Reproducibility and Peer Review

Daniel Nüst

Keynote at virtual kick off meeting of the **ORDS network**, December 1st 2020



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About me

Self-identified research software engineer and *Open X* fan

Diploma Geoinformatics (Münster)

Software developer/consultant @ 52°North GmbH, Münster

Researcher in project **Opening Reproducible Research** (o2r, https://o2r.info)

Founding member and deputy chair of de-RSE e. V., ms-RSE

Reproducibility Chair AGILE conference 2020, 2021

Co-Pl of **CODECHECK**

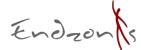
https://orcid.org/0000-0002-0024-5046

GitHub.com/nuest | GitLab.com/nuest

@nordholmen

Open Science, #ReproducibleResearch, R, containerisation (Docker), Python, ...









Messy Laboratory Stock Photos & Mess...











essy Desk Is a Sign of Genius, According to Scienc...



The World's Best Photos of lab and mes...







Mes alan









Messy Laboratory Stock Photos & Messy L...



ssy offices - ...



Messy Laboratory Stock Pho... alamy.com



How to Handle Untidy, Messy Employees | Inc.com

Untidy Kitchenware Pile Dirty Dishes Sink Sto...



Messy Laboratory Stock Photos & Mes... alamy.com



Untidiness Cartoons and C...



Are You Messy? Here's Why It Might Mean



Top 10 Office Decluttering Tricks lifehacker.com



The Messy Desks Behind These Creati... designnews.com









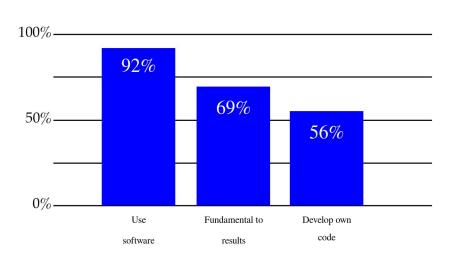






Back to 2010 The Software Sustainability Institute (SSI, UK) run a study (1000 randomly chosen researchers) ...

"It's impossible to conduct research without software, say 7 out of 10 UK researchers"



A study of Nature papers from Jan-March 2016 reveals that

"32 of the 40 papers examined mention software, and the 32 papers contain 211 mentions of distinct pieces of software, for an average of 6.5 mentions per paper."

Nangia, Udit; Katz, Daniel S. (2017): Understanding Software in Research: Initial Results from Examining Nature and a Call for Collaboration. doi:10.1109/eScience.2017.78



https://giphy.com/gifs/with-computers-fascination-PxSFAnuubLkSA



https://theconversation.com/how-computers-broke-scienceand-what-we-can-do-to-fix-it-49938



https://giphy.com/gifs/david-hasselhoff-M3o3fL9nnxG4o

Crisis? Crisis of what?



Credibility crisis?
Replicability crisis?
Reproducibility crisis?
Robustness crisis?
Generalisability crisis?

THE PARTY OF THE P		Data		
		Same	Different	
nalysis	Same	Reproducible	Replicable	
Ana	Different	Robust	Generalisable	

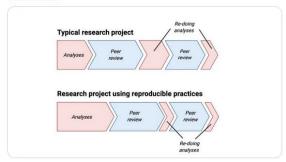
https://the-turing-way.netlify.app/reproducible-research/overview/overview-definitions.html



Dan Quintana

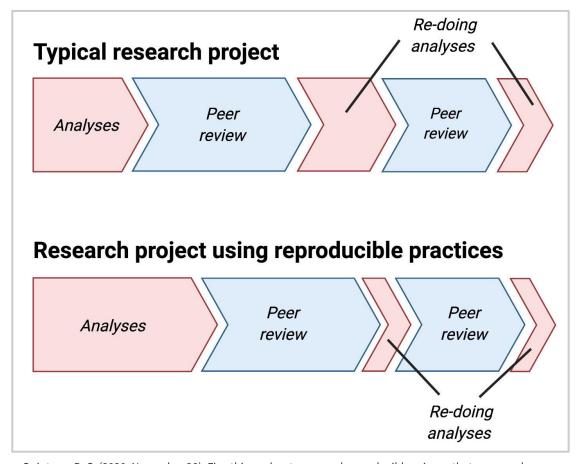
In my experience, you don't lose time doing reproducible science—you just *relocate* how you're spending it

