Reproducibility and Open Research Software

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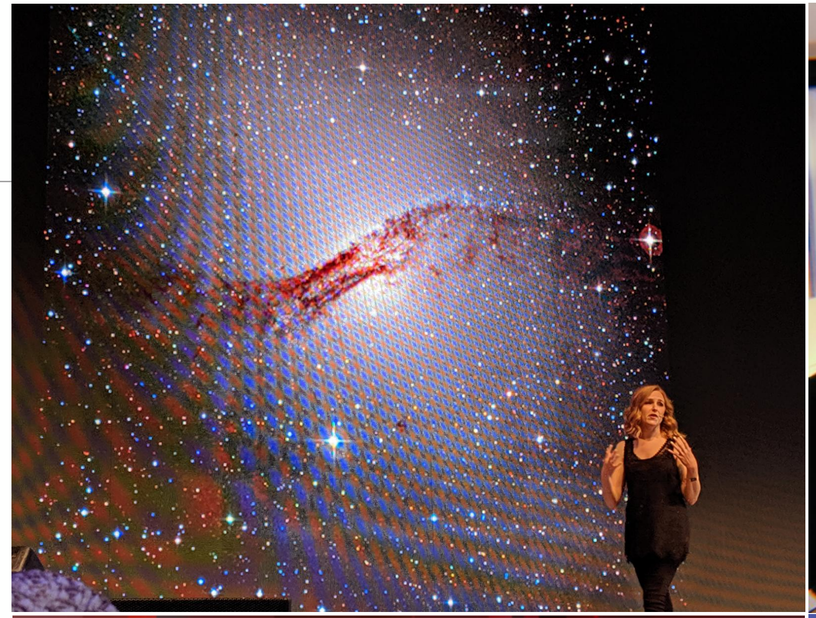
Outline

- About me and the Software Sustainability Institute
- Reproducibility and research culture
- Barriers to sharing research software
- Benefits to sharing research software
- How to share your research software and get credit
- Takeaways

About me and the Software Sustainability Institute

About me

- Community Manager for the Software Sustainability Institute at the University of Manchester
- Research background in Astrophysics
- Passionate about openness, transparency, reproducibility, wellbeing and inclusion in STEM/research
- TEDx speaker: youtu.be/c-bemNZ-IqA
- Was a cartoon in the UK's National Science and Media Museum Hello Universe exhibition
- Organise the Manchester women in data meetup group HER+Data MCR meetup.com/HER-Data-MCR



Software Sustainability Institute

- A national facility promoting the advancement of software in research by cultivating better, more sustainable, research software to enable world-class research: ***“Better software, better research”***

- Based at the Universities of Edinburgh, Manchester, Oxford and Southampton, and we have Software, Policy, Outreach, Training and Community teams to support the community developing and using research software

- Fellowship Programme to engage with and support natural ambassadors of better software practice in their research domains

- https://www.software.ac.uk/

Collaborations Workshop 2020 (CW20) #CollabW20

Software Sustainability Institute

- March 31 - April 2, 2020 at Queen's University Belfast, Northern Ireland
- Bringing together researchers, developers, innovators, managers, funders, publishers, leaders and educators to explore best practices and the future of research software
- Unconference: keynote presentations, mini-workshop/demo sessions, discussion groups, lightning talks, panel sessions, collaborative ideas and a hack day
- Themes: Open Research, Data Privacy and Software Sustainability
- http://bit.ly/ssi-cw20

Dr. Rachael Ainsworth, SSI @rachaelevelyn @OpenResLDN #ResearchSoftware

https://doi.org/10.6084/m9.figshare.11762121

Reproducibility and research culture

nature International weekly journal of science

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Archive > Volume 533 > Issue 7604 > News Feature > Article

