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Infrastructures and Practices for Reproducible Research in Geography, Geosciences, and GIScience

PhD Thesis Defense | 2022-02-14 | **Daniel Nüst**, Dipl-Geoinf.

This document: **http://go.wwu.de/wklef**

Full reference: 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

ifgi
Institute for Geoinformatics
University of Münster

living.knowledge

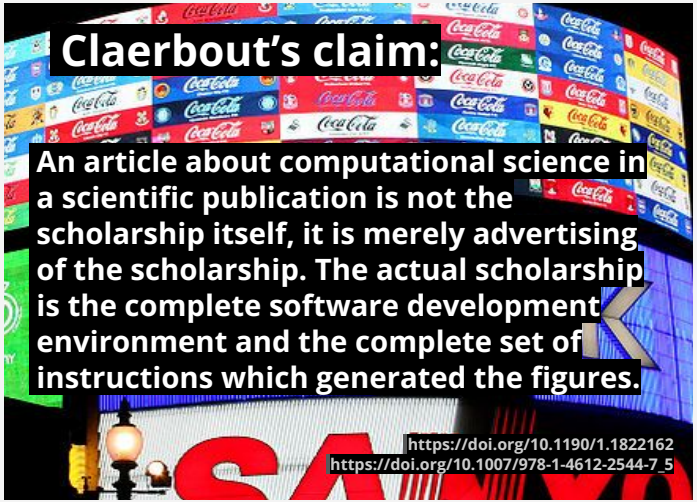
Scope & motivation

A problematic situation

https://giphy.com/gifs/usnationalarchives-nasa-scientist-scientists-1F1JGyGZhiSAA8Vuhn

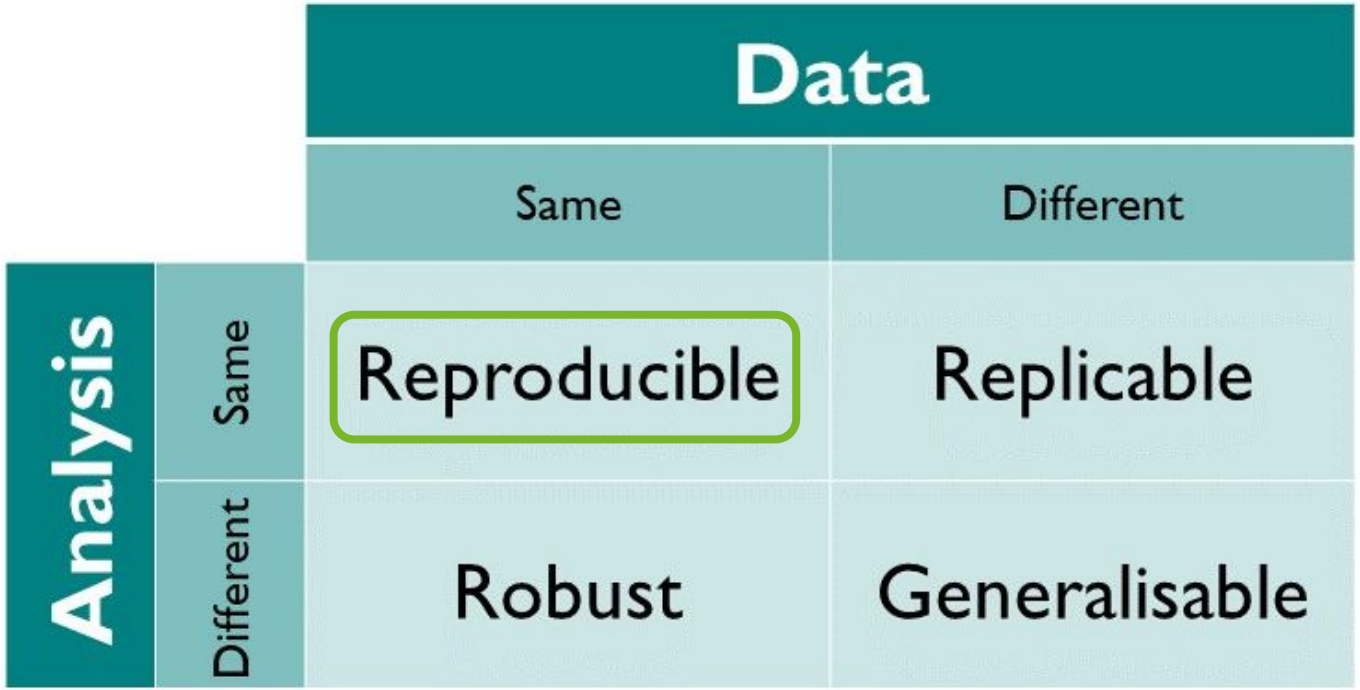
https://giphy.com/gifs/with-computers-fascination-PxSFAnuubLkSA

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



CC-BY 3.0, Sebastian Bertalan, Wikimedia Commons

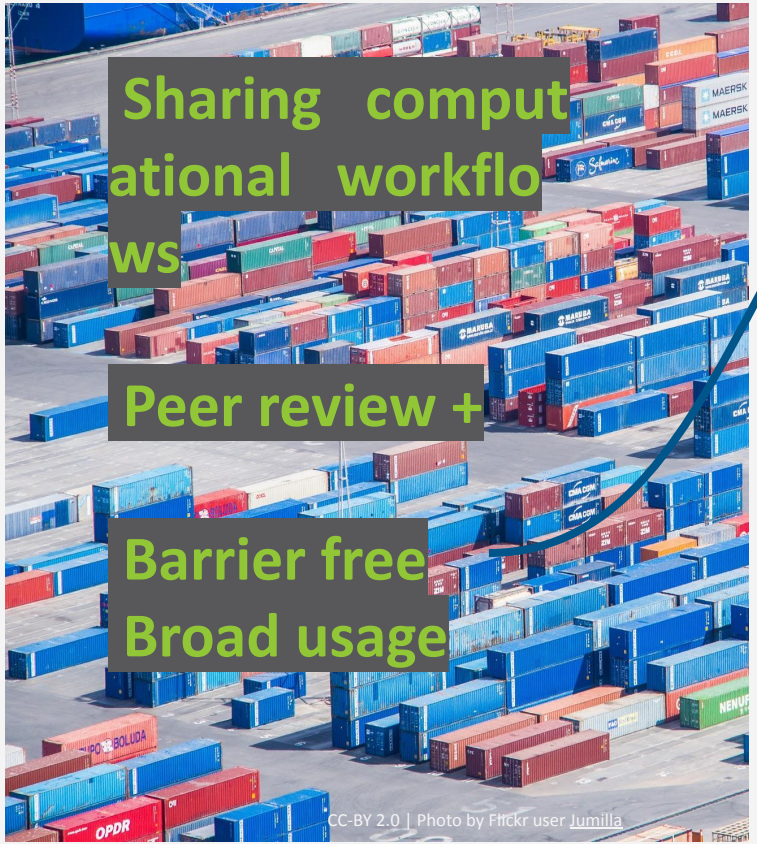
Definition



Closed and irreproducible research




Approach



Technological

Individual

Structural

Cultural

Policy

The culture change pyramid (Nosek et al.)

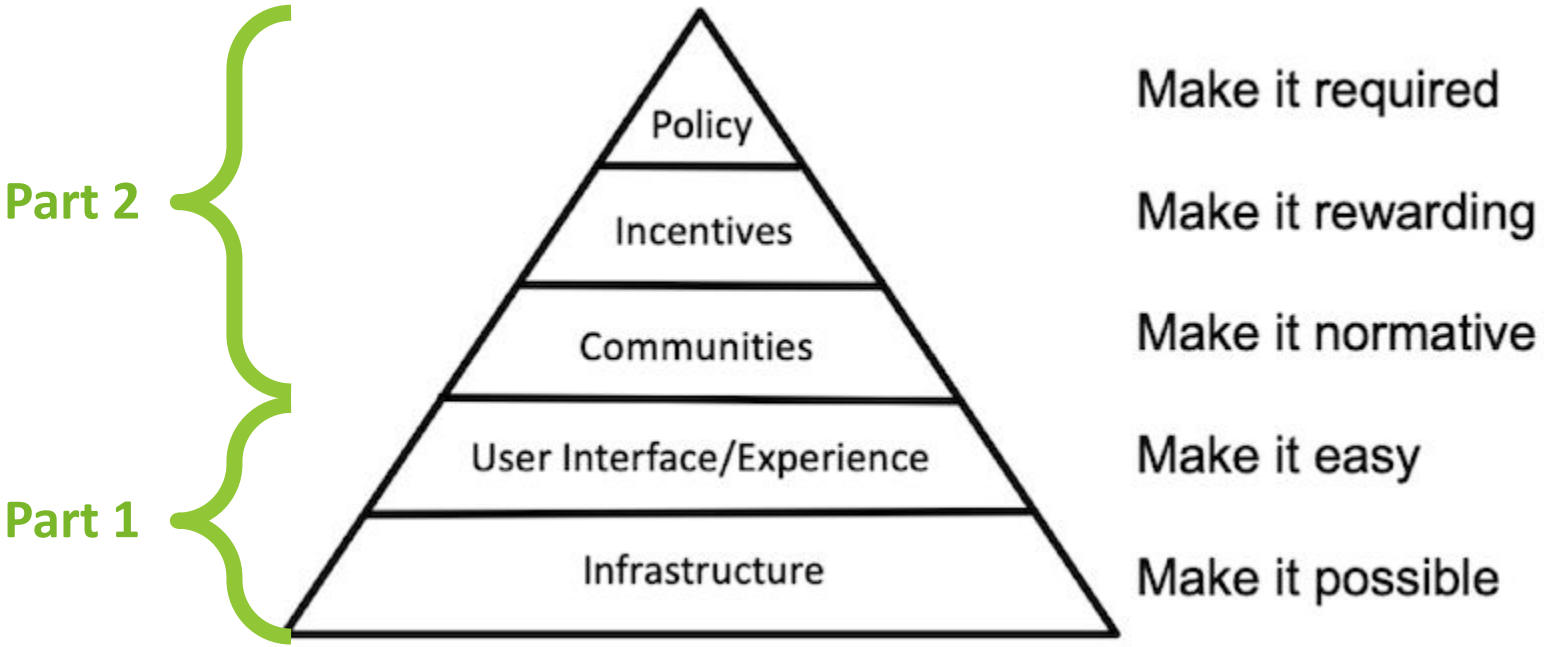
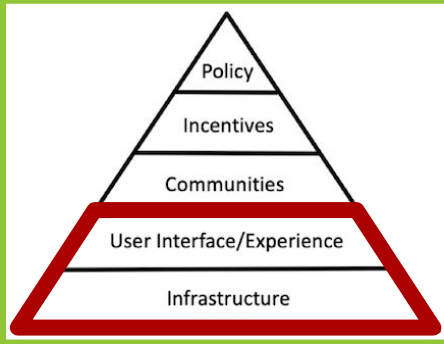
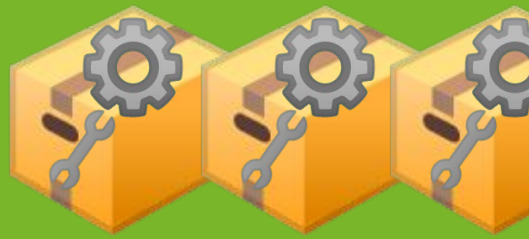


Image by Brian Nosek; licensed under CC BY-ND 4.0, reproduced from the blog post **Strategy for Culture Change**.

Part 1: Infrastructure & user experience

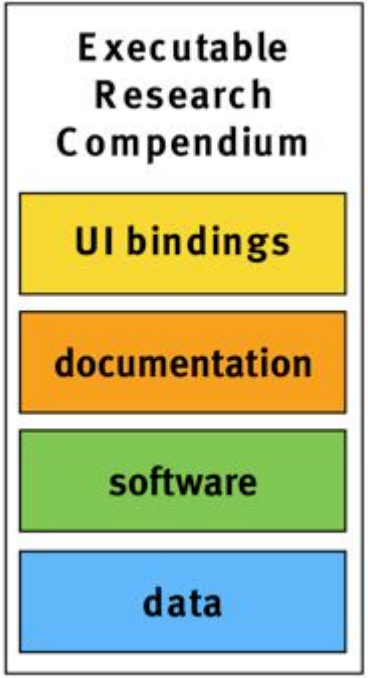




ERC

- links/connections
- UI widgets w/o coding
- entrypoints

- computational environment
- executable
- Open Source



- article/manuscript as notebook
- metadata (licenses, …)
- tech. instructions

- raw (ideal) or preprocessed
- files
- Open Data

Nüst, D., Konkol, M., Pebesma, E., Kray, C., Schutzeichel, M., Przibytzin, H., & Lorenz, J. (2017). **Opening the Publication Process with Executable Research Compendia**. D-Lib Magazine, 23(1/2). https://doi.org/10.1045/january2017-nuest

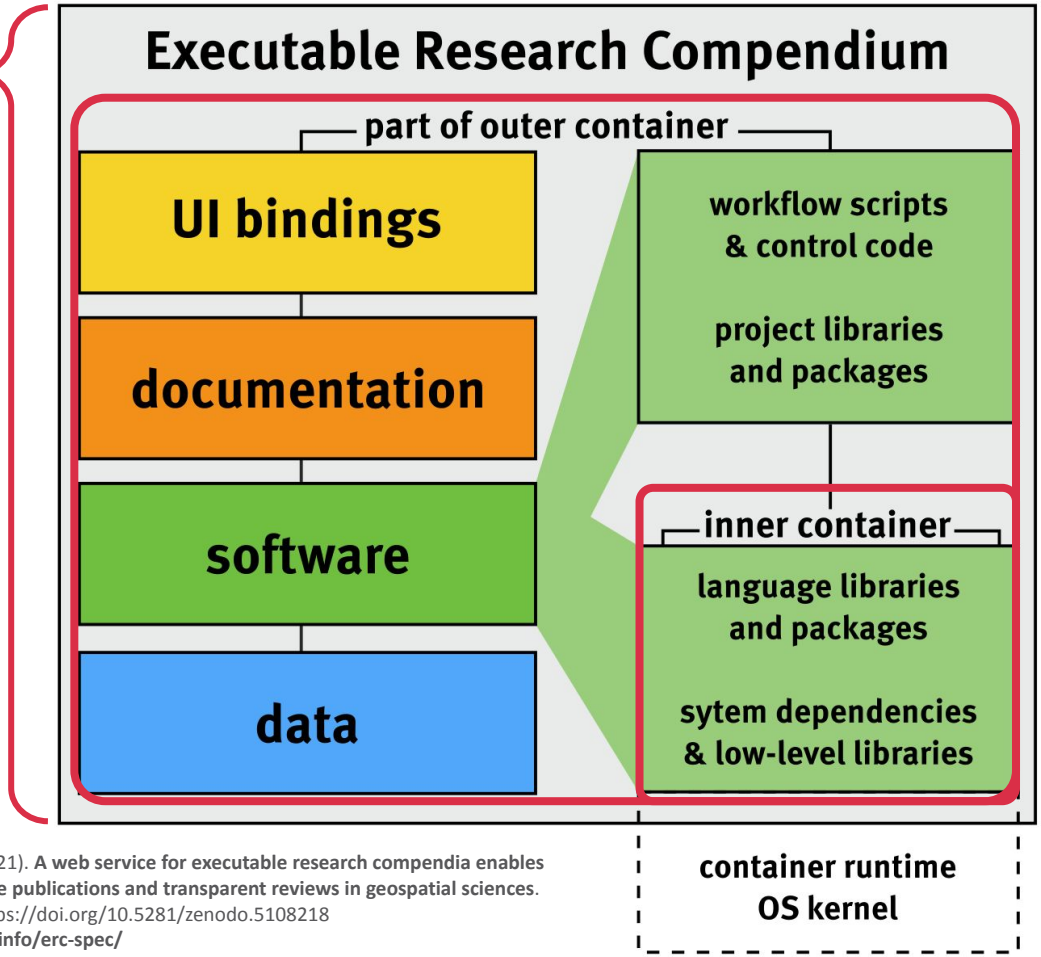
Contents

```
main.Rmd
display.html
Dockerfile
image.tar
erc.yml
```

erc.yml

```yaml
id: b9b0099e-9f8d-4a33-8acf-cb0c062
spec_version: 1
main: main.Rmd
display: display.html
licenses:
  code: MIT
  data: "data_licenses_info.pdf"
  text: CC-BY-4.0
  metadata: CC0-1.0
```

BagIt
IETF
RFC 8493



Nüst, D. (2021). **A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences**. Zenodo. https://doi.org/10.5281/zenodo.5108218
https://o2r.info/erc-spec/

containerit

Nüst, D., & Hinz, M. (2019). **containerit: Generating Dockerfiles for reproducible research with R**. Journal of Open Source Software, 4(40), 1603. https://doi.org/10.21105/joss.01603

Capturing an R session (script, Rmd) in a Dockerfile

User only uses **R functions**
System **dependency** resolving

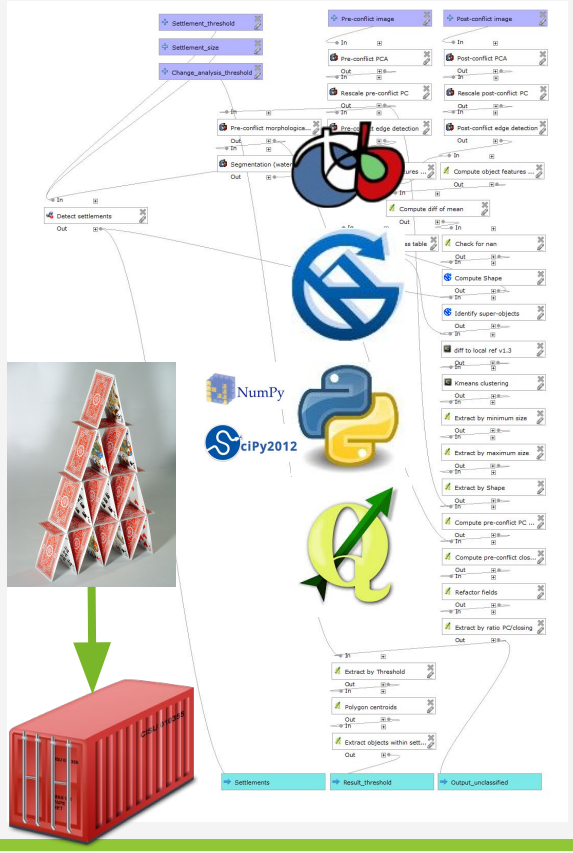
Always **executes** script (`callr`), hard to fool (unlike static progr. anal.)

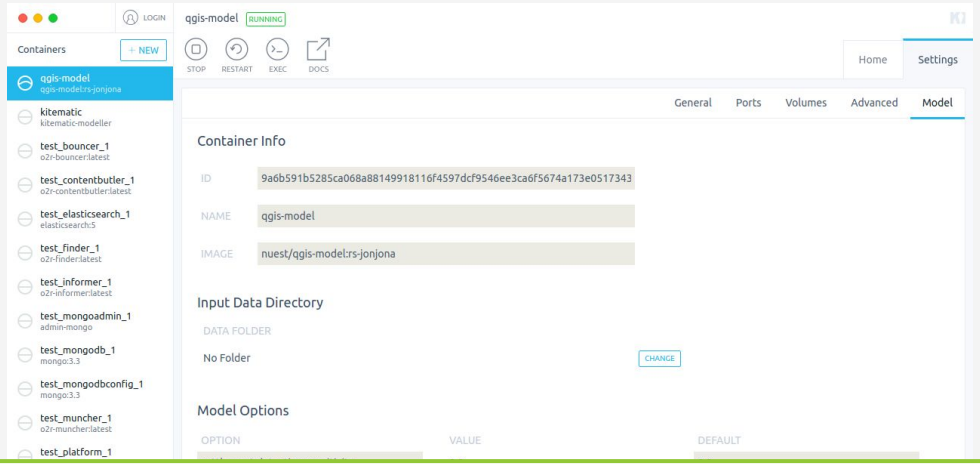
github.com/o2r-project/containerit

```
> suppressPackageStartupMessages(library("containerit"))
> my_dockerfile <- containerit::dockerfile(from = utils::sessionInfo())
> print(my_dockerfile)
FROM rocker/r-ver:3.5.2
LABEL maintainer="daniel"
RUN export DEBIAN_FRONTEND=noninteractive; apt-get -y update \
  && apt-get install -y git-core \
    libcurl4-openssl-dev \
    libssl-dev \
    pandoc \
    pandoc-citeproc
RUN ["install2.r", "curl", "digest", "evaluate", "formatR", \
  "futile.logger", "futile.options", "htmltools", "jsonlite", \
  "knitr", "lambda.r", "magrittr", "Rcpp", "rjson", \
  "rmarkdown", "rsconnect", "semver", "stevedore", "stringi", \
  "stringr", "xfun", "yaml"]
WORKDIR /payload/
CMD ["R"]
```

Reproducible GEOBIA workflow

Knoth, C., & Nüst, D. (2017). **Reproducibility and Practical Adoption of GEOBIA with Open-Source Software in Docker Containers**. Remote Sensing, 9(3), 290. https://doi.org/10.3390/rs9030290





Model Options

OPTION	VALUE	DEFAULT
settlement detection sensitivity	0.3	0.3
minimum settlement size	0	0
change sensitivity	0.3	0.3

minimum change in edge intensity for objects to be flagged as changed

SAVE AND RUN

Nüst, D., Sochat, V., Marwick, B., Eglen, S. J., Head, T., Hirst, T., & Evans, B. D. (2020).
Ten simple rules for writing Dockerfiles for reproducible data science.
PLOS Computational Biology, 16(11), 1–24. https://doi.org/10.1371/journal.pcbi.1008316

Ten “simple” rules for bespoke hand-crafted computing environments for smaller-scale data science

1. - 2. Use only if no tool works and don’t reinvent the wheel

3. - 4. Dockerfiles are for humans and machines (communication!)

5. - 6. Pinning and versioning

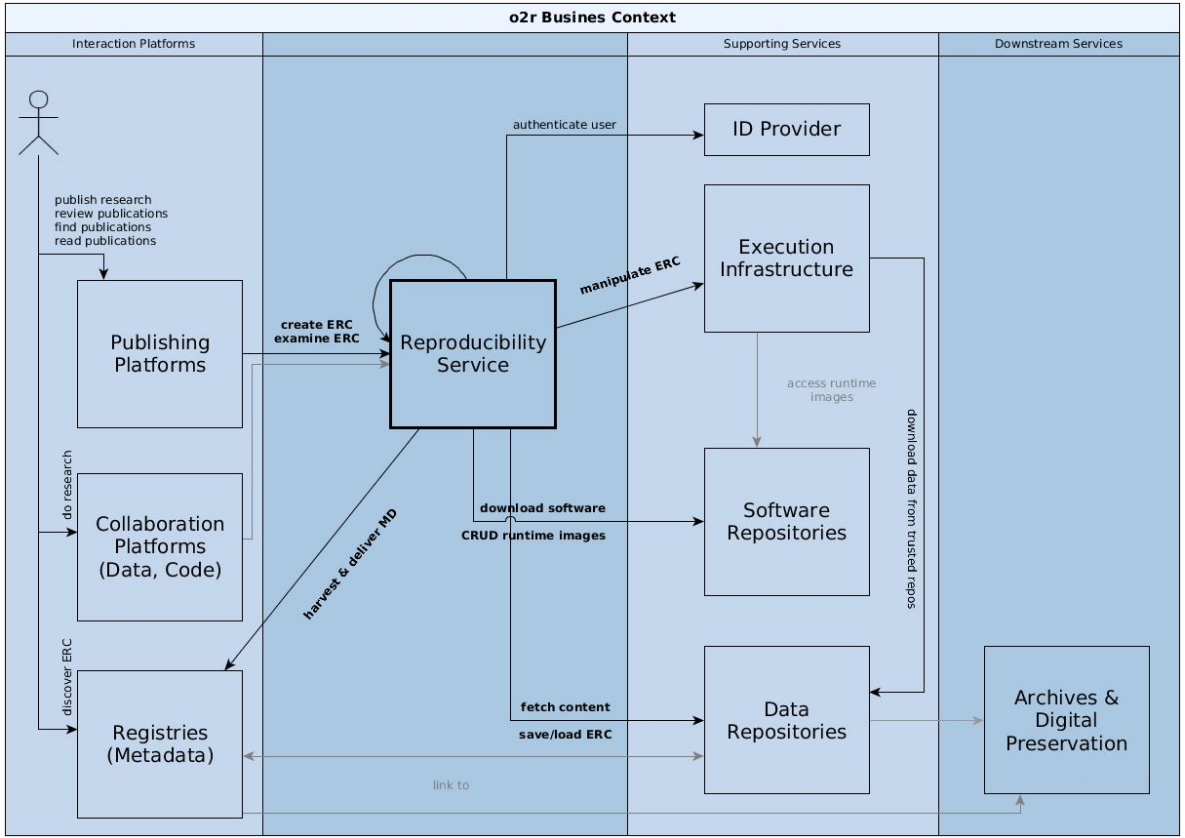
7. - 10. Habits & tricks for usability and stability

o2r web service for reproducibility

Nüst, D. (2021). **A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences**. Zenodo. https://doi.org/10.5281/zenodo.5108218

ERC Reproducibility Service (ERS):

- Context
- Architecture
- Specification
- Web API



ERS Architecture

https://o2r.info/architecture/#527-whitebox-reproducibility-service

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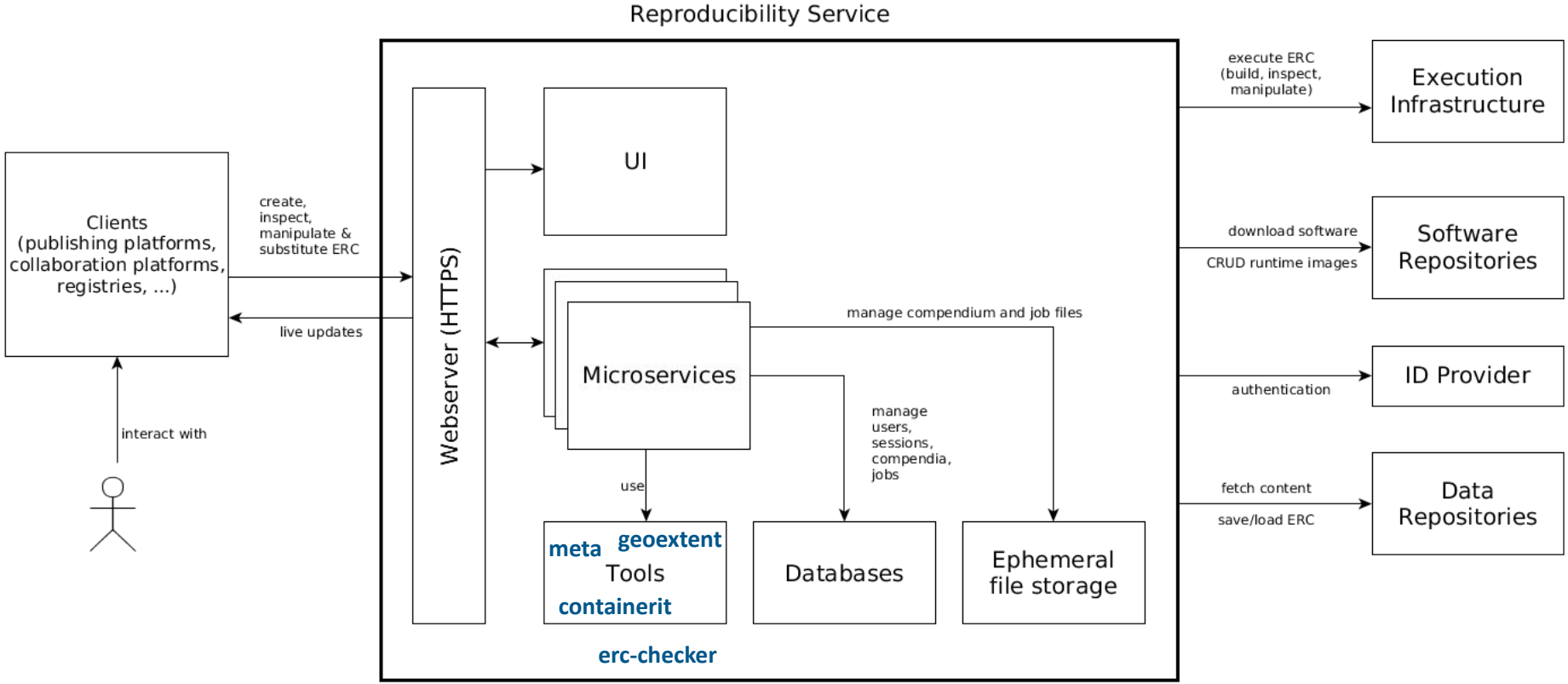


ERS reference implementation

Nüst, D. (2021). **A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences**. Zenodo. https://doi.org/10.5281/zenodo.5108218

Original results

Capacity of container ships in seaborne trade from 1980 to 2016 (in million dwt)*

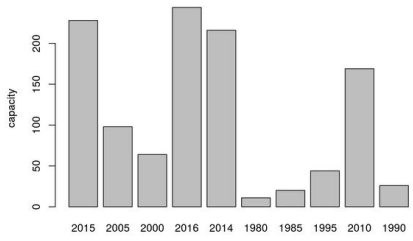
Daniel Nüst

o2r team

2017

Abstract

Capacity of container ships in seaborne trade of the world container ship fleet.



This statistic portrays the capacity of the world

Reproduced results

Capacity of container ships in seaborne trade from 1980 to 2016 (in million dwt)*

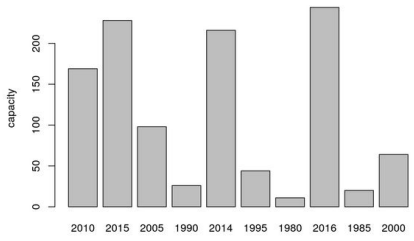
Daniel Nüst

o2r team

2017

Abstract

Capacity of container ships in seaborne trade of the world container ship fleet.



This statistic portrays the capacity of the world

Differences between original and reproduced results

Capacity of container ships in seaborne trade from 1980 to 2016 (in million dwt)*

Daniel Nüst

o2r team

2017

Abstract

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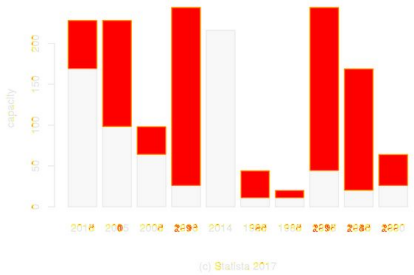
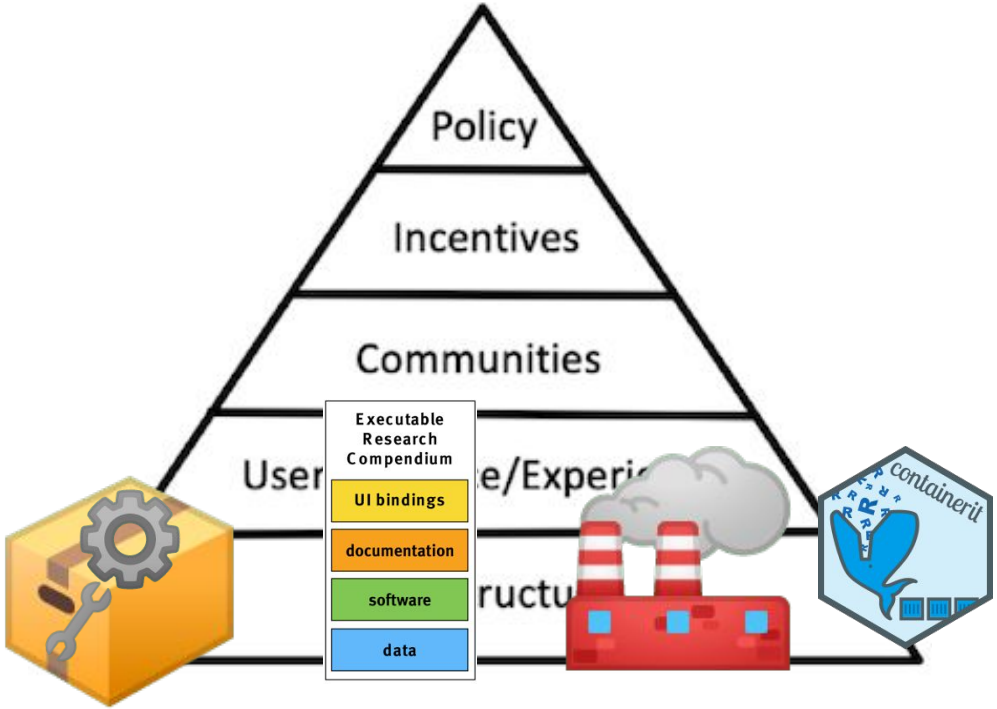


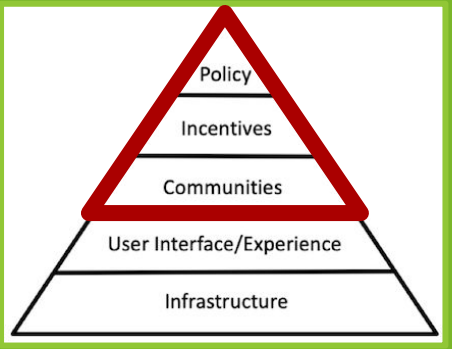
This statistic portrays the capacity of the world

https://o2r.uni-muenster.de/erc/q7Eje/job/9YCzy#result

Nüst, D. (2021). **A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences**. Zenodo. https://doi.org/10.5281/zenodo.5108218


Policy
Incentives
Communities
Executable Research Compendium
UI bindings
documentation
software
data
containerit

Part 2: Communities, incentives & policy




NEW

State of reproducibility in GIScience?

AGILE Association of Geographic Information Laboratories in Europe

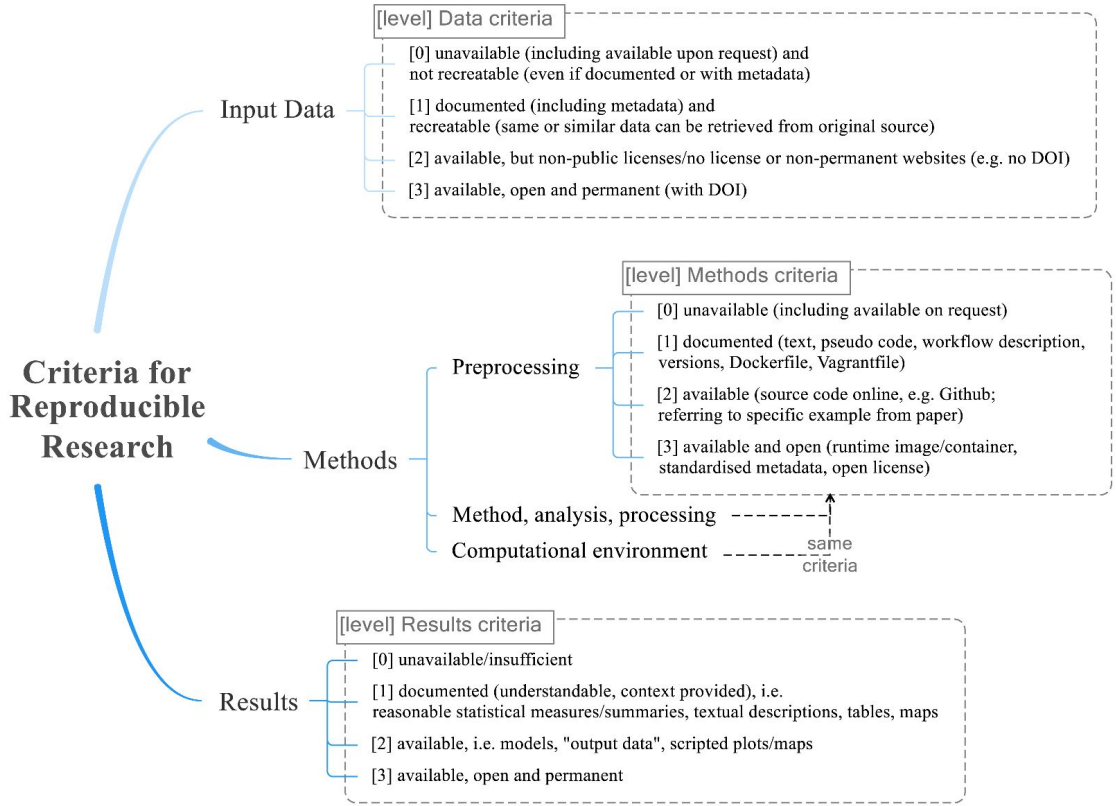
32 “best papers” nominees (20/12); 2010-17

Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018). **Reproducible research and GIScience: An evaluation using AGILE conference papers**. PeerJ, 6, e5072. https://doi.org/10.7717/peerj.5072

GIScience

75 papers; 2012-2018

Ostermann, F. O., 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 (dissertation version)
> 11th International Conference on Geographic Information Science (GIScience 2021) - Part II. Schloss Dagstuhl - Leibniz-Zentrum Für Informatik. https://doi.org/10.4230/LIPICS.GISCIENCE.2021.II.2 (accepted)



https://doi.org/10.7717/peerj.5072/fig-2

State of reproducibility?