Tweet übersetzen



4:13 nachm. · 26. Nov. 2020 · TweetDeck

107 Retweets 20 Zitierte Tweets 536 "Gefällt mir"-Angaben



Quintana, D. S. (2020, November 28). Five things about open and reproducible science that every early career researcher should know. https://doi.org/10.17605/OSF.IO/DZTVQ

Comment | Open Access | Published: 08 December 2015

Five selfish reasons to work reproducibly

Florian Markowetz 🗠

Genome Biology 16, Article number: 274 (2015) Cite this article

15k Accesses 28 Citations 443 Altmetric Metrics

https://doi.org/10.1186/s13059-015-0850-7

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

Reproducible Research & research software

Peer Review





Reproducible research and peer review are cornerstones of science. But are they getting along?

The many problems of science

Publish or perish **Broken metrics (citations, JIF)** Structural change not considering senior academics **Publication bias** Long-term funding for tools & infrastructure **HARKing** p-Hacking **Scholarly communication 1.0** Lack of reusability **Lack of transparency** Lack of reproducibility Reinventing the wheel **Retraction practices** Not invented here syndrome Fraud **Imposter syndrome**

No "negative" citation



https://giphy.com/gifs/bbcamerica-cute-animals-lifestory-Ze3RpHue7qkwvcYOOf

Open Science (OER, OA, OS, OPR) **Registered reports/preregistration Altmetrics Preprints Leiden Manifesto DORA Vienna Principles** Citing data and software **Software papers** Data and software as products of research RSEng & RSEs (software sustainability) **CRediT Research Compendia Ten Hot Topics Around Scholarly Publishing** Code review (PyOpenSci, ROpenSci, JOSS)

•••

Traditional and modern scientists

Deep knowledge: expertise and

Broad knowledge: across disciplines collaborate with other experts, apply outside of own field

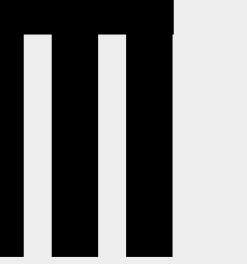












Code Review



Boettiger, C., Chamberlain, S., Hart, E., & Ram, K. (2015). Building Software, Building Community: Lessons from the rOpenSci Project. Journal of Open Research Software, 3(1), e8. doi:10.5334/jors.bu







Code Review Community Working Group

How to get reproducible research and peer review to get along?

Reproducible computational research in journals & conferences

ACM Transactions on Mathematical Software

Journal of Statistical Software









Reproducibility Initiative





AGILE Reproducible Paper Guidelines



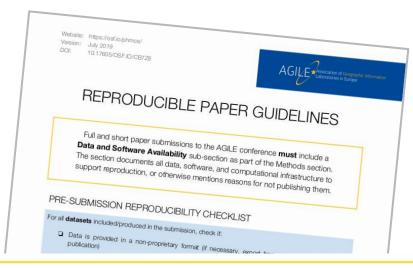
https://doi.org/10.17605/OSF.IO/CB7Z8

Created by AGILE Initiative in 2019, see report at https://osf.io/hupxr/

Transparency & Reproducibility GIScience

https://osf.io/phmce/wiki/home/

Promotion Acknowledge spectrum



Full and short paper submissions to the AGILE conference **must** include a **Data and Software Availability** sub-section as part of the Methods section. The section documents all data, software, and computational infrastructure to support reproduction, or otherwise mentions reasons for not publishing them.

The guidelines

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

Author guidelines

Data in Research Papers
Computational workflows
in Research Papers
Pre-submission checklist
Writing DASA section

Rationale/Motivation/Vision

Reviewer guidelines

Reproducibility reviewer guidelines (WIP)

Website: https://osf.io/phmce/ Version: July 2019 DOI: 10.17605/OSF.IO/CB7Z8



REPRODUCIBLE PAPER GUIDELINES

Full and short paper submissions to the AGILE conference **must** include a **Data and Software Availability** sub-section as part of the Methods section. The section documents all data, software, and computational infrastructure to support reproduction, or otherwise mentions reasons for not publishing them.