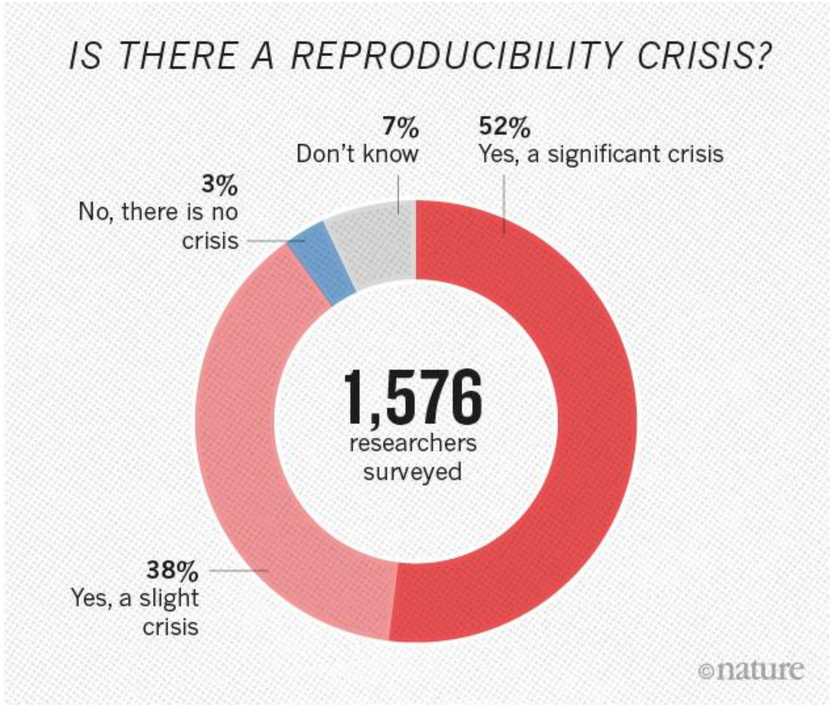
NATURE | NEWS FEATURE

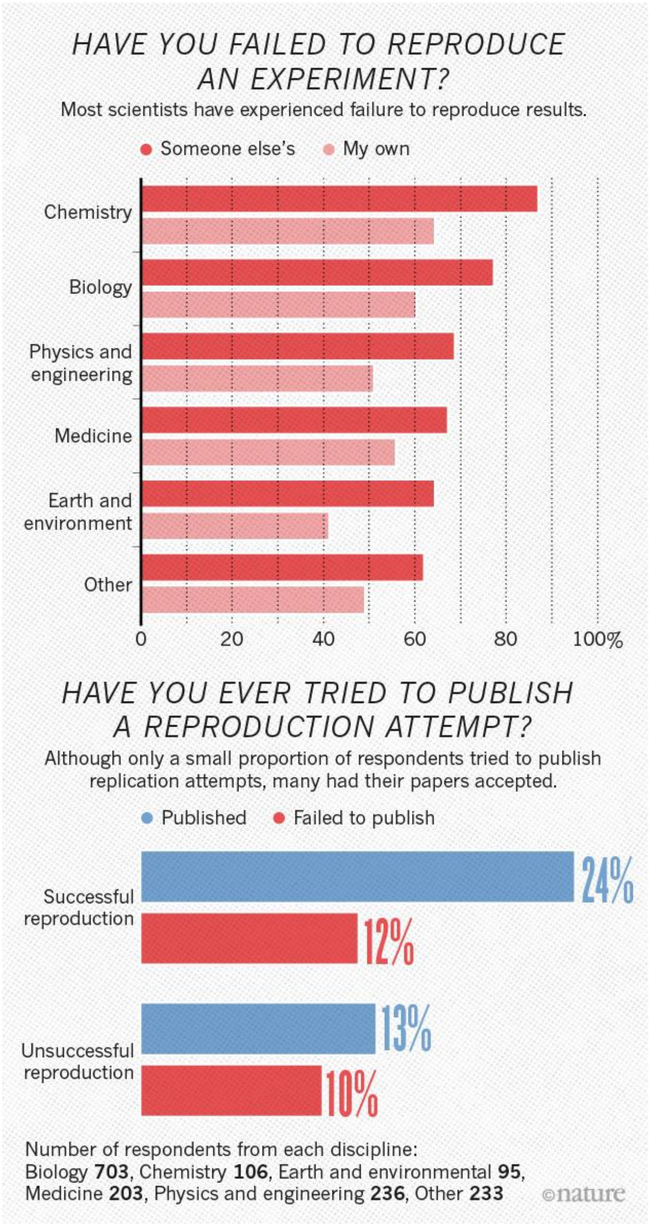
1,500 scientists lift the lid on reproducibility

