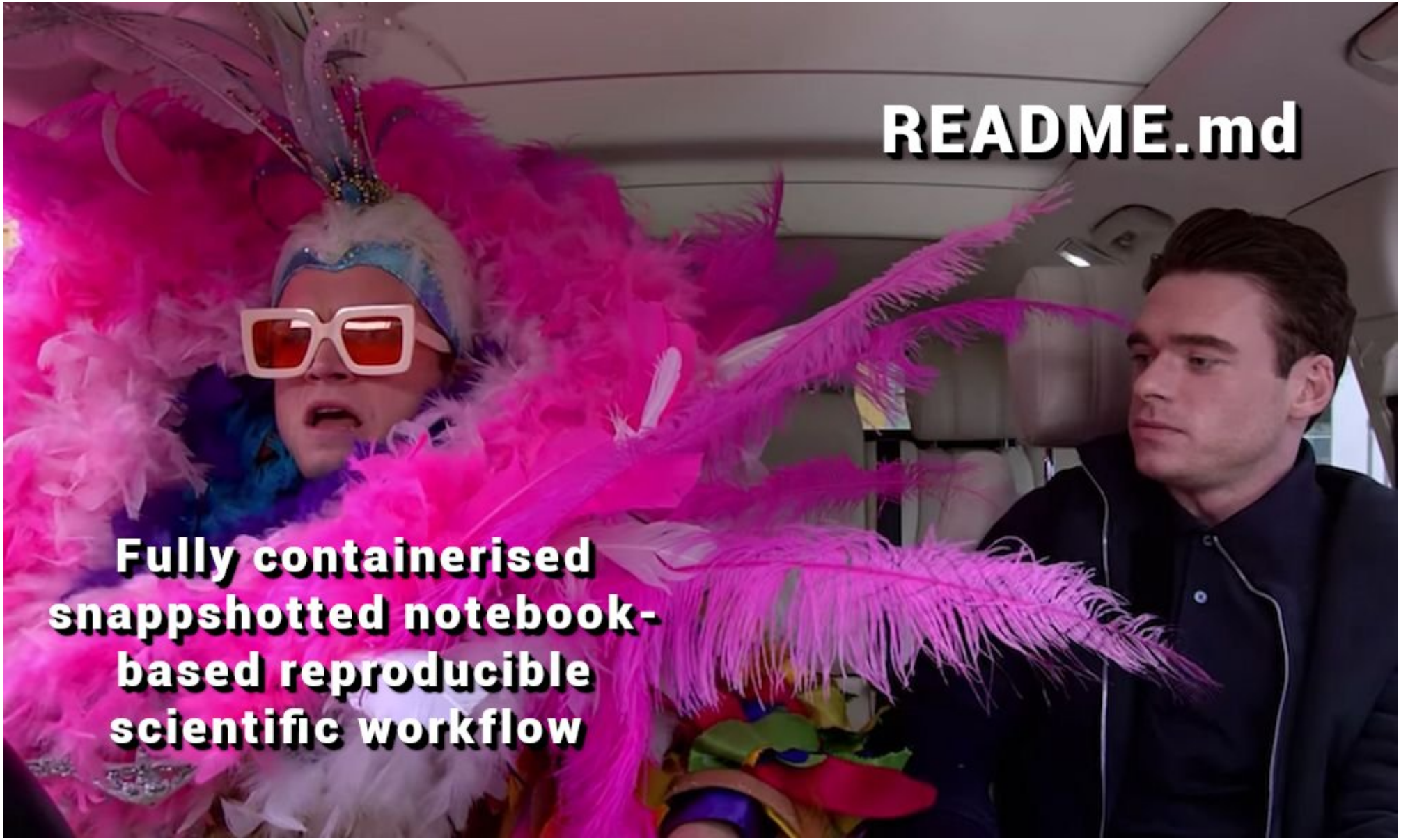
Thank you! Questions?

HTML slides: https://bit.ly/cw22-keynote-daniel | PDF slides: https://doi.org/10.6084/m9.figshare.19487573