PRE-SUBMISSION REPRODUCIBILITY CHECKLIST

For all datasets included/produced in the submission, check if:

- Data is provided in a non-proprietary format (if necessary, export from proprietary format for publication)
- Data is documented (at least description of collection query and field or column names, ideally using complete metadata following established standards)
- Data is accessible in a public repository
- Data has a clear licence

For any software tool/library/package used or produced, check if:

- Computational environment (including hardware) is documented or provided in the most appropriate format given its complexity
- The versions of relevant software components (libraries, packages) are provided
- Software is available in a public repository
- Software has a clear license
- Computational steps are explained in a text file, flowchart, or script
- All parameters needed to run the computational workflow are provided

In the Data and Software Availability section, check if you include:

- Data and software statements according to the template
- The reasons, if any, for not being able to share (parts of) data or code.

For properly acknowledging data and software by both you and others check that:

All datasets and code used or mentioned are cited throughout the paper and included in the references with DOIs.

AGILE conference review process

Proceedings:

https://www.agile-giscience-series.net/review_process.html

Process documentation:

https://osf.io/7rjpe/

Reproducibility review *after* accept/reject decisions, triggered by regular reviewer

Reproducibility review & communication

Community conference & coronavirus

Badges on proceedings page

Presentation at conference

Read full report at https://osf.io/7rjpe/



Reproducibility review results

6 reproducibility reports published

16 not possible/not attempted

(5 of which after communication with authors):

- no starting point in the paper
- documentation insufficient for third party
- sensitive/confidential/commercial data
- proprietary software
- software paper
- (conceptual papers)

■■ Reproducibility review of: Integrating cellular automata and discrete global grid systems: a case study into wildfire modelling

Nüst

Reproduction report and material.

■ Reproducibility review of: Extracting interrogative intents and concepts from geo-analytic questions

Nüst

Reproduction report and material.

■ Reproducibility review of: Tracking Hurricane Dorian in GDELT and Twitter

Ostermann & Nüst

Reproduction report and material.

■ Reproducibility Review of: Comparing supervised learning algorithms for Spatial Nominal Entity recognition

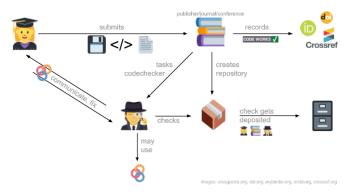
Ostermann & Nüst
Reproduction report and material.

■ Reproducibility review of: Window Operators for Processing Spatio-Temporal Data Streams on Unmanned Vehicles

Nüst & Ostermann Reproduction report and material.

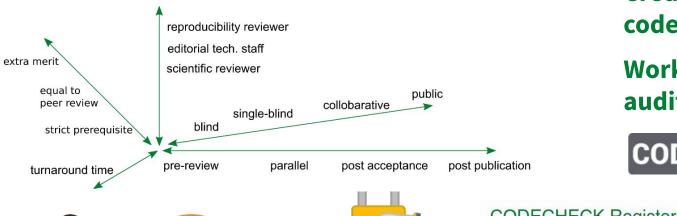
Reproducibility review of: What to do in the Meantime: A Service Coverage Analysis for Parked Autonomous Vehicles

Nüst & Granell Reproduction report and material. attps://osf.io/6k5fh/





Independent execution of computations underlying research articles.



Codecheckers record but don't investigate or fix.

Communication between humans is key.

Credit is given to codecheckers.

Workflows must be auditable.









Certificate	Repository	Туре	Issue	Report
2020-001	O codecheckers/Piccolo-2020	journal (GigaScience)	NA	http://doi.org/10.5281/zenodo.3674056
2020-002	O codecheckers/Reproduction-Hancock	community	2	http://doi.org/10.5281/zenodo.3750741
2020-003	O codecheckers/Hopfield-1982	community	1	https://doi.org/10.5281/zenodo.3741797
2020-004	O codecheckers/Barto-Sutton-Anderson-1983	community	4	https://doi.org/10.5281/zenodo.3827371
2020-005	O codecheckers/Larisch-reproduction	community	5	https://doi.org/10.5281/zenodo.3959175
2020-006	O codecheckers/Detorakis-reproduction	community	6	https://doi.org/10.5281/zenodo.3948353

Reproducible AGILE and CODECHECK: Highlights of Lessons learned





Spectrum or layers of reproducibility

Effect of guidelines at AGILE: improved reproducibility

Reproducibility reports/CODECHECK certificates full of **recommendations** for improvement, well received by authors, even included in revision before publication

Good practices spread slowly, establishing a **process** is tedious

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

Reproductions are **rewarding** and educational, matching expertises tricky

Safety net (**●●**), not **security**

What can you do today?