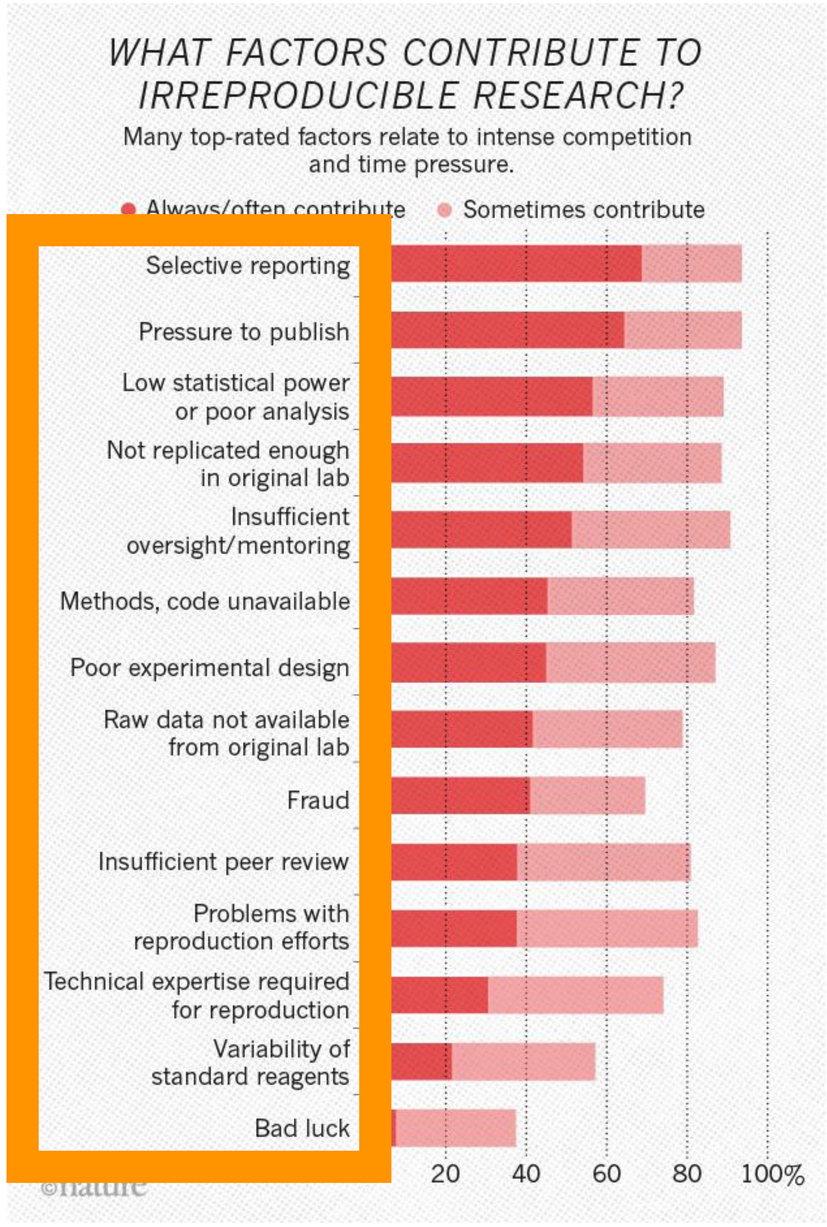
Survey sheds light on the 'crisis' rocking research.