0 papers were readily reproducible.
Majority not even at time of publication.
🥴

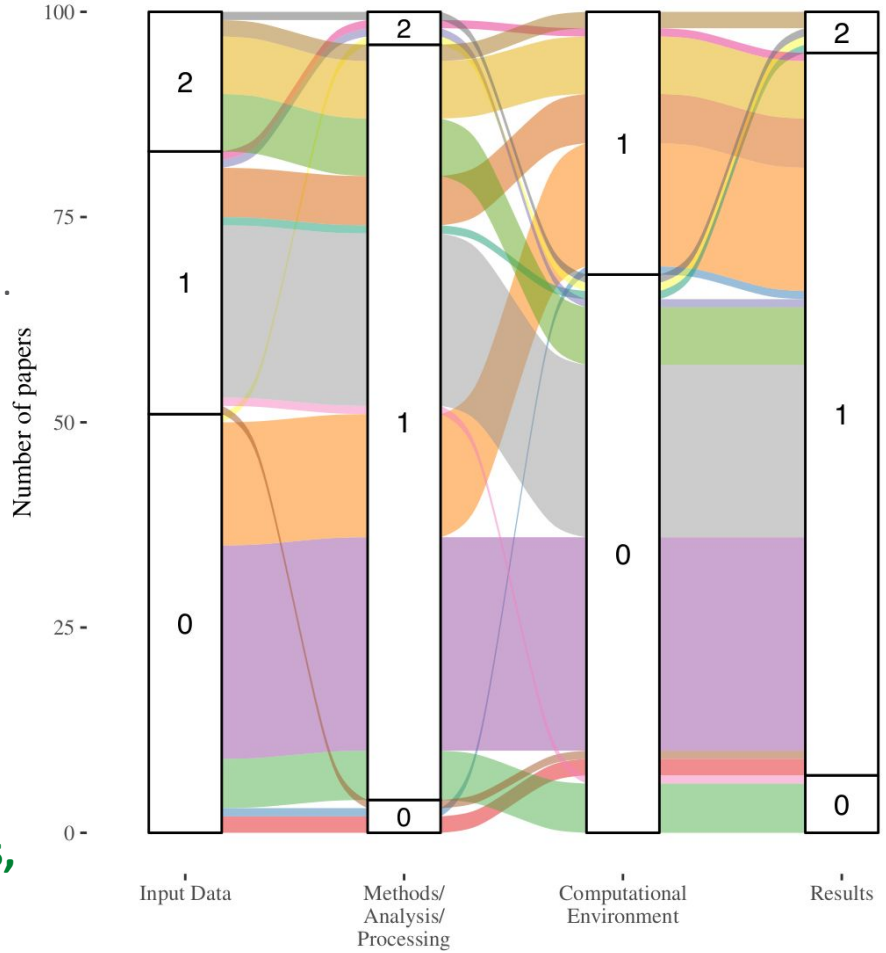
Few “Level 2”, **no** “Level 3”.

Majority of papers **describe** methods/results (Level “1”).

Comp. env. largely **neglected**.

Variations partly reaching Level “2” > **no common practice**.

No recognition, no requirements, no details, no reproductions.



Change peer review

AGILE Reproducible Paper Guidelines

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

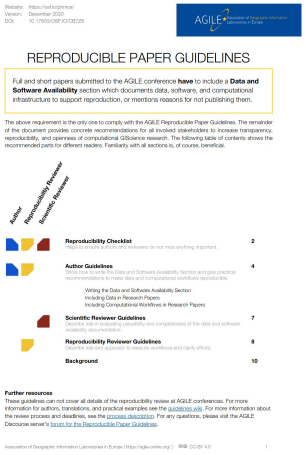
Promotion, not exclusion

Data and software availability section

Author & reviewer guidelines; Reproducibility checklist

AGILE Reproducibility Review 2020, 2021

14 reproductions, guidelines mandatory since 2021


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

Reproducibility Checklist 2

Author Guidelines 4

Writing the Data and Software Availability Section
Including Data in Research Papers
Including Computational Workflows in Research Papers

Scientific Reviewer Guidelines 7

Reproducibility Reviewer Guidelines 8

Background 10

Further resources

Nüst, D., & Eglen, S. J. (2021). **CODECHECK: An Open Science initiative for the independent execution of computations underlying research articles during peer review to improve reproducibility**
[version 1; peer review: 1 approved, 1 approved with reservations]. F1000Research, 10, 253.
https://doi.org/10.12688/f1000research.51738.1 (dissertation version)
[version 2; peer review: 2 approved]
https://doi.org/10.12688/f1000research.51738.2 (published)

Independent execution of computations underlying research articles.

One re-execution by codechecker during peer review

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.**

30+ Certificates

https://codecheck.org.uk/register/

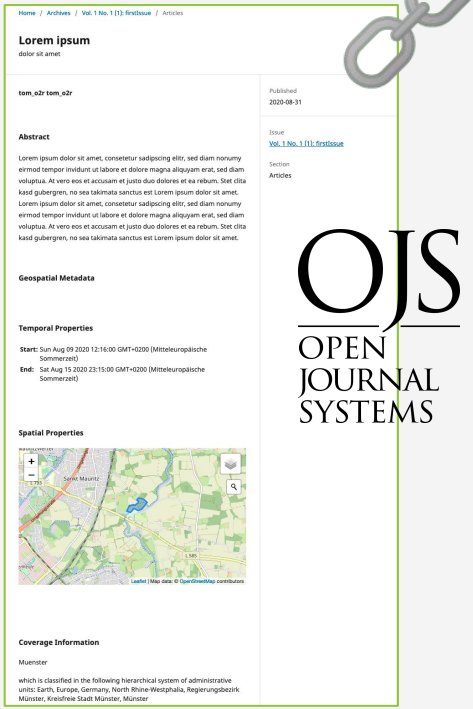
What are challenges for practical reproducibility in geography and geosciences?

Nüst, D., & Pebesma, E. (2021). **Practical reproducibility in geography and geosciences**. Annals of the American Association of Geographers, 111(5), 1300–1310. https://doi.org/10.1080/24694452.2020.1806028

SDI

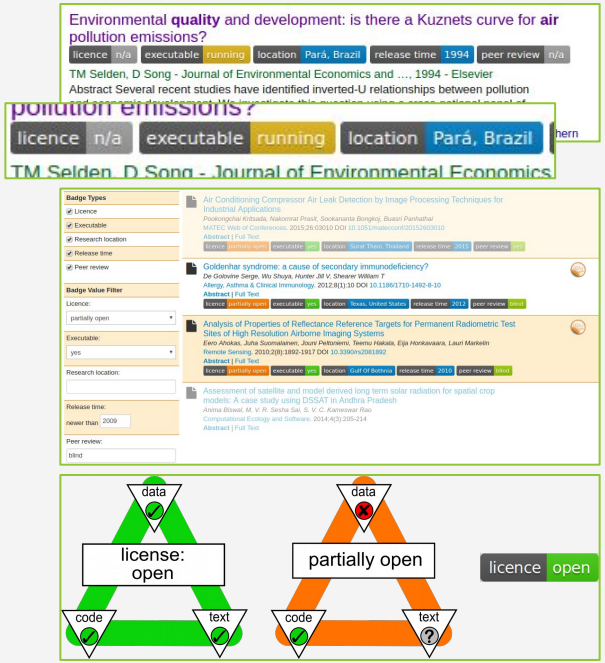
Downstream applications

Geospatial Metadata



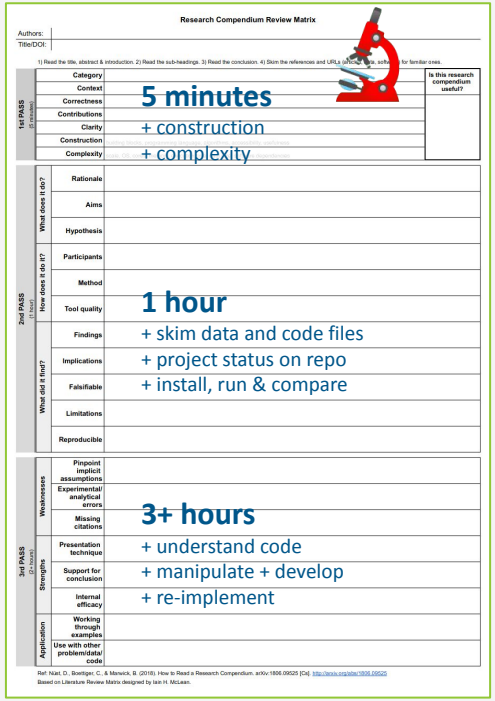
Niers, T., & Nüst, D. (2020). **Geospatial Metadata for Discovery in Scholarly Publishing**. Septentrio Conference Series, 4. https://doi.org/10.7557/5.5590

Badges

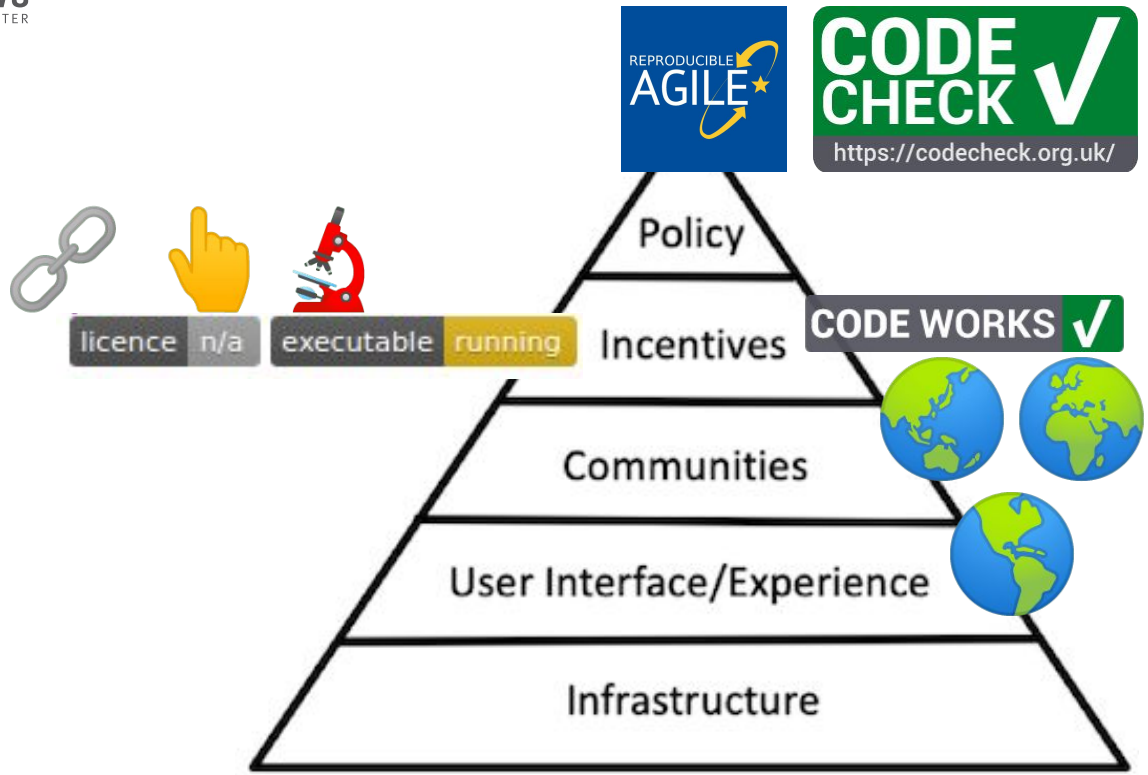


Nüst, D., Lohoff, L., Einfeldt, L., Gavish, N., Götza, M., Jaswal, S. T., Khalid, S., Meierkort, L., Mohr, M., Rendel, C., & Eek, A. van. (2019). **Guerrilla Badges for Reproducible Geospatial Data Science**. AGILE Short Papers. https://doi.org/10.31223/osf.io/xtsqh

Interaction



Nüst, D., Boettiger, C., & Marwick, B. (2018). **How to Read a Research Compendium**. arXiv:1806.09525 [Cs]. http://arxiv.org/abs/1806.09525


REPRODUCIBLE AGILE
CODE CHECK
https://codecheck.org.uk/
licence n/a
executable running
Policy
Incentives
CODE WORKS
Communities
User Interface/Experience
Infrastructure

Key contributions

WWU
MÜNSTER


infrastructure


captured &
crafted containers


?


state & path


introduce RR

Citation & Publications

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

Infrastructure & use experience

Knoth, C., & Nüst, D. (2017). Reproducibility and Practical Adoption of GEOBIA with Open-Source Software in Docker Containers. Remote Sensing, 9(3), 290. https://doi.org/10.3390/rs9030290

Konkol, M., Nüst, D., & Goulier, L. (2020). Publishing computational research - a review of infrastructures for reproducible and transparent scholarly communication. Research Integrity and Peer Review, 5(1), 10. https://doi.org/10.1186/s41073-020-00095-y

Nüst, D. (2021). A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences. Zenodo. https://doi.org/10.5281/zenodo.5108218

Nüst, D., Eddelbuettel, D., Bennett, D., Cannoodt, R., Clark, D., Daróczi, G., Edmondson, M., Fay, C., Hughes, E., Kjeldgaard, L., Lopp, S., Marwick, B., Nolis, H., Nolis, J., Ooi, H., Ram, K., Ross, N., Shepherd, L., Sólymos, P., Swetnam, T. L., Turaga, N., Petegem, C. V., Williams, J., Willis, C., & Xiao, N. (2020). The Rockerverse: Packages and Applications for Containerisation with R. The R Journal, 12(1). https://doi.org/10.32614/RJ-2020-007

Nüst, D., & Hinz, M. (2019). containerit: Generating Dockerfiles for reproducible research with R. Journal of Open Source Software, 4(40), 1603. https://doi.org/10.21105/joss.01603

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Nüst, D., & Pebesma, E. (2021). Practical reproducibility in geography and geosciences. Annals of the American Association of Geographers, 111(5), 1300–1310. https://doi.org/10.1080/24694452.2020.1806028

Nüst, D., Sochat, V., Marwick, B., Eglen, S. J., Head, T., Hirst, T., & Evans, B. D. (2020). Ten simple rules for writing Dockerfiles for reproducible data science. PLOS Computational Biology, 16(11), 1–24. https://doi.org/10.1371/journal.pcbi.1008316

Communities, incentives & policy

Niers, T., & Nüst, D. (2020). Geospatial Metadata for Discovery in Scholarly Publishing. Septentrio Conference Series, 4. https://doi.org/10.7557/5.5590

Nüst, D., Boettiger, C., & Marwick, B. (2018). How to Read a Research Compendium. arXiv:1806.09525 [Cs]. http://arxiv.org/abs/1806.09525

Nüst, D., & Eglen, S. J. (2021). CODECHECK: An Open Science initiative for the independent execution of computations underlying research articles during peer review to improve reproducibility. F1000Research, 10, 253. https://doi.org/10.12688/f1000research.51738.1

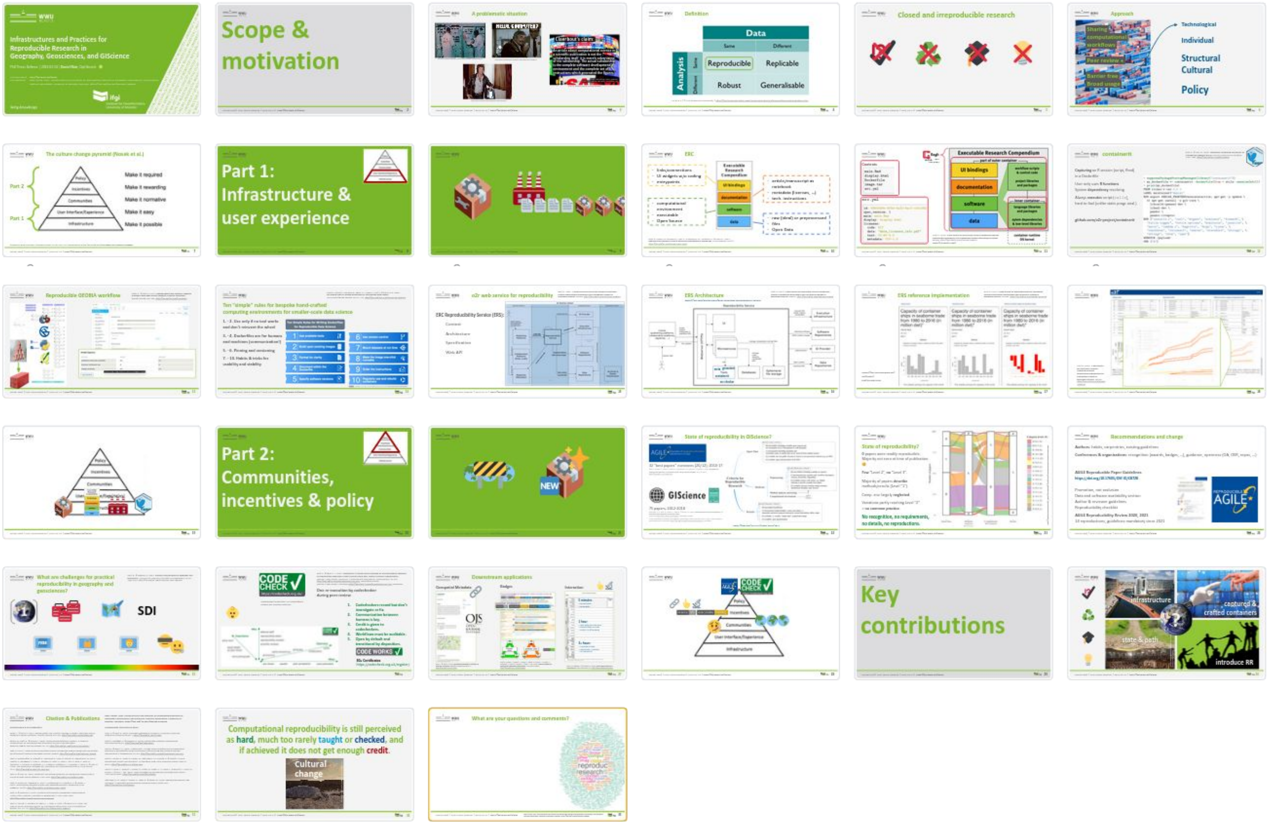
Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018). Reproducible research and GIScience: An evaluation using AGILE conference papers. PeerJ, 6, e5072. https://doi.org/10.7717/peerj.5072

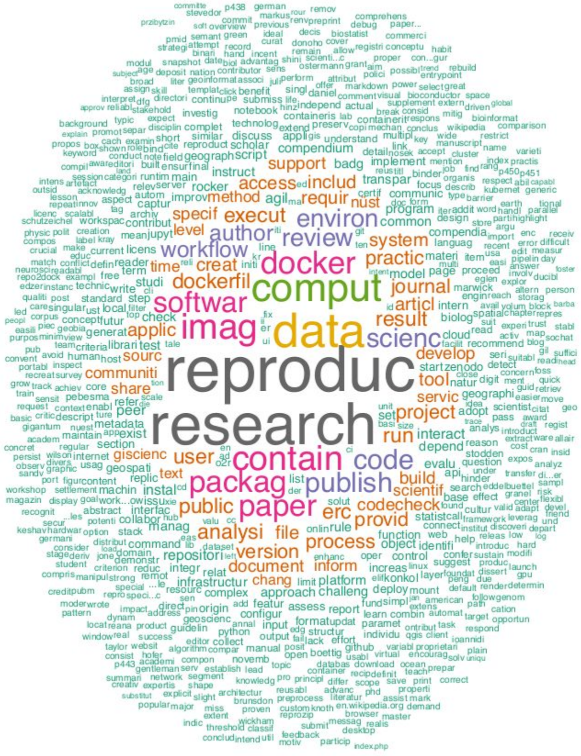
Nüst, D., Lohoff, L., Einfeldt, L., Gavish, N., Götza, M., Jaswal, S. T., Khalid, S., Meierkort, L., Mohr, M., Rendel, C., & Eek, A. van. (2019). Guerrilla Badges for Reproducible Geospatial Data Science. AGILE Short Papers. https://doi.org/10.31223/osf.io/xtsqh

Ostermann, F. O., 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

Computational reproducibility is still perceived as **hard**, much too rarely **taught** or **checked**, and if achieved it does not get enough **credit**.

What are your questions and comments?





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Encore

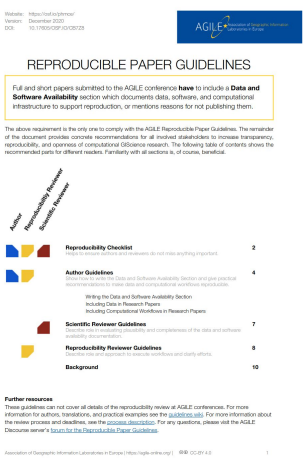
1. GI solves geospatial problems with IT, the problem: **computational reproducibility**
2. Adaptation and transfer of mainstream IT to domain: **containerisation**
   (little needed, future work re. maps?!)
3. ERC infrastructure & metascience are **transferable**, the direct addressing (examples, community membership) is **not** - without domain focus just a **theoretical exercise**
4. Geoinformatitians **translate and interpret** between geo-scientists and developers

Recommendations and change

Authors: habits, carpentries, existing guidelines

Conferences & organisations: recognition (awards, badges, …), guidance, openness (OA, OER, repos, …)

AGILE Reproducible Paper Guidelines
https://doi.org/10.17605/OSF.IO/CB7Z8


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 this 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.

AGILE Reproducibility Review 2020, 2021
14 reproductions, guidelines mandatory since 2021

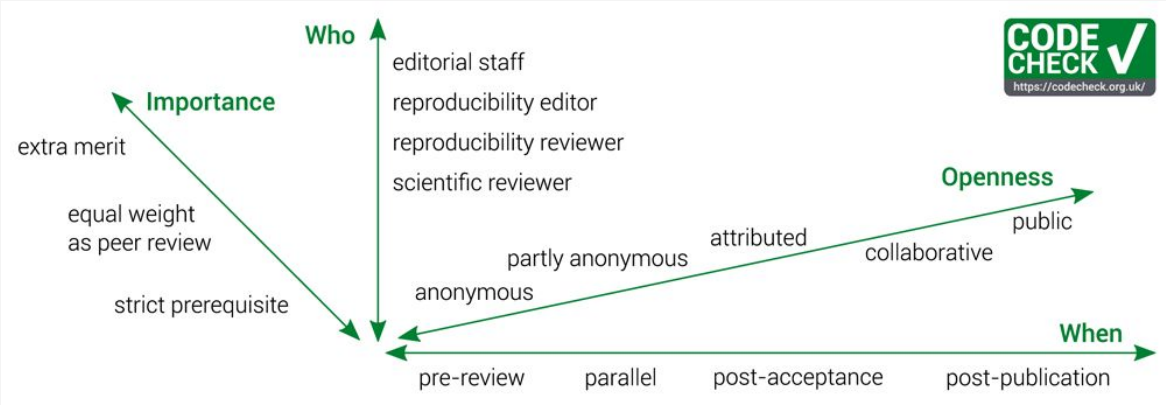
WWU MÜNSTER

CODE CHECK ✓
https://codecheck.org.uk/

Independent execution of computations underlying research articles.

Nüst, D., & Eglen, S. J. (2021). **CODECHECK: An Open Science initiative for the independent execution of computations underlying research articles during peer review to improve reproducibility** [version 1; peer review: 1 approved, 1 approved with reservations]. F1000Research, 10, 253. https://doi.org/10.12688/f1000research.51738.1 (dissertation version)
[version 2; peer review: 2 approved] https://doi.org/10.12688/f1000research.51738.2 (published)

One re-execution by codechecker during peer review



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.**

CODE WORKS ✓

30+ Certificates
https://codecheck.org.uk/register/

Nüst, D., & Pebesma, E. (2021). **Practical reproducibility in geography and geosciences**. Annals of the American Association of Geographers, 111(5), 1300–1310. https://doi.org/10.1080/24694452.2020.1806028

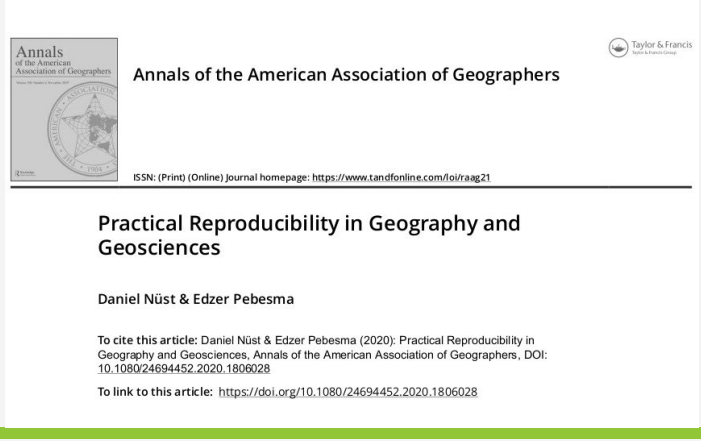
Practical Reproducibility in Geography and Geosciences

Review of **common** guidance for RR

Core idea: consciously control & share computing environment

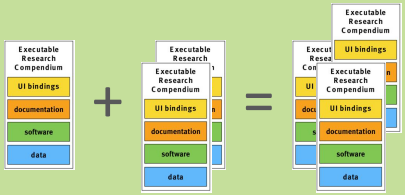
- physical,
- logical, and
- cultural components

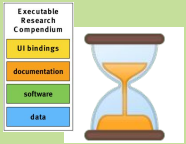
Use scripts and notebooks, create research compendia.

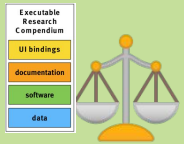


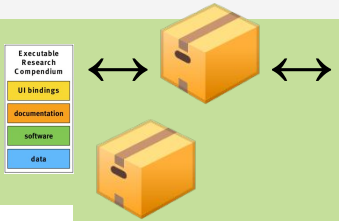
Outlook

Outlook

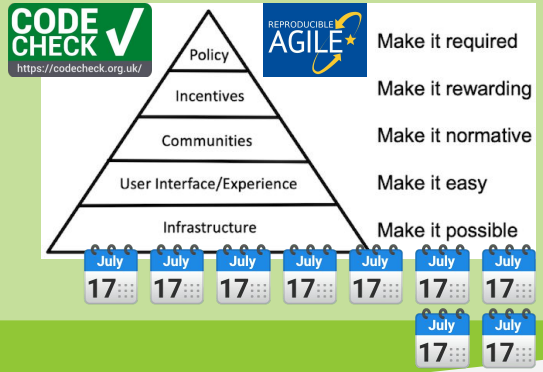








What works?



Why has it not happened yet? Landmark papers

Electronic Documents Give Reproducible Research a New Meaning RE1.3

Jon F. Claerbout and Martin Karrenbach, Stanford Univ.

SUMMARY

A revolution in education and technology transfer follows from the marriage of word processing and software command scripts. In this marriage an author attaches to every figure caption a pushbutton or a name tag usable to recalculate the figure from all its data, parameters, and programs. This provides a concrete definition of reproducibility in computationally oriented research. Experience at the Stanford Exploration Project shows that preparing such electronic documents is little effort beyond our customary report writing; mainly, we need to file everything in a systematic way.

In 1990 we began experimenting with electronic documents that merge our scientific software with our word-processing software. A year later we manufactured a CD-ROM containing a new textbook, Joe Dellinger's doctoral dissertation, and two progress reports of the Stanford Exploration Project. We distributed these CD-ROMs[1] to sponsors and many friends at the 1991 SEG meeting.

In 1990, we set this sequence of goals:

- Learn how to merge a publication with its underlying computational analysis.
- Teach researchers how to prepare a document in a form where they themselves can reproduce their own research results a year or more later by "pressing a single button".
- Learn how to leave finished work in a condition where coworkers can reproduce the calculation including the final illustration by pressing a button in its caption.
- Prepare a complete copy of our local software environment so that graduating students can take their work away with them to other sites, press a button, and reproduce their Stanford work.
- Merge electronic documents written by multiple authors (SEP reports).
- Export electronic documents to numerous other sites (sponsors) so they can readily reproduce a substantial portion of our Stanford research.

We met all these goals and set new ones:

- produce all new documents in this form, including lab reports in formal classes and "lab notebooks" of research progress.
- make incremental improvements in electronic-document software
- seek partners for broadening standards (and making incremental improvements).

Our basic goal is reproducible research. The electronic document is our means to this end. In principle, reproducibility in research can be achieved without electronic documents and that is how we started. Our first nonelectronic reproducible document was a textbook in which the paper document contained the name of a program script in every figure caption. The program scripts were organized by book chapter and section so they could be correlated to an accompanying magnetic tape dump of the file system. The magnetic tape also contained all the necessary data to feed the program script.

Now that we have begun using CD-ROM publication, we can go much further. Every figure caption contains a pushbutton that jumps to the appropriate science directory (folder) and initiates a figure rebuild command and then displays the figure, possibly as a movie or interactive program. We normally display seismic images of the earth's interior, but to reach wider audiences, Figure 1 shows a satellite weather picture which the pushbutton will animate as seen on commerical television. We include all our plot software as well as freely available software from many sources, including compilers and the LaTeX word processing system. Naturally we cannot include licensed software, but with the exception of Fortran and C compilers and the UNIX system itself, our publication includes source code for everything needed. The CD-ROM, at 680 megabytes, is so large we have had room for many executable programs on popular brands of workstations. The presence of these executables gives our readers a fast start.

Nearly everyone would rather read a paper book than the bitmapped page images on a screen that you see with an electronic document. But the illustrations in the electronic book are mostly in color, many are movies, and some are interactive. So the electronic book gives the reader a better understanding of the results. We typically use an interactive movie program to compare seismic sections where successive frames include processing with various parameters. The movie medium is much more informative than comparing seismic sections side by side. 3-D volumes are much better exhibited by movies than static paper illustrations. We are delivering a volume of software that is accessed like a book.

[1]SEP-CD-1 is available from Stanford University Press, $15 plus shipping, tel 415-723-1593

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Claerbout, J., & Karrenbach, M. (**1992**). **Electronic documents give reproducible research a new meaning**. SEG Technical Program Expanded Abstracts, 601–604. https://doi.org/10.1190/1.1822162

Gentleman, R., & Temple Lang, D. (**2007**). **Statistical analyses and reproducible research**. Journal of Computational and Graphical Statistics, 16(1), 1–23. https://doi.org/10.1198/106186007X178663

Statistical Analyses and Reproducible Research

Robert GENTLEMAN and Duncan TEMPLE LANG

It is important, if not essential, to integrate the computations and code used in data analyses, methodological descriptions, simulations, and so on with the documents that describe and rely on them. This integration allows readers to both verify and adapt the claims in the documents. Authors can easily reproduce the results in the future, and they can present the document's contents in a different medium, for example, with interactive controls. This article describes a software framework for both authoring and distributing these integrated, dynamic documents that contain text, code, data, and any auxiliary content needed to recreate the computations. The documents are dynamic in that the contents—including figures, tables, and so on—can be recalculated each time a view of the document is generated. Our model treats a dynamic document as a master or "source" document from which one can generate different views in the form of traditional, derived documents for different audiences.

We introduce the concept of a *compendium* as a container for one or more dynamic documents and the different elements needed when processing them, such as code and data. The compendium serves as a means for distributing, managing, and updating the collection.

The step from disseminating analyses via a compendium to *reproducible research* is a small one. By reproducible research, we mean research papers with accompanying software tools that allow the reader to directly reproduce the results and employ the computational methods that are presented in the research paper. Some of the issues involved in paradigms for the production, distribution, and use of such reproducible research are discussed.

Key Words: Compendium; Dynamic documents; Literate programming; Markup language; Perl; Python; R.

1. INTRODUCTION

Statistical methodology generally involves algorithmic concepts. The descriptions of how to perform a specific analysis for a given dataset or generally how to perform a type of analysis tend to be similarly procedural or algorithmic. Expressing these concepts in a

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Journal of Computational and Graphical Statistics, Volume 16, Number 1, Pages 1–23
DOI: 10.1198/106186007X178663

1

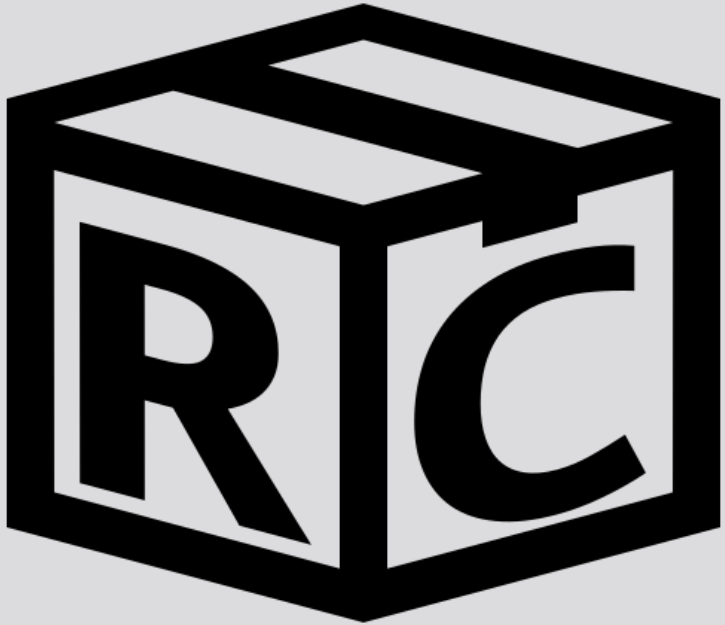
One thing

Have a README: all else is details.

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

Research Compendia

research-compendium.science



Is there a *reproducibility crisis* in

geography?
geosciences?
GIScience?

https://www.incaseofpeace.org/currencies-in-academia/

Crisis narrative useful?

Unclear!

A lot of work to proof on the **technical/practical** side, even not separable from general **academic crisis**?

How likely is it that these disciplines are so different from others (psychology) that there really is nothing?

Generalisability

Yes, CODECHECK, Reproducible AGILE, and the o2r ERS should work across all disciplines.

“Geo” is already very mixed discipline, manifold methods and specialisations.
E.g., qualitative research? Make reproducible what is based on code.

Other documents? Atlases, books (Jupyter Book), …

Limitations

ERCs

Big data, long workflows

User evaluation of ERC/ERS
> proof benefits

Small # workflows

Long term study

Prototype

Bindings environment != ERC image

Real world deployment missing
- BagIt profile + real archive

Research Questions

All Research Questions

Infrastructure & user experience

1) How can packaging of computational analyses serve the needs of authors, publishers, readers, and preservationists?
2) To what extent can the process of capturing the runtime, software, data, and metadata of reproducible research packages be automated in geoscientific analyses?
3) How can the ERC fit into the existing practices and infrastructure for research and publishing in geography, geosciences, and GIScience?

Communities, incentives & policy

1) What are domain-specific challenges and solutions for the geography, geosciences, and GIScience domains in the context of reproducible publications?
2) What new services and features can be built upon reproducible workflows, e.g., when packaged as an ERC?

How can packaging of computational analyses serve the needs of authors, publishers, readers, and preservationists?

To what extent can the process of capturing the runtime, software, data, and metadata of reproducible research packages be automated in geoscientific analyses?

✍️ efficiency in (self-)collaboration, understandability = persuading/accessibility

🏛️ Innovative leadership position, more interesting product, costs unclear; ERC: adaptable and flexible

📖 Reduced barriers to understanding/evaluation, extend workflows, become collaborator

👩‍💻 Assume completeness, ERC (plain text, meaningful links & entrypoints; snapshot with consistent packaging = one preservation strategy)

Automation of ERC creation for large majority of workflows *starting from a notebook or fully scripted workflow* is possible **with containerisation**

Capturing **large data** and **HPC** environments challenging

Manual alternative important for researcher freedom

Manual checks for crucial metadata needed

How can the ERC fit into the existing practices and infrastructure for research and publishing in geography, geosciences, and GIScience?

ERS can make the ERC the **unit of publication**, interacting with existing open or even closed services, **no duplication of services**

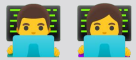
ERC can alleviate the issues of **procedural and cultural shift** in publication practices

Notebooks are established practice for reproducibility

Missing (for ERC): private data (solutions exist),
huge data (under development),
commercial support
uptake/investment by publishers

Unique ERS: full openness (spec, impl), substitutions, bindings

What are domain-specific *challenges* and *solutions* for the geography, geosciences, and GIScience domains in the context of reproducible publications?

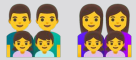


Technical: generally none, some at concrete level

All recommendations draw from other disciplines

Incentives & policy: same as academia at a whole?

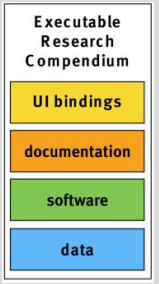
CAN change within our communities



Communities: have a lot of technical literacy

What new services and features can be built upon reproducible workflows, e.g., when packaged as an ERC?