What can scientists do?

Do what Heidi tells you! [slides] One step at a time.

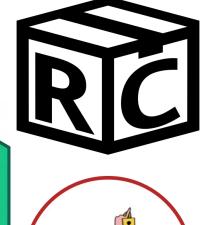
Create and publish Research Compendia (Your code is good enough!): https://research-compendium.science/

Become a **codechecker** or **reprohacker**.

Strive to be open science champion **especially** if you're in a senior position in your field (hiring, contributorship, funding & openness).

[RIOT Science Club Talk by Gavin Buckinham; preprint by Sam Westwood]







What can communities and institutions do?

Introduce reproducibility reviews - CODECHECK (or not)!

Workshops on RCR, ReproHacks

Provide support (**R2S2**, Anja)

Rewards and incentives

Awareness > Change



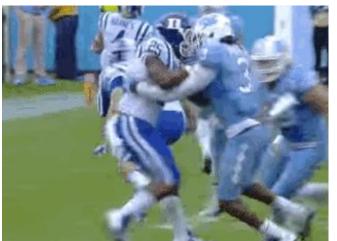
https://giphy.com/gifs/chicagodancecrash-KCqjrcPfL55q3MkgHZ

How does the future of reproducible research in peer review look like?

Reproducibility is **possible**, but disciplines/communities must agree what "peer review" entails and acknowledge the **efforts** (ECRs, RSEs) in a **positive** way.

Help each other! Move together as a community through disruptive changes. Then reproducible research and peer review will get along just fine.







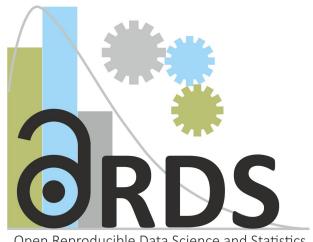
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Thank you!

What are your questions?

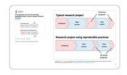


https://giphy.com/gifs/mrw-save-counting-wvWJOoYmFnSp2



Open Reproducible Data Science and Statistics













https://doi.org/10.17001/08/10/CB128





Keynote at virtual kick off meeting of the **ORDS**

Reproducibility and





5. reproductionly helps

continuity of your work. 5. remote hits/select









research without autoware

pay 7 out of 10 UK



Traditional and modern scientists.



· Immediatel papers





CODE WORKS V



doi.org/10.5281/zenodo.4292263

network, December 1st 2020

orcid.org/0000-0002-0024-5046















bonus slides

Published online 13 October 2010 | Nature 467, 753 (2010) | doi:10.1038/467753a





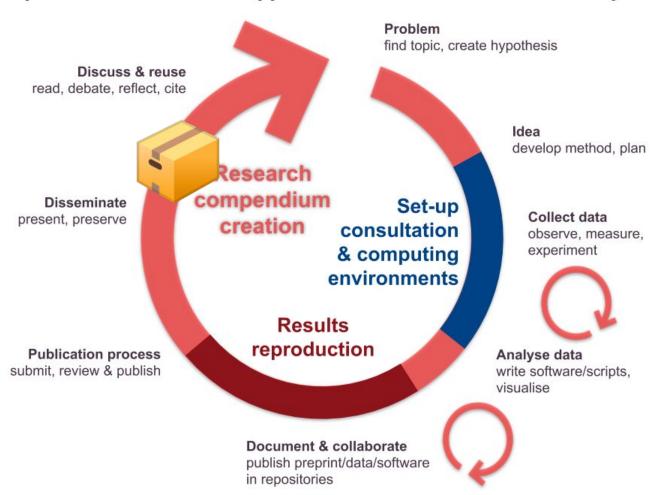
Freely provided working code — whatever its quality improves programming and enables others to engage with your research, says Nick Barnes.