Monya Baker

25 May 2016 | Corrected: 28 July 2016





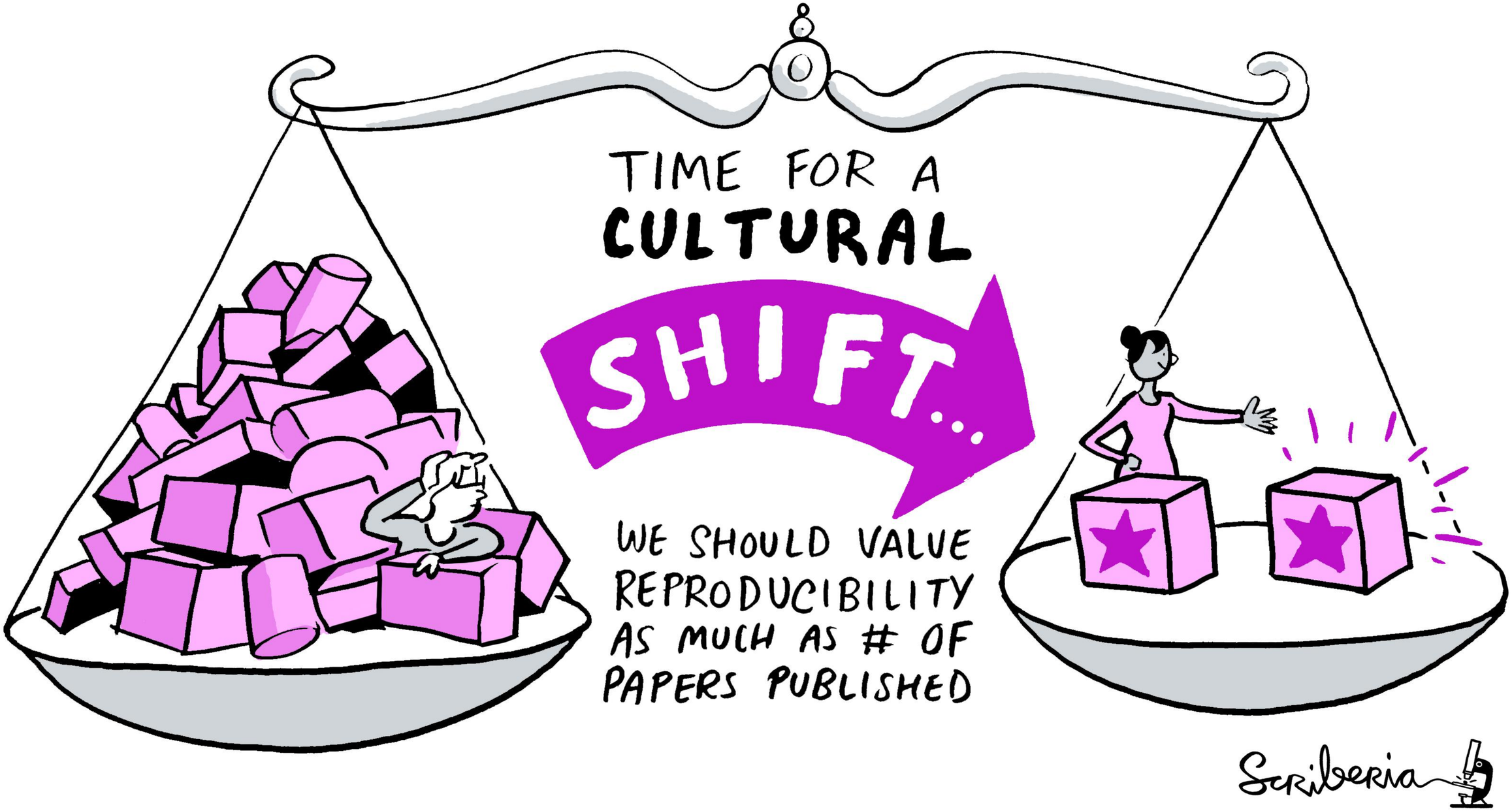


Baker (2016) https://doi.org/10.1038/533452a

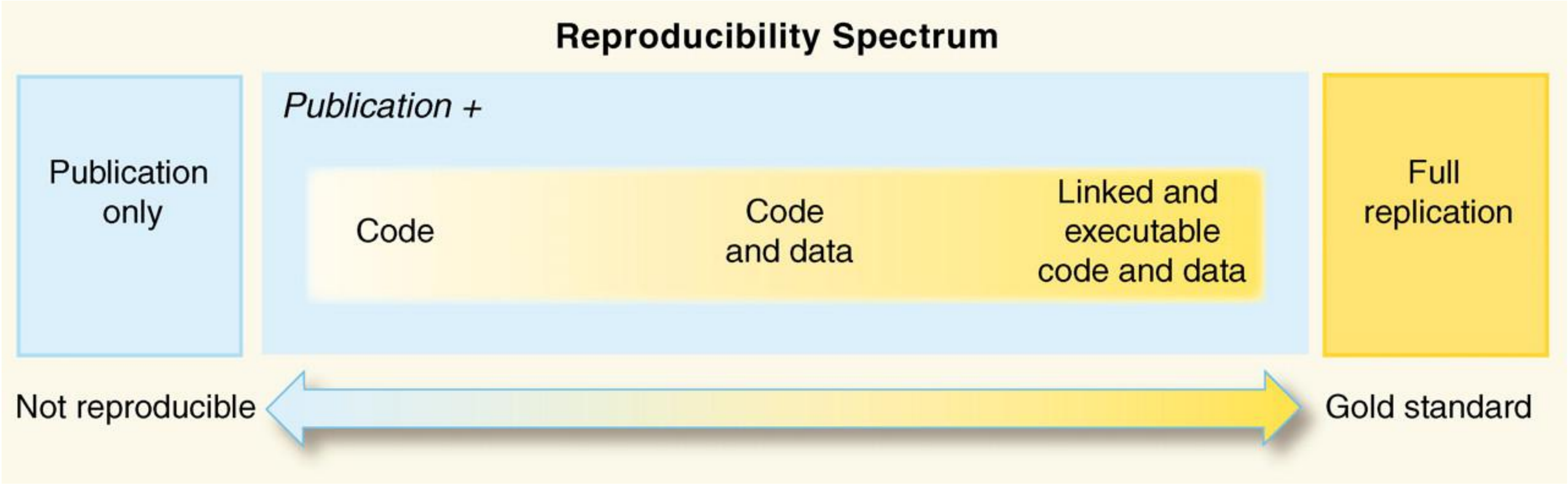
Research Culture

- Royal Society policy project on research culture: https://royalsociety.org/topics-policy/projects/research-culture/
    - There are ongoing concerns around issues such as: research integrity, career paths, permeability between sectors, recognition and reward, diversity, and support for collaboration and interdisciplinarity
- Wellcome key issue and report on research culture: https://wellcome.ac.uk/what-we-do/our-work/research-culture
    - Poor research culture is leading to unhealthy competition, bullying and harassment, and mental health issues

Words that researchers would use to describe research culture. (Wellcome, https://wellcome.ac.uk/reports/what-researchers-think-about-research-culture)



The Turing Way Community and Scriberia, http://doi.org/10.5281/zenodo.3332808



"Computational science has led to exciting new developments, but the nature of the work has exposed limitations in our ability to evaluate published findings. Reproducibility has the potential to serve as a minimum standard for judging scientific claims when full independent replication of a study is not possible."