CODE WORKS ✓



Reproducibility technology & humans in peer review

for improving the odds for high quality and reusability of work

Enhanced **search** engines and novel recombination of works (more than text, search, recommend, filter)

Higher understanding and more collaboration

= **Better science**

Platforms

Reproducibility Platform Landscape

Konkol, M., Nüst, D., & Goulier, L. (2020). **Publishing computational research - a review of infrastructures for reproducible and transparent scholarly communication**. Research Integrity and Peer Review, 5(1), 10. https://doi.org/10.1186/s41073-020-00095-y

Table 1 Overview of applications we included in the analysis

Application	Description
Authorea	In Authorea, authors can create executable papers collaboratively. They can attach code and data to figures to make them reproducible. Authors can also directly submit to a journal and, at the same time, publish a preprint.
Binder	Binder creates a containerized executable environment based on a repository (e.g., on GitHub/Lab, Zenodo) including a Jupyter Notebook [24]. Readers can launch the analysis and inspect the workflow in a browser.
Code Ocean	Code Ocean creates "capsules" containing code, data, and the computational environment. While reading, users can execute and inspect the analysis in a separate window below the article or on Code Ocean's website [25].
eLife Reproducible Document Stack (RDS)	RDS originates from the life sciences. Authors can publish executable documents based on Stencila (https://stenci.la/), an open-source editor for articles. The executable document, which contains the whole narrative and executable code snippets, is not only a supplement but the actual scientific article.
Galaxy	Galaxy [26] provides features tailored to use cases in the life sciences. It is a web app for developing comput. Analyses without programming expertise. Scientists can upload and analyze data using Jupyter Notebooks [27].
Gigantum	Gigantum packages code, data, the computational environment, and the work history into a Git repository. Gigantum is composed of a client app for creating as well as executing analyses locally and a cloud-based infrastructure for sharing computations and collaborating with peers.
Manuscripts	Manuscripts is an online tool for writing executable documents collaboratively based on the concept of literate programming, but featuring a "What you see is what you get" user interface. The runtime environment of the author is, however, not considered.
o2r	o2r [22] originates from the geosciences and addresses publishers who want to extend their infrastructure via a reproducibility service during the process of paper submission [28]. Authors can create interactive figures, allowing readers to change model parameters using a slider [29].
REANA	REANA [4, 30] originates from particle physics and provides a specification for capturing data, code, and the comput. Environment. Based on this structure and manually created configuration files, REANA provides command line interface (CLI) commands to run large analyses on a remote REANA cloud.
ReproZip	ReproZip [31, 32] provides a set of CLI commands for encapsulating data, code, and the computational environment. Users can execute the resulting bundle on a server provided by ReproZip [33] or locally on different systems.
Whole Tale	With Whole Tale [34], authors can create so-called "Tales" that combine narrative, data, code, and the computational environment. Readers can inspect the materials and execute the analysis in the original environment.

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

	Authorea	Binder	Code Ocean	eLife RDS	Galaxy	Gigantum	Manuscripts	o2r	REANA	Repro Zip	Whole Tale
Free self-hosting	–	+	–	+*	+	–	+	+	+*	+	+
Open license	–	+	–	+	+	+/–	+	+	+	+	+
In use	in use [40]	in use [2]	in use [41]	in use [42]	in use [43]	–	–	–	in use [44]	in use [31]	–
Grant-based	–	+	–	+	+	–	N/D	+	+	+	+
R Markdown	–	+	+	+	–	+	–	+	–	–	+
Jupyter Notebooks	+	+	+	+	+	+	–	–	+	+	+
Extensible	–	+	+	+	+	–	–	–	+	+	+
Upload	+	+	+	–	+	–	+	+	–	–	+
Copyright	+	N/D	+	N/D	+	+	N/D	+	N/D	N/D	+
Sensitive data	–	–	–	–	–	–	–	–	–	–	–
Discovery	+	–	+	+	+	–	–	+	–	–	+
Inspection	+	+	+	+	+	+	+	+	–	–	+
Execution	+	+	+	+	+	+	+	+	+	+	+
Manipulation	+	+	+	+	+	+	+	+	+	+	+
Substitution	–	–	–	–	–	–	–	+	–	+	–
Download	+	+	+	+	+	+	+	+	–	+	+
Modify/Delete after publishing	–	+	–	–	+	+	+	–	+	+	–
Shared via DOI	+	–	+	+	–	–	–	–	–	–	+
Shared via URL	+	+	+	+	+	+	+	+	–	+	–

Rockerverse

Rockerverse

I) Packaging research reproducibly benefits from other use cases applying containerisation

II) Usability vs. Diversity vs. Stability vs. Uptake vs. Innovation vs. Funding

Interfaces for Docker in R

Image stacks for communities of practice

Capture and create environments

Development, debugging, and testing

Processing

Deployment and continuous delivery

Using R to power enterprise software in production environments

Common or public work environments

Teaching

Packaging research reproducibly

Functionality	AzureContainers	babelwhale	dockermachine	dockyard	googleCloudRunner	harbor	stevedore
Generate a Dockerfile				✓			
Build an image	✓			✓	✓		
Execute a container locally or remotely	✓	✓	✓	✓	✓	✓	✓
Deploy or manage instances in the cloud	✓		✓		✓	✓	✓
Interact with an instance (e.g., file transfer)		✓	✓				✓
Manage storage of images						✓	✓
Supports Docker and Singularity		✓					
Direct access to Docker API instead of using the CLI							✓
Installing Docker software			✓				

Nüst, D., Eddelbuettel, D., Bennett, D., Cannoodt, R., Clark, D., Daróczi, G., Edmondson, M., Fay, C., Hughes, E., Kjeldgaard, L., Lopp, S., Marwick, B., Nolis, H., Nolis, J., Ooi, H., Ram, K., Ross, N., Shepherd, L., Sólymos, P., Swetnam, T. L., Turaga, N., Petegem, C. V., Williams, J., Willis, C., & Xiao, N. (2020). **The Rockerverse: Packages and Applications for Containerisation with R**. The R Journal, 12(1). https://doi.org/10.32614/RJ-2020-007

GEOBIA

Reproducible GEOBIA workflow

Knoth, C., & Nüst, D. (2017). **Reproducibility and Practical Adoption of GEOBIA with Open-Source Software in Docker Containers**. Remote Sensing, 9(3), 290. https://doi.org/10.3390/rs9030290

1) `docker run` starts a container and executes the entry point script `/qgis/model.sh` using a Bash shell
2) `/qgis/model.sh` ...
    a) copies model and script files
       from `/workspace/models/*` to `/root/.qgis2/processing/models`
       from `/workspace/scripts/*` to `/root/.qgis2/processing/sripts`
    b) executes `model.py` as a Python file with a virtual frame buffer
3) `/workspace/model.py` ...
    a) initiates QGIS application
    b) loads manipulation parameters and construct input and output paths
    c) runs the model `example_analysis_linux_v3.1.model` using the QGIS Python API passing configuration parameters
4) `/root/.qgis/processing/models/example_analysis_linux_v3.1.model` ...
    a) executes the model steps, using user scripts from `/root/.qgis/processing/scripts`
    b) saves the files to the result directory
5) `/results` holds the output files for user access

GEOBIA

Knoth, C., & Nüst, D. (2017). **Reproducibility and Practical Adoption of GEOBIA with Open-Source Software in Docker Containers**. Remote Sensing, 9(3), 290. https://doi.org/10.3390/rs9030290

Listing 1: Excerpt of workspace directory tree; the full workspace is available on GitHub [62] and in the reproducibility package, see Section 3.4.

```
/workspace
|-- data
| |-- COPYRIGHT
| |-- jonjona_pos_conflict_proj.tif
| `-- jonjona_pre_conflict_proj.tif
|-- model.py
|-- models
| |-- detect_settlements_on_edgelayer.model
| `-- example_analysis_linux_v3.1.model
`-- scripts
  |-- diff_to_local_ref_v1.3.py
  `-- kmeans_clustering_v2.3.py
```

Listing 6: Full reproduction commands: run the container from Docker Hub and extract the result.

```
docker run -it --name repro nuest/qgis-model:rs-jonjona
docker cp repro:/workspace/results /tmp/repro_results
```

Listing 7: Result directory tree after execution, supplementary shapefile files, i.e., .dbf, .prj, .qpj, and .shx, and workspace files (see previous Listing 1) not shown.

```
|/result
|`-- 20161212-172947
|  |-- result_threshold.shp
|  |-- result_unclassified.shp
|  |-- settlements.shp
```

Listing 8: Analysis control and data switching examples. From top to bottom: (a) mounting another workspace; (b) mounting only input files; (c) changing model options via environment variables.

```
# (a)
docker run -it -v /my/analysis:/workspace nuest/qgis-model:rs-jonjona

# (b)
docker run -it -v mypreconflict.tif:/workspace/data/pre_conflict.tif
  -v mypostconflict.tif:/workspace/data/pos_conflict.tif nuest/qgis-model:rs-jonjona

# (c)
docker run -it -e change_analysis_threshold=0.28 nuest/qgis-model:rs-jonjona
```

GEOBIA

Knoth, C., & Nüst, D. (2017). **Reproducibility and Practical Adoption of GEOBIA with Open-Source Software in Docker Containers**. Remote Sensing, 9(3), 290. https://doi.org/10.3390/rs9030290

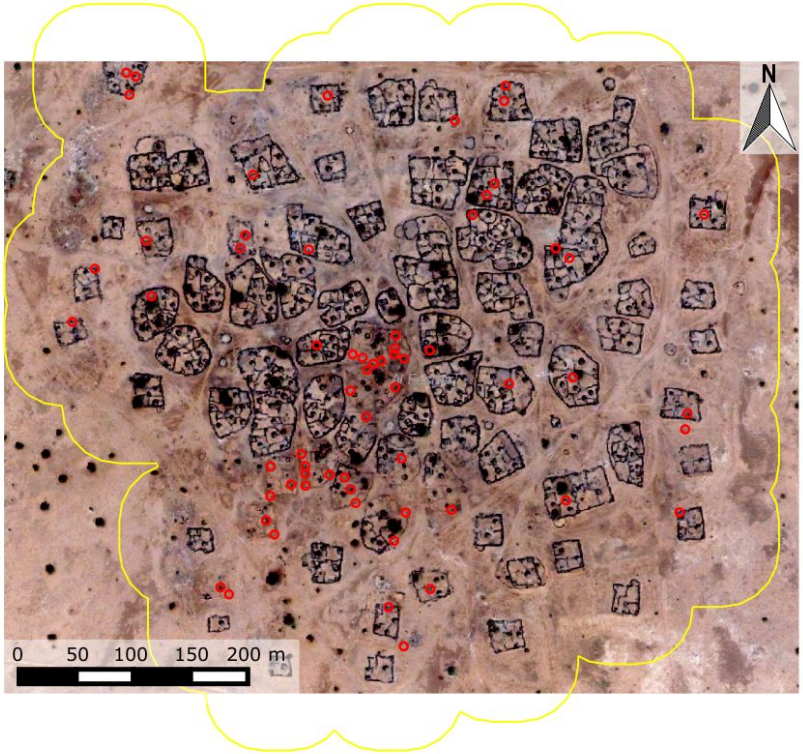


Figure 4. Post-conflict image (location: 13.686°N, 24.979°E) with two results of the example analysis. The detected settlement area is the yellow polygon. The results of the damage assessment, i.e., the disappeared dwellings, are the red circles (image © 2016 DigitalGlobe).

AGILE conference

AGILE paper corpus

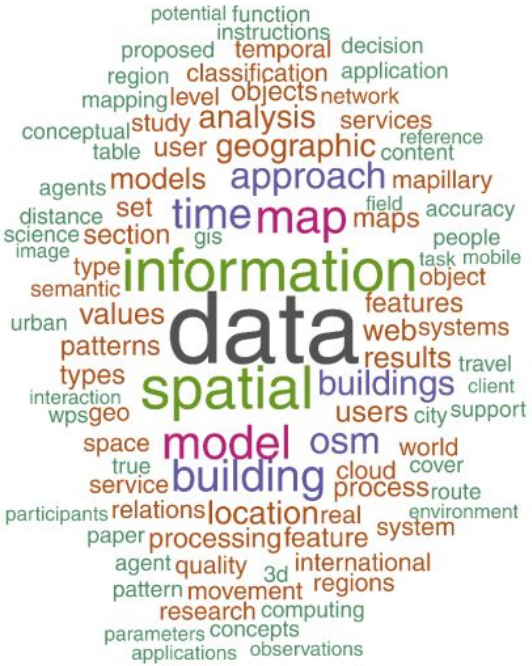
Table 1 Reproducibility-related keywords in the corpus, ordered by sum of matches per paper. For full references of the corpus papers see Supplemental Material.

Citation	Reproduc.	Replic.	Repeatab.	Code	Software	Algorithm(s)	(pre)process.	Data	Result(s)	All
Foerster et al. (2012)	0	0	0	2	3	11	140	129	41	326
Wiemann & Bernard (2014)	0	0	0	0	0	0	20	98	3	123
Mazimpaka & Timpf (2015)	0	0	0	3	0	4	4	97	10	118
Steuer et al. (2015)	0	0	0	0	0	25	12	64	17	118
Schäffer et al. (2010)	0	0	0	0	10	1	26	65	6	108
Rosser et al. (2016)	0	0	0	0	2	1	42	51	6	105
Gröchening et al. (2014)	0	0	0	0	0	3	2	69	27	101
Almer et al. (2016)	0	0	0	1	1	1	22	53	22	100
Magalhães et al. (2012)	0	0	0	2	1	20	52	9	1	85
Juhász & Hochmair (2016)	0	0	0	0	1	1	2	55	11	70
Wiemann (2016)	0	0	0	0	3	0	8	55	1	69
Fan et al. (2014)	0	0	0	0	0	3	8	44	12	67
Merki & Laube (2012)	0	0	0	0	0	9	6	40	6	62
Zhu et al. (2017)	2	2	0	2	0	10	7	32	6	61
Kuhn & Ballatore (2015)	0	0	1	2	14	1	5	26	8	58
Soleymani et al. (2014)	1	0	0	0	0	0	4	39	9	56
Fogliaroni & Hobel (2015)	0	0	0	0	0	3	14	30	5	52
Osaragi & Hoshino (2012)	0	0	0	0	0	0	5	36	7	48
Stein & Schlieder (2013)	0	0	0	0	0	0	3	42	3	48
Körner et al. (2010)	0	0	0	0	0	6	5	30	4	45
Knoth et al. (2017)	0	0	0	3	2	1	6	25	7	44
Raubal & Winter (2010)	0	0	0	1	1	1	18	0	13	34
Konkol et al. (2017)	1	0	0	3	1	1	2	4	19	31
Kiefer et al. (2012)	1	0	0	0	2	1	9	10	8	31
Haumann et al. (2017)	0	0	0	0	0	6	8	10	2	26
Josselin et al. (2016)	0	0	0	0	2	1	9	5	8	25
Heinz & Schlieder (2015)	1	0	0	2	1	3	2	14	2	25
Osaragi & Tsuda (2013)	0	0	0	1	1	0	3	16	2	23
Baglatzi & Kuhn (2013)	1	0	0	0	0	0	6	12	3	22
Scheider et al. (2014)	0	0	0	0	1	0	0	13	4	19
Brinkhoff (2017)	0	0	0	0	1	9	2	3	2	17
Schwering et al. (2013)	0	0	0	0	0	4	2	3	5	14
Total	7	2	1	22	47	126	454	1,179	280	2,131

Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018). **Reproducible research and GIScience: An evaluation using AGILE conference papers**. PeerJ, 6, e5072. https://doi.org/10.7717/peerj.5072

AGILE paper corpus

A



B

place	word	n	# papers
1	data	1058	31
2	information	589	32
3	spatial	577	30
4	map	411	25
5	model	411	25
6	building	381	24
7	time	378	30
8	approach	297	32
9	osm	292	8
10	buildings	266	15
11	geographic	249	28
12	location	239	26
13	analysis	229	28
14	users	225	19
15	results	207	30
16	web	206	21
17	models	202	20
18	values	202	23
19	patterns	196	16
20	maps	189	20

Figure 1 **Two illustrations of the test corpus papers: word cloud, scaled and coloured by number of occurrence of words with at least 100 occurrences (96 unique words) (A); top words sorted by overall occurrence and number of papers including the word at least once (B).**

Full-size DOI: 10.7717/peerj.5072/fig-1

Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018). **Reproducible research and GIScience: An evaluation using AGILE conference papers**. PeerJ, 6, e5072. https://doi.org/10.7717/peerj.5072

AGILE paper corpus levels

Table 3 **Reproducibility levels for paper corpus; '-' is category not available.** For full references of the corpus papers see Supplemental Material.

Author	Short paper	Input data	Preprocessing	Method/analysis/ processing	Computational environment	Results
Zhu et al. (2017)		0	1	1	1	1
Knoth et al. (2017)		0	–	0	1	1
Konkol et al. (2017)		2	2	1	1	1
Haumann et al. (2017)	X	0	1	1	0	1
Brinkhoff (2017)	X	0	–	1	0	0
Almer et al. (2016)		0	–	1	1	1
Wiemann (2016)		2	–	1	1	1
Juhász & Hochmair (2016)		0	1	1	0	0
Josselin et al. (2016)	X	1	–	0	0	1
Rosser et al. (2016)	X	0	–	1	0	0
Kuhn & Ballatore (2015)		–	–	–	–	–
Mazimpaka & Timpf (2015)		2	1	1	1	1
Steuer et al. (2015)		2	0	1	1	1
Fogliaroni & Hobel (2015)	X	–	–	–	–	–
Heinz & Schlieder (2015)	X	0	0	1	1	1
Scheider et al. (2014)		1	1	2	1	1
Gröchening et al. (2014)		2	0	1	0	1
Fan et al. (2014)		0	1	1	0	1
Soleymani et al. (2014)	X	0	0	1	0	0
Wiemann & Bernard (2014)	X	0	0	1	0	0
Osaragi & Tsuda (2013)		0	1	1	0	1
Baglatzi & Kuhn (2013)		–	–	–	–	–
Li et al. (2013)	X	0	0	1	–	1
Stein & Schlieder (2013)	X	0	–	1	0	1
Osaragi & Hoshino (2012)		0	0	1	0	1
Magalhães et al. (2012)		0	0	1	0	0
Foerster et al. (2012)		1	–	1	1	1
Merki & Laube (2012)	X	0	–	1	1	1
Kiefer et al. (2012)	X	0	1	1	0	1
Raubal & Winter (2010)		–	–	–	–	–
Schäffer et al. (2010)		0	0	1	1	1
Körner et al. (2010)		–	–	–	–	–

Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018). **Reproducible research and GIScience: An evaluation using AGILE conference papers**. PeerJ, 6, e5072. https://doi.org/10.7717/peerj.5072

AGILE assessment results

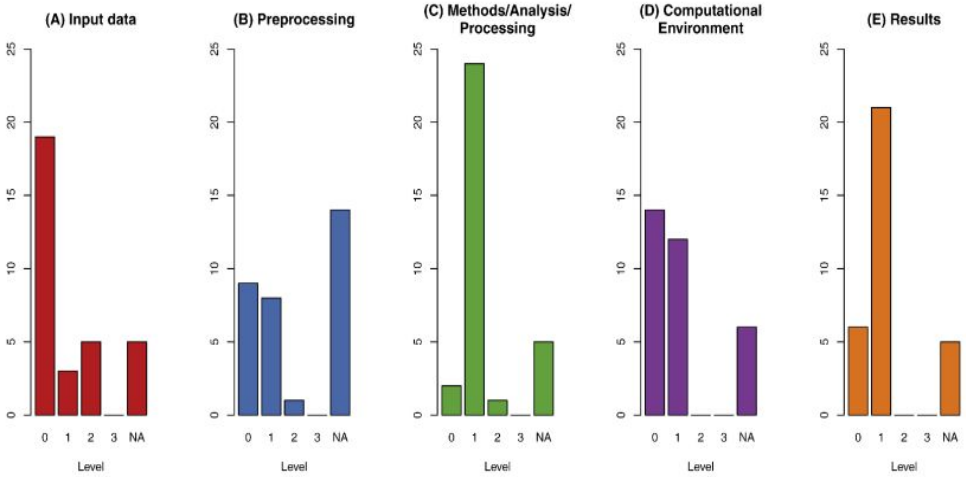


Figure 3 **Results of reproducibility assessment across all categories for the assessment of reproducibility: *Data* (A), *Methods* with sub-categories preprocessing (B), method/analysis/processing (C) and computational environment (D), and *Results* (E).** The level of reproducibility ranges from 0 (not reproducible) to 3 (fully reproducible); NAs include 5 conceptual papers (all categories are NA).

Full-size DOI: 10.7717/peerj.5072/fig-3

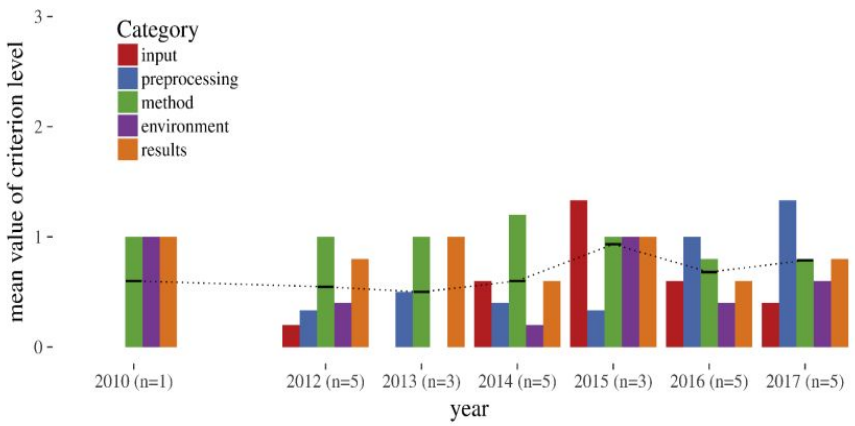


Figure 4 **Mean reproducibility levels per category over time; black dotted line connects the mean per year over all categories (in 2010 only one of three papers could be assessed, reaching level 1 for methods).**

Full-size DOI: 10.7717/peerj.5072/fig-4

Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018).
Reproducible research and GIScience: An evaluation using AGILE conference papers.
PeerJ, 6, e5072. https://doi.org/10.7717/peerj.5072

AGILE survey results

Table 6 Hindering circumstances for reproducibility for each survey response ($n = 17$) sorted by barrier type for the category with most "Main reason" occurences; each line is one response and background colour corresponds to cell text.

Legal restrictions	Lack of time	Lack of tools	Lack of knowledge	Lack of incentive
Main reason	Strongly hindered	Not at all	Not at all	Strongly hindered
Main reason	Not at all	Not at all	Not at all	Moderately hindered
Main reason	Slightly hindered	Strongly hindered	Moderately hindered	Strongly hindered
Main reason	Not at all	Slightly hindered	Not at all	Not at all
Strongly hindered	Strongly hindered	Strongly hindered	Moderately hindered	Strongly hindered
Moderately hindered	Main reason	Not at all	Not at all	Not at all
Slightly hindered	Moderately hindered	Slightly hindered	Slightly hindered	Moderately hindered
Slightly hindered	Not at all	Main reason	Strongly hindered	Not at all
Not at all	Moderately hindered	Not at all	Moderately hindered	Not at all
Not at all	Strongly hindered	Strongly hindered	Strongly hindered	Slightly hindered
Not at all	Moderately hindered	Not at all	Not at all	Not at all
Not at all	Slightly hindered	Main reason	Not at all	Strongly hindered
Not at all	Main reason	Not at all	Not at all	Not at all
Not at all	Main reason	Not at all	Not at all	Not at all
Not at all	Moderately hindered	Moderately hindered	Not at all	Strongly hindered
Not at all	Not at all	Not at all	Not at all	Not at all
Not at all	Slightly hindered	Not at all	Slightly hindered	Not at all

Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018).
Reproducible research and GIScience: An evaluation using AGILE conference papers.
PeerJ, 6, e5072. https://doi.org/10.7717/peerj.5072

GIScience conference

GIScience assessment results

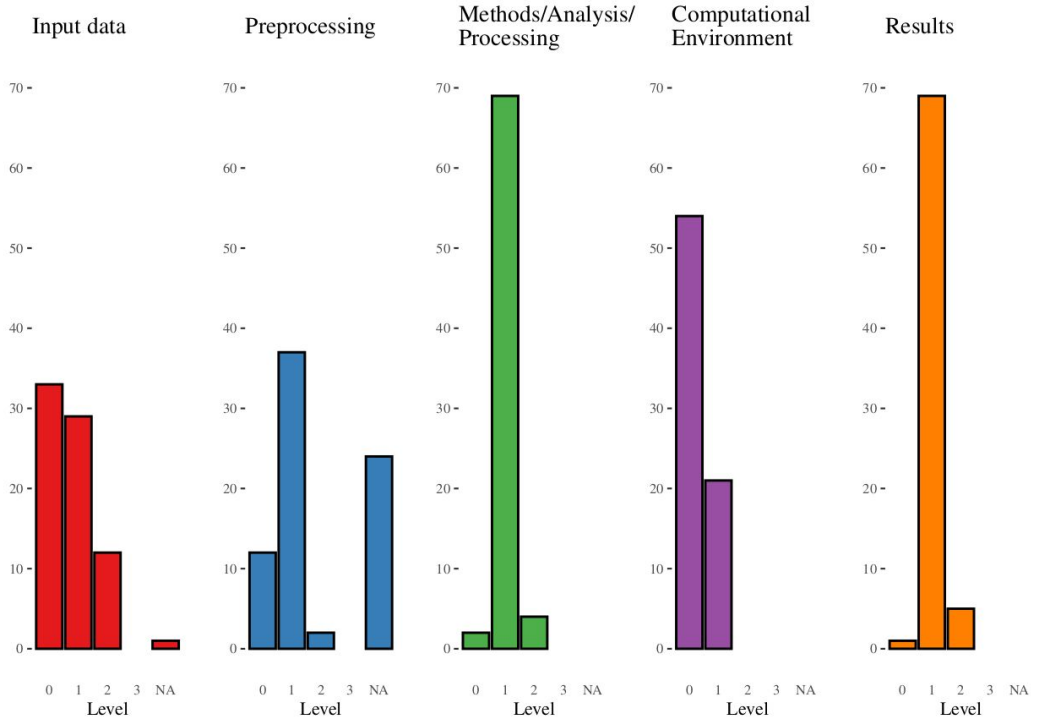


Figure 1 Barplots of reproducibility assessment results; levels range from 0 (leftmost bar) to 'not applicable' (rightmost bar).

Ostermann, F. O., 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 (dissertation version)
> 11th International Conference on Geographic Information Science (GIScience 2021) - Part II. Schloss Dagstuhl - Leibniz-Zentrum Für Informatik. https://doi.org/10.4230/LIPICS.GISCIENCE.2021.II.2 (accepted)

GIScience assessment results

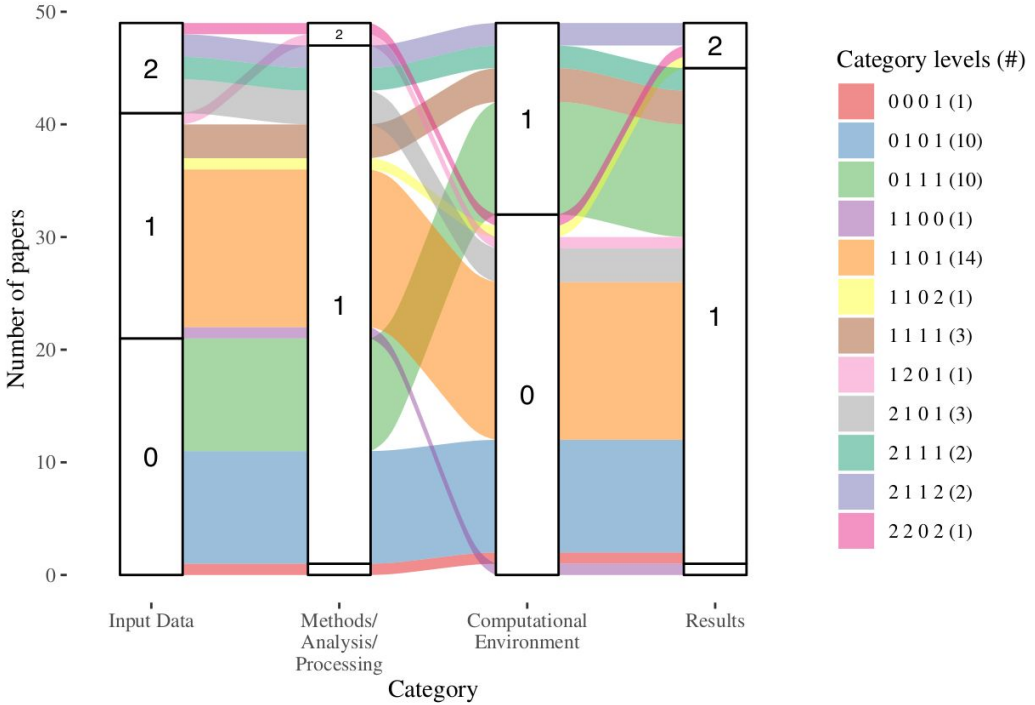
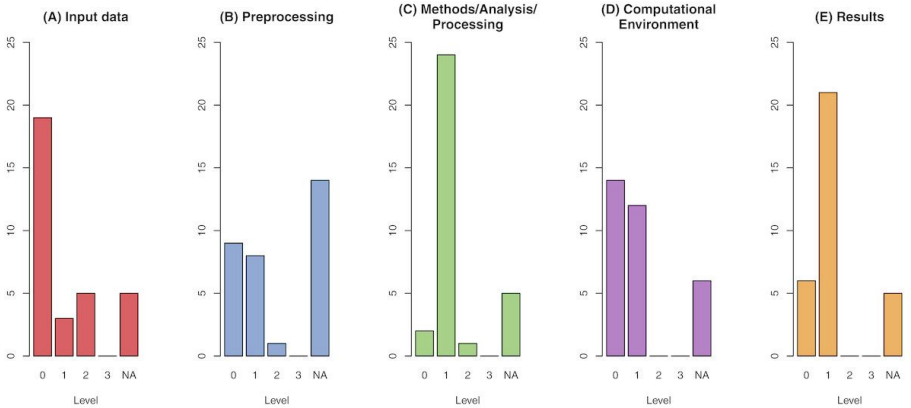
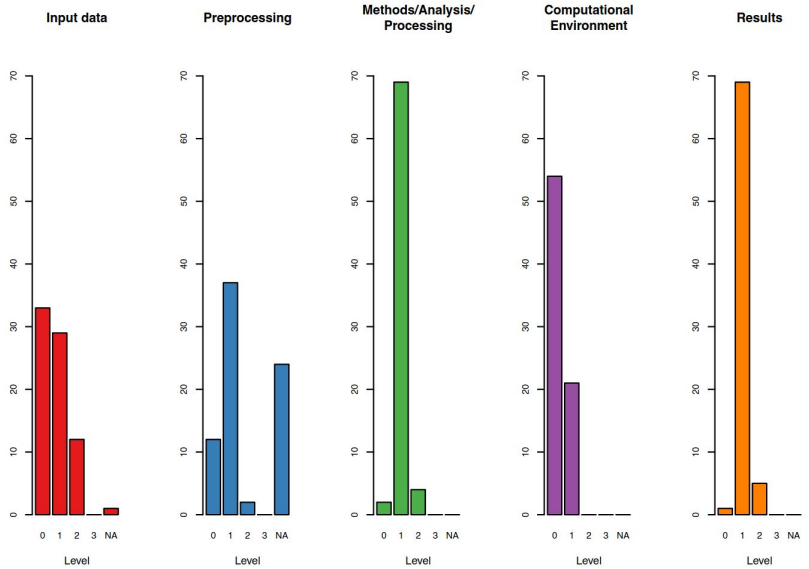


Figure 2 Alluvial diagram of common groups of papers throughout 4 of 5 categories including only papers without any "not applicable" *(Level NA)* value; category *Preprocessing* was dropped because difficulty to clearly assess it lead to many "not applicable" values.

Ostermann, F. O., 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 (dissertation version)
> 11th International Conference on Geographic Information Science (GIScience 2021) - Part II. Schloss Dagstuhl - Leibniz-Zentrum Für Informatik. https://doi.org/10.4230/LIPICS.GISCIENCE.2021.II.2 (accepted)

Assessment of GIScience papers: AGILE & GIScience





Nüst, D., Granell, C., Hofer, B., Konkol, M., Ostermann, F. O., Sileryte, R., & Cerutti, V. (2018). *Reproducible research and GIScience: an evaluation using AGILE conference papers.* PeerJ, 6, e5072. **https://doi.org/10.7717/peerj.5072**

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** | *pub. pending at GIScience conf.*

Posters

WWU MÜNSTER

Nüst, D., & Schutzeichel, M. (2017). **An Architecture for Reproducible Computational Geosciences**. 20th AGILE Conference for Geoinformation Science poster session. **https://doi.org/10.5281/zenodo.1478542**

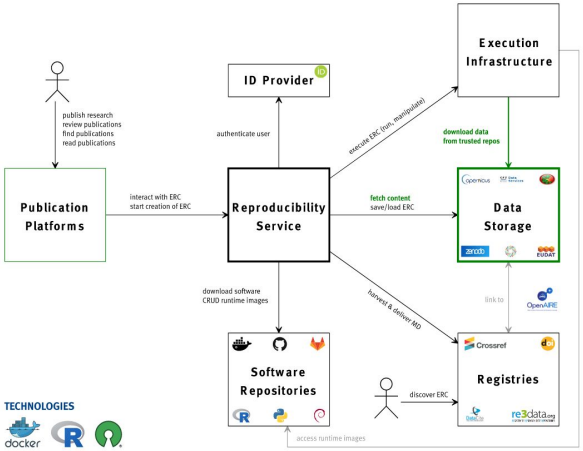
An Architecture for Reproducible Computational Geosciences

Daniel Nüst
Institute for Geoinformatics (ifgi)
Marc Schutzeichel
University and State Library Münster (ULB)

MOTIVATION & THE REPRODUCIBILITY SERVICE

Data, methods and products of geoscience research today are digital: from inception/measurement, via algorithmic analyses to static and interactive online publications. The triplet of Open Source Software, Open Science projects and Open Access publications has created *unprecedented potential to collaborate* in all steps of a scientific process: idea, implementation, scholarly review, publication, and preservation.
There should be more scrutiny of existing work, less repetition of basics, and higher degree and quality of collaboration, but the *pressure of academia* leads to publishing first and foremost articles and rarely complete workflows.
To break the modus operandi, we see *supporting technical solutions*, i.e. tools and services making it easier to conduct reproducible research and to leverage the advantages of reproducible analyses, as a crucial point towards reproducible scientific publications. The must be accompanied by improvements in education, scholarly accreditation mechanisms, and **scientific culture**.

By **preserving knowledge** instead of collecting citations, the geosciences community can reach new levels with respect to how reviews are being conducted and how publications can be used. This work introduces a novel technical building block, the reproducibility service.
Two of its qualities are crucial in the scientific setting: **transparency** allows scrutiny required by a rigorous scientific process; **integration** with existing platforms ensures quality through focus on the core functionality and easier adoption.
The service does not replicate the complex tasks of data storage, peer-review procedures, preservation, or interdisciplinary efforts such as persistent identifiers. It enhances current practices in computational geosciences from publishing static documents to sharing executable research compendia.



GEO-READY

The reproducibility service integrates with existing services and platforms involved in the publication and archival of geosciences research by providing the following functions:

- create ERC from provided workspaces initiated from publication platforms
- save ERC to data repositories and archives
- execute ERC in scalable computing infrastructures **allowing connections** to trusted data repositories
- save ERC metadata in registries to facilitate discovery

This comprises *a relevant extension of the ERC's self-containment idea at the execution stage*, which is crucial for geosciences.

The **data repositories** are also specific to geoscience domains, because they must be accepted by domain members and provide the required data.

TECHNOLOGIES

docker

PROJECT

o2r opening reproducible research
http://o2r.info
@o2r_project

Opening Reproducible Research is a joint project by the Institute for Geoinformatics and the University and Regional Library Münster funded by the German Research Foundation aims to improve the exchange and archiving of geoscience research results that are published over the Internet, by facilitating access to them and by simplifying their reuse in the form of a research compendium. The project focuses on the publication process and the interaction with digital research objects as technical challenges to increase publication of open reproducible research.Combining these goals will set a clear innovation in the area of reproducibility, which is at the heart of the scientific method.

WWU DFG

SUMMARY

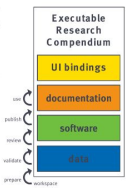
Reproducibility is a cornerstone of science but poses a large challenge when it comes to modern computational sciences. Initiatives for openness must be accompanied by an infrastructure going beyond the state of the art in scientific publications and preservation of knowledge. Building on the concept of Executable Research Compendia (ERC), this work presents an architecture to support a scholarly process for computational geosciences. In this architecture the novel **reproducibility service** enriches scientific publications and integrates with the existing platforms.
The architecture presented here is a work in progress report on software and concepts. It identifies domain-agnostic conceptual components and points out those **functions specific to the geosciences**, namely data storage platforms & data service access during execution of ERC. Following the spirit of Open Science, the architecture is developed publicly in a repository on GitHub. Suggestions and improvements by the geospatial community are welcome.