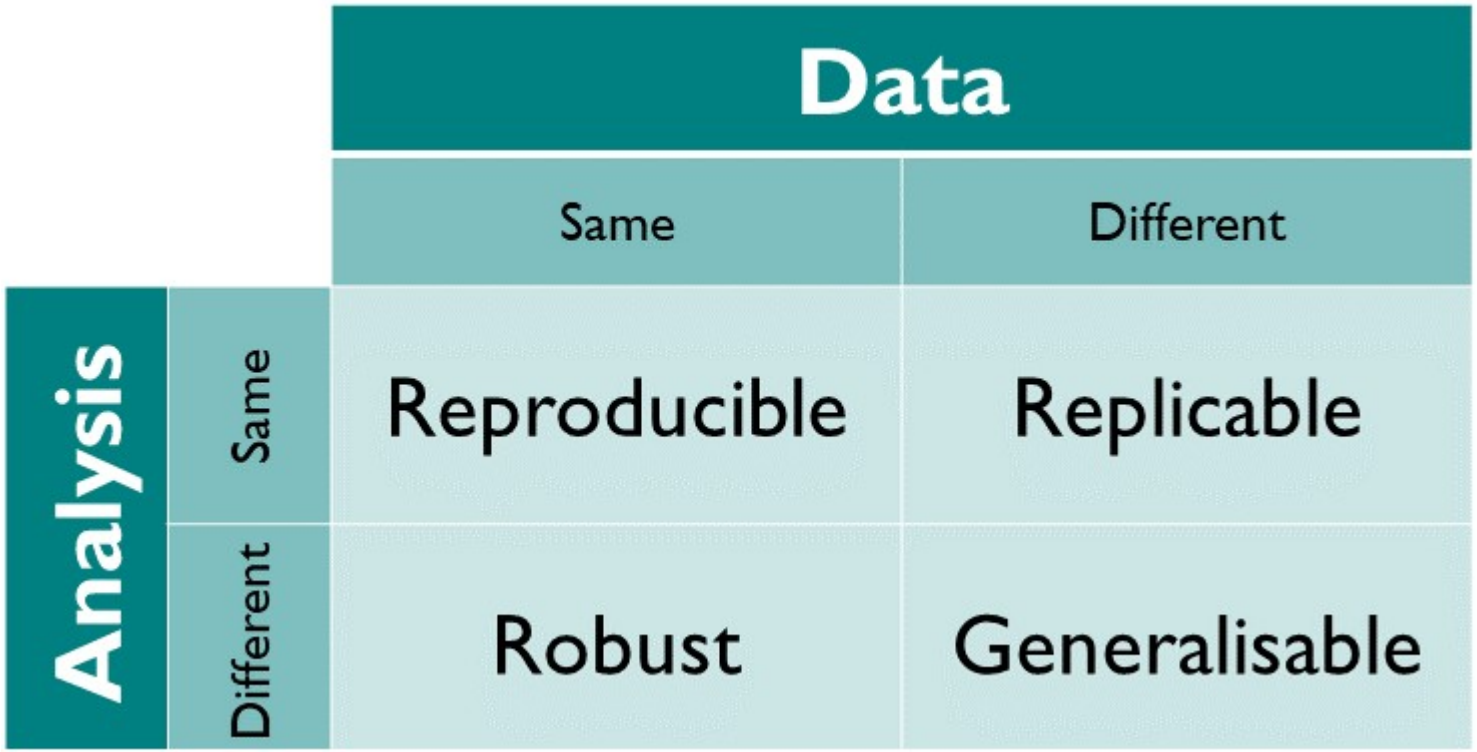
Encore

"It ain't pretty, but it works" (H. Bastian)

(The most prominent check until today!)


README.md
Fully containerised
snappshotted notebook-
based reproducible
scientific workflow

Definition



Learn more about code execution practices at journals and conferences

https://osf.io/x32nc

Daniel Nüst, Heidi Seibold, Stephen Eglen, Lea Schulz-Vanheyden, Limor Peer, Josef Spillner

TODO more

Deep dive

Knowledge Exchange

Chiarelli, Andrea, Loffreda, Lucia, & Johnson, Rob. (2021). The Art of Publishing Reproducible Research Outputs: Supporting emerging practices through cultural and technological innovation. Zenodo. https://doi.org/10.5281/zenodo.5521077

Chiarelli, Andrea, Loffreda, Lucia, & Johnson, Rob. (2021). Executive Summary: The Art of Publishing Reproducible Research Outputs: Supporting emerging practices through cultural and technological innovation. Zenodo. https://doi.org/10.5281/zenodo.5639384

https://knowledge-exchange.info/event/publishing-reproducible-research-output

Reproducible AGILE and CODECHECK: Highlights of Lessons learned

Spectrum or layers of reproducibility very apparent

Effect of guidelines at AGILE: improved reproducibility, community discourse

Reproducibility reports/CODECHECK certificates full of recommendations for improvement, often well received by authors, many included in revised submission

Good practices spread slowly, establishing a process is tedious, needs time until familiarity

Challenges for reproducibility reviewer: Inconsistencies and disconnects (figures), lack of documentation, unknown runtimes vs. no subsets of data, lack of reprod. guidance

Reproductions are rewarding and educational, matching expertises tricky

Communication is without alternative

Safety net (👀), not security

What can communities & institutions do?