Nick Barnes

I am a professional software engineer and I want to share a trade secret with scientists: most professional computer software isn't very good. The code inside your laptop, television, phone or car is often badly documented, inconsistent and poorly tested.

Why does this matter to science? Because to turn raw data into published research papers often requires a little programming, which means that most scientists write software. And you scientists generally think the code you write is poor. It doesn't contain good comments, have sensible variable names or proper indentation. It breaks if you introduce badly formatted data, and you need to edit the output by hand to get the columns to line up. It includes a routine written by a graduate student which you never completely understood, and so on. Sound familiar? Well, those things don't matter.

Reproducible Research Support Services in the Research Lifecycle





Reproducible Research Support Service

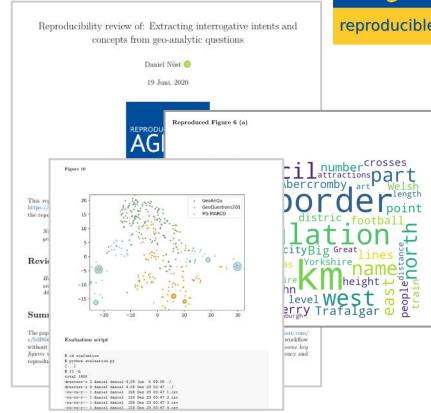
https://go.wwu.de/r2s2

EDUCATION OF CONDITIONS FOR RESEARCHERS USING SOFTWARE DEVELOPERS LEAD TO RESEARCH

Reproducibility review reports

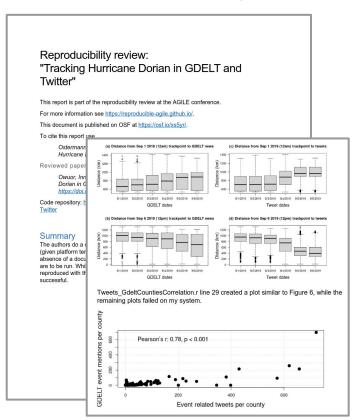


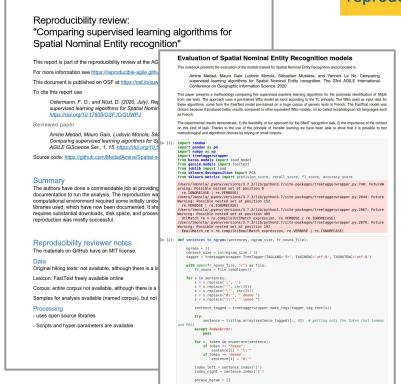




Reproducibility review reports

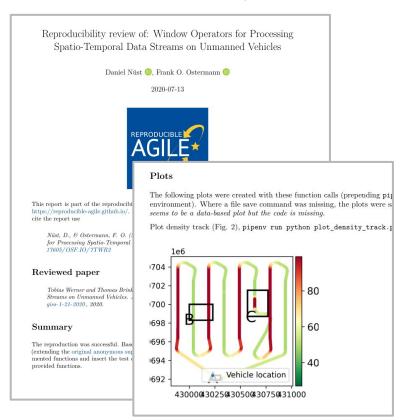


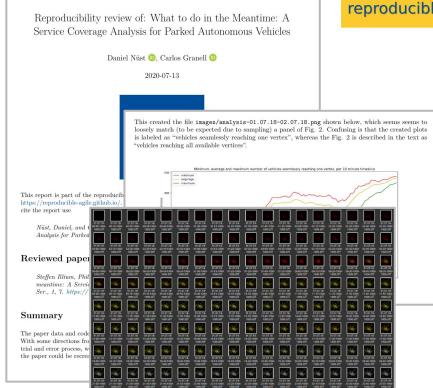




Reproducibility review reports







The guidelines for reproducibility reviewers (WIP)

Ideal vs. realistic

Role

Skills

Do's & dont's

https://docs.google.com/document/d/1Kc-ToUVcrdsq6aB8Qy2J_rlluFwDniv6GHGtZuPvlEo/edit#