Contribute at **https://github.com/o2r-project/architecture**

BACKGROUND: ERC

Executable Research Compendia (ERC) support requirements of authors, readers, publishers, curators, as well as preservationists. They are a new way to package computational research combining data, software, text, and a user interface description and provide a novel potential to find, explore, reuse, and archive computer-based research. [1]

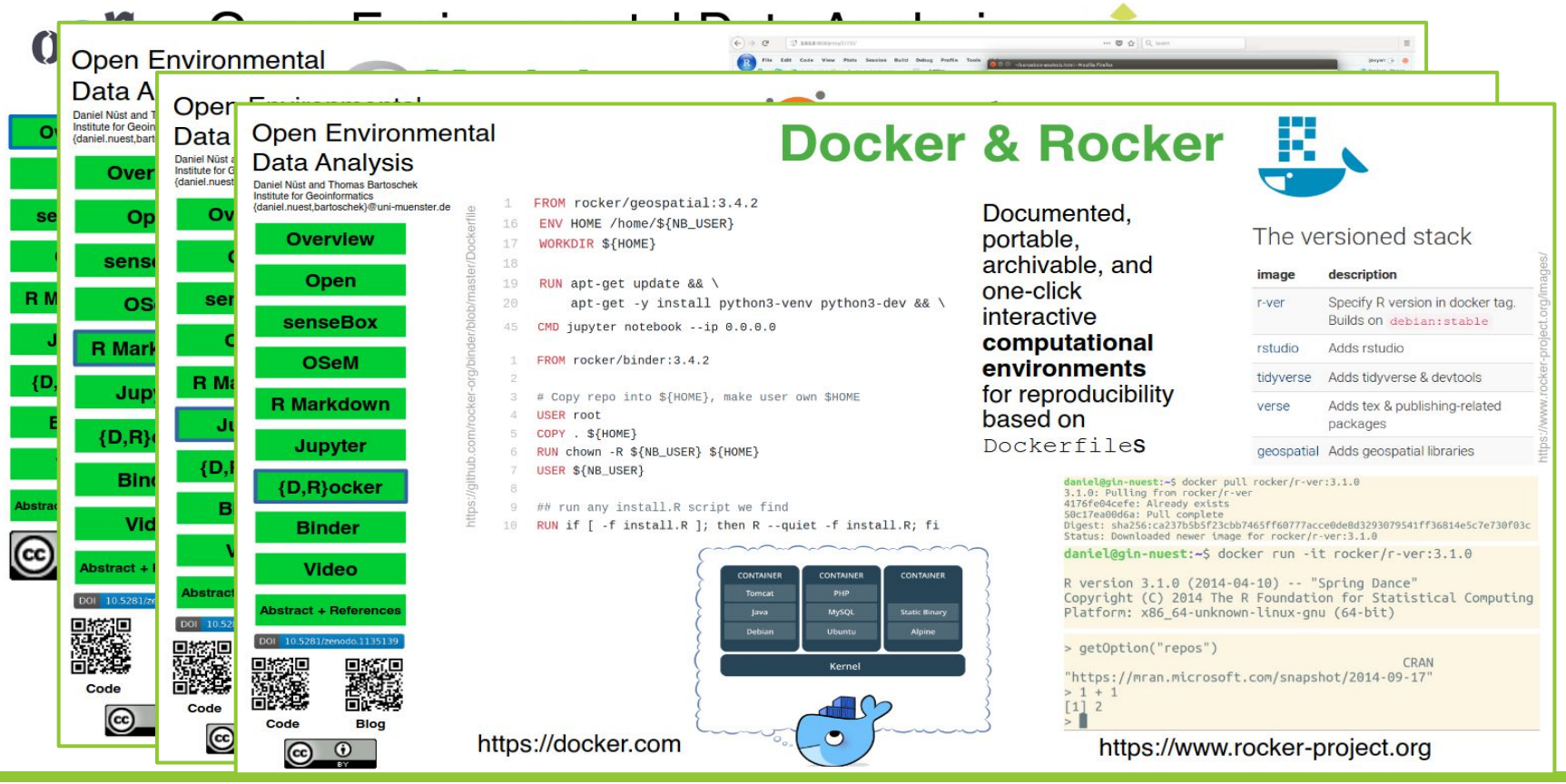
Data comprises all inputs for an analysis, ideally starting with raw measurements, in form of text files, or databases. **Software** comprises analysis code/scripts created by a researcher and the complete runtime environment as an executable Docker image and a Dockerfile as the manifest. **Documentation** comprises both instructions (e.g. a README), the actual scientific publication, and metadata in standardized formats (licenses, discovery metadata). The actual publication comes in a source format (i.e. based on literate programming) and a viewable format (e.g. an HTML document). **UI bindings** open up the compendium. They allow reviewers to interact with diagrams and manipulate formerly hidden parameters for a comprehensive understanding of the underlying data and code. A **formal specification** for ERC connects these building blocks in a meaningful way. It enables technical checking of computation outputs of an ERC and closes the gap of dependency preservation for computational scholarly works.



[1] Opening the Publication Process with Executable Research Compendia
Nüst, D., Konkol, M. et al.
D-Lib Magazine, 2017
doi: 10.1045/january2017-nuest

EGU 2018 Poster

Nüst, D., & Bartoschek, T. (2018). Open Environmental Data Analysis. Geophysical Research Abstracts, Vol. 20; archived on Zenodo; ERC: https://o2r.uni-muenster.de/erc/Phbla. https://doi.org/10.5281/zenodo.1217912



BSc & Msc theses

https://o2r.info/theses/

Developing and Evaluating Infrastructure for ERC to Communicate with Data Repositories and Computing Services

Niklas George, 2021, MSc

Open up ERCs to allow controlled access to specific computing or data services; expert interviews and prototyping approaches (proxy, **DNS**, firewall) for Docker container/networks.

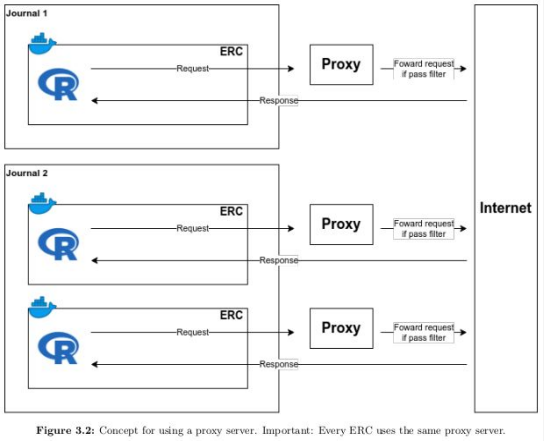


Figure 3.2: Concept for using a proxy server. Important: Every ERC uses the same proxy server.

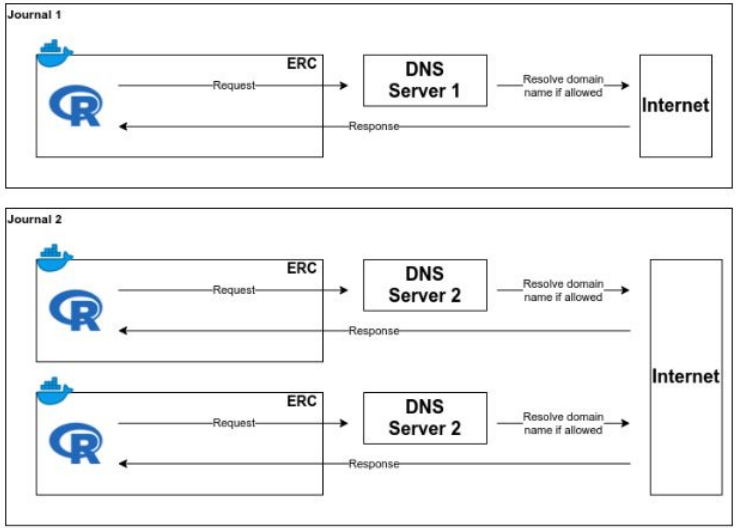


Figure 3.3: Concept for using a DNS server.

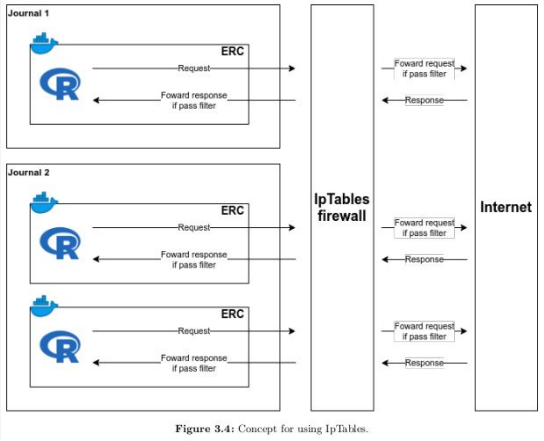


Figure 3.4: Concept for using IpTables.

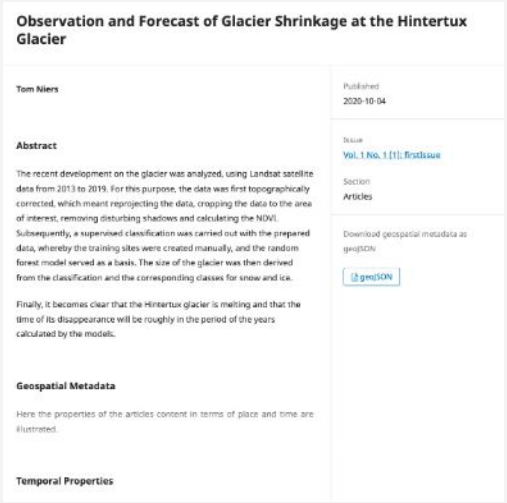
Geospatial Metadata for Discovery in Scholarly Publishing

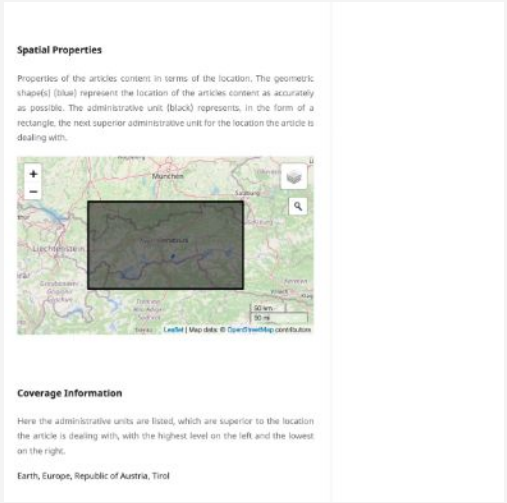
Tom Niers, 2020, BSc

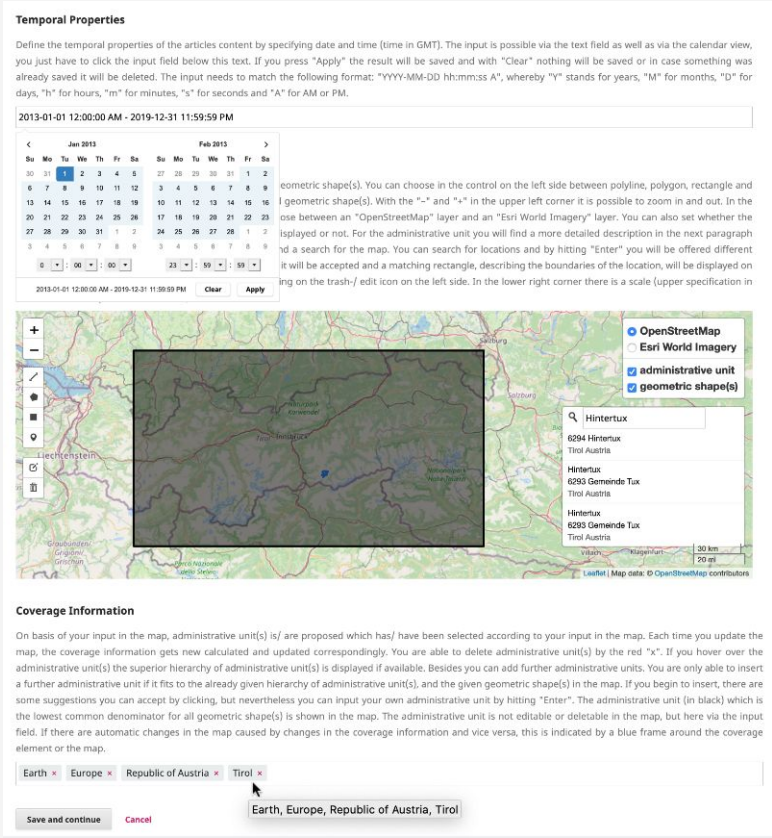
http://nbn-resolving.de/urn:nbn:de:hbz:6-69029469735

https://github.com/tnier01/geoOJS

Geospatial metadata for articles as part of OJS; innovative matching of text and coordinate metadata.







Testing Geospatial R Packages on Implementations of the R language and Platforms

Ismail Sunni, 2020, MSc GeoTech

http://hdl.handle.net/10362/95140 | https://github.com/ismailsunni/altRnative/

Using containers for R implementations (GNU R, MRO, Renjin, FastR, pqR, TERR) across several distributions (Debian, Fedora, Ubuntu, Arch), including benchmarking; challenging installations!

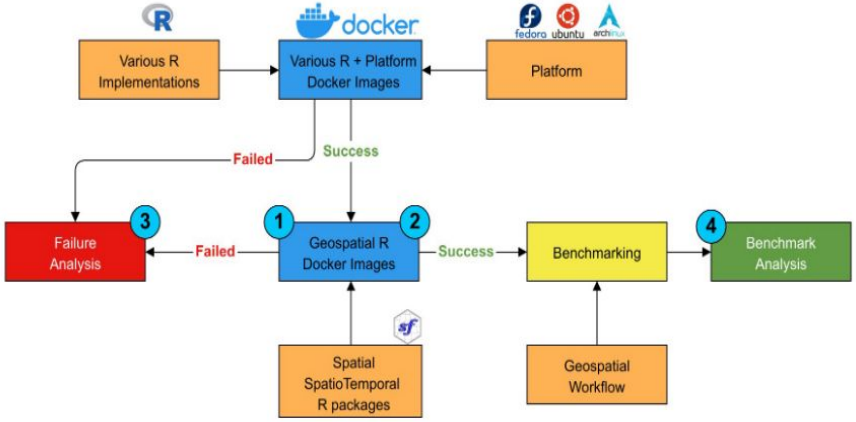


Figure 3.1: Methodology

Table 4.1: Vanilla R Docker Images

	GNU R	MRO	Renjin	FastR	pqR	TERR
Debian	Yes	Yes	Yes	Yes	Yes	Yes
Fedora	Yes	Yes	Stop	Yes	Stop	Stop
Arch Linux	Yes	Yes	Stop	Stop	Stop	Stop

Table 4.2: Geospatial R Docker Images

	GNU R	MRO	Renjin	FastR	pqR	TERR
Debian	Yes	Yes	No	No	No	No
Fedora	Yes	Yes	No	No	No	No
Arch Linux	Yes	?	No	No	No	No

Testing Geospatial R Packages on Implementations of the R language and Platforms (cont.)

Ismail Sunni, 2020, MSc GeoTech

http://hdl.handle.net/10362/95140 | https://github.com/ismailsunni/altRnative/

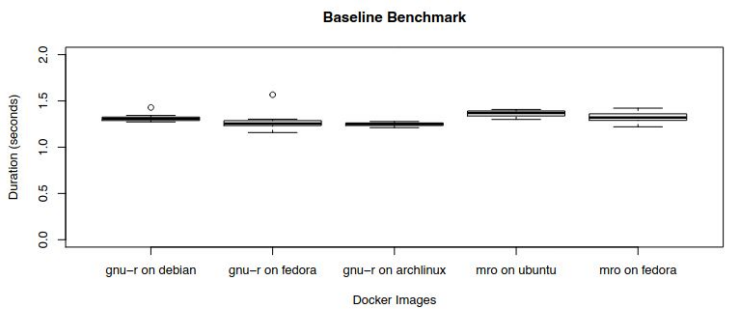


Figure 4.1: Baseline Benchmark

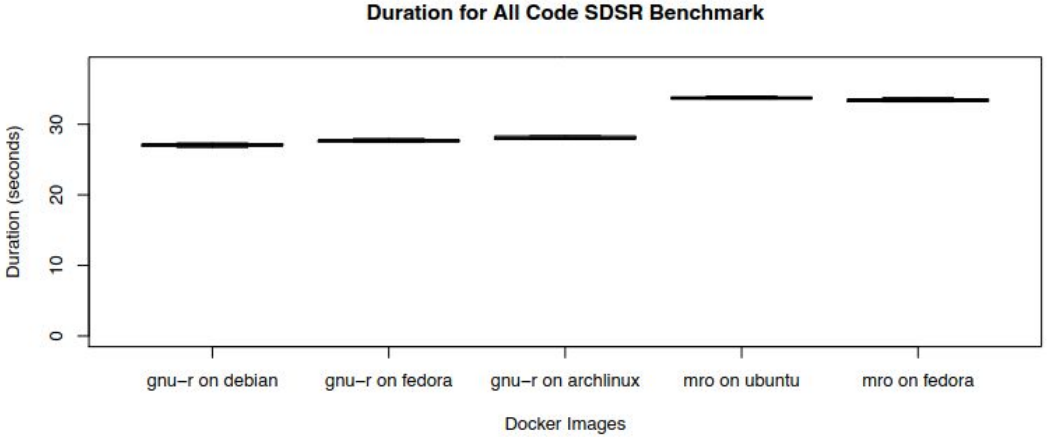
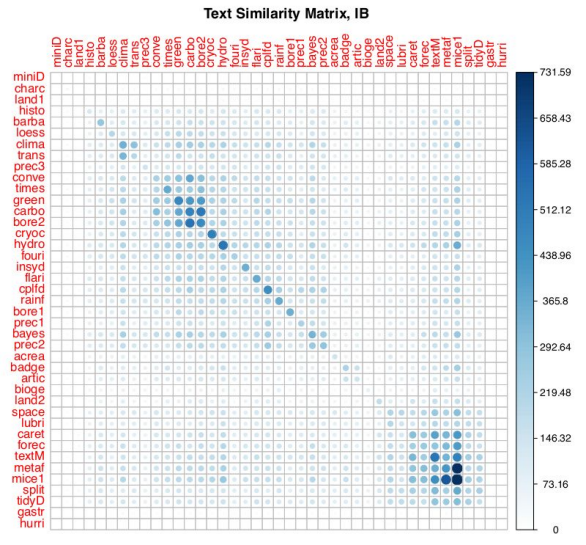


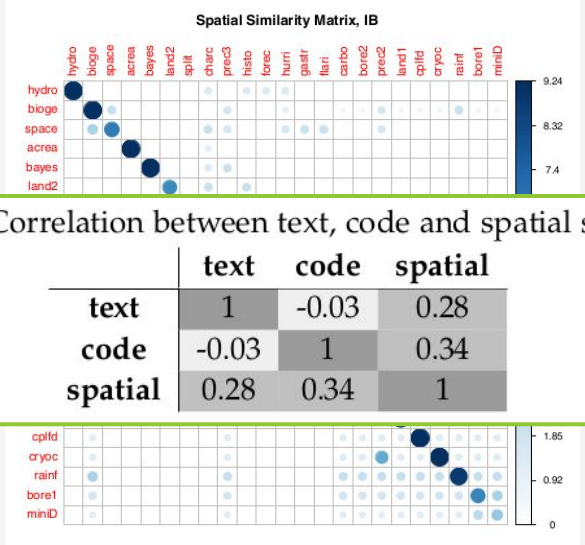
Figure 4.2: Duration for All Code SDSR Benchmark

Similarity Measurements for Executable Research Compendia

Lukas Lohoff, 2018, MSc

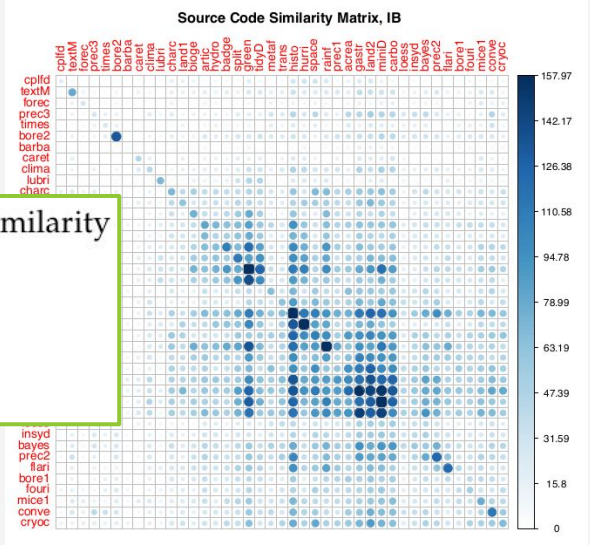
Use components of an ERC, code and geospatial metadata, to enhance search, i.e., find spatially (Geohash + Text similarity) and computationally similar works (e.g., loaded libraries)





Correlation between text, code and spatial similarity

	text	code	spatial
text	1	-0.03	0.28
code	-0.03	1	0.34
spatial	0.28	0.34	1



Serverless GEO Labels for the Semantic Sensor Web

Graupner, A., & Nüst, D. (2020). **Serverless GEO Labels for the Semantic Sensor Web**. Schloss Dagstuhl - Leibniz-Zentrum Für Informatik. https://doi.org/10.4230/LIPICS.GISCIENCE.2021.I.4

Scalable generation of meaningful and rich metadata visualisations with labels (GIScience '20)

> Adaptable to ERC badges!

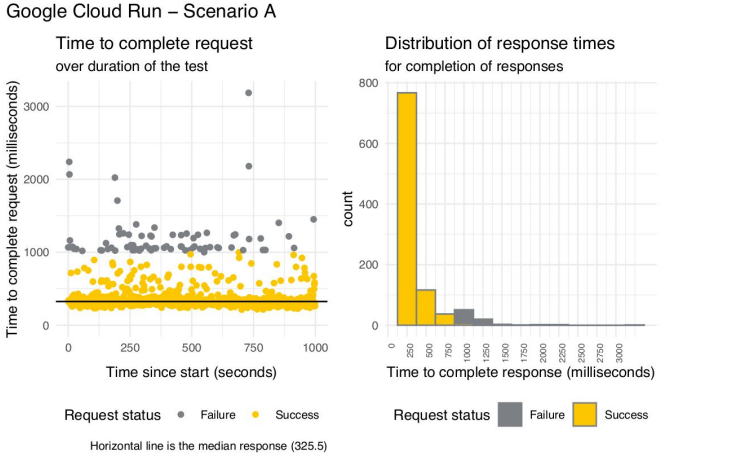


Figure 2 Plots of response time for GCR deployment under scenario A: elapsed time to complete requests (left); histrogram with distribution of response times (right); result data file: `GCR_Scenario_2_V1`.

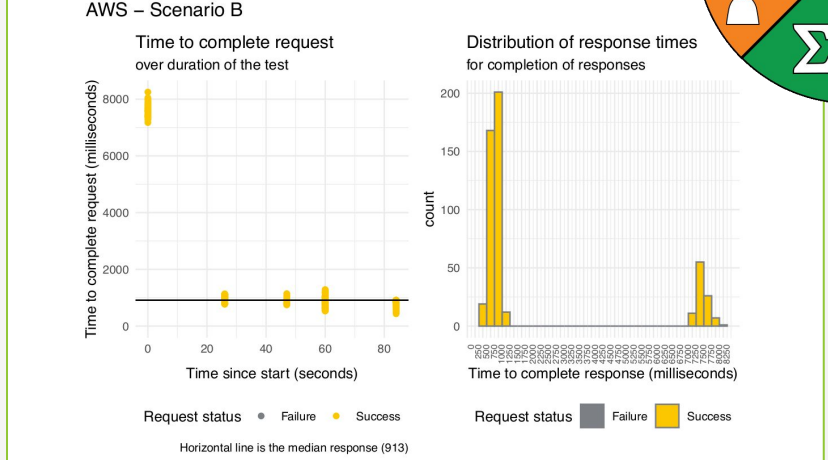
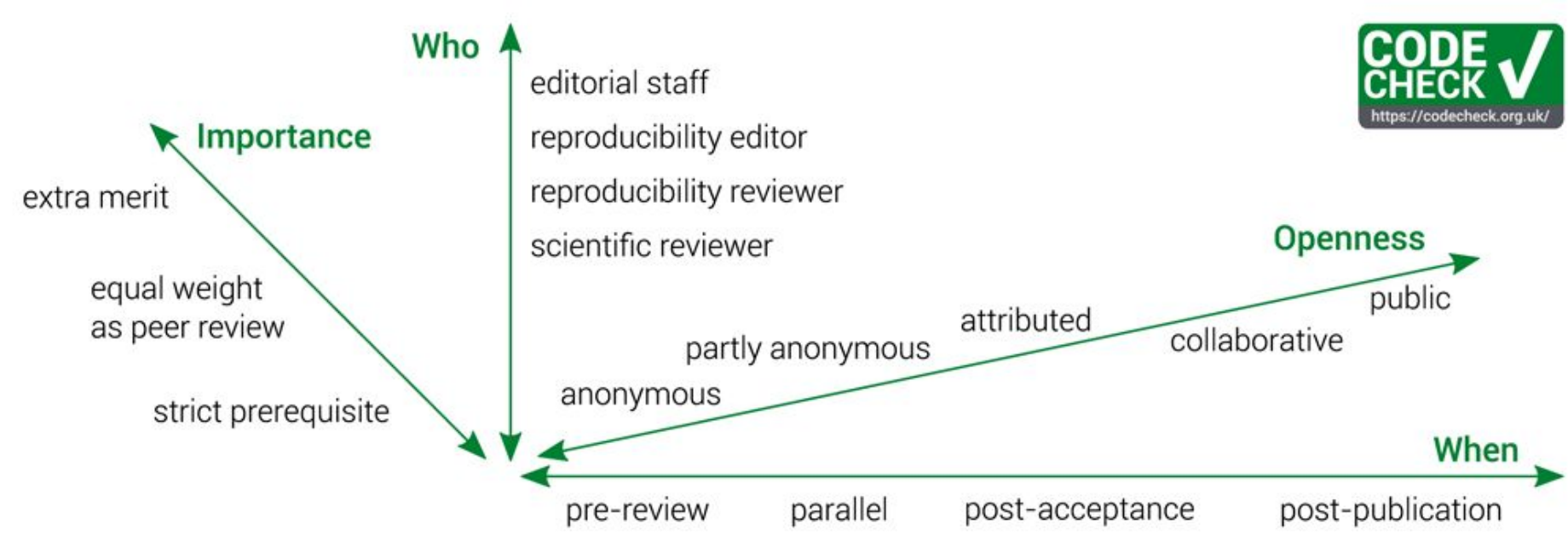


Figure 5 Plots of response time for AWS deployment in scenario A: elapsed time to complete requests (left); histrogram with distribution of response times (right); result data file: `AWS_Scenario_3_V2`.

CODECHECK


Who
editorial staff
reproducibility editor
reproducibility reviewer
scientific reviewer
CODE CHECK
https://codecheck.org.uk/
Importance
extra merit
equal weight as peer review
strict prerequisite
Openness
anonymous
partly anonymous
attributed
collaborative
public
When
pre-review
parallel
post-acceptance
post-publication

CODECHECK Experiences

Independent execution of computations underlying research articles.

30+ certificates

Several journals, one conference > ongoing contacts

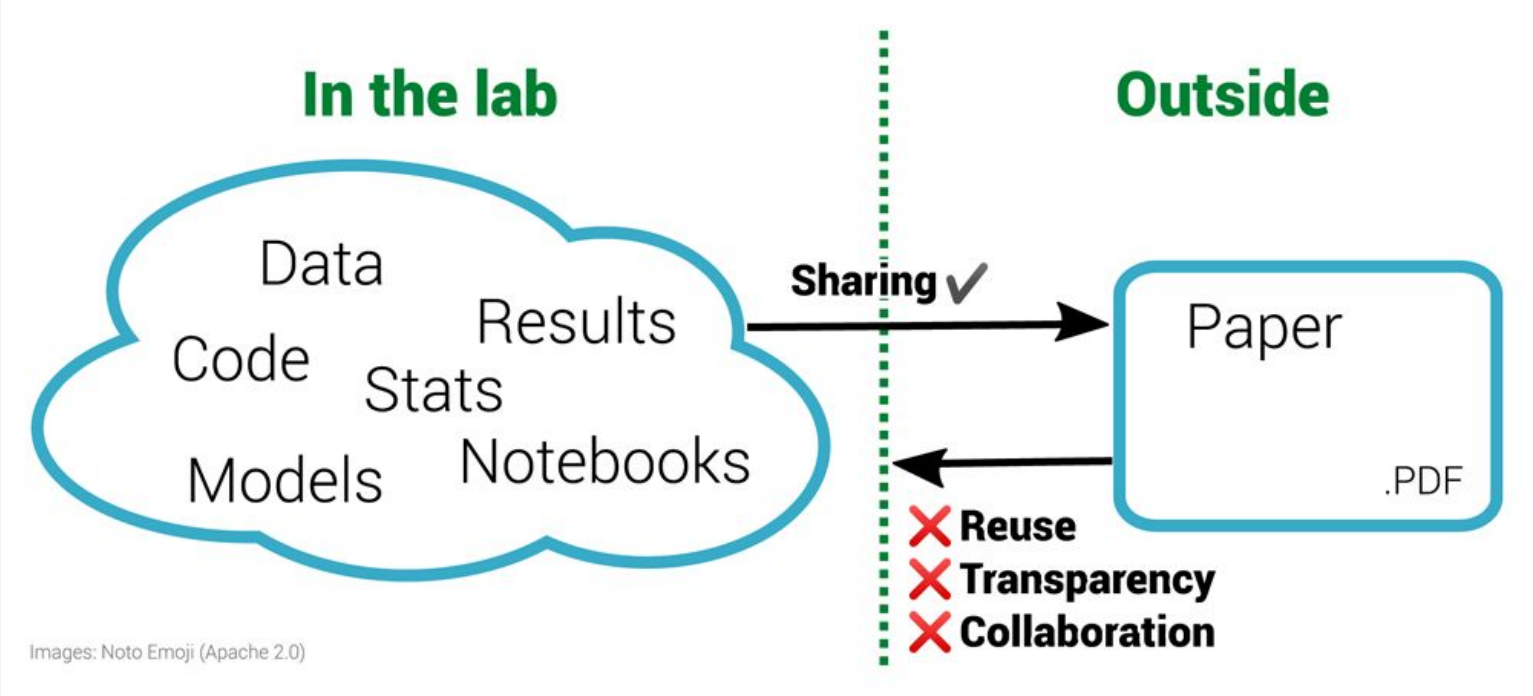
25+ codecheckers signed up, 1 check from not core team member

Next

Mentoring + practical experiences (ReproHack collaboration?), funding! (codechecks for diamond OA journals?)

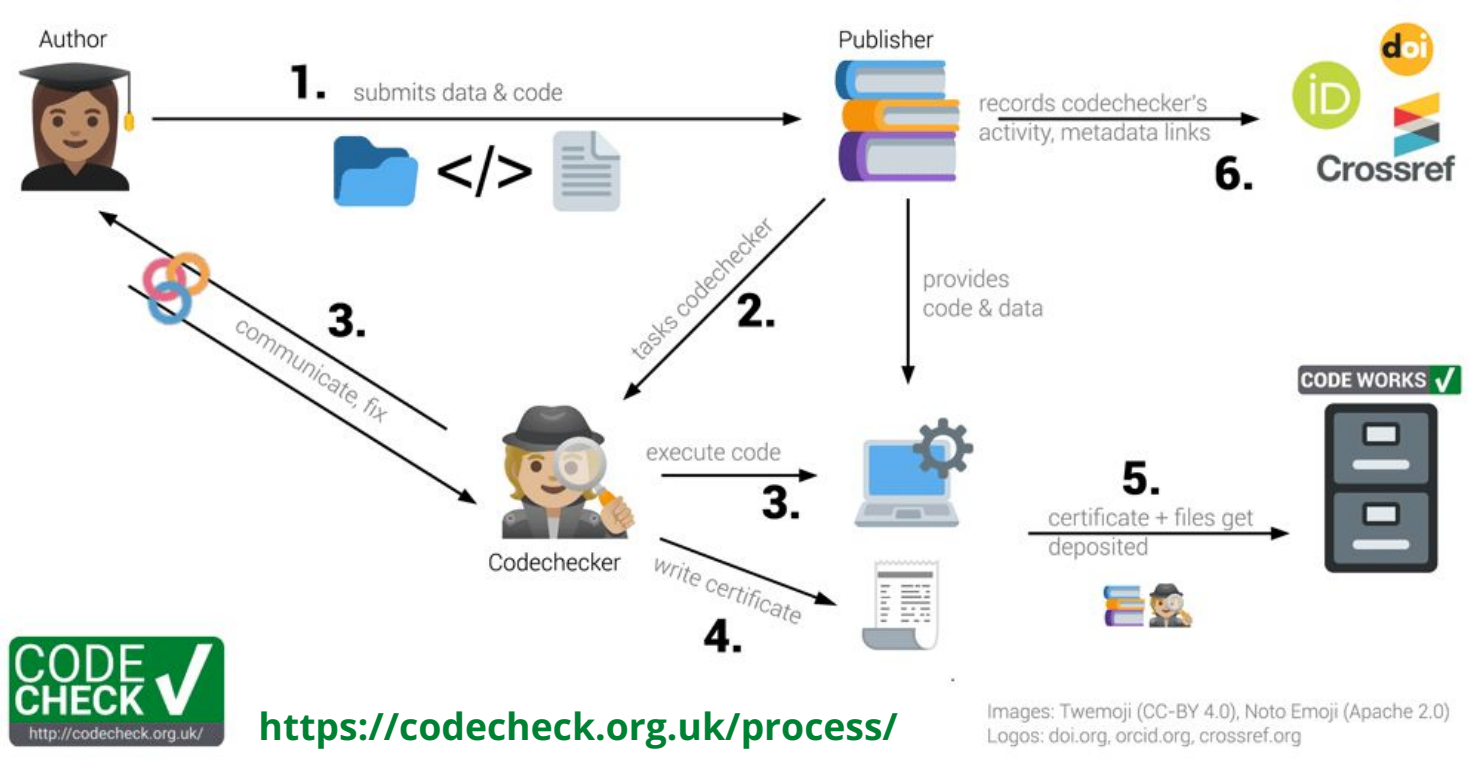
CODECHECK + R2S2 @ ITC: https://www.itc.nl/research/open-science/codecheck/

CODECHECK: The inverse problem in research



The inverse problem in reproducible research. Figure 1 of https://doi.org/10.12688/f1000research.51738.1

The left half of the diagram shows a diverse range of materials used within a laboratory. These materials are often then condensed for sharing with the outside world via the research paper, a static PDF document. Working backwards from the PDF to the underlying materials is impossible. This prohibits reuse and is not only non-transparent for a specific paper but is also ineffective for science as a whole. By sharing the materials on the left, others outside the lab can enhance this work.



The CODECHECK example process implementation. Figure 2 of https://doi.org/10.12688/f1000research.51738.1

The left half of the diagram shows a diverse range of materials used within a laboratory. These materials are often then condensed for sharing with the outside world via the research paper, a static PDF document. Working backwards from the PDF to the underlying materials is impossible. This prohibits reuse and is not only non-transparent for a specific paper but is also ineffective for science as a whole. By sharing the materials on the left, others outside the lab can enhance this work.

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

The AGILE guidelines

Reproducibility checklist

Author guidelines
Writing DASA section
Data in Research Papers
Computational workflows in Research Papers

Reviewer guidelines

Reproducibility reviewer guidelines

Background

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

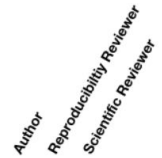
Website: https://osf.io/phmce/
Version: December 2020
DOI: 10.17605/OSF.IO/CB7Z8

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.



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.

Checklist & Writing the DASA section

REPRODUCIBILITY CHECKLIST

For all **datasets** included/produced in the paper, check if data:

- ❑ Is provided in a non-proprietary format
- ❑ Is documented for third parties to reuse
- ❑ Is accessible in a public repository and has an open data licence

For all **software tools/libraries/packages** and **computational workflows** included/produced, check if:

- ❑ Reproduction steps are explained in a README (plain text file), flowchart, or script
- ❑ Computational environments (including hardware) are documented or provided
- ❑ Versions of relevant software components (libraries, packages) are provided
- ❑ All parameters and expected execution times for the computational workflow are provided
- ❑ Software developed by the authors is available in a public repository and has an open licence
- ❑ There is a clear connection between **tables, figures, maps, and statistical values** and the data and code that they are based on, e.g., using file names or documentation in the README

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

- ❑ Data and software statements (see examples below)
- ❑ The reasons, if any, for not being able to share (parts of) data or code

For all **data and software** check that:

- ❑ All datasets and code (used or mentioned) are assigned DOIs
- ❑ Datasets and code are cited throughout the paper

After acceptance in the **camera-ready paper** check that:

- ❑ If data has been shared privately or anonymously for peer review, they are updated with all metadata and accessible via a DOI and referenced from the paper
- ❑ If a reproducibility review report will be published for your paper, a DOI URL in the Data and Software Availability section is included using the following template:
  A reproducibility report for this paper is available confirming that [considerable parts of the computational workflow / all results / Figures 1 and 4] could be independently reproduced, see https://doi.org/link_to_report.

WRITING THE DATA AND SOFTWARE AVAILABILITY SECTION

The DASA section provides references to where data, software and documentation is available (e.g., paper section or README file) and under what conditions (e.g., copyright, licenses or access procedures for protected data). It should be concise and contain persistent links to repositories using Digital Object Identifiers[7] (DOI). You may remove links for anonymity during peer review ("xxx"), or share anonymized links[8] if your repository supports them. Data, software and (third-party) tools should be cited following recommended citation or standard citation guidelines. Possible statements for the DASA section are provided below. You may include one of these statements or draft your own.