Introduce reproducibility reviews - CODECHECK (or not) - at your journals, labs, collaborations!

Workshops on RCR, ReproHacks

Provide support (R2S2, PhD edu.)

Rewards and incentives

Community discourse

Awareness > Change

Throw technology at it

Digital information lasts forever, or five years - whichever comes first.

Rothenberg, Jeff. 1995. “Ensuring the Longevity of Digital Documents.” Scientific American 272 (1): 42–47. JSTOR via https://twitter.com/snet_jklump/status/1141934045820887040?s=09

"Preproducibility" - Philip Stark

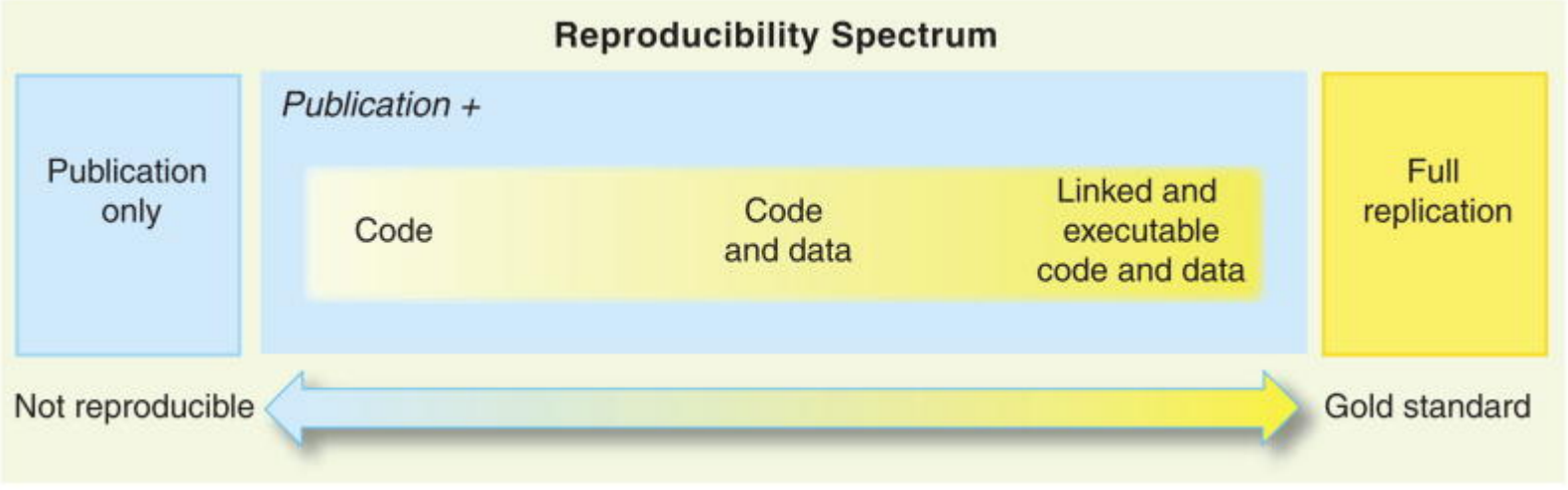
"Science should be 'show me', not 'trust me'; it should be 'help me if you can', not 'catch me if you can'."

[...]

"*If you and I get different results, preproducibility can help us to identify why — and the answer might be fascinating.*"

Nature 557, 613 (2018).
https://doi.org/10.1038/d41586-018-05256-0

Reproducibility spectrum



Peng R. D. (2011). Reproducible research in computational science. Science (New York, N.Y.), 334(6060), 1226–1227. https://doi.org/10.1126/science.1213847