Peng (2011) https://doi.org/10.1126/science.1213847

Barriers to sharing research software

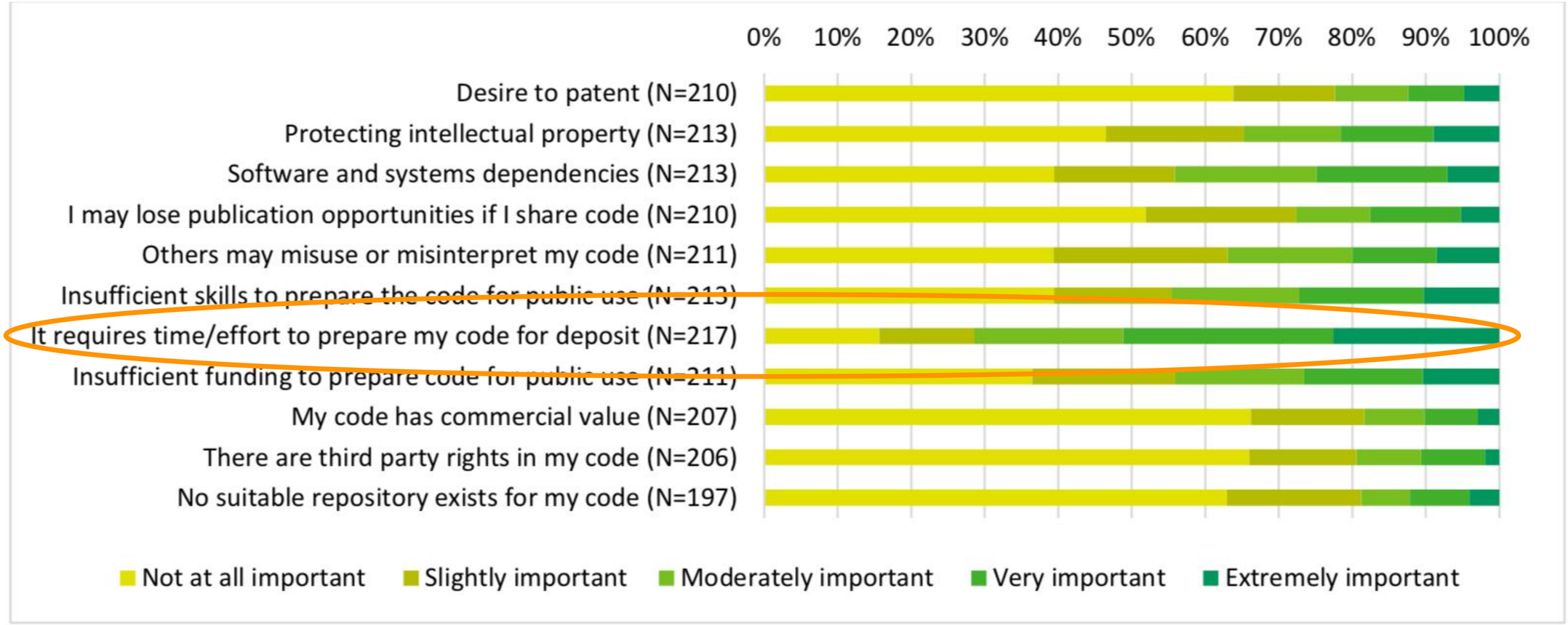
Barriers to Open Research

- Lack of awareness and training
- Cultural inertia and misinformation
- Challenging the establishment
- Follow the status quo to succeed
- Perceived lack of reward
- Not considered for promotion
- Requires additional skills
- Takes time
- Publication bias towards novel findings