Statements for non-computational or conceptual work

No data or code was collected, developed, or used in this work.

The full list of reviewed literature is available at [link to attachment or citable deposit of bibliography].

The full concept maps are available at [link] *and the ideas were first sketched in a blog post at* [link].

Research data/code supporting this publication ...

… is available in [name of the repository(-ies)] *and is accessible via the following DOI* [DOI link(s)]

… was accessed on [date of dataset access/download] *with the following* [query parameters, if applicable] *under the license* [dataset license].

… was downloaded manually using the services at [name of organisation] *(using a departmental subscription for costs) and* [name of organisation]. *The compiled dataset cannot be redistributed due to licensing restrictions.*

...is not available due to [indicate reasons, e.g., licenses, sensitive data on human subjects, privacy statements; if there are processes to obtain the data, describe them].

The computational workflow supporting this publication ...

… is executed via [choose, e.g., a single command/file, a workflow management software, a set of numbered scripts] *published under license* [the license] *at* [DOI of repository].

… is published in a [language] *module/package at* [link of software project]. *The used version is archived at* [DOI of repository].

… is provided as a [container/VM] *published at* [DOI of repository] *with instructions included in the file README.md in the repository.*

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

The guidelines for data

"What if…"

Examples

INCLUDING DATA IN RESEARCH PAPERS

	Minimum requirements	Recommended practices
What?	• All input data and configuration • Data description/documentation, including provenance, field or column types, etc. • If data is retrieved from an external source, documentation on collection queries and download steps	• Standardised, discipline-specific metadata[8] and ontologies to describe your data • Data download scripts
Where?	• Publish data in a public repository providing a DOI • Cite data (including date and version) in the paper	• Discipline- or data type-specific repository[9] • Include recommended citation in dataset description (unless already provided by repository) • Create a registration for OSF projects[10] and use the DOI to cite it
How?	• Use open data formats; export from proprietary format for publication • Specify the license	• Use plain text-based file formats

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

The guidelines for computational workflows

INCLUDING COMPUTATIONAL WORKFLOWS IN RESEARCH PAPERS

	Minimum requirements	Recommended practices
What? Computational environment	• Describe the used environment and computational infrastructure, e.g., hardware specs, operating system • List software versions • Cite used software[14]	• Provide the actual environment, e.g., a Dockerfile + container[15] or a Virtual Machine (e.g., using OSGeo-Live) • Provide a pinned freeze of your dependencies (structured configuration files with dependency information) • Add a colophon or "reproducibility receipt"[16] to your notebooks • Installation and execution instructions for different operating systems
Computation steps	• Document the detailed steps in a text file and/or flowchart (every action/click) • Document expected execution times given computing power unless negligible • Ask a colleague to try out the instructions	• Scripts/models and a README file that explains their use • All figures are fully scripted and a peer has read your README's instructions (incl. interactive visualisations and interactive adjustments • Multi-panel plots are composited with scripts[17] • Software package with structured metadata[18], tests/CI[19], and a pipeline framework[20] or workflow language[21] • Live documents for analyses, e.g., Binder[22] • Live demo of APIs/online applications (e.g., anonymous cloud resources, such as Google Cloud Run or AWS) • Subset or a synthetic dataset for quick evaluation
Where?	• Repository providing a persistent identifier, e.g., a DOI or SWHID[23]	• Versioned code repository, such as GitHub or GitLab, and ongoing open development
How? Tools used	• Use generally available tools (avoid proprietary tools that are not available to reviewers and other researchers)	• Use and create Open Source tools • Cite core modules/tools/language used
Development practices	• Use clear licenses[24] that fit your environment • Follow one of "Good enough practices in scientific computing"[25]	• Follow all "Good enough practices.." Use development guidelines for your environment / language of choice (e.g., for R[26])

REPRODUCIBLE AGILE

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

WWU MÜNSTER

Scientific reviewer guidelines… concerning the reproducibility review only!

REPRODUCIBLE AGILE

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

SCIENTIFIC REVIEWER GUIDELINES

This section clarifies the expectations and role of the scientific reviewer with respect to the reproducible paper guidelines. For information for the Reproducibility Reviewer, please see the following section.

Reproducibility is considered good scientific practice that provides input for the quality assessment of a paper. Therefore, reviewers of AGILE papers should be aware of the **author guidelines on reproducibility** and be familiar with the **reproducibility checklist**, as well as the expected content of the **mandatory data and software availability section.** Using this information, reviewers should evaluate the plausibility and completeness of the data and software availability documentation, and whenever possible and readily available **include feedback on reproducibility aspects** in their comments. Scientific reviewers are free to but **are not expected to attempt reproductions of computations**.

Data and software availability documentation provide an additional set of information for assessing the quality of research presented in a manuscript. Reviewers are asked to know about the AGILE reproducible paper guidelines and to consider the level of reproducibility reached in a manuscript. To do so, they shall assume the position of someone who would like to reproduce the submitted work to assess whether the provided material is likely to allow reproduction of the submitted work. Based on this impression, reviewers may challenge authors regarding the level of reproducibility reached, if any statements are made regarding reproducibility in a manuscript.

Scientific reviewers are not required to actually reproduce a manuscript, but, if the data and code are provided in an anonymous format, and if a reviewer attempts to reproduce all or parts of the submitted work, then they are asked to document the process and outcomes (see Reproducibility Reviewer Guidelines below). Please reach out to the reproducibility chair if you are keen on conducting a reproducibility review for a paper you are reviewing.

The peer review of AGILE papers is a fully anonymous peer review, i.e. authors and reviewers do not know each other's identity. Reviewers should be supportive to authors and consider potential limitations in access to resources due to anonymisation. Since the provision of information to help reproduction of a paper can accidentally lead to disclosure of an author's identity, the reviewers should not use any such additional information to the disadvantage of the authors. The reviewers' comments provided to the authors are expected to be neutral[28] and contribute to improved reproducibility of the reported findings.

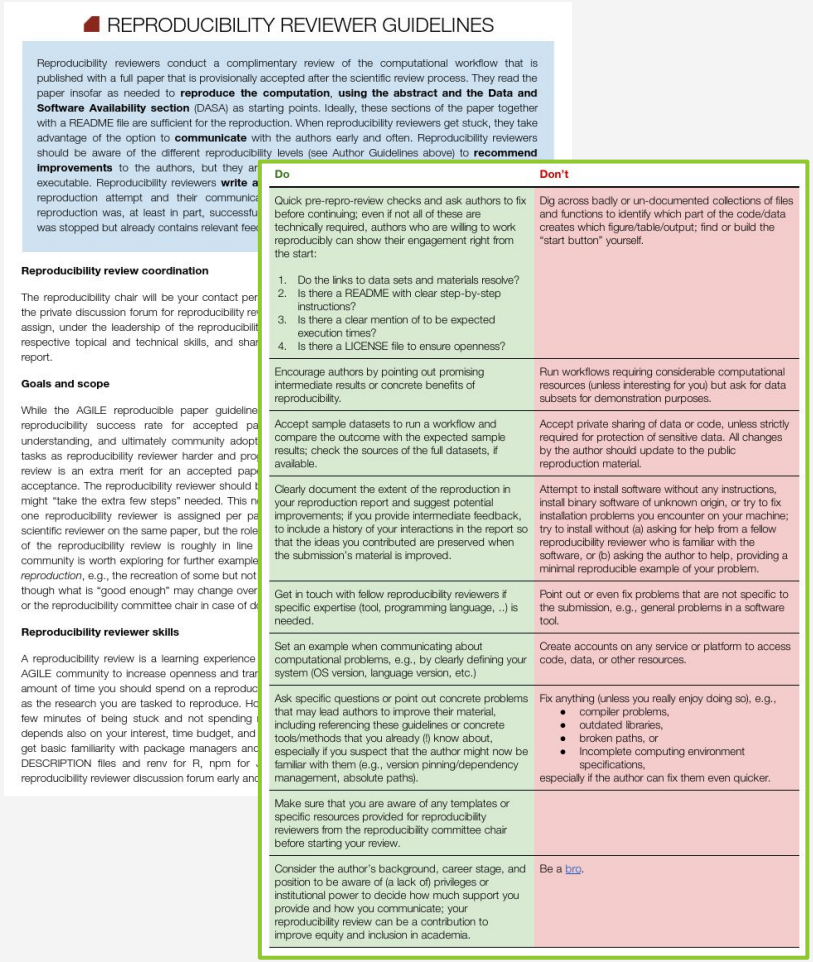
The guidelines for reproducibility reviewers

Ideal vs. realistic

Role & skills

Examples for “Do’s and Don’ts”:

- Do shift burden to author
- Do encourage and s
- Private data/code sharing last resort
- Document your work in report (impact)
- Be kind (career stage, knowledge, privileges)
- No rummaging



REPRODUCIBILITY REVIEWER GUIDELINES

Reproducibility reviewers conduct a complimentary review of the computational workflow that is published with a full paper that is provisionally accepted after the scientific review process. They read the paper insofar as needed to **reproduce the computation**, **using the abstract and the Data and Software Availability section** (DASA) as starting points. Ideally, these sections of the paper together with a README file are sufficient for the reproduction. 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 reproducibility levels (see Author Guidelines above) to **recommend improvements** to the authors, but they ar
executable. Reproducibility reviewers **write a**
reproduction attempt and their communic
reproduction was, at least in part, successfu
was stopped but already contains relevant fee

Reproducibility review coordination

The reproducibility chair will be your contact per
the private discussion forum for reproducibility re
assign, under the leadership of the reproducibilit
respective topical and technical skills, and shar
report.

Goals and scope

While the AGILE reproducible paper guideline
reproducibility success rate for accepted pa
understanding, and ultimately community adopt
tasks as reproducibility reviewer harder and pro
review is an extra merit for an accepted pap
acceptance. The reproducibility reviewer should b
might “take the extra few steps” needed. This n
one reproducibility reviewer is assigned per pa
scientific reviewer on the same paper, but the role
of the reproducibility review is roughly in line
community is worth exploring for further example
reproduction, e.g., the recreation of some but not
though what is “good enough” may change over
or the reproducibility committee chair in case of d

Reproducibility reviewer skills

A reproducibility review is a learning experience
AGILE community to increase openness and tra
amount of time you should spend on a reproduc
as the research you are tasked to reproduce. Ho
few minutes of being stuck and not spending
depends also on your interest, time budget, and
get basic familiarity with package managers and
DESCRIPTION files and renv for R, npm for
reproducibility reviewer discussion forum early and

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? 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, 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., • compiler problems, • outdated libraries, • broken paths, or • Incomplete computing environment specifications, especially if the author can fix them even quicker.
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 reproducibility review can be a contribution to improve equity and inclusion in academia.	Be a bro.

Review process

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

Process documentation:
https://osf.io/7rjpe/

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!)

Reproducibility Reports

Published on OSF with a DOI
Title page, cites the paper

Paper links to report via URL (no citation)

Automatically added to ORCID profile

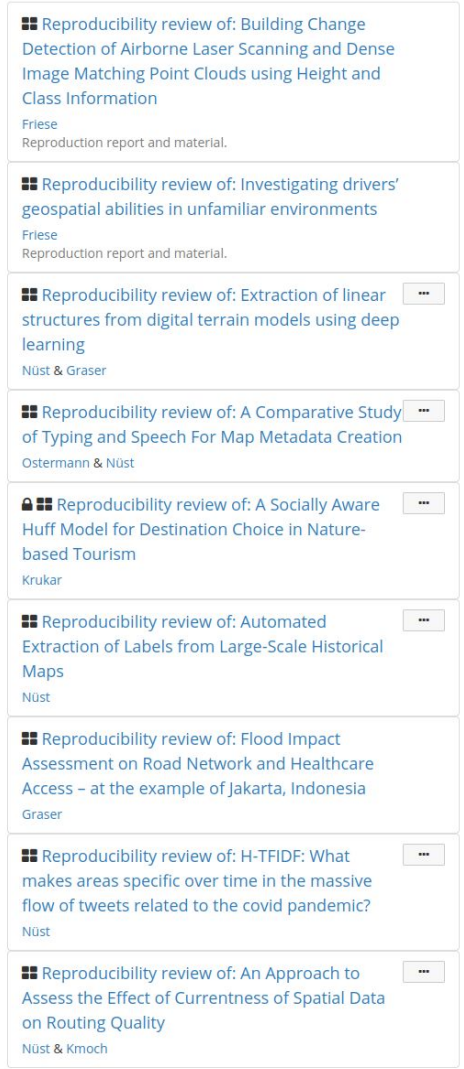
Reproducibility review results 2021

9 reproducibility reports published (2020: 6)

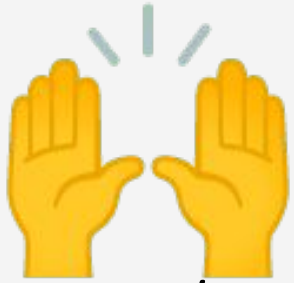
- no starting point in the paper
- documentation insufficient for third party

8 not reproducible:

- conceptual papers
- data not shared (choice, licence)
- code not shared (choice) or proprietary software (repro reviewer matching failed)



https://osf.io/h64sd/



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

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

Next steps for reproducible AGILE

Do it again in 2022 🎉

Grow reproducibility reviewer team

Opportunity ECRs (mentoring/workshops/…)

Continue discourse (meaning of rprdcblty)

Re-assess new papers > impact?

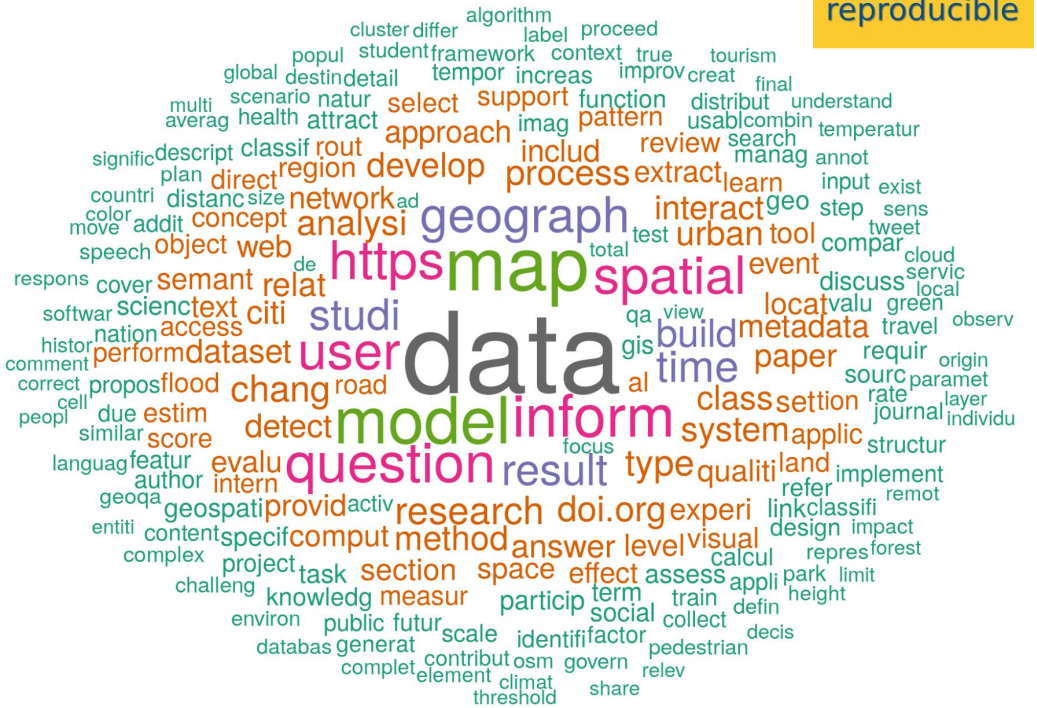
Towards opening scholarship

Scope, requirements, acceptance condition?

Open review if tenured? Format-free first submission

CRediT

Phase out when standard practice...



Word-stem cloud of all AGILE 2021 submissions (full/short/poster & accepted/rejected)

Reproducible AGILE and CODECHECK: Highlights of Lessons learned

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

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 and 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

Concepts, metaphors, memes

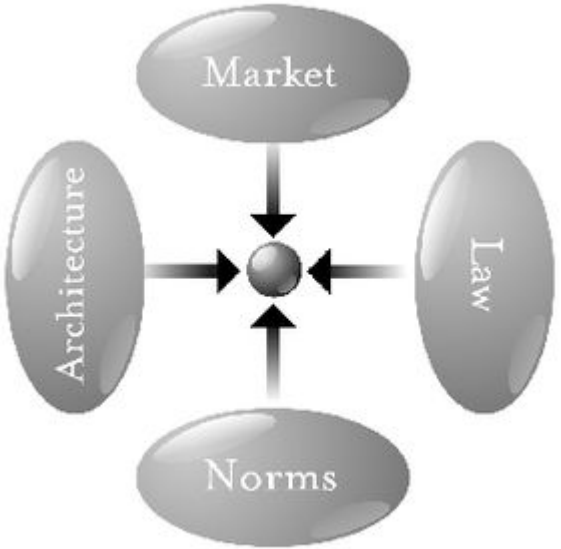
Lessig's pathetic dot theory

Law
policies, sanctions

Social norms
community enforcement

Markets
supply & demand > price of items & behaviours

(Social) Architecture
Made or found features & properties & infrastructure (biology, physics, major social/cultural forces); constraints



https://en.wikipedia.org/wiki/Pathetic_dot_theory

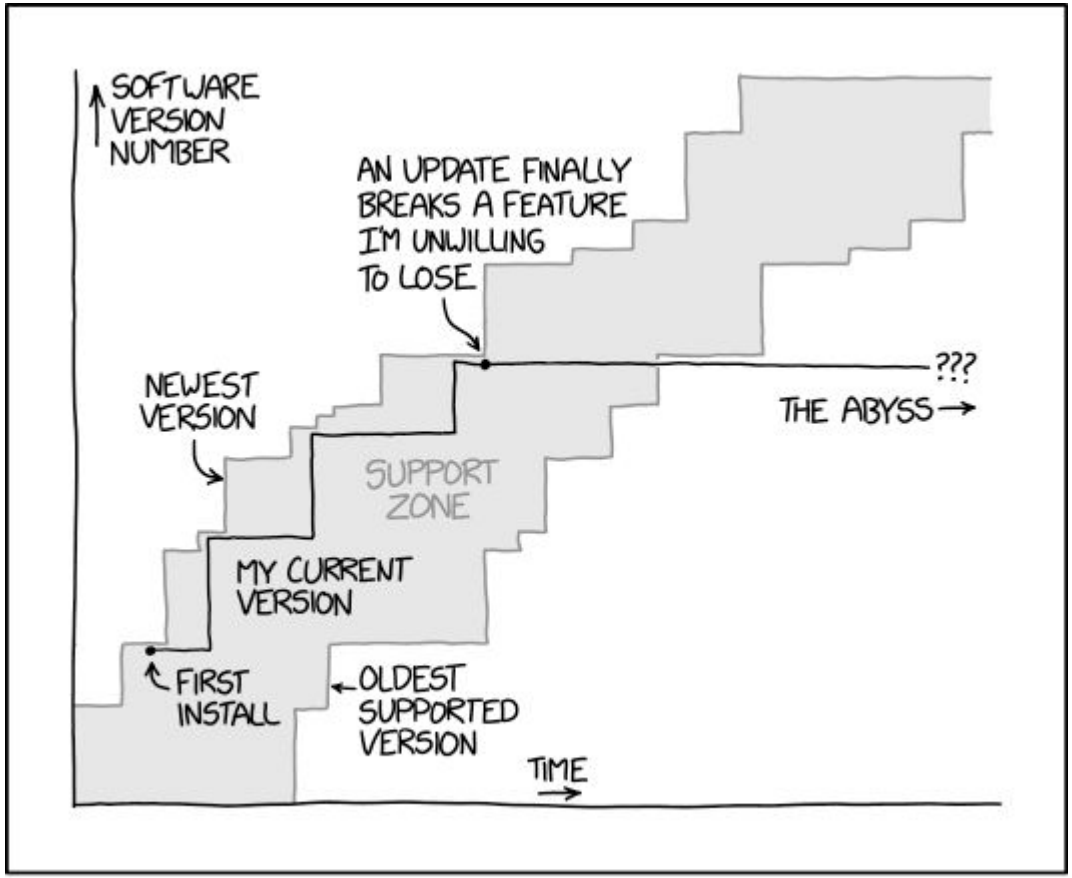
Theory of regulation, applied to internet *but also fitting scholarly communication* > unlike real world, architecture (= code) is created and controlled by humans resp. *scientists*, yet still are a force on our behaviour.

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.

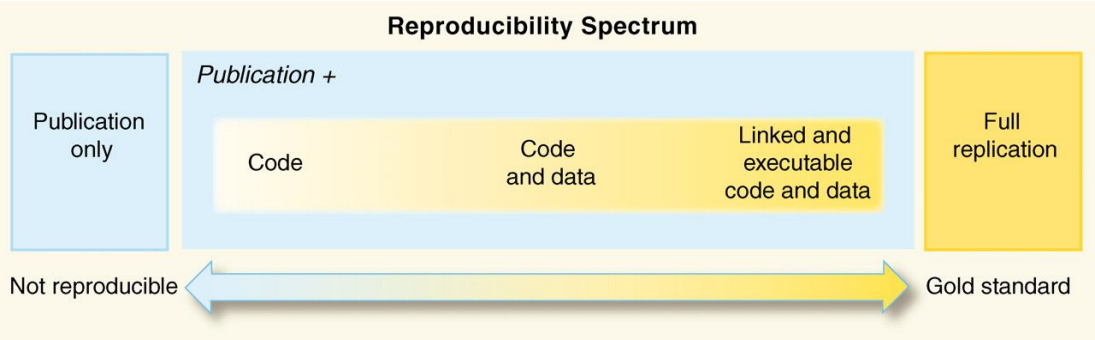
via https://twitter.com/snet_jklump/status/1141934045820887040?s=09

http://phdcomics.com/comics.php?f=1689

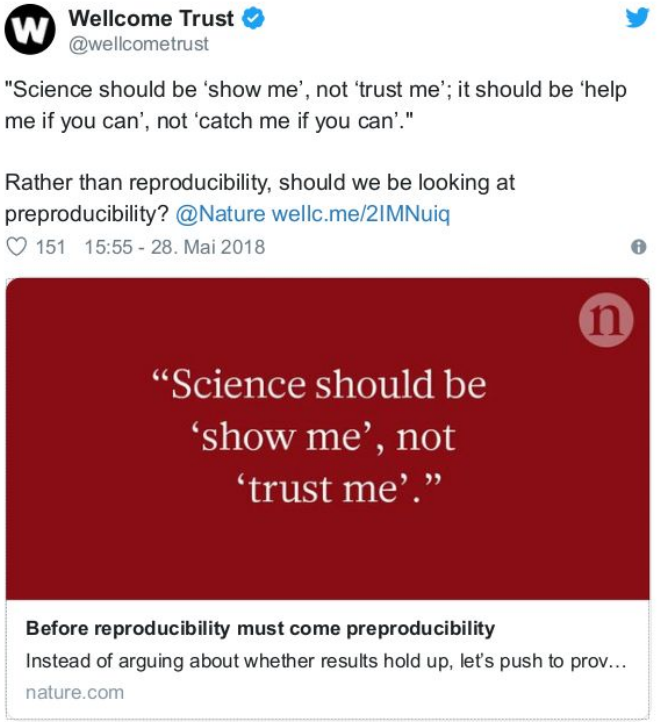


https://xkcd.com/2224/

Reproducibility Spectrum & Preproducibility



https://doi.org/10.1126/science.1213847



https://www.nature.com/articles/d41586-018-05256-0

Traditional and modern scientists

https://en.wikipedia.org/wiki/T-shaped_skills

https://doi.org/10.1007/s10816-015-9272-9

https://jakevdp.github.io/blog/2014/08/22/hacking-academia/
https://www.sciencemag.org/careers/2013/05/when-all-science-becomes-data-science
https://escience.washington.edu/community-level-data-science-and-its-spheres-of-influence-beyond-novelty-squared/

http://dx.doi.org/10.1190/1.1822162

RE1.3

Electronic Documents Give Reproducible Research a New Meaning

Jon F. Claerbout and Martin Karrenbach, Stanford Univ.

SUMMARY

A revolution in education and technology transfer follows from the marriage of word processing and software command scripts. In this marriage an author attaches to every figure caption a pushbutton or a name tag usable to recalculate the figure from all its data, parameters, and programs. This provides a concrete definition of reproducibility in computationally oriented research. Experience at the Stanford Exploration Project shows that preparing such electronic documents is little effort beyond our customary report writing; mainly, we need to file everything in a systematic way.

In [redacted] we began experimenting with electronic documents that merge our scientific software with our word-processing software. A year later we manufactured a CD-ROM containing a new textbook, Joe Dellinger's doctoral dissertation, and two progress reports of the Stanford Exploration Project. We distributed these CD-ROMs[1] to sponsors and many friends at the [redacted] SEG meeting.

In [redacted] we set this sequence of goals:

- Learn how to merge a publication with its underlying computational analysis.
- Teach researchers how to prepare a document in a form where they themselves can reproduce their own research results a year or more later by "pressing a single button".
- Learn how to leave finished work in a condition where coworkers can reproduce the calculation including the final illustration by pressing a button in its caption.

In [redacted] we set this sequence of goals:

- Learn how to merge a publication with its underlying computational analysis.
- Teach researchers how to prepare a document in a form where they themselves can reproduce their own research results a year or more later by "pressing a single button".
- Learn how to leave
coworkers can repr
final illustration by
- Prepare a complete
ment so that gradu
away with them t
reproduce their Sta
- Merge electronic d
thors (SEP reports
- Export electronic
(sponsors) so they
portion of our Star

We met all these goals a

- produce all new documents in this form, including lab reports in formal classes and "lab notebooks" of research progress.

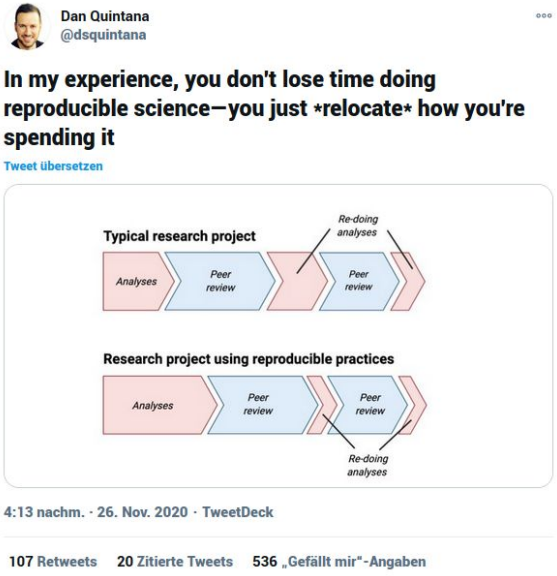
CD-ROM, at 680 megabytes, is so large we have

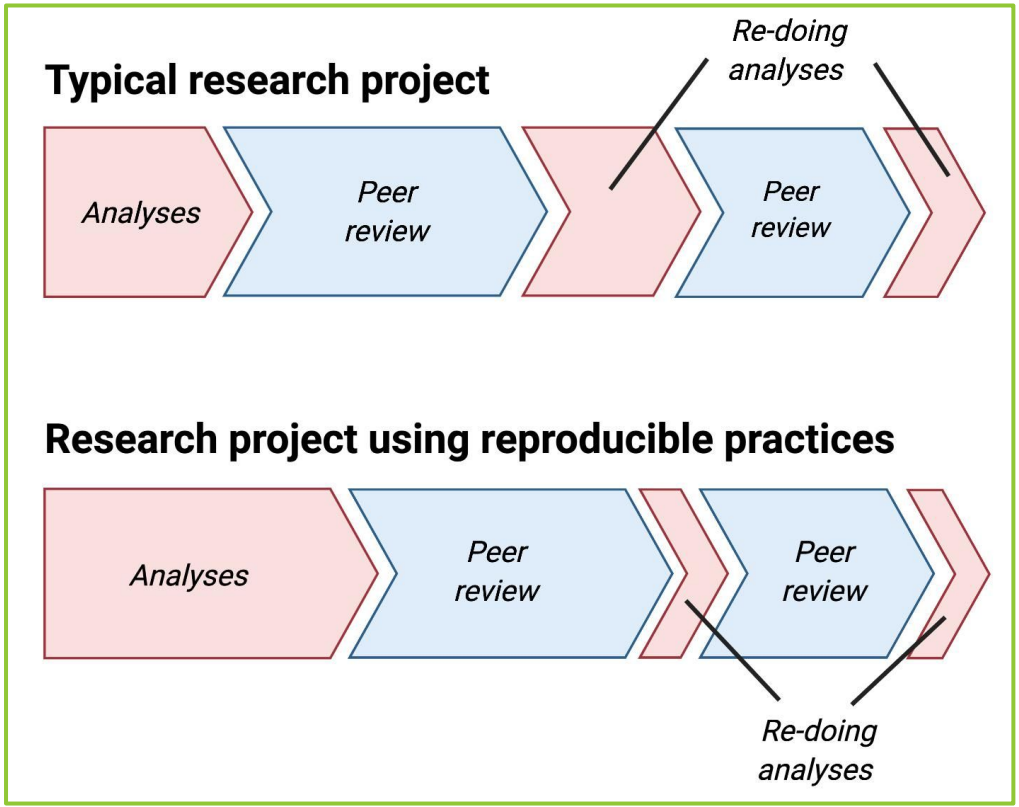
1992

We met all these goals and set new ones:

- produce all new documents in this form, including lab reports in formal classes and "lab notebooks" of research progress.
- make incremental improvements in electronic-document software
- seek partners for broadening standards (and making incremental improvements).

Reproducibility is “more work”?





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**

RSEng = create research software
RSEs = people behind research softw
RSEs ≠ IT !!!

Reproducibility guru dives deeply into manifold software and tools to make his research reproducible and develops his own software in a sustainable way.

Researcher uses scripts for data analysis and needs working stable software for her work. She learns what is necessary to achieve her research goals.

”Software is 95% human and only 5% code” *

Person for tough problems knows how to solve all kinds of computer-related issues; he was not hired for that, but enjoys to help and spends time to get to the bottom of other people’s challenges.

Software developer was hired to implement software for a research project and contributes to large collaborative software projects to realise the next generation of digital infrastructure for science.

Geek writes software as part of her research project and would like to code more, but must keep an eye on her career in science and needs to write papers.

* Eric Albers, CCC2019, https://media.ccc.de/v/thms-49-ber-die-nachhaltigkeit-von-software | Bilder © H. Seibold, S. Janosch, OSD2019

Professionalisation

≠

Images: https://pxhere.com/en/photo/477458 https://pxhere.com/en/photo/1087259 https://pxhere.com/en/photo/703106 https://pxhere.com/en/photo/103038


EDUCATION OF
CONDITIONS FOR
DEVELOPERS
RESEARCHERS USING
BETTER
SOFTWARE
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RESEARCH

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Sylvain Deville

Freezing
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@DevilleSy

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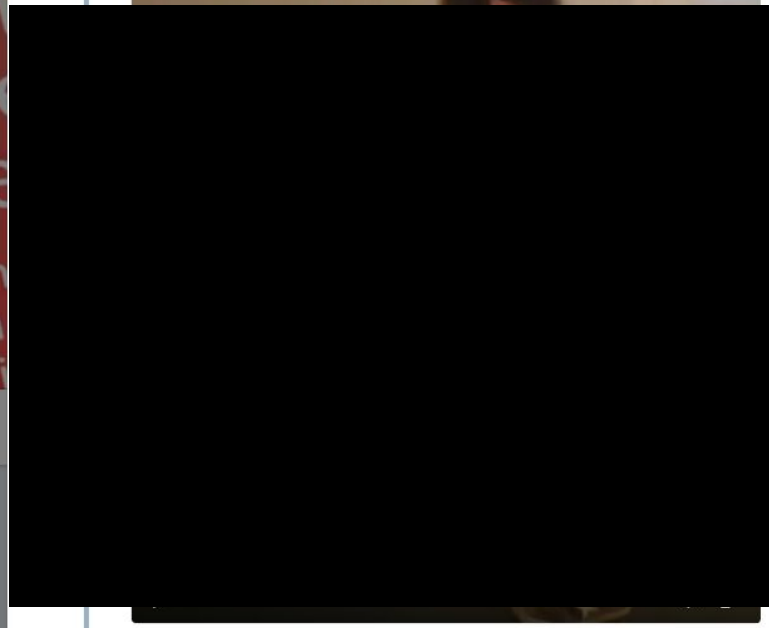
France

sylvaindeville.net

Sylvain ❄️👨‍🎓
@DevilleSy

Follow

When you try to replicate a paper using the methods section



9:56 AM - 31 Jan 2018

2,605 Retweets **5,877** Likes

54 2.6K 5.9K

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https://twitter.com/DevilleSy/status/958761021421903872

Code review, journals, crisis

Code Review != Reproduction/Reproducibility 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

Reproducible computational research in journals & conferences

ACM Transactions on Mathematical Software

SC19 PROGRAM

Reproducibility Initiative

Journal of Statistical Software

ReproZip

Biostatistics

NEURAL INFORMATION PROCESSING SYSTEMS

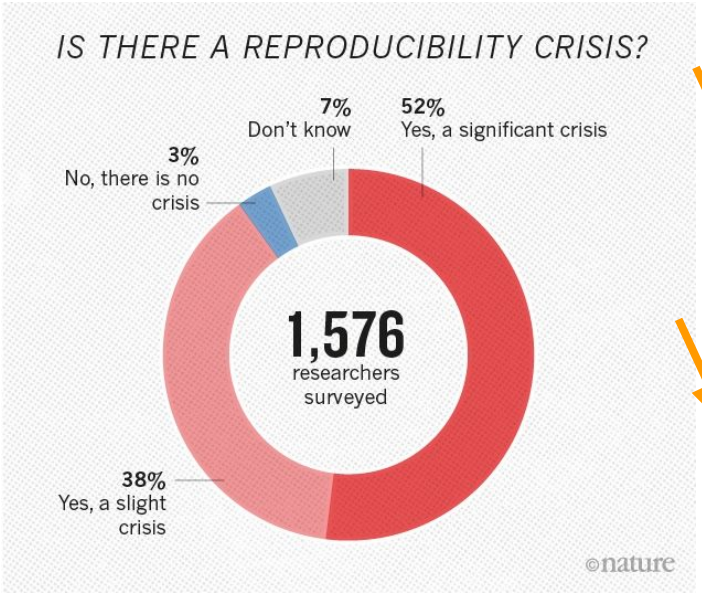
https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970

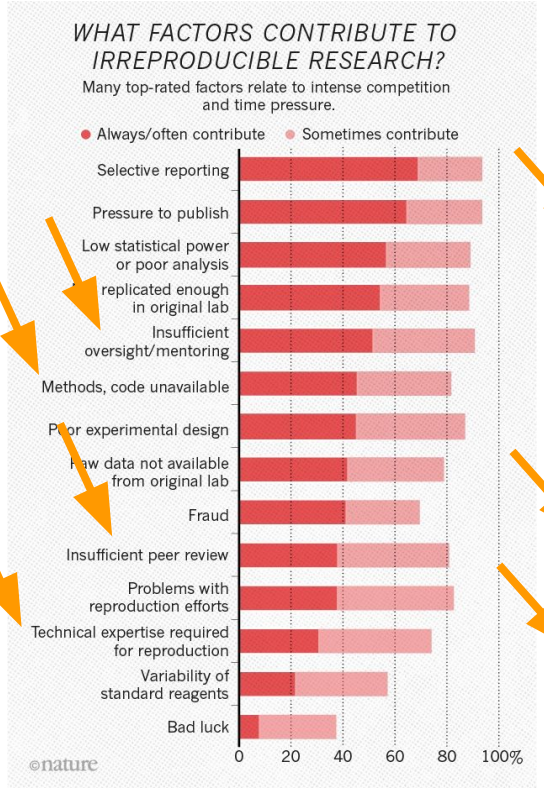
1,500 scientists lift the lid on reproducibility

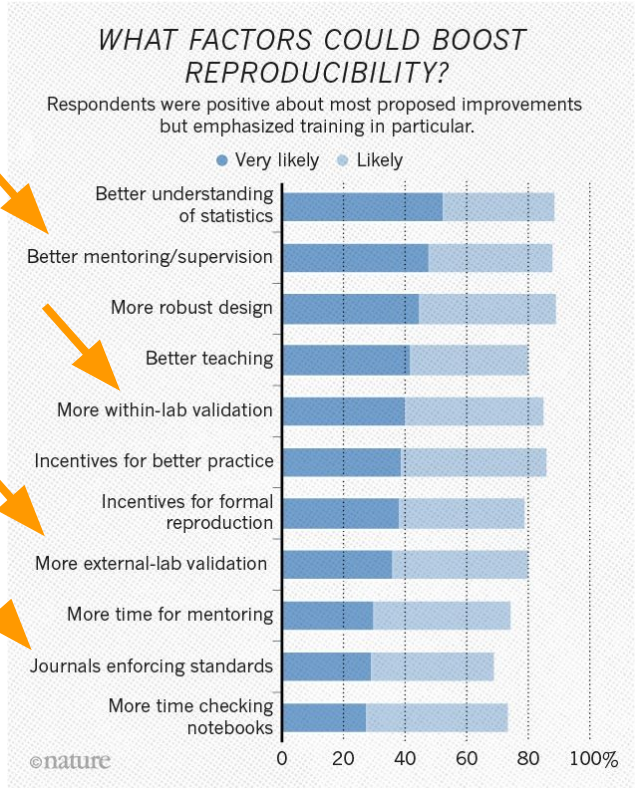
Survey sheds light on the 'crisis' rocking research.