REPRODUCIBILITY REVIEWER GUIDELINES

Reproducibility reviewers conduct a complimentary review of the workflow that is published with a manuscript. Ideally, reproducibility reviewers only read the abstract and the Data and Software Availability section (DASA) of an article. They may read other sections referenced in the latter. Then they follow the authors' instructions for executing the workflow, ideally starting from the DASA or a README file in the referenced reproduction material. When reproducibility reviewers get stuck, they take advantage of the option to communicate with the authors early and often. Reproducibility reviewers should be aware of the different levels for making research reproducible in the author guidelines (see above) to be able to recommend improvements to the author and at the same time have the skillset and tools to conduct their review efficiently. Reproducibility reviewers are not responsible for making a workflow transparent or executable. Reproducibility reviewers write a short reproducibility report documenting their communication and the results of their reproduction attempt. The report is published if the reproduction was, at least in part, successful.

Do	Don't	
Ouick pre-repro-review checks and ask authors to fix before continuing; even if not all of these are technically required, authors who are willing to work reproducibly can show their engagement right from the start: 1. Do the links to data sets and materials resolve? 2. Is there a README with clear step-by-step instructions? 3. Is there a clear mention of to be expected execution times? 4. Is there a LICENSE file to ensure openness?	Dig across badly or un-documented collections of files and functions to identify which part of the code/data creates which figure/table/output; find or build the "start button" yourself.	
Encourage authors by pointing out promising intermediate results or concrete benefits of reproducibility.	Run workflows requiring considerable computational resources (unless interesting for you) but ask for data subsets for demonstration purposes.	
Accept sample datasets to run a workflow and compare the outcome with the expected sample results; check the sources of the full datasets, if available.	Accept private sharing of data or code, unless strictly required for protection of sensitive data. All changes by the author should update to the public reproduction material.	
Clearly document the extent of the reproduction in your reproduction report and suggest potential improvements; if you provide intermediate feedback, to include a history of your interactions in the report so that the ideas you contributed are preserved when the submission's material is improved.	Attempt to install software without any instructions, install binary software of unknown origin, or try to fix installation problems you encounter on your machine; try to install without (a) asking for help from a fellow reproducibility reviewer who is familiar with the software, or (b) asking the author to help, providing a minimal reproducible example of your problem.	
Get in touch with fellow reproducibility reviewers if specific expertise (tool, programming language,) is needed.	Point out or even fix problems that are not specific to the submission, e.g., general problems in a software tool.	
Set an example when communicating about computational problems, e.g., by clearly defining your system (OS version, language version, etc.)	Create accounts on any service or platform to access code, data, or other resources.	
Ask specific questions or point out concrete problems that may lead authors to improve their material,	Fix anything (unless you really enjoy doing so), e.g., • compiler problems,	

eventually have 100% of is positive encouragement, is a clear definition of your iew is an extra merit for an The reproducibility reviewer nor not to "go the extra few ected in the fact that only be both the reproducibility

oles and the CODECHECK onducting a reproducibility tall of them, should still be e. Please consult with your

and part of a process for idelines do not mention a tare just as unique as the my problem" if you cannot not don't spend more than r documentation should be honing are all the different da and very for Python, Docker.



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

- Build a team of enthusiasts (workshop, social events)
- 2. Assess the current state and raise awareness (workshop, paper)
- 3. Institutional support (A AGILE Council A + committee chairs)
- 4. Positive encouragement (no reproduction != bad science)
- 5. Keep at it!



Next steps





Revise guidelines 🎢 🔲 🔲 📁

Grow reproducibility reviewer team

ECRs, credit @ ORCID, skills

Continue research 🍒

Ostermann, F., Nüst, D., Granell, C., Hofer, B., & Konkol, M. (2020). Reproducible Research and GIScience: an evaluation using GIScience conference papers.

EarthArXiv. https://doi.org/10.31223/x5zk5v

Continue community engagement towards opening scholarship

Scope

Requirements

Acceptance condition?

Open review if tenured

Format-free submission

CRediT

Phase out when standard practice...