Five selfish reasons to work reproducibly

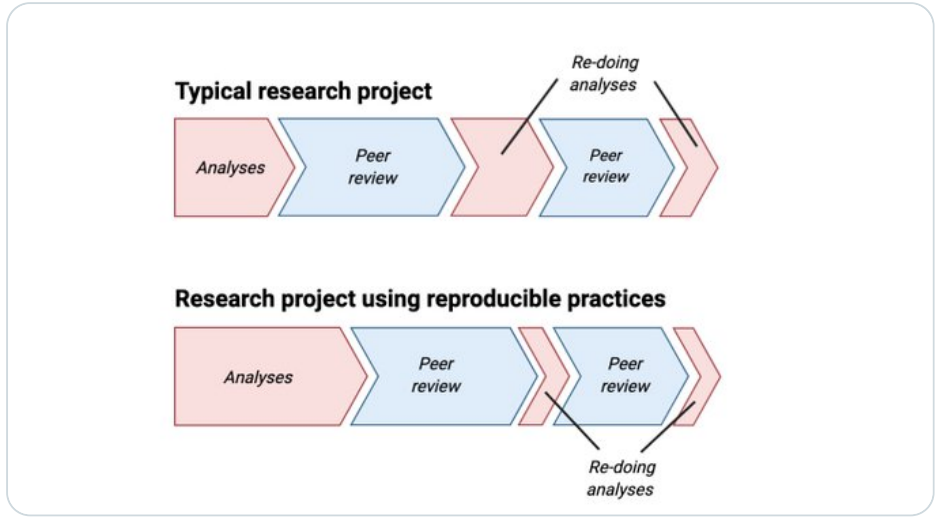
1. reproducibility helps to avoid disaster
2. reproducibility makes it easier to write papers
3. reproducibility helps reviewers see it your way
4. reproducibility enables continuity of your work
5. reproducibility helps to build your reputation

Markowetz, F. Five selfish reasons to work reproducibly. Genome Biol 16, 274 (2015). https://doi.org/10.1186/s13059-015-0850-7

Reproducibility is "more work"

Dan Quintana
@dsquintana

In my experience, you don't lose time doing reproducible science—you just *relocate* how you're spending it



3:13 PM · Nov 26, 2020

Read the full conversation on Twitter

GIScience assessment

Nüst, Daniel. 2021. Infrastructures and Practices for Reproducible Research in Geography, Geosciences, and GIScience. Doctoral dissertation, University of Münster, Germany. https://doi.org/10.5281/zenodo.4768096

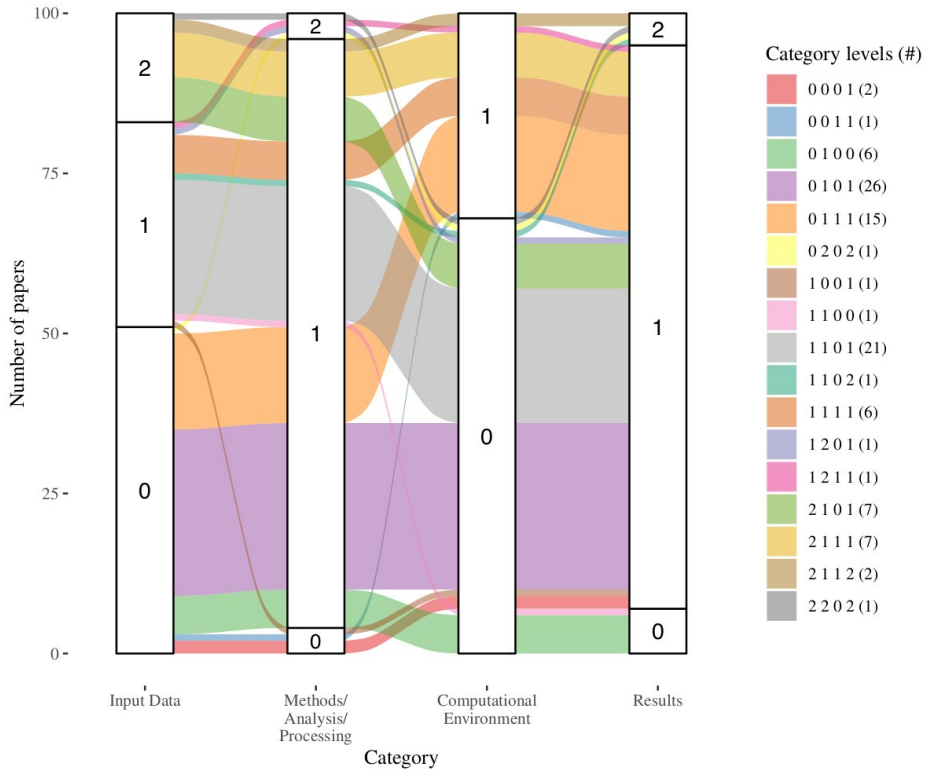


Figure 4: Combined alluvial diagram. Includes groups of papers across four categories for the merged AGILE (Chapter 11) and GIScience (Chapter 12) datasets; the category *Preprocessing* was dropped because of difficulties to clearly assess it; included are 100 papers without any "not applicable" value from 2010 to 2018; see analysis notebook at https://zivgitlab.uni-muenster.de/d_nues01/phd-package/-/blob/master/combined-giscience-assessment-figure.Rmd.