Monya Baker

https://www.youtube.com/watch?v=j7K3s_vi_1Y

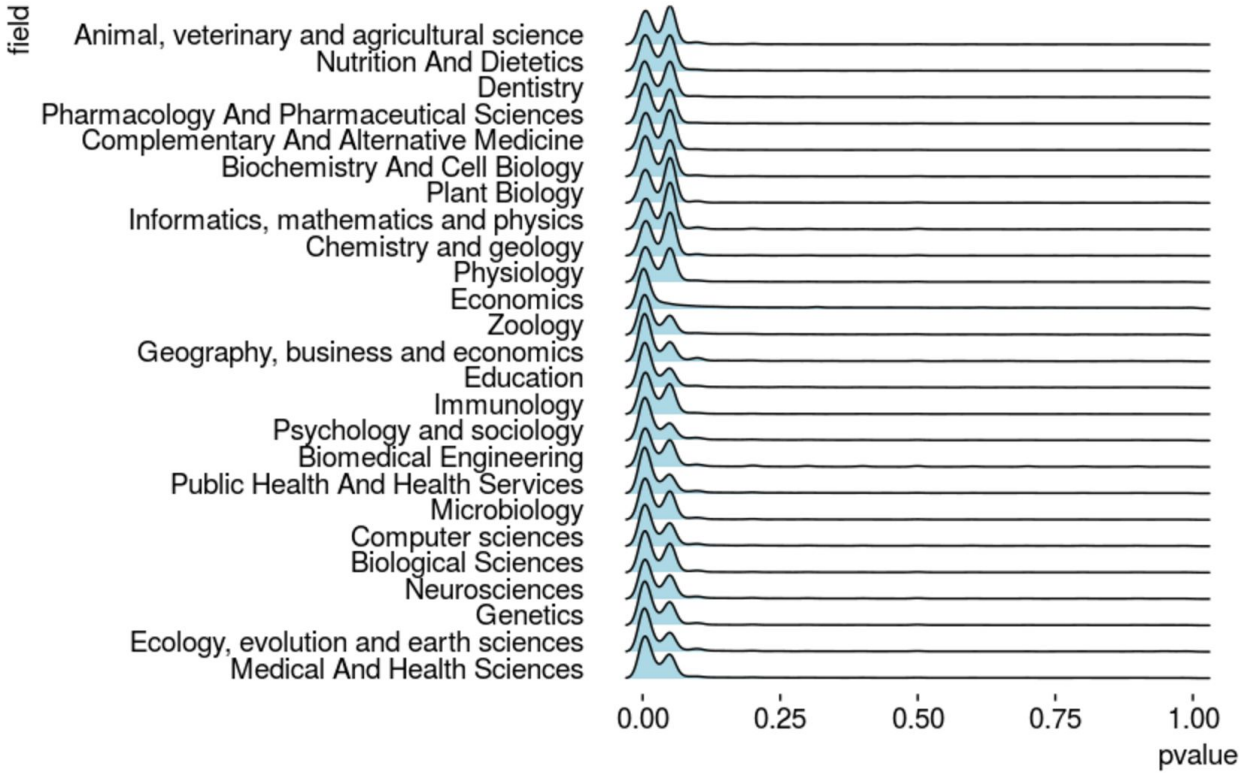






J. Leek's tidypvals

The tidypvals package is an effort to find previous collections of published p-values, synthesize them, and tidy them into one analyzable data set. The currently available p-value data sets in this package are:



"Notice Anything funny?"

https://**simplystatistics.org**/2017/07/26/announcing-the-tidypvals-package/

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

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

nature International weekly journal of science

Publish your computer code: it is good enough

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.

https://doi.org/10.1038/467753a

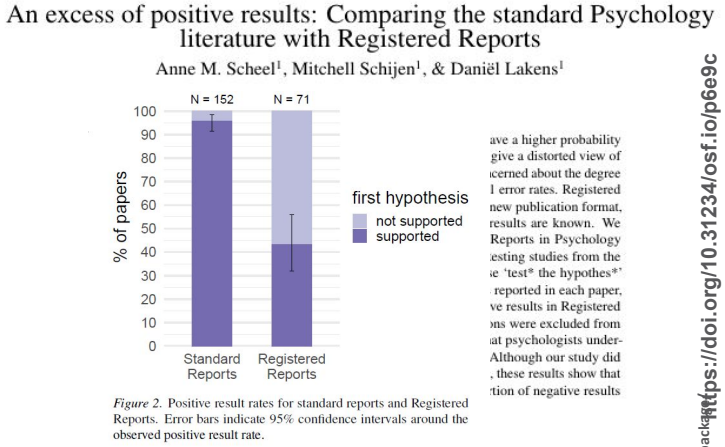
Structural challenges

Metrics for acknowledging/measuring impact in science **are broken** (impact factor, ..) and they lead to publication bias, HARKing, p-Hacking, intransparency and lack of reproducibility

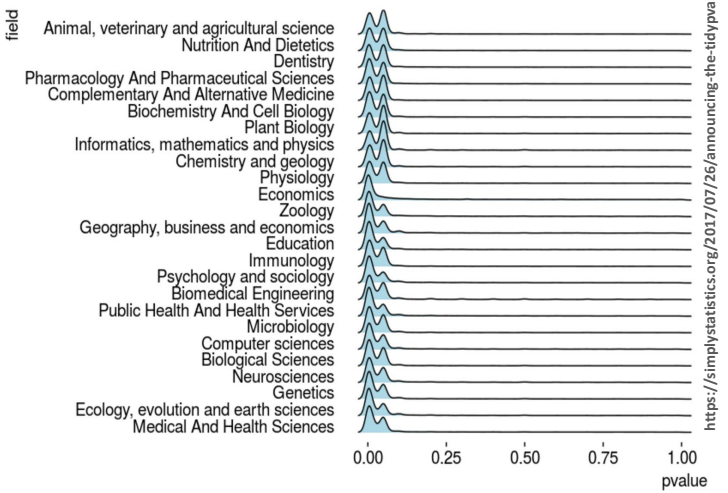
Leiden Manifesto: **http://www.leidenmanifesto.org**
DORA: **https://sfdora.org**
Vienna Principles: **https://viennaprinciples.org**

Acknowledging data and software as valuable products of research (instead of shoehorning software into papers)

http://doi.org/10.5334/dsj-2020-003



https://doi.org/10.31234/osf.io/p6e9c

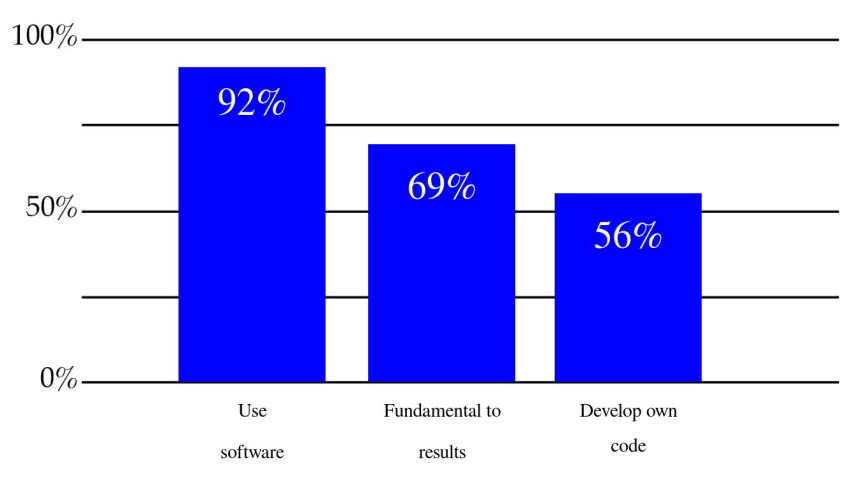


https://simplystatistics.org/2017/07/26/announcing-the-tidypvals-package/

Motivation for RSE

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”



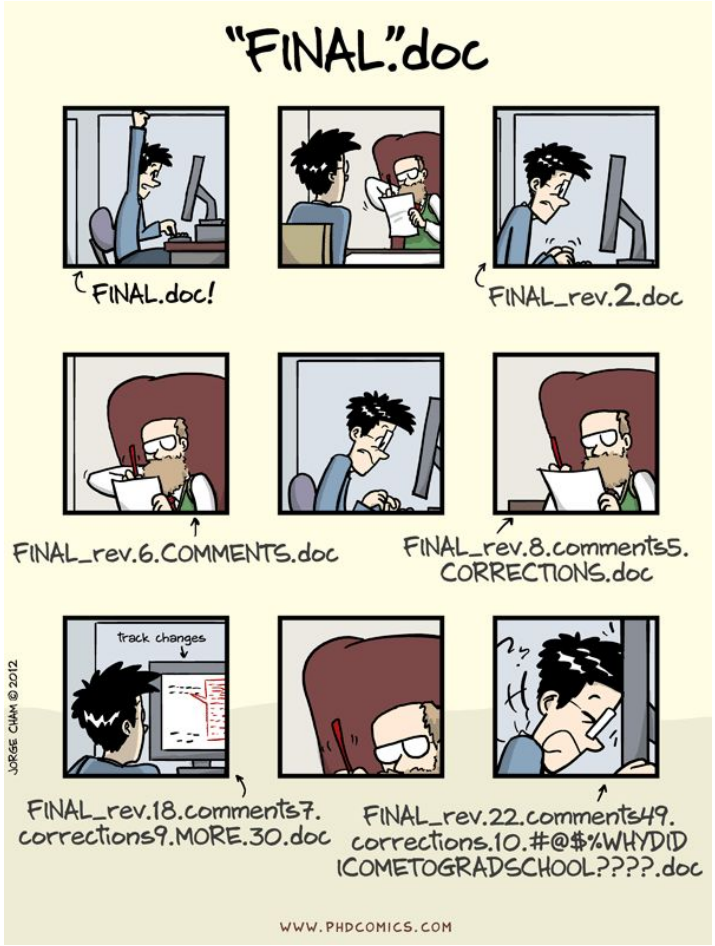
https://www.software.ac.uk/blog/2014-12-04-its-impossible-conduct-research-without-software-say-7-out-10-uk-researchers

Motivation for RSEng

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.”

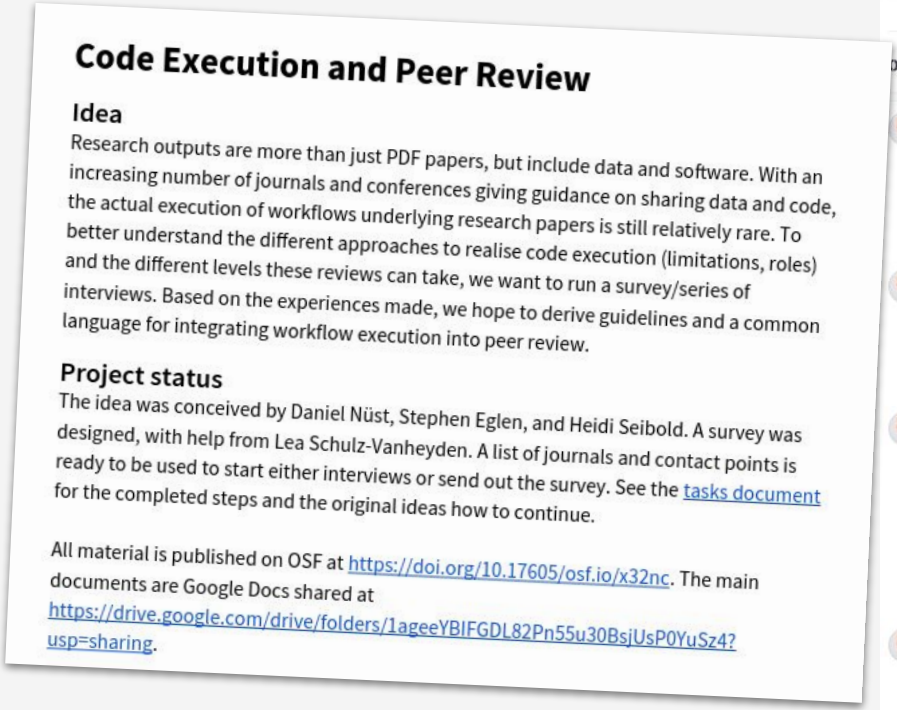
[2] Nangia, Udit; Katz, Daniel S. (2017): Understanding Software in Research: Initial Results from Examining Nature and a Call for Collaboration. doi:**10.1109/eScience.2017.78**



http://phdcomics.com/comics/archive.php?comicid=1531

Learn more about code execution practices at journals and conferences

osf.io/x32nc



Code Execution and Peer Review

Idea

Research outputs are more than just PDF papers, but include data and software. With an increasing number of journals and conferences giving guidance on sharing data and code, the actual execution of workflows underlying research papers is still relatively rare. To better understand the different approaches to realise code execution (limitations, roles) and the different levels these reviews can take, we want to run a survey/series of interviews. Based on the experiences made, we hope to derive guidelines and a common language for integrating workflow execution into peer review.

Project status

The idea was conceived by Daniel Nüst, Stephen Eglen, and Heidi Seibold. A survey was designed, with help from Lea Schulz-Vanheyden. A list of journals and contact points is ready to be used to start either interviews or send out the survey. See the tasks document for the completed steps and the original ideas how to continue.

All material is published on OSF at https://doi.org/10.17605/osf.io/x32nc. The main documents are Google Docs shared at https://drive.google.com/drive/folders/1ageeYBIFGDL82Pn55u30BsjUsP0YuSz4?usp=sharing.

Daniel Nüst
@nordholmen

Sometimes the idea & the people are right, but the timing is bad. No question about the people: @HeidiBaya & @StephenEglen are awesome collaborators and great supporters of #OpenScience & #ReproducibleResearch. Here is our idea that we cannot pursue. You tell us if it is good:

Tweet übersetzen

4:49 nachm. · 1. Juni 2021 · Typefully

23 Retweets 3 Zitierte Tweets 31 „Gefällt mir"-Angaben

Twittere deine Antwort

Antworten

Daniel Nüst @nordholmen · 1. Juni
Antwort an @nordholmen
Data and code are first class research outputs. No doubt about it! Is there a long way to go to broad recognition? Sure. Do we need more rewards for open practices and transparency? Definitely. Do we need more pressure? Possibly.

What about simply trying out stuff during review?

Daniel Nüst @nordholmen · 1. Juni
It's great that peer review practices are challenged in academia (#preprints, #OpenPeerReview, post publication review). We need to improve them.

Sadly, one thing is often missing from reviews: the attempt to actually execute the workflow underlying a research paper.

Daniel Nüst @nordholmen · 1. Juni
There are reasons for code & data review not commonly being part of peer review, but this thread is not them. Based on the simple #CODECHECK perspective (codecheck.org.uk) we want to learn more about journals and conferences who simply try to execute a paper's code.

CODECHECK
CODECHECK is a process for independent execution of computations underlying scholarly ...
codecheck.org.uk

Daniel Nüst @nordholmen · 1. Juni
So we came up with a survey and collected a long list of journals and events that include workflow evaluation and code execution. We realised the survey might not be a great fit to learn what we want to know: to understand what works, who must be involved, and how to sustain.

Daniel Nüst @nordholmen · 1. Juni
To understand code execution practices during peer review we decided the best approach is to conduct semi-structured interviews with associated editors for reproducibility, reproducibility chairs... But we don't have the time atm. Do you think it is a worthwhile project?

Code execution in peer review

https://osf.io/x32nc/

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

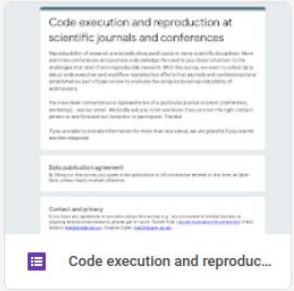
Survey practices of code execution as part of peer review

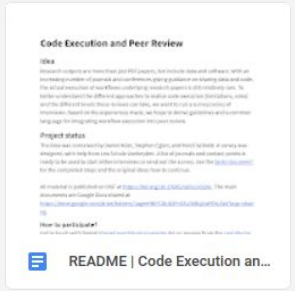
Text survey design ✔

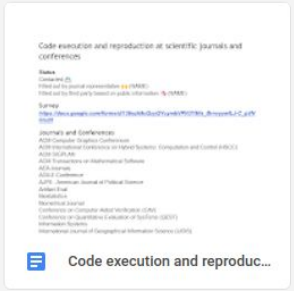
Manuscript outline ✔

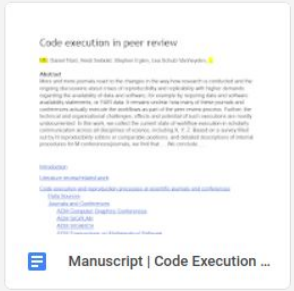
List of journals and events ✔

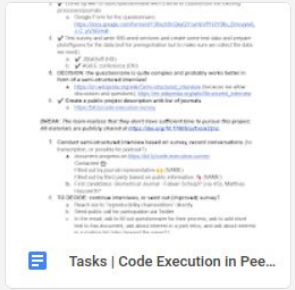
Surveying ❌ (interviews?)

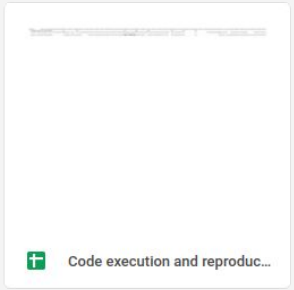










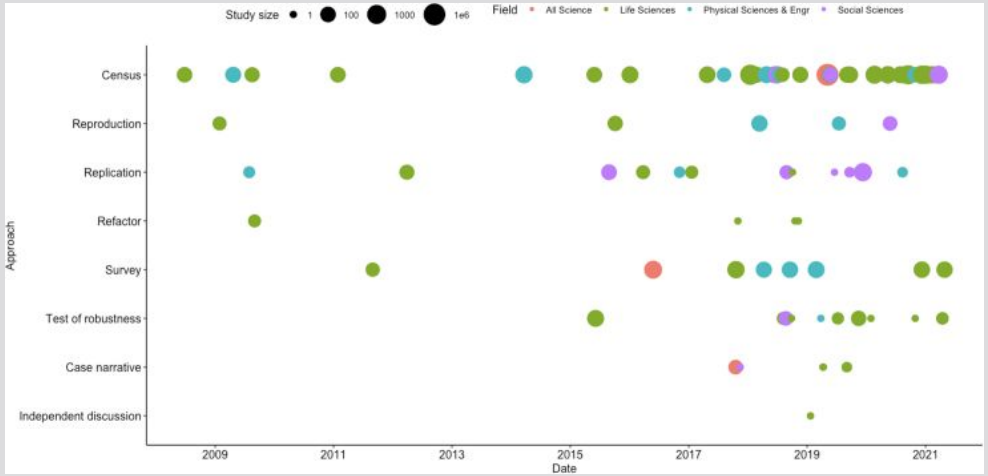


Metadata

The role of metadata in reproducible computational research

Jeremy Leipzig, Daniel Nüst, Charles Tapley Hoyt, Karthik Ram, Jane Greenberg

Patterns (N Y). 2021 Sep 10;2(9):100322. **https://doi.org/10.1016/j.patter.2021.100322**



Type of standard	Purpose
Reporting standards	Ensure adequate metadata for reproduction
Terminology artifacts or semantics	Concept disambiguation and semantic relationships
Models and formats	Interoperability
Identifier schemata	Discovery

Metadata level	Description	Examples of metacontent	Examples of standards	Projects and organizations
1. Input	metadata related to raw data and intermediates	sequencing parameters, instrumentation, spatiotemporal extent	MIAME, • EML, • DICOM • , GBIF CIF ThermoML, CellML, DATS, FAANG, ISO/TC 276, NetCDF, OGC, GO	OBO, NCBO, FAIRsharing, Allotrope
2.Tools	metadata related to executable and script tools	version, dependencies, license, scientific domain	CRAN DESCRIPTION file, • Conda • meta.yaml/environment.yml, pip requirements.txt, • pipenv Pipfile/Pipfile.lock, Poetry pyproject.toml/poetry.lock, EDAM, • CodeMeta, • Biotoolsxsd, DOAP, ontosoft, SWO	Dockstore, Biocontainers
3.Statistical reports and notebooks	literate statistical analysis documents in Jupyter or knitr, overall statistical approach or rationale	session variables, ML parameters, inline statistical concepts	OBCS, STATO • SDMX DDI, MEX, • MLSchema, MLFlow, • Rmd YAML •	Neural Information Processing Systems Foundation
4.Pipelines, preservation, and binding	dependencies and deliverables of the pipeline, provenance	file intermediates, tool versions, deliverables	CWL, • CWLProv, • RO-Crate, • RO, WICUS, OPM, PROV-O, ReproZip Config, ProvOne, WES, BagIt, BCO, ERC	GA4GH, ResearchObjects, WholeTale, ReproZip
5.Publication	research domain, keywords, attribution	bibliographic, scientific field, scientific approach (e.g., "GWAS")	BEL, • Dublin Core, JATS, ONIX, MeSH, LCSH, MP, Open PHACTS, SWAN, SPAR, PWO, PAV	NeuroLibre, JOSS, ReScience, Manubot

Metadata standards, including MIAME,[46] EML,[50] DICOM,[51] GBIF,[52] CIF,[53] ThermoML,[54] CellML,[55] DATS,[56] FAANG,[57] ISO/TC 276,[58] GO,[41] Biotoolsxsd,[59] meta.yaml,[60] DOAP,[61] ontosoft,[62] EDAM,[63] SWO,[64] OBCS,[65] STATO,[66] SDMX,[67] DDI),[68] MEX,[69] MLSchema,[70] CWL,[71] WICUS,[72] OPM,[73] PROV-O,[74] CWLProv,[75] ProvOne,[76] PAV,[77] BagIt,[78] RO,[47] RO-Crate (abstract by Sefton et al., 2019), BCO,[79] Dublin Core,[80] JATS,[81] ONIX,[82] MeSH,[83] LCSH,[84] MP,[85] Open PHACTS,[86] BEL,[87] SWAN,[88] SPAR,[89] PWO.[90] • Standards that are featured within this article. Examples of all standards can be found at https://github.com/leipzig/metadata-in-rcr.

Knowledge Exchange

The Art of Publishing Reproducible Research Outputs: Supporting emerging practices through cultural and technological innovation.

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

Five take-away messages

Reproducibility is part of the vision for open science, alongside concepts such as replication, robustness and the generalisation of research findings. It is difficult to pursue culture change with regard to reproducibility without considering this broader context.

Stakeholder collaboration is needed to continue developing reproducible publication practices. All players from the individual researcher to national and international bodies have a role to play, including in the context of policy development and implementation.

Incentives for reproducible publication practices are currently limited. Research performing organisations are beginning to support researchers in meeting their growing reproducibility expectations, and there is increasing demand for new training and support pathways in this area.

The management, curation and sharing of research data and methods are necessary conditions for reproducible publication. It is essential for these practices to become the norm to push the reproducibility agenda forward, and some dedicated institutional roles such as data stewards may be required to keep up with the demand for support.

Reproducible publication practices require a range of technological solutions, but most contributors agreed that these are already available in today's research landscape. The key technical gap appears to be the interoperability between available tools and workflows; however, we also note that technological solutions for reproducibility are not currently covered as part of training curricula.

The Art of Publishing Reproducible Research Outputs: Supporting emerging practices through cultural and technological innovation.

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

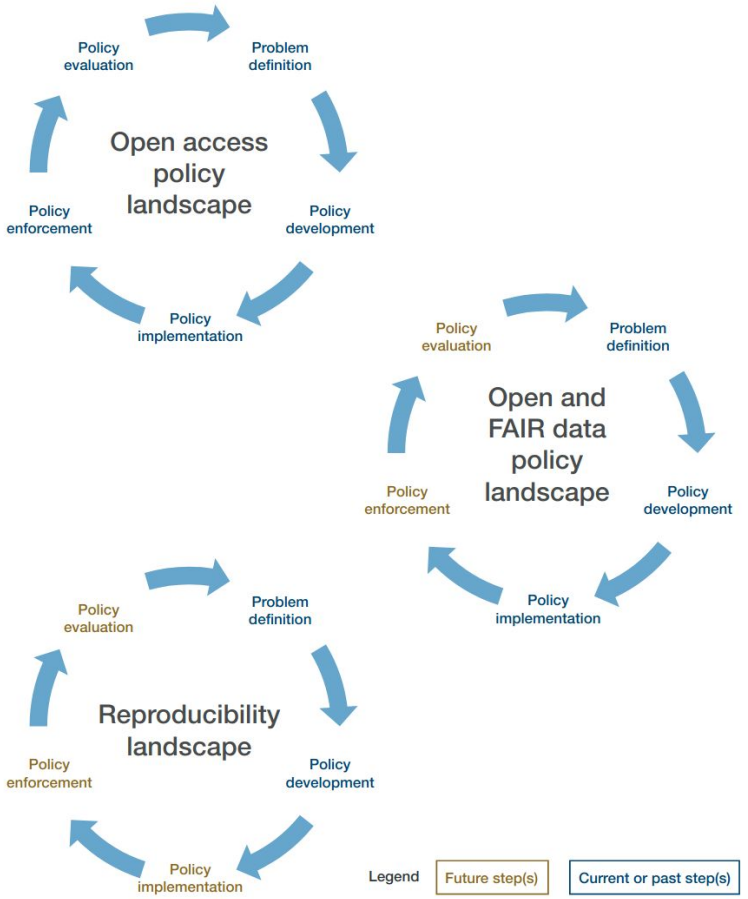
Stakeholders, roles and responsibilities
(awesome contributor list)

Incentivising and supporting reproducible publication practices (tech./struct. pathways)

Technological innovation

Covering the costs of reproducible publication practices

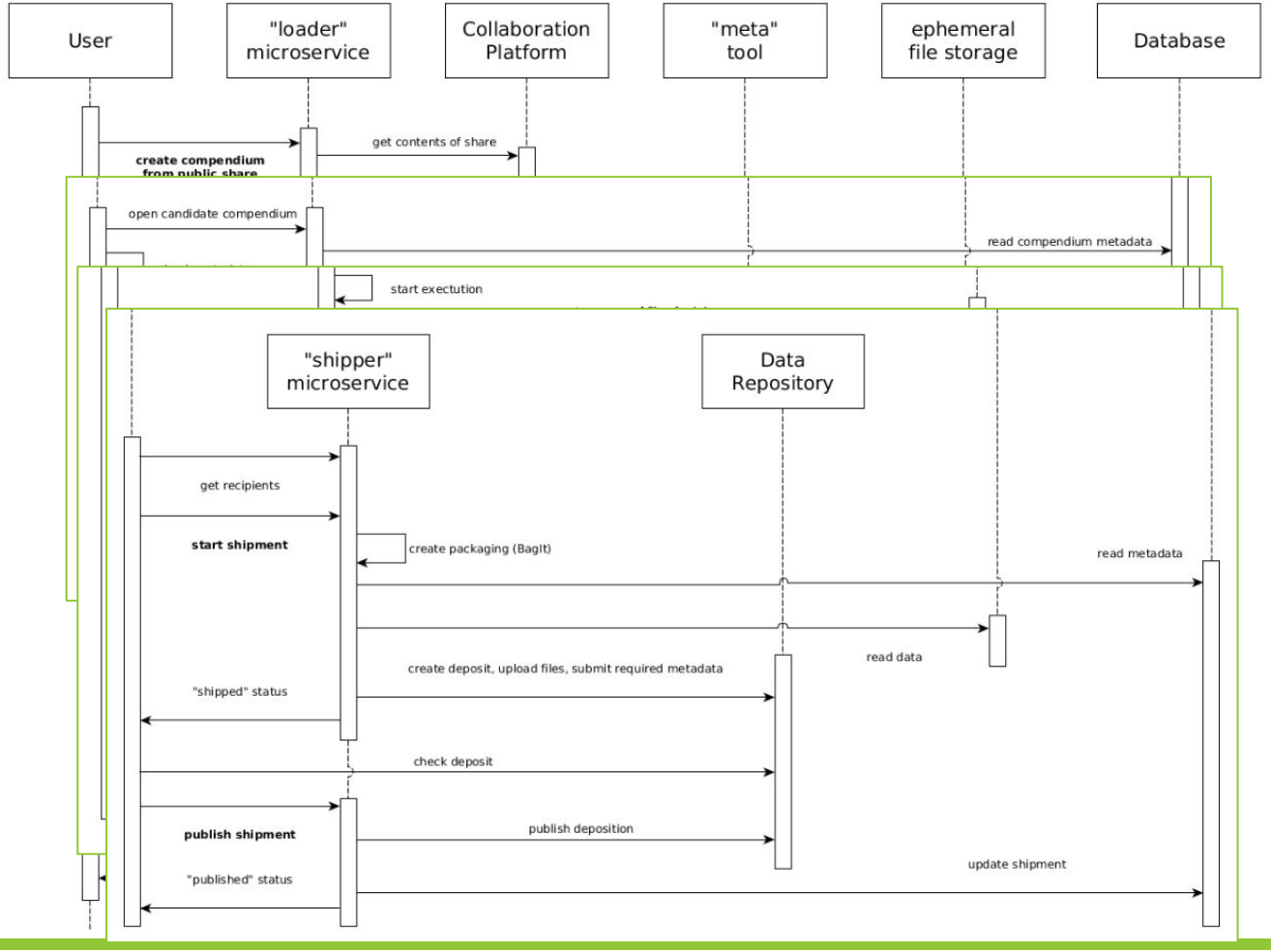
Figure 4. Comparison between open science policy landscapes



o2rX

ERC creation sequence

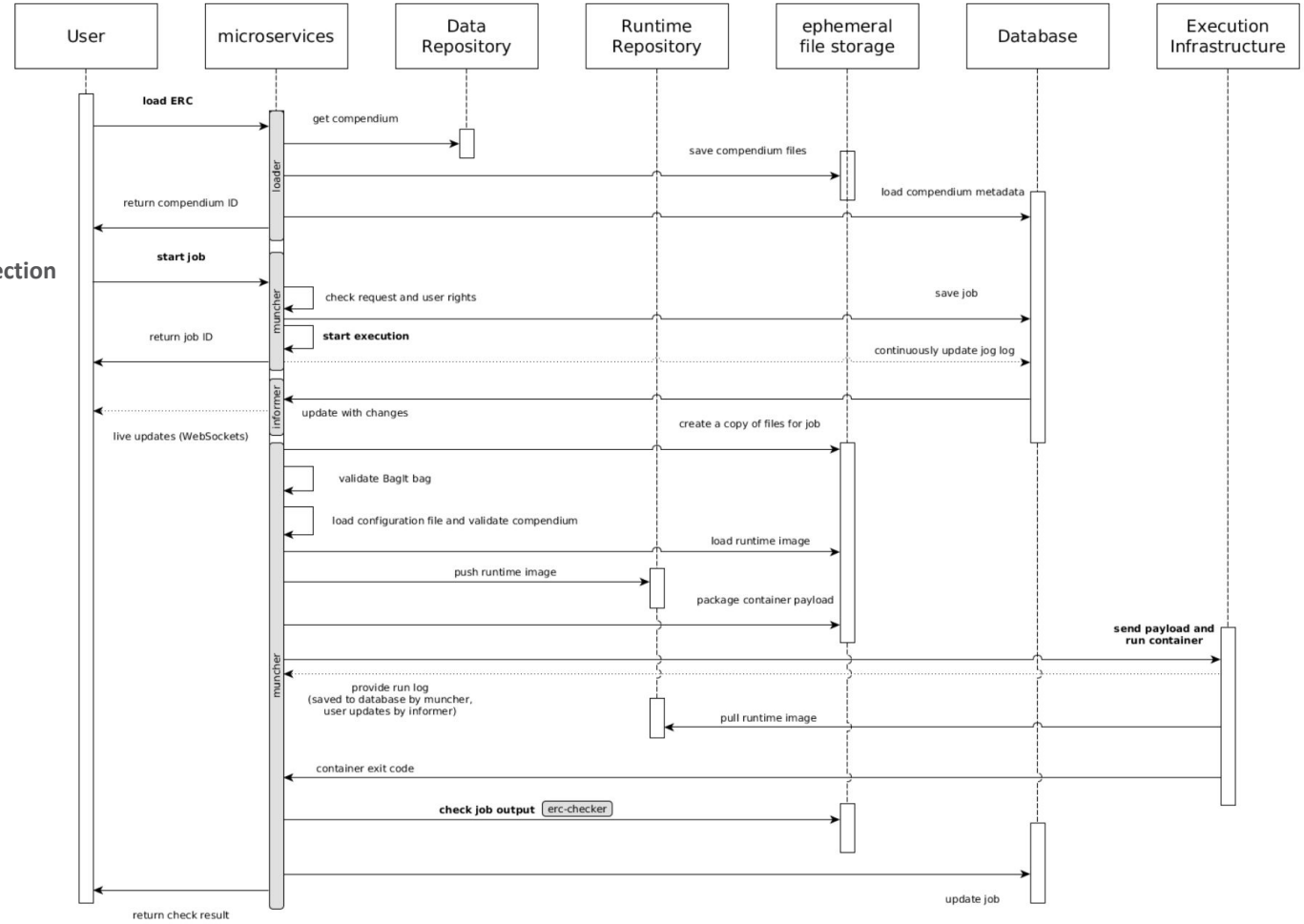
https://o2r.info/architecture/#61-erc-creation



Nüst, D. (2021). **A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences**. Zenodo. https://doi.org/10.5281/zenodo.5108218

ERC examination sequence

https://o2r.info/architecture/#62-erc-inspection



Nüst, D. (2021). **A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences**. Zenodo. https://doi.org/10.5281/zenodo.5108218

ERS Web API

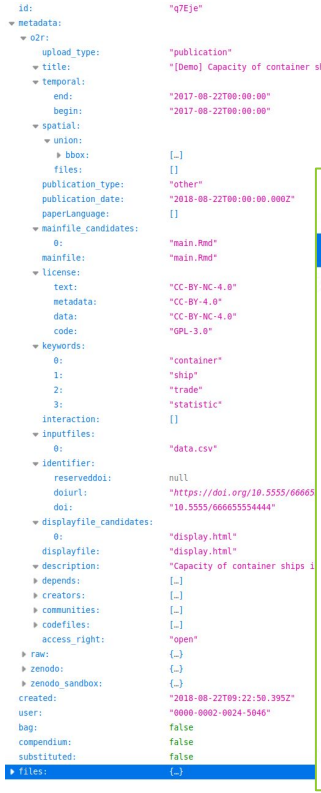
Nüst, D. (2021). **A web service for executable research compendia enables reproducible publications and transparent reviews in geospatial sciences**. Zenodo. https://doi.org/10.5281/zenodo.5108218

OpenAPI Spec: **https://o2r.info/api/**

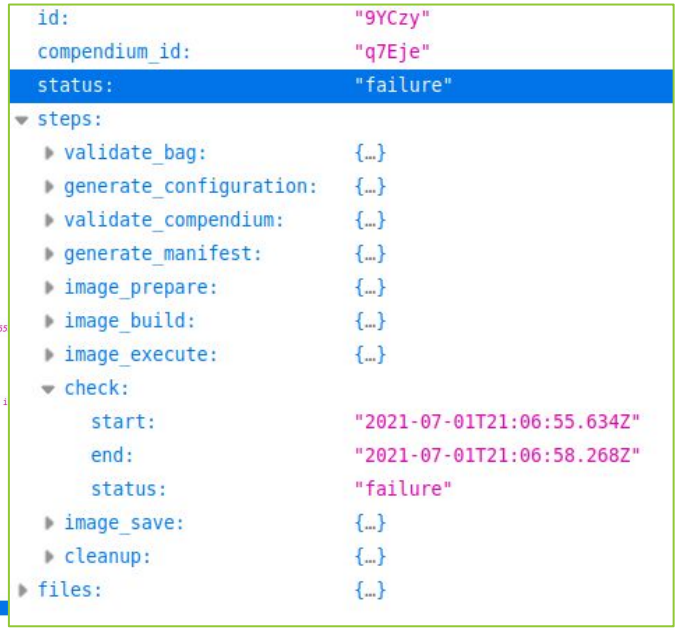
Demo: **https://o2r.uni-muenster.de/api/v1/**

```
{
  "auth": "/api/v1/auth",
  "compendia": "/api/v1/compendium",
  "jobs": "/api/v1/job",
  "users": "/api/v1/user",
  "search": "/api/v1/search",
  "shipments": "/api/v1/shipment",
  "recipients": "/api/v1/recipient",
  "substitutions": "/api/v1/substitution",
  "links": "/api/v1/link"
}
```

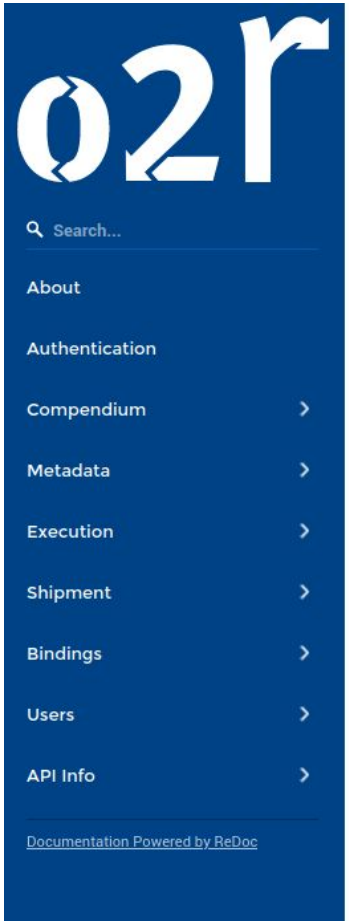
https://o2r.uni-muenster.de/api/v1/compendium/q7Eje (/jobs)



https://o2r.uni-muenster.de/erc/q7Eje/job/9YCzy#result



https://o2r.info/api/



o2r web API (1.0)

Download OpenAPI specification: Download

o2r project: o2r.team@uni-muenster.de | URL: https://o2r.info/about | License: Creative Commons CC0 1.0 Universal License

Find more info in our documentation.