The guidelines for data



DATA IN RESEARCH PAPERS

	Minimum	Ideal
What?	Publish all input data + data description / documentation	Publish all data and adhere to standardised, discipline-specific metadata ² to describe your data
Where?	Use a data repository providing a DOI ³	Use a discipline-specific repository ⁴ with a DOI
How?	Use open data formats + specify a license	Make your data FAIR (Findable, Accessible, Interoperable and Reusable) and as open as possible

"What if..." and Examples (not shown)

The guidelines for workflows



Examples (not shown)

COMPUTATIONAL WORKFLOWS IN RESEARCH PAPERS

	Minimum	Intermediate	Ideal
What? Computational environment	Describe the environment and computational infrastructure, e.g. computer specs, operating system + software versions	Provide live documents (structured configuration files with dependency information, e.g. a Binder ⁹)	Provide the actual environment, e.g. a container created by a Dockerfile ¹⁰ or a Virtual Machine (VM, e.g. OSGeo-Live)
Computation steps	Document the detailed steps in a text file and/or flowchart (every action/click)	Provide scripts / models and a README file that explains their use	Provide a software package with structured metadata ¹¹ , tests/Cl ¹² , and an automated workflow ¹³ + If applicable: Add link to running instance of software
Where?	Repository providing a DOI, such as Zenodo, OSF, b2share, or FigShare		Minimum + versioned code repository, such as GitHub or GitLab
How? Tools used	Use generally available proprietary tools (avoid tools that are not available to reviewers and other researchers)		Use (and create) open source tools; cite core modules/tools/language used, including your own
Development practices	Use clear licenses ¹⁴ that fit your environment	Follow "Good enough practices" for scientific computing software ¹⁵	Use development guidelines for your environment / language of choice (e.g. for R ¹⁶) 39

The guidelines for reproducibility reviewers (WIP)

Examples for "Do's and Don'ts":

- Do shift burden to author
- Do encourage and s
- Do not accept private data sharing
- Document your work in report (impact)
- Be kind (career stage, knowledge, privileges)
- No rummaging

https://docs.google.com/document/d/1Kc-ToUVcrdsq6aB8Qy2J_rlluFwDniv6GHGtZuPvlEo/edit#

Do	Don't
Quick pre-repro-review checks and ask authors to fix before continuing; even if not all of these are technically required, authors who are willing to work reproducibly can show their engagement right from the start: 1. Do the links to data sets and materials resolve?	Dig across badly or un-documented collections of files and functions to identify which part of the code/data creates which figure/table/output; find or build the "start button" yourself.
2. Is there a README with clear step-by-step instructions? 3. Is there a clear mention of to be expected execution times? 4. Is there a LICENSE file to ensure openness?	
Encourage authors by pointing out promising intermediate results or concrete benefits of reproducibility.	Run workflows requiring considerable computational resources (unless interesting for you) but ask for data subsets for demonstration purposes.
Accept sample datasets to run a workflow and compare the outcome with the expected sample results; check the sources of the full datasets, if available.	Accept private sharing of data or code, unless strictly required for protection of sensitive data. All changes by the author should update to the public reproduction material.
Clearly document the extent of the reproduction in your reproduction report and suggest potential improvements; if you provide intermediate feedback, to include a history of your interactions in the report so that the ideas you contributed are preserved when the submission's material is improved.	Attempt to install software without any instructions, install binary software of unknown origin, or try to fix installation problems you encounter on your machine; try to install without (a) asking for help from a fellow reproducibility reviewer who is familiar with the software, or (b) asking the author to help, providing a minimal reproducible example of your problem.
Get in touch with fellow reproducibility reviewers if specific expertise (tool, programming language,) is needed.	Point out or even fix problems that are not specific to the submission, e.g., general problems in a software tool.
Set an example when communicating about computational problems, e.g., by clearly defining your system (OS version, language version, etc.)	Create accounts on any service or platform to access code, data, or other resources.
Ask specific questions or point out concrete problems that may lead authors to improve their material, including referencing these guidelines or concrete tools/methods that you already (!) know about, especially if you suspect that the author might now be familiar with them (e.g., version pinning/dependency management, absolute paths).	Fix anything (unless you really enjoy doing so), e.g.,
Make sure that you are aware of any templates or specific resources provided for reproducibility reviewers from the reproducibility committee chair before starting your review.	
Consider the author's background, career stage, and position to be aware of (a lack of) privileges or institutional power to decide how much support you provide and how you communicate; your	Be a <u>bro</u> .
reproducibility review can be a contribution to improve equity and inclusion in academia.	40