About

The o2r web API acts as the interface between the o2r microservices and the web interface.

The API provides services around the executable research compendium (ERC), or "compendium" for short, which is documented in the ERC spec.

A good starting point for understanding the different parts of the API is the compendium life-cycle. The API is implemented as a RESTful API. The entrypoint for the current version is /api/v1. Unless specified otherwise, responses are always in JSON format. Body parameters in `POST` requests are expected in `multipart/form-data format.` Requests to the API should always be made with a secure connection using `HTTPS` . Some requests require authentication with a specific user level.

To cite this specification please use

> *Nüst, Daniel, 2018. Reproducibility Service for Executable Research Compendia: Technical Specifications and Reference Implementation. Zenodo. doi:10.5281/zenodo.2203844*

For a complete list of publications, posters, presentations, and software projects from the o2r project please visit https://o2r.info/results/.

Secondary metadata in the ERC & preservation

More formats, higher chance of long-term meaningful access

https://o2r.info/erc-spec/spec/#preservation-of-erc

Leaflet

.erc folder

- DateCite
- Zenodo
- o2r (extraction, options)

Example package leaflet

```
{
    "standards_used": [
        {
            "o2r": {
                "map_description": "maps raw extracted metadata to
                    o2r schema compliant metadata",
                "mode": "json",
                "name": "o2r",
                "outputfile": "metadata_o2r.json",
                "root": ""
            }
        },
        {
            "zenodo_sandbox": {
                "map_description": "maps o2r schema compliant MD to
                    Zenodo Sandbox for deposition creation",
                "mode": "json",
                "name": "zenodo_sandbox",
                "outputfile": "metadata_zenodo_sandbox.json",
                "root": "metadata"
            }
        }
    ]
}
```

BagIt example & profile


```
{
  "BagIt-Profile-Info":{
  "BagIt-Profile-Identifier":"https://o2r.info/erc-bagit-v1.json",
  "Source-Organization":"o2r.info",
  "Contact-Name":"o2r Team",
  "Contact-Email":"o2r@uni-muenster.de",
  "External-Description":"BagIt profile for packaging
       executable research compendia.",
  "Version":"1"
  },
  "Bag-Info":{
    "Contact-Name":{
       "required":true
    },
    "Contact-Email":{
       "required":true
    },
    "External-Identifier":{
       "required":true
    },
    "Bag-Size":{
       "required":true
    },
    "Payload-Oxum":{
       "required":true
    }
  },
  "Manifests-Required":[
    "md5"
  ],
  "Allow-Fetch.txt":false,
  "Serialization":"optional",
  "Accept-Serialization":[
     "application/zip"
  ],
  "Tag-Manifests-Required":[
    "md5"
  ],
  "Tag-Files-Required":[
     "erc/metadata.json",
     "erc.yml"
  ],
  "Accept-BagIt-Version":[
     "0.96"
  ]
}
```


Example `bagit.txt`

```
Payload-Oxum: 2172457623.43
Bagging-Date: 2016-02-01
Bag-Size: 2 GB
Is-Executable-Research-Compendium: true
```

Example file tree for a bagged ERC

```
├── bag-info.txt
├── bagit.txt
├── data
│   ├── 2016-07-17-sf2.Rmd
│   ├── erc.yml
│   ├── metadata.json
│   ├── Dockerfile
│   └── image.tar
├── manifest-md5.txt
└── tagmanifest-md5.txt
```

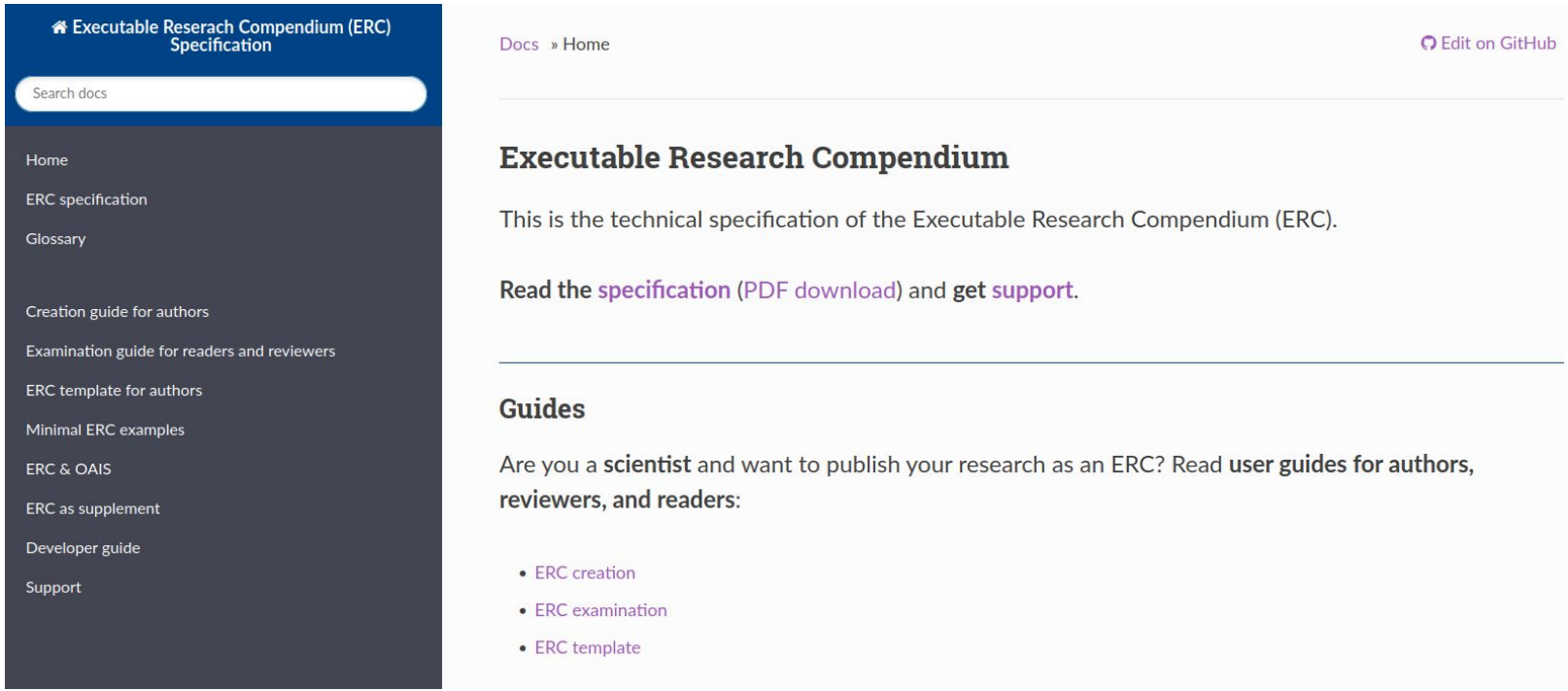
https://o2r.info/erc-spec/spec/#preservation-of-erc

erc.yml

```yaml
id: b9b0099e-9f8d-4a33-8acf-cb0c062efaec
spec_version: 1
main: paper.rmd
display: paper.html
execution:
  bind_mounts: ...
licenses:
  code: MIT
  data: ODbL-1.0
  text: "data_licenses_info.pdf"
  metadata: CC0-1.0
convention: https://github.com/ropensci/rrrpkg
ui_bindings:
  interactive: true
  bindings:
    - purpose: http://.../data-inspection
      widget: http://.../tabular-browser
      code: [...]
      data: [...]
      text: [...]
    - purpose: http://.../parameter-manipulation
      widget: http://.../dropdown
```

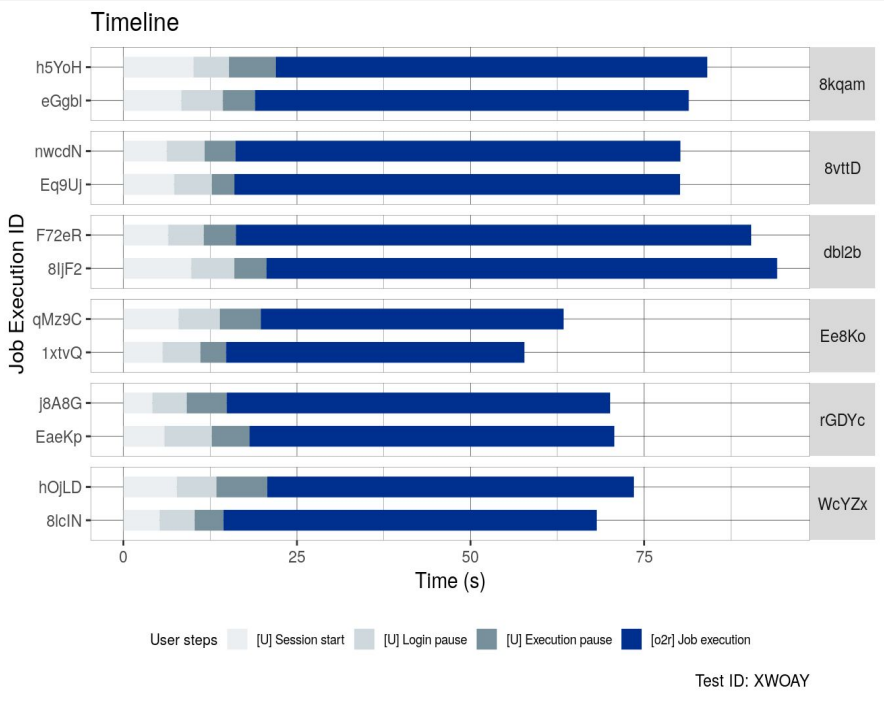
ERC specification

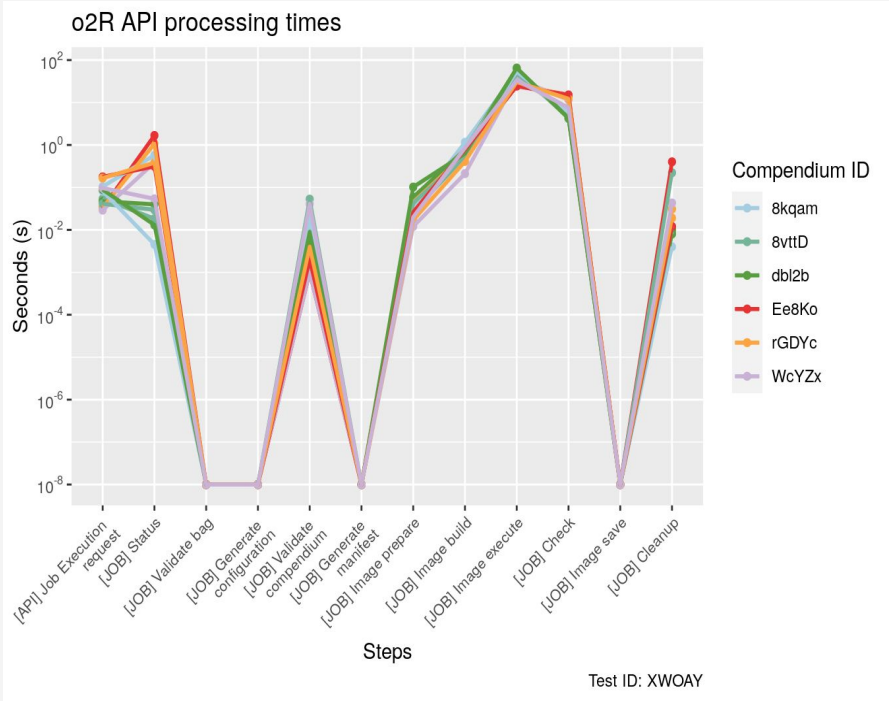
https://o2r.info/erc-spec/

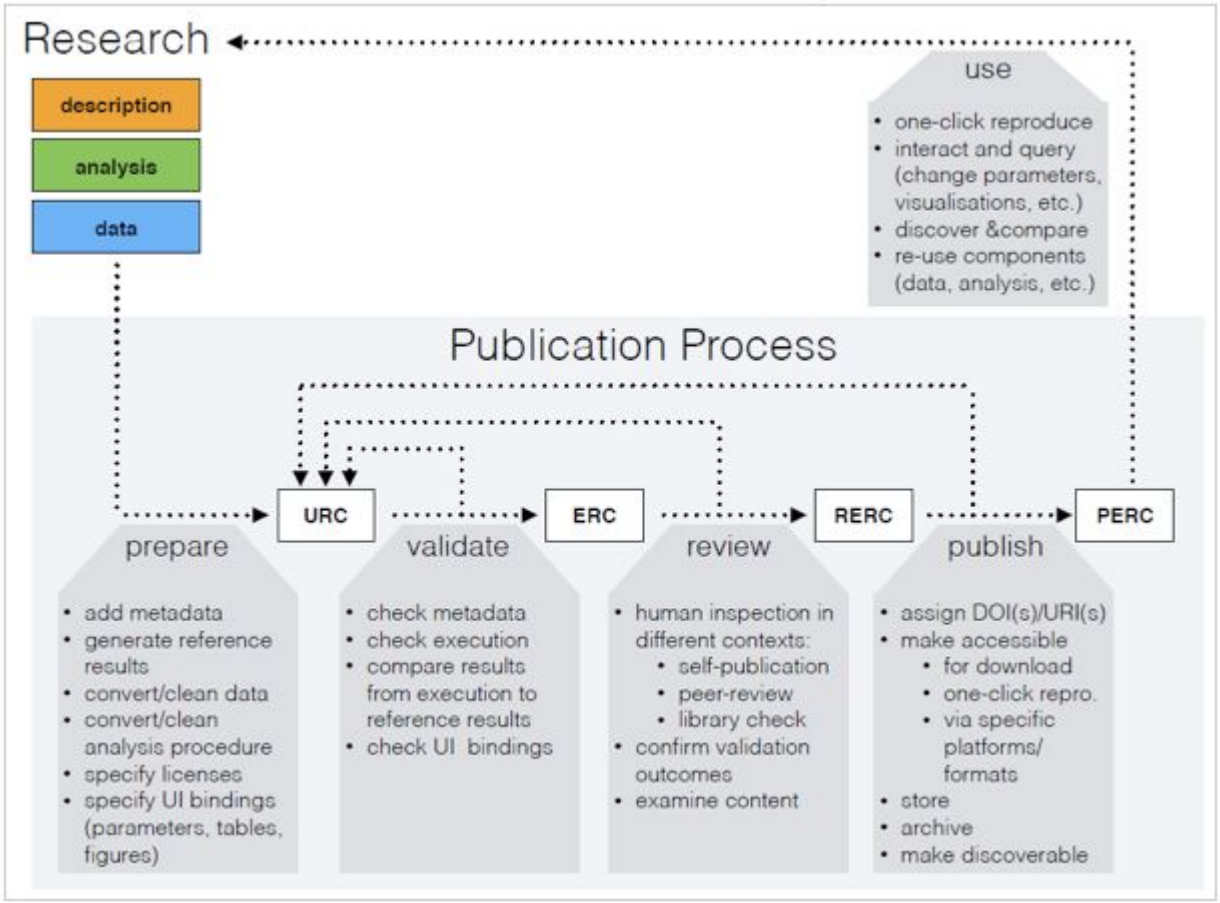


Load test of o2r ERS

https://github.com/o2r-project/api/pull/84







Nüst, D., Konkol, M., Pebesma, E., Kray, C., Schutzeichel, M., Przibytzin, H., & Lorenz, J. (2017). **Opening the Publication Process with Executable Research Compendia**. D-Lib Magazine, 23(1/2). https://doi.org/10.1045/january2017-nuest

ERC Vision

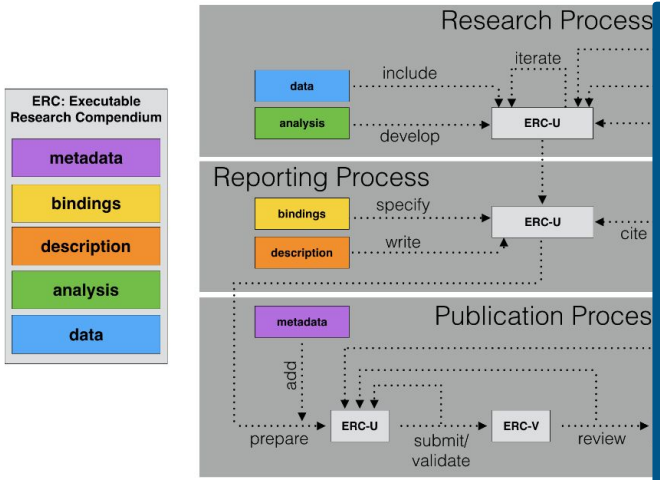


Figure 1 Executable Research Compendium (ERC) with its five
ERCs can be integrated into the research, reporting and publicati
stands for an unvalidated ERC, ERC-V for a validated one, ERC-R fo
for a published one. Processes are sequentialised to make the figure

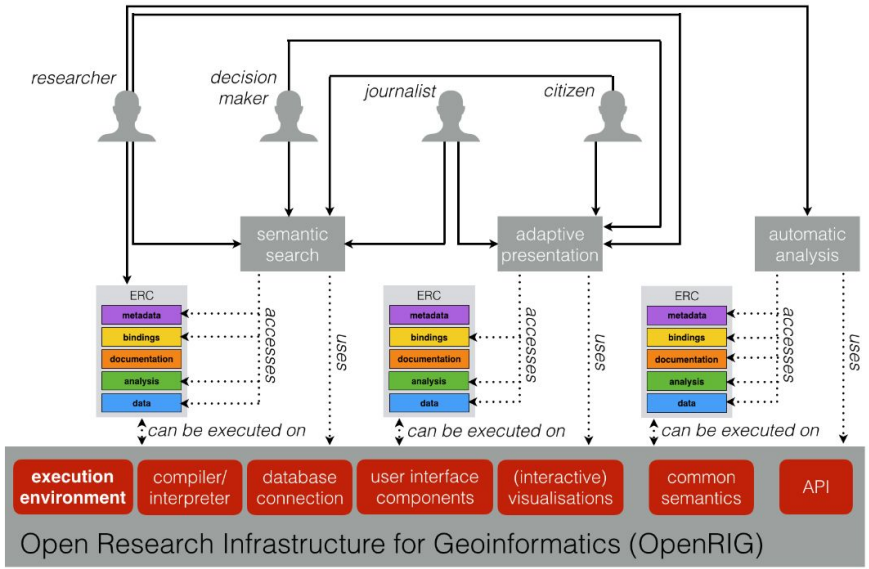


Figure 2 Open Research Infrastructure for Geoinformatics (OpenRIG): key components (red), essential functionalities enabled by it (grey boxes) and different stakeholders wanting to access them.

Reproducible Research in Geoinformatics: Concepts, Challenges and Benefits (Vision Paper) *Kray C, Pebesma E, Konkol M, Nüst D.* doi:10.4230/LIPIcs.COSIT.2019.8
GenR blog: https://genr.eu/wp/a-vision-for-reproducible-research-in-geoinformatics-geography-and-geosciences/

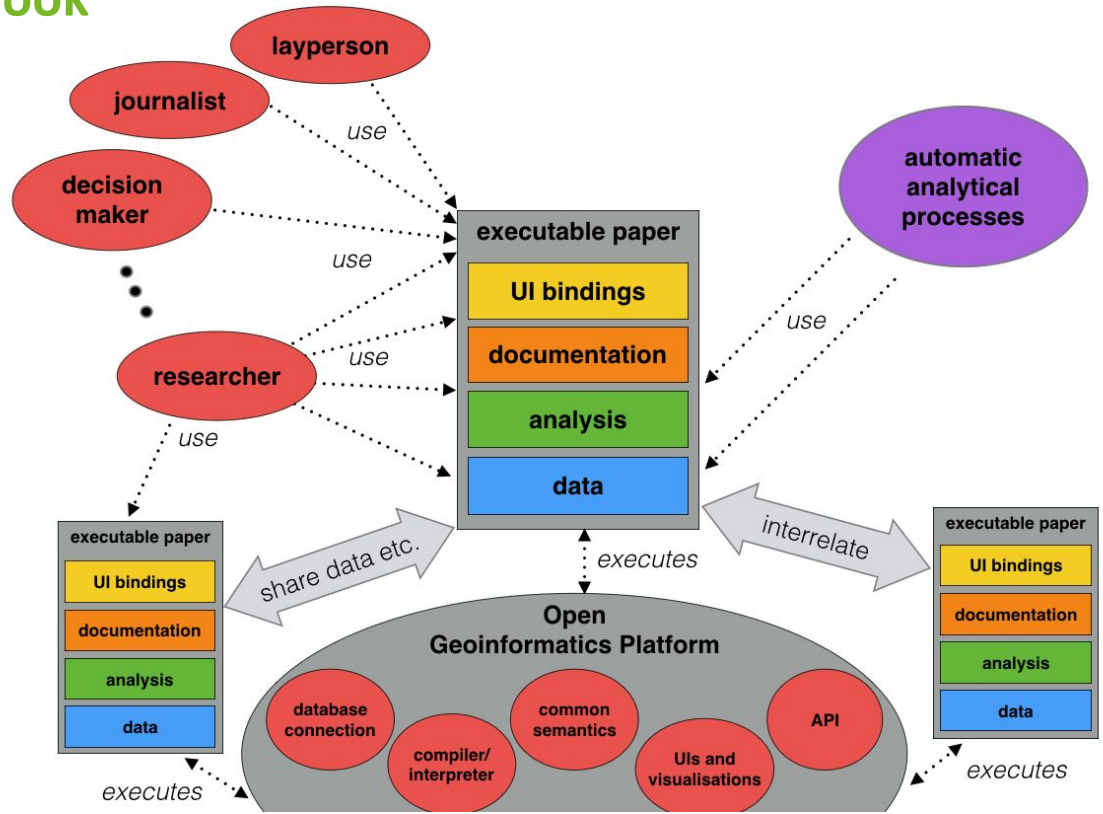
ERC Vision: Outlook

Explore further options such as other tech interactions

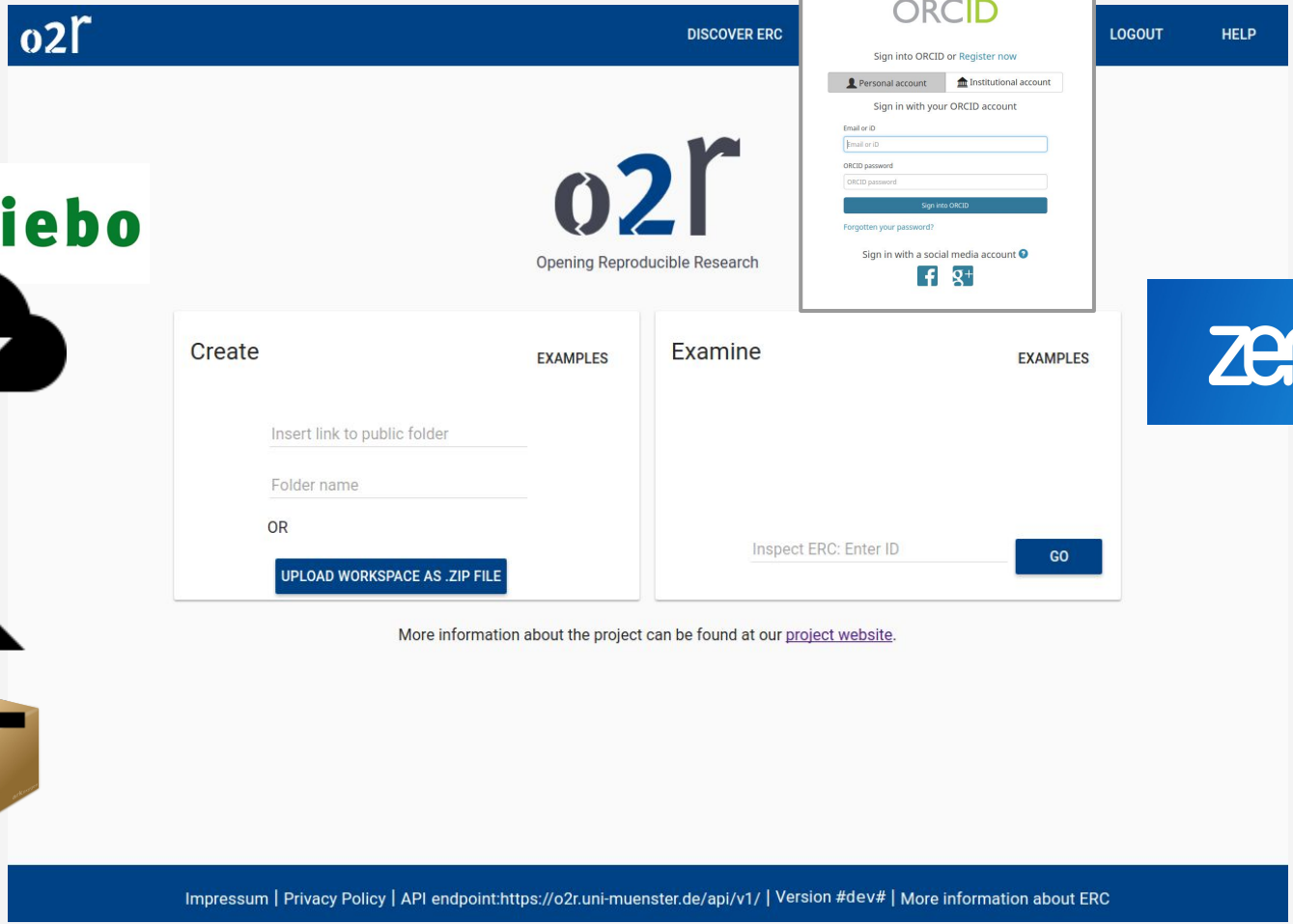
Deploy in practice

Use in teaching

Towards Vision of Geoinformatics V2



Reproducible Research in Geoinformatics: Concepts, Challenges and Benefits (Vision Paper) *Kray C, Pebesma E, Konkol M, Nüst D.* doi:10.4230/LIPIcs.COSIT.2019.8


o2r
DISCOVER ERC
LOGOUT
HELP
ORCID
Sign into ORCID or Register now
Personal account
Institutional account
Sign in with your ORCID account
Email or iD
ORCID password
Sign into ORCID
Forgotten your password?
Sign in with a social media account
o2r
Opening Reproducible Research
Create
EXAMPLES
Insert link to public folder
Folder name
OR
UPLOAD WORKSPACE AS .ZIP FILE
Examine
EXAMPLES
Inspect ERC: Enter ID
GO
More information about the project can be found at our project website.
Impressum | Privacy Policy | API endpoint:https://o2r.uni-muenster.de/api/v1/ | Version #dev# | More information about ERC

SHIP TO...

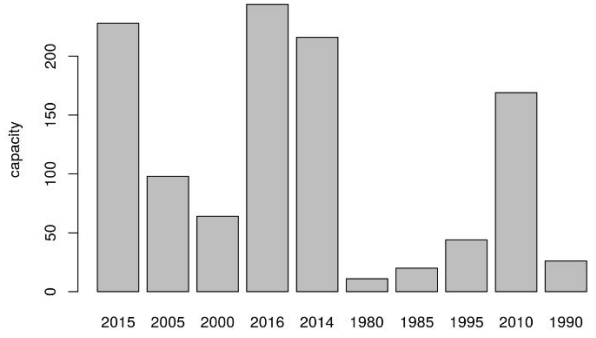
display.html

Capacity of container ships in seaborne trade from 1980 to 2016 (in million dwt)*

Daniel Nüst
o2r team
2017

Abstract

Capacity of container ships in seaborne trade of the world container ship fleet.



(c) Statista 2017

This statistic portrays the capacity of the world container ship fleet from 1980 through 2016

CHECK INSPECT MANIPULATE SUBSTITUTE

RUN ANALYSIS JOB (RAW) ERC (RAW)

Last finished analysis

cleanup	success ✓	Running regular cleanup Removed image with tag erc:Iee4f: [{"Untagged":"erc:Iee4f"},{"Dele {"Deleted":"sha256:58fe0c6657d3a3b805c9a6344f4b01609e940ddb6159f5 {"Deleted":"sha256:68f098069dacf60cb94f4e33144f365c333134461a7bb0 {"Deleted":"sha256:72117b430a92302deeca8e9466cc0069ca80e8c7e46e66 Deleted temporary payload file.
check	failure ✗	Check fai [started R version redistrib R package > rmarkdo processin | | 0% | |..... | 33% ordinary text without R code | |..... label: plot (with options)
image execute	success ✓	List of 1 $ echo: logi FALSE | |..... inline R code fragments output file: main.knit.md /usr/bin/pandoc +RTS -K512m -RTS main.utf8.md --to html --from mar section-divs --template /usr/local/lib/R/site-library/rmarkdown/rm variable 'mathjax-url:https://mathjax.rstudio.com/latest/MathJax.j Output created: /erc/display.html > > [finished image execution]
		Step 1/6 : FROM rocker/r-ver:3.4.3 ---> 933de9d8cc93 Step 2/6 : LABEL maintainer "o2r <http://o2r.info>" ---> Running in 9986044e14b2 ---> 68d293c25b60 Removing intermediate container 9986044e14b2 Step 3/6 : RUN export DEBIAN_FRONTEND=noninteractive; apt-get -y u ---> Running in be3915e6711b Ign:1 http://deb.debian.org/debian stretch InRelease Get:2 http://security.debian.org stretch/updates InRelease [63.0 k Get:3 http://deb.debian.org/debian stretch-updates InRelease [91.0 Get:4 http://deb.debian.org/debian stretch Release [118 kB] Get:5 http://deb.debian.org/debian stretch Release.gpg [2,434 B] Get:6 http://deb.debian.org/debian stretch-updates/main amd64 Pack Get:7 http://security.debian.org stretch/updates/main amd64 Packag Get:8 http://deb.debian.org/debian stretch/main amd64 Packages [9.

failure ✗ Check failed

o2r

DISCOVER ERC CHRIS NIX | orcid.org/0000-0001-6523-2935 LOGOUT HELP

Check Results

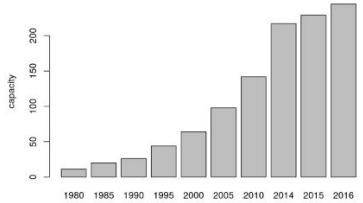
Daniel Nüst

o2r team

2017

Abstract

Capacity of container ships in seaborne trade of the world container ship fleet.



(c) Statista 2017

This statistic portrays the capacity of the world container ship fleet from 1980 through 2016. In 2016, the world merchant container ship fleet had a capacity of around 244 million metric tons deadweight. As of January 2016, there were 5,239 container ships in the world's merchant fleet (source).

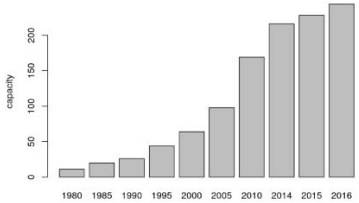
Sources: UNCTAD; Clarkson Research Services, via statista.

o2r team

2017

Abstract

Capacity of container ships in seaborne trade of the world container ship fleet.



(c) Statista 2017

This statistic portrays the capacity of the world container ship fleet from 1980 through 2016. In 2016, the world merchant container ship fleet had a capacity of around 244 million metric tons deadweight. As of January 2016, there were 5,239 container ships in the world's merchant fleet (source).

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Daniel Nüst

o2r team

2017

Abstract

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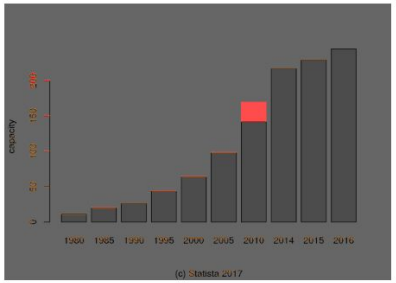


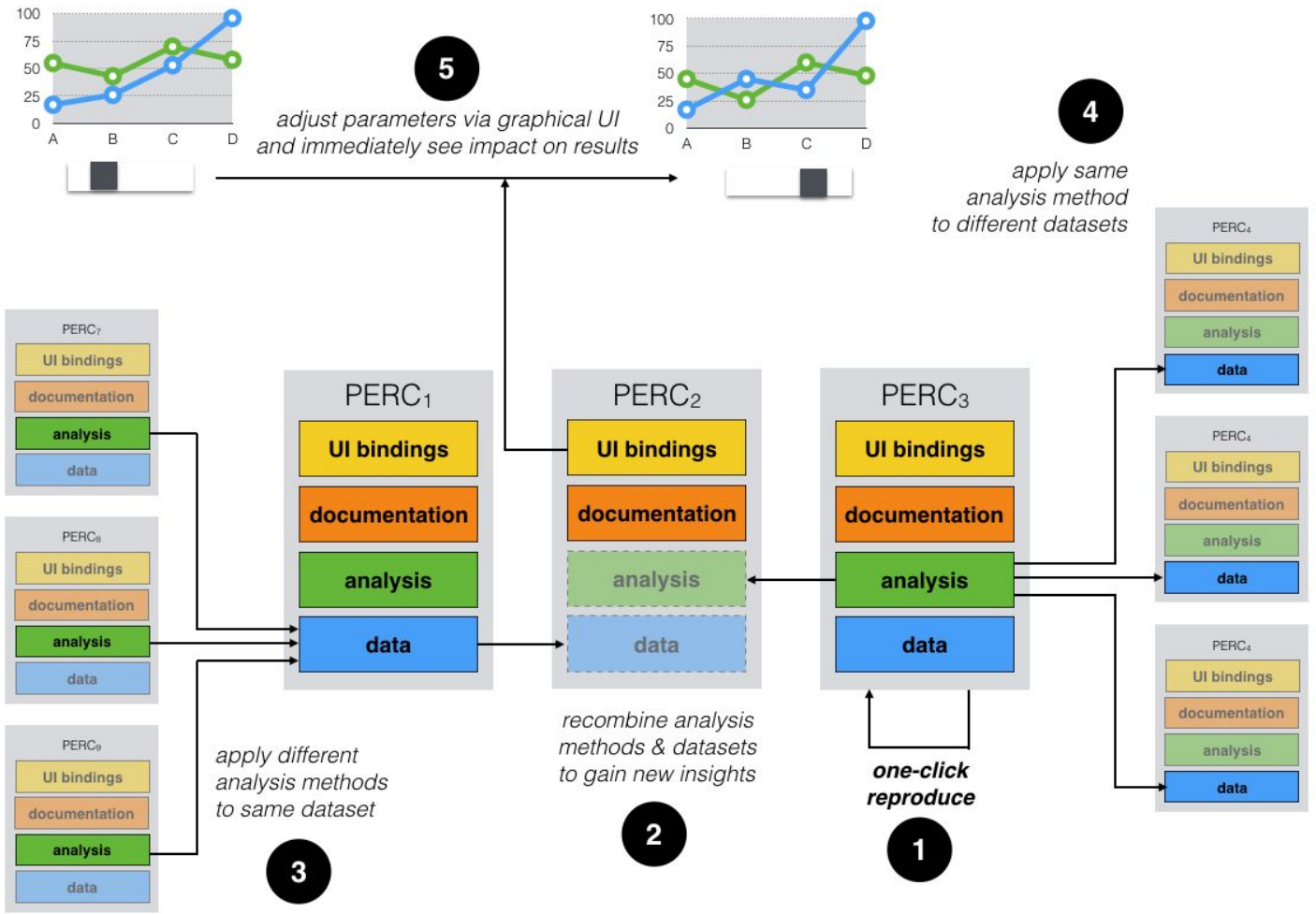
(c) Statista 2017

This statistic portrays the capacity of the world container ship fleet from 1980 through 2016. In 2016, the world merchant container ship fleet had a capacity of around 244 million metric tons deadweight. As of January 2016, there were 5,239 container ships in the world's merchant fleet (source).

Sources: UNCTAD; Clarkson Research Services, via statista.

```
Successfully built e031b03dfd2b
Removing intermediate container 4e20a84808cd
```

ERC benefits



geoextent

https://o2r.info/geoextent/

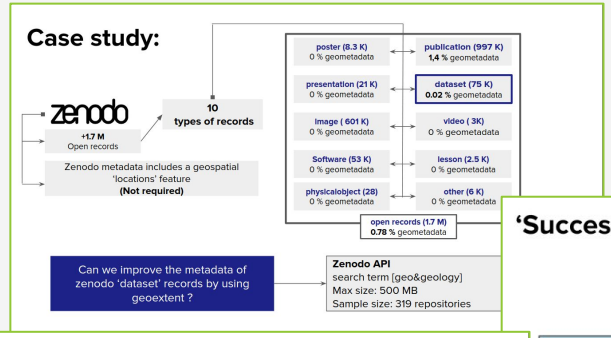
Sebastian Garzón and Nüst, Daniel. 2021. **Exploring Research Data Repositories with geoextent**. EarthCube annual meeting. https://doi.org/10.5281/zenodo.5496311

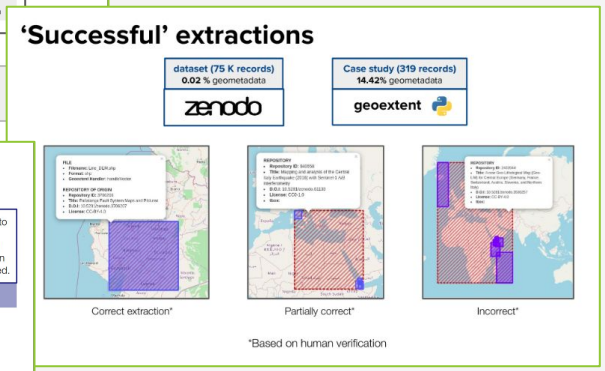
Extraction of geospatial metadata (spatial and temporal extent) from data files in workspaces submitted to the ERC reproducibility service. *Integrated in ERS as containerised CLI tool via o2r-meta.*

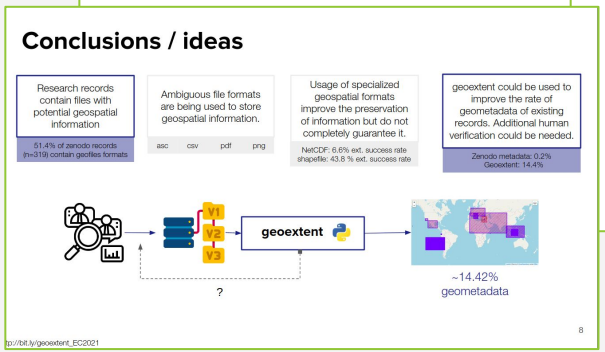
File formats (via GDAL):
GeoJSON, CSV, GeoTIFF, Shapefile,
GeoPackage, GPX, GML, KML, (tbc)

```
geoextent -b -t muenster_ring_zeit.geojson
```

```
{'format': 'geojson',
 'geoextent_handler': 'handleVector',
 'tbox': ['2018-11-14', '2018-11-14'],
 'bbox': [7.6016807556152335,
  51.94881477206191,
  7.647256851196289,
  51.974624029877454],
 'crs': '4326'}
```







o2r meta

https://github.com/o2r-project/o2r-meta

Extraction of metadata (publication, geospatial, code, licenses, …) from workspaces submitted to the ERC reproducibility service,

Mapping of metadata documents from one schema to another for target systems (Zenodo, archives, …),

Validation of metadata, and

Harvesting of catalogues for metadata completion (OAI-PMH).

Integrated in ERC reproducibility service as a containerised CLI tool.

ERC in peer review in o2r pilots

https://o2r.info/pilots/

Copernicus journal **Earth System Science Data**

Deep-sea sediments of the global ocean by Markus Diesing (Data description paper)
https://essd.copernicus.org/articles/12/3367/2020/essd-12-3367-2020-discussion.html

Referee comment
https://essd.copernicus.org/preprints/essd-2020-22/essd-2020-22-RC1.pdf

introduction, data, methods, results, limitations of the approach, potential usage, data availability, and conclusion. These sections are streamlined towards the understanding of the algorithmic implementation and its results; they retain completeness while remaining pleasantly concise, "Limitations of the approach" being the only exception to this. All accompanying figures and tables are clear and understandable, both, in digital form and in paper.

The software was tested for reproducibility using the ERC tool under https://o2r.uni-muenster.de/#/erc/GWME2voTDb5oeaQFuTWMCEMveKS1MiXm, and performed positively in this aspect. Upon closer examination, the discrepancies that led to it being flagged with failed reproducibility multiple times, appear to be minor formatting changes. The data products found under https://doi.pangaea.de/10.1594/PANGAEA.911692 are accessible, complete, and use standard file types.

For the most part, the methodology was clearly explained, with enough references to the sources for the used techniques as well as a clear specification of the software

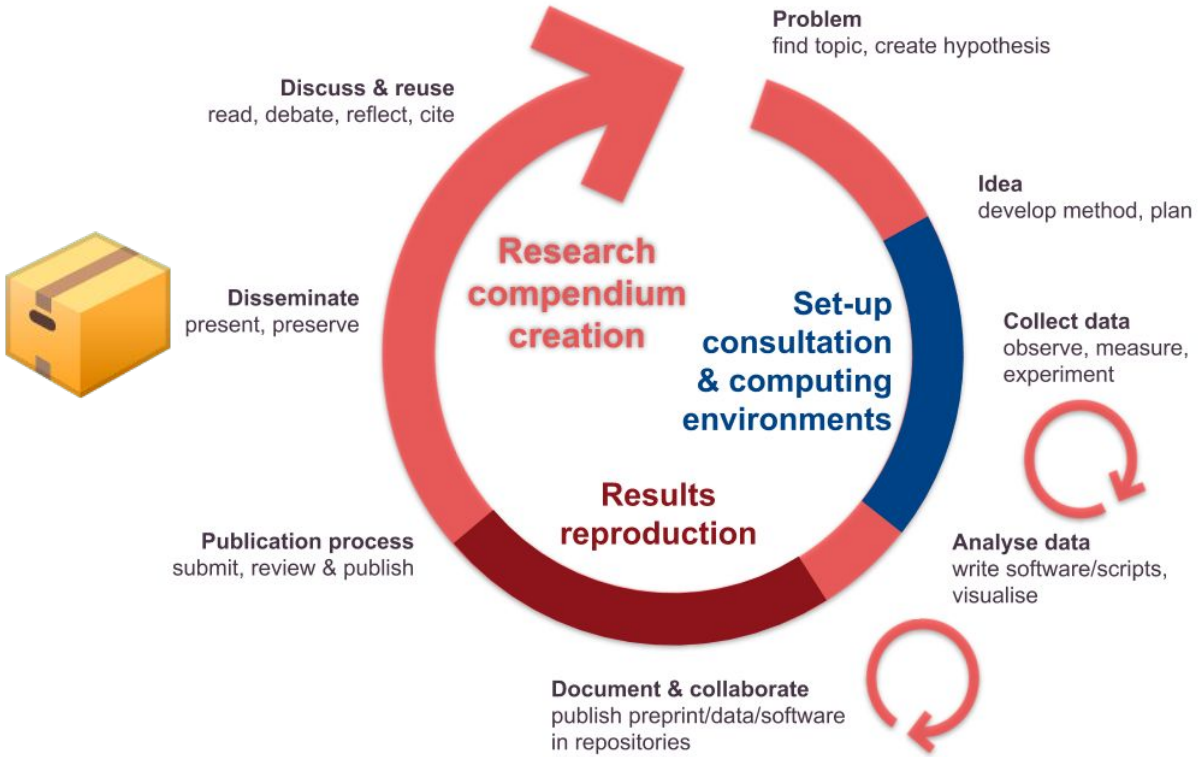
ESSDD

Interactive comment

WWU
MÜNSTER

R2S2

Reproducible Research Support Services in the Research Lifecycle

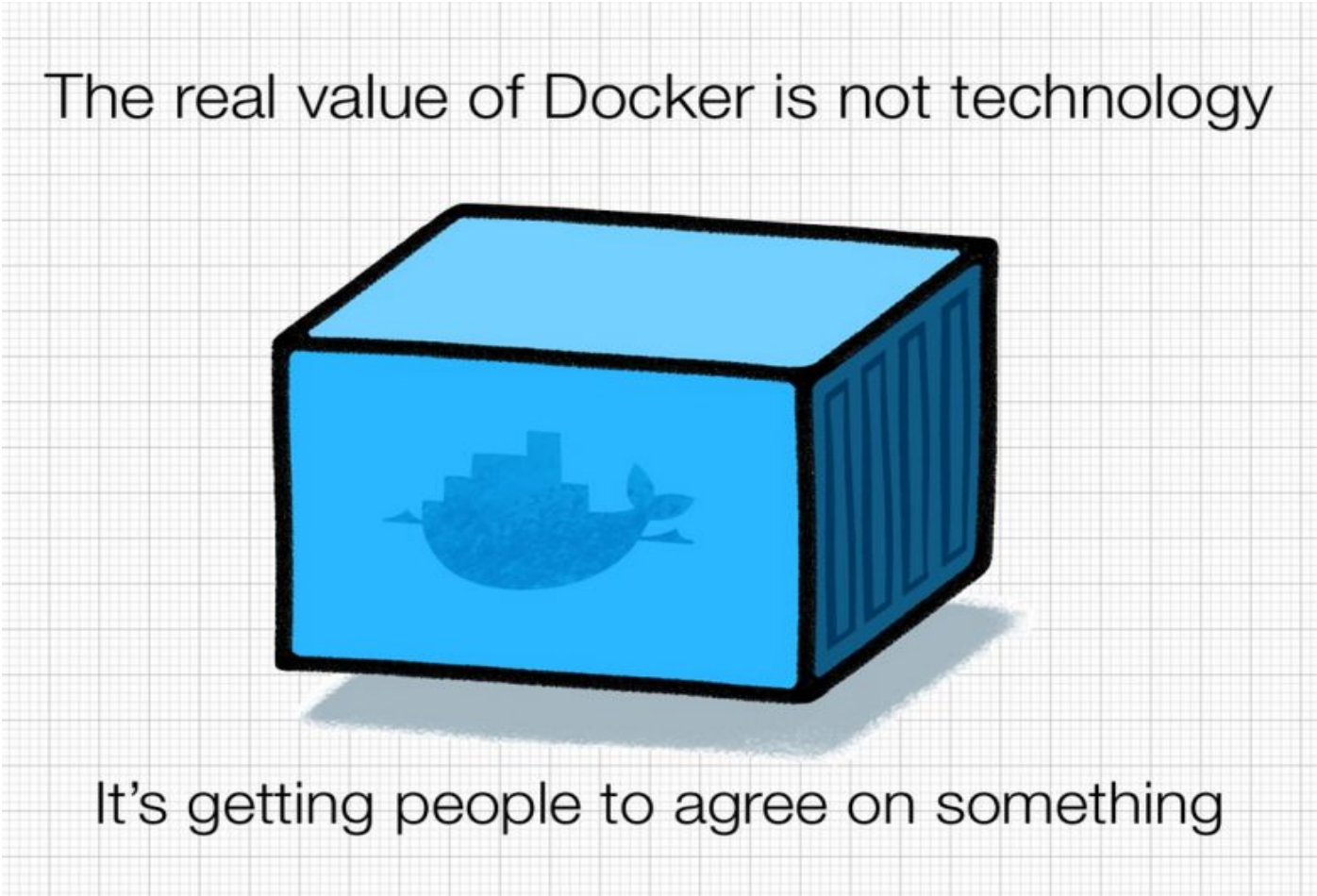


R2S2

Reproducible **R**esearch **S**upport **S**ervice

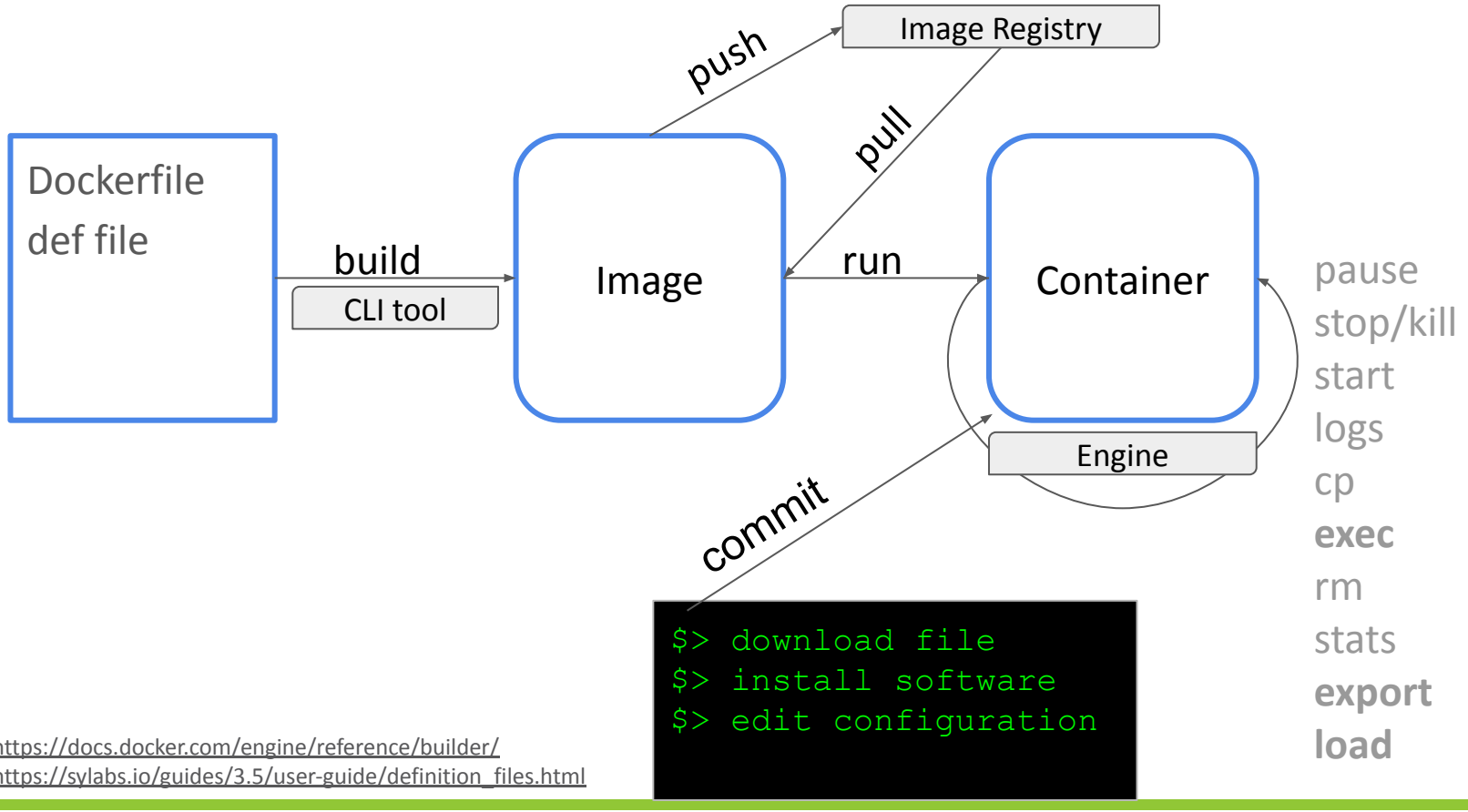
https://go.wwu.de/r2s2

Containers



Slide by Docker inventor & Docker, Inc. CTO Solomon Hykes, DockerCon 2014

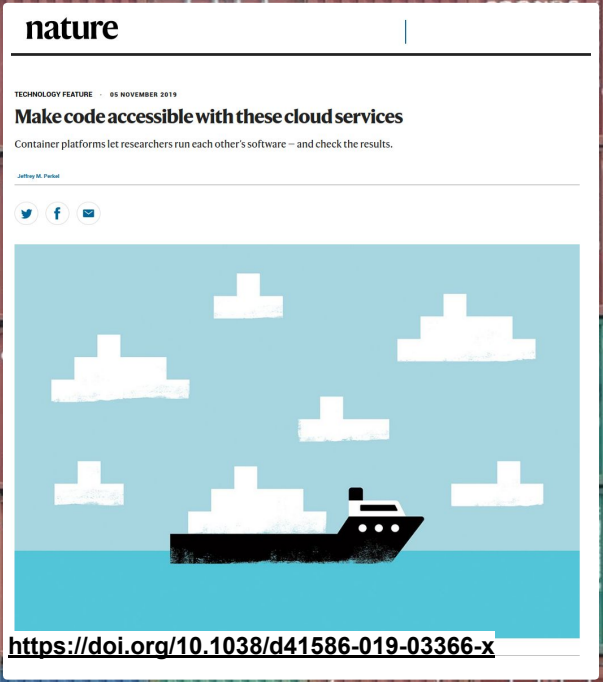
Containerisation Basics



https://docs.docker.com/engine/reference/builder/
https://sylabs.io/guides/3.5/user-guide/definition_files.html

Containers in Scholarly Communication

1. **Data Science!**
   - **Reproducibility**
   - **Project** separation
   - Computing environment **documentation**
   - **Collaboration**
   - “Live” **papers**
2. **Tools** to support users and automate creating environments from containers
3. **Platforms** built on containers



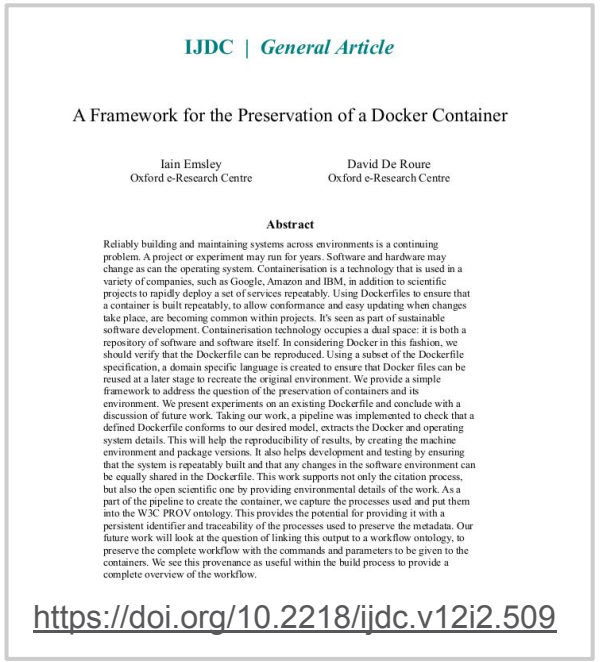
https://doi.org/10.1038/d41586-019-03366-x

binder o2r ReproZip WHOLE TALE

https://mybinder.org/ https://o2r.info/ https://www.reprozip.org/ https://wholetale.org/

Container preservation

1. Saving the image + the Dockerfile is a good idea!
2. Remaining risk: availability of hardware to host container runtime



IJDC | *General Article*

A Framework for the Preservation of a Docker Container

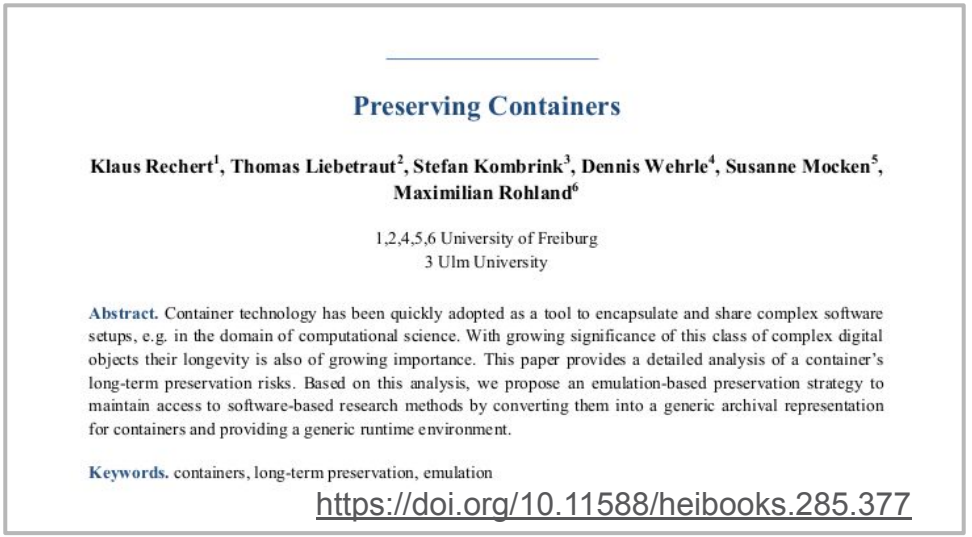
Iain Emsley
Oxford e-Research Centre

David De Roure
Oxford e-Research Centre

Abstract

Reliably building and maintaining systems across environments is a continuing problem. A project or experiment may run for years. Software and hardware may change as can the operating system. Containerisation is a technology that is used in a variety of companies, such as Google, Amazon and IBM, in addition to scientific projects to rapidly deploy a set of services repeatably. Using Dockerfiles to ensure that a container is built repeatably, to allow conformance and easy updating when changes take place, are becoming common within projects. It's seen as part of sustainable software development. Containerisation technology occupies a dual space: it is both a repository of software and software itself. In considering Docker in this fashion, we should verify that the Dockerfile can be reproduced. Using a subset of the Dockerfile specification, a domain specific language is created to ensure that Docker files can be reused at a later stage to recreate the original environment. We provide a simple framework to address the question of the preservation of containers and its environment. We present experiments on an existing Dockerfile and conclude with a discussion of future work. Taking our work, a pipeline was implemented to check that a defined Dockerfile conforms to our desired model, extracts the Docker and operating system details. This will help the reproducibility of results, by creating the machine environment and package versions. It also helps development and testing by ensuring that the system is repeatably built and that any changes in the software environment can be equally shared in the Dockerfile. This work supports not only the citation process, but also the open scientific one by providing environmental details of the work. As a part of the pipeline to create the container, we capture the processes used and put them into the W3C PROV ontology. This provides the potential for providing it with a persistent identifier and traceability of the processes used to preserve the metadata. Our future work will look at the question of linking this output to a workflow ontology, to preserve the complete workflow with the commands and parameters to be given to the containers. We see this provenance as useful within the build process to provide a complete overview of the workflow.

https://doi.org/10.2218/ijdc.v12i2.509



Preserving Containers

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Abstract. Container technology has been quickly adopted as a tool to encapsulate and share complex software setups, e.g. in the domain of computational science. With growing significance of this class of complex digital objects their longevity is also of growing importance. This paper provides a detailed analysis of a container's long-term preservation risks. Based on this analysis, we propose an emulation-based preservation strategy to maintain access to software-based research methods by converting them into a generic archival representation for containers and providing a generic runtime environment.

Keywords. containers, long-term preservation, emulation

https://doi.org/10.11588/heibooks.285.377

Challenges

High **potential** to abstract away problems with computing environments in science, but risk to add **“yet another layer”** / containers all the way down

Almost too easy to build your own image > **fragmentation**

Need practices (e.g., how/if to mount volumes) to ensure preservation - **no “one-click” by default**

Tooling still fluid, “standards” outside of preservation domain

Is there a critical mass for OCI-based “own” **standard for research**?

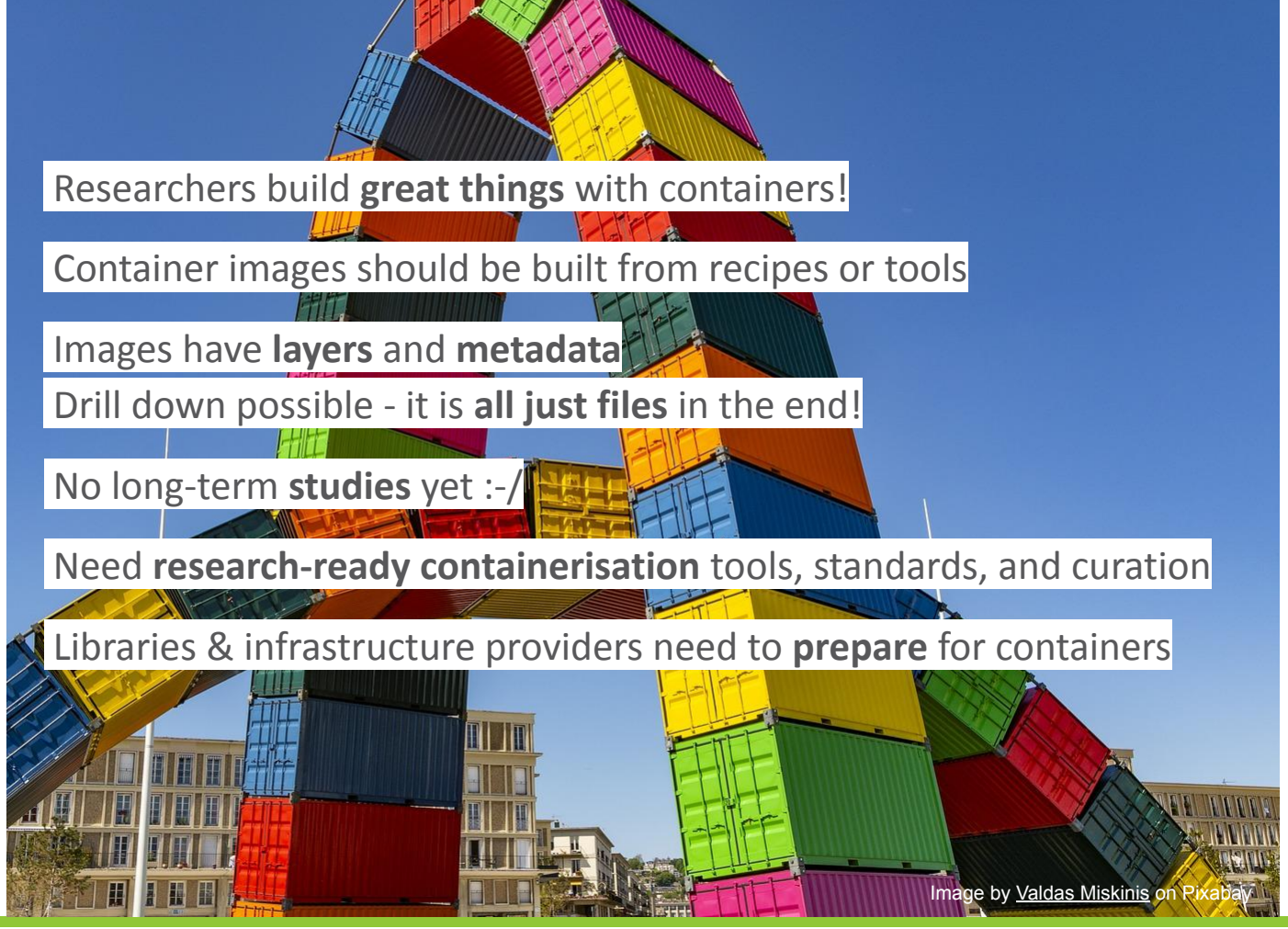
Docker main actor, who does not care about scientific usage

Best practices based on **Singularity** must catch up

Resources for science-grade and preservation-ready tools missing

Cross-cutting nature and ubiquity of containers lead to **diverse practices**

Solutions: Library leadership + author guidelines.



Researchers build **great things** with containers!

Container images should be built from recipes or tools

Images have **layers** and **metadata**

Drill down possible - it is **all just files** in the end!

No long-term **studies** yet :-/

Need **research-ready containerisation** tools, standards, and curation

Libraries & infrastructure providers need to **prepare** for containers

Image by Valdas Miskinis on Pixabay

Abstracts

Abstract (for indexing and search)

Reproducibility of computational research, i.e., research based on code and data, poses enormous challenges to all branches of science. In this dissertation, technologies and practices are developed to increase reproducibility and to connect it better with the process of scholarly communication with a particular focus on geography, geosciences, and GIScience. Based on containerisation, this body of work creates a platform that connects existing academic infrastructures with a newly established executable research compendium (ERC). It is shown how the ERC can improve transparency, understandability, reproducibility, and reusability of research outcomes, e.g., for peer review, by capturing all parts of a workflow for computational research. The core part of the ERC platform is software that can automatically capture the computing environment, requiring authors only to create computational notebooks, which are digital documents that combine text and analysis code. The work further investigates how containerisation can be applied independent of ERCs to package complex workflows using the example of remote sensing, to support data science in general, and to facilitate diverse use cases within the R language community. Based on these technical foundations, the work concludes that functioning practical solutions exist for making reproducibility possible through infrastructure and making reproducibility easy through user experience. Several downstream applications built on top of ERCs provide novel ways to discover and inspect the next generation of publications.

To understand why reproducible research has not been widely adopted and to contribute to the propagation of reproducible research practices, the dissertation continues to investigate the state of reproducibility in GIScience and develops and demonstrates workflows that can better integrate the execution of computational analyses into peer review procedures.

We make recommendations for how to (re)introduce reproducible research into peer reviewing and how to make practices to achieve the highest possible reproducibility normative, rewarding, and, ultimately, required in science. These recommendations are rest upon over 100 GIScience papers which were assessed as irreproducible, the experiences from over 30 successful reproductions of workflows across diverse scientific fields, and the lessons learned from implementing the ERC.

Besides continuing the development of the contributed concepts and infrastructure, the dissertation points out broader topics of future work, such as surveying practices for code execution during peer review of manuscripts, or reproduction and replication studies of the fundamental works in the considered scientific disciplines. The technical and social barriers to higher reproducibility are strongly intertwined with other transformations in academia, and, therefore, improving reproducibility meets similar challenges around culture change and sustainability. However, we clearly show that reproducible research is achievable today using the newly developed infrastructures and practices. The transferability of cross-disciplinary lessons facilitates the establishment of reproducible research practices and, more than other transformations, the movement towards greater reproducibility can draw from accessible and convincing arguments both for individual researchers as well as for their communities.

Zusammenfassung

Die Reproduzierbarkeit von rechnergestützter Forschung stellt alle Wissenschaftszweige vor enorme Herausforderungen. In dieser Dissertation werden Technologien und Praktiken entwickelt, um die Reproduzierbarkeit zu erhöhen und sie besser mit dem Prozess der wissenschaftlichen Kommunikation zu verbinden, mit besonderem Fokus auf Geographie, Geowissenschaften und GIScience. Basierend auf Containerisierung wird in dieser Arbeit eine Plattform geschaffen, die bestehende akademische Infrastrukturen mit einem neuartigen ausführbarem Forschungskompendium (Executable Research Compendium; ERC) verbindet. Es wird gezeigt, dass das ERC die Transparenz, Verständlichkeit, Reproduzierbarkeit und Wiederverwendbarkeit von Forschungsergebnissen, zum Beispiel für Peer-Reviews, verbessert, indem es alle Teile eines computergestützten Arbeitsablaufs erfasst. Das Kernstück der ERC-Plattform ist eine Software, welche die Rechenumgebung automatisch erfassen kann, so dass die Autoren nur noch sogenannte computational notebooks, digitale Notizbücher die Text und Analysecode verbinden, erstellen müssen. Die Arbeit untersucht weiter, wie Containerisierung unabhängig von ERCs angewendet wird und werden kann, unter anderem bei einer komplexen Analyse aus der Fernerkundung, für Datenwissenschaften im Allgemeinen sowie innerhalb der Anwenderschaft der Programmiersprache R. Basierend auf diesen technischen Grundlagen kommt die Arbeit zu dem Schluss, dass es funktionierende praktische Lösungen gibt, die Reproduzierbarkeit durch geeignete Infrastruktur möglich machen und die Benutzung deutlich vereinfachen. Mehrere nachgelagerte Anwendungen, die auf ERCs aufbauen, bieten neuartige Möglichkeiten, die nächste Generation von Publikationen besser suchen und inspizieren zu können.

Um zu verstehen, warum reproduzierbare Forschung nicht weit verbreitet ist, und um zur Verbreitung reproduzierbarer Forschungspraktiken beizutragen, untersucht die Dissertation weiterhin den Stand der Reproduzierbarkeit in der wissenschaftlichen Disziplin GIScience. Sie entwickelt und demonstriert Arbeitsabläufe, mit welchen die Durchführung von rechnerischen Analysen besser in Peer-Review-Verfahren integriert werden können. Es werden Empfehlungen gegeben, wie reproduzierbare Forschung in Peer-Review-Verfahren (wieder) eingeführt werden kann und wie Praktiken um die höchstmögliche Reproduzierbarkeit zu erreichen in der Wissenschaft normativ, lohnend und letztlich verpflichtend werden können. Diese Empfehlungen stützen sich auf über 100 als irreproduzierbar befundenen Artikeln aus der GIScience, auf die Erfahrungen aus über 30 erfolgreichen Reproduktionen von computerbasierten Arbeitsabläufen in verschiedenen Wissenschaftsbereichen und auf die Erkenntnisse von der Implementierung des ERC.

Neben der Weiterentwicklung der eingebrachten Konzepte und der Infrastruktur weist die Dissertation auf weitergehende Themen zukünftiger Arbeit hin, wie zum Beispiel die Untersuchung von Prozessen für Code-Ausführung als Teil von Begutachtungen von Manuskripten, oder Reproduktions- und Replikationsstudien für grundlegende Arbeiten in den betrachteten Wissenschaftsdisziplinen. Die technischen und sozialen Barrieren für höhere Reproduzierbarkeit sind stark mit anderen Transformationsprozessen in der Wissenschaft verwoben und daher trifft die Verbesserung der Reproduzierbarkeit auf ähnliche Herausforderungen rund um Kulturwandel und Nachhaltigkeit. Die Arbeit zeigt jedoch klar, dass reproduzierbare Forschung jedoch schon heute auf Basis der neu entwickelten Infrastrukturen und Praktiken realisierbar ist. Die Übertragbarkeit von disziplinübergreifenden Erkenntnissen begünstigt die Etablierung reproduzierbarer Forschungspraktiken, und mehr als andere Transformationen kann die Bewegung hin zu mehr Reproduzierbarkeit aus zugänglichen und überzeugenden Argumenten sowohl für einzelne Forscher als auch für ihre Gemeinschaften schöpfen.

Acknowledgements & Thanks

Thanks!

Throughout the writing of this dissertation I have received a great deal of support, met interesting people, enjoyed collaborating with many different minds, and even made new friends. This dissertation bears one name but captures the efforts of many. I would first like to thank my supervisor, **Edzer Pebesma**, who not only trusted me with an exciting project to work on, but also always helped me with insightful feedback, patience, and wisdom when I needed it, but mostly gave me more leeway than any young scholar would dare to ask for. Thank you Edzer, I'm very lucky to have you as my boss! I would like to acknowledge my colleagues at the **o2r project, ifgi, and WWU** whose expertise and personalities made our little attempt at changing how science is done both educational and fun, be they professor, librarian, researcher, or student. I will do some people injustice by omission, but nevertheless would like to thank a few people by name: **Markus Konkol**, who sharing an office with made the good times of getting a PhD enjoyable and the bad times bearable. Thank you dear **Mark Schutzeichel, Christian Kray, Christian Knoth, Marius Appel, Thomas Bartoschek, Holger Przibytzin, Jörg Lorenz, my fellow GSGI students of all years, Matthias Mohr, Fabian Fermazin, Juan Sebastian Garzón Alvarado, Laura Goulier, Matthias Hinz, Nick Jakuschona, Jan Koppe, Timm Kühnel, Torben Kraft, Lukas Lohoff, Tom Niers, Jan Suleiman, and Yousef Qamaz**. I am extremely lucky to not only have colleagues in the same institute, but that I can rely on excellent and enjoyable collaborators from all over the world. I was not good at setting up a straight line to follow, but in all detours and digressions I learned a lot and I am very appreciative of the opportunities and leaps of faith that were extended to me. The papers and events I could contribute to, make me proud. Big thanks for the great times go to **Stephen Eglen, Frank O. Ostermann, Barbara Hofer, Carlos Granell, Rusnė Šilerytė, Vicky & Remi Rampin, Vanessa Sochat, Heidi Seibold, Dirk Eddelbuettel, Ben Marwick, Marta Teperek, Anita Graser, Karl Broman, Niels Drost, David Topping, Lesley Wyborn, Xenia van Edig, Martin Rasmussen, Dirk Fleischer, Tim Head, Tony Hirst, Ben Evans, Bernadette Fritzsch, Martin Hammitzsch, Peter Kedron, Werner Kuhn, Alexis Comber, Jeremy Leipzig, Carl Boettiger, Alexander Kmoch, and the eLife sprints' teams and participants (Thanks, Naomi & Emmy)**. It is a testament to Open Science's power and its brilliant inspirational kind communities, such as the Binder team, that the list above is incomplete. Like-minded researchers and developers from many different disciplines, backgrounds, and locations contributed to big parts of this dissertation. I would also like to thank **Celeste R. Brennecka** for proofreading almost all manuscripts and helping me to find better words. I would not have had the energy to pursue a career in research to this point without the awesome local and national **Ultimate Frisbee** communities, the great teams I could play with (InDISCutabel, UMS, Monster Mix, Deine Mudder Bremen), and the many friends I found while throwing and catching discs. Ultimate delivered a way to rest my mind outside of my research. You should try it, too! In particular, I thank the **Braun family** and **Katja & Simon** for generously welcoming me in their homes in Münster whenever I needed it. Much closer to work, the RSE community is the best support network and inspirational crowd of nerds there is—we will change how things are done to the better! To all my colleagues, collaborators, professional contacts, who luckily not always stayed strictly professional, and those of you who I missed to recognise here (Sorry!), I would like to restate my thanks—it has been an honour and a privilege. Finally and most importantly, I would like to thank my beloved wife **Maria** for her unconditional support, sympathetic ear, and wise counsel. And on top of that, you even helped with this dissertation—I am grateful, now if not then, for every little and much needed push. I also want to thank my parents, my sister, my extended **family**, and my closest friends who are always there for me and are always understanding—I could not have completed a single bit of this research work without your backing. Danke! This work is dedicated to you.

Big thanks go also to the second assessor **Ben Marwick** and the committee members Professors **Daniel Sui, Christian Kray, and Norbert Hölzel**.