Fig: https://doi.org/10.6084/m9.figshare.5558653

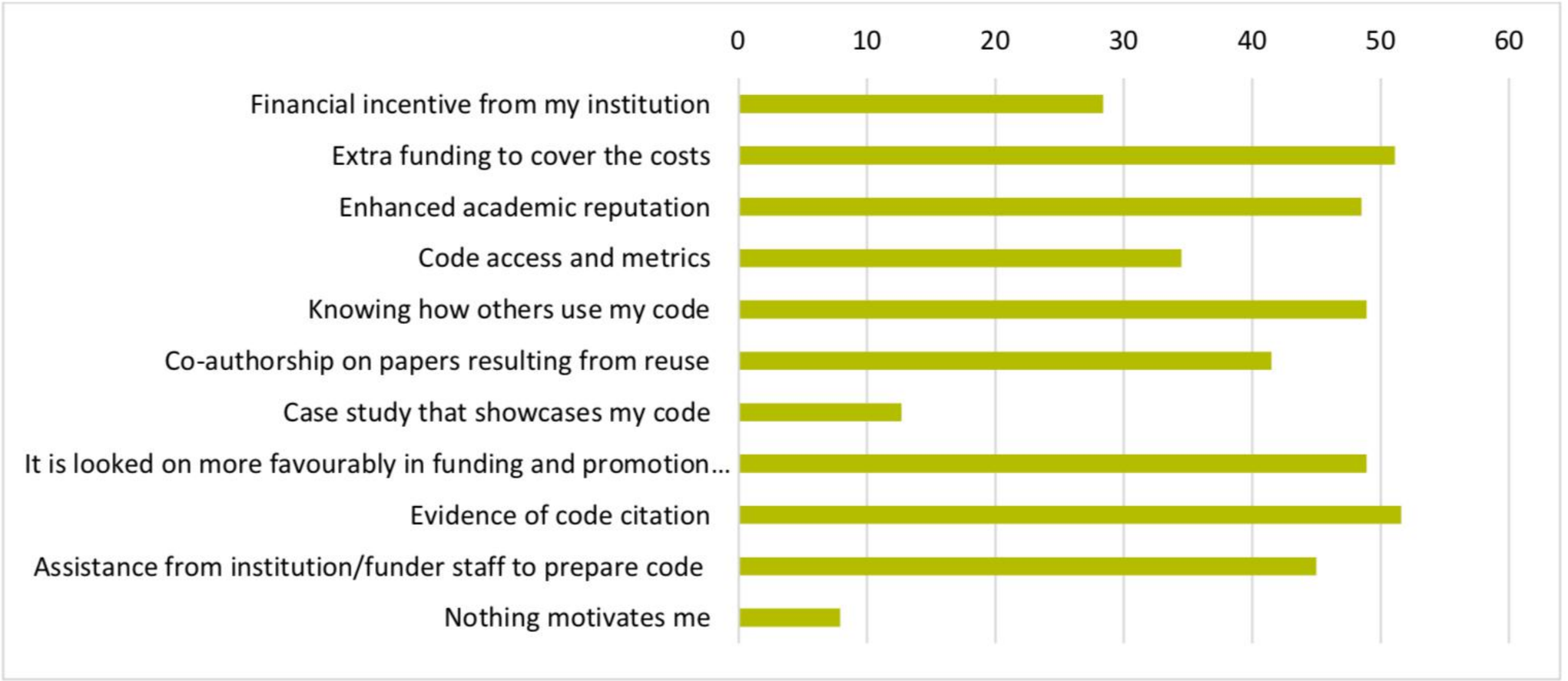
Whitaker (2018) https://doi.org/10.6084/m9.figshare.7140050.v2

FIGURE 25 RESPONDENT EVALUATION OF CODE SHARING BARRIERS



Van den Eynden, Veerle; Knight, Gareth; Vlad, Anca; Radler, Barry; Tenopir, Carol; Leon, David; et al. (2016): Survey of Wellcome researchers and their attitudes to open research. figshare. Journal contribution. https://doi.org/10.6084/m9.figshare.4055448.v1

FIGURE 26 FACTORS THAT WOULD MOTIVATE THE RESPONDENT TO MAKE MORE CODE AVAILABLE, AS PERCENTAGE OF RESPONDENTS (N=229)



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“Give some indication that sharing code is valued when funding decisions are made. Editing code from the state where it works on my computer to where it can be used by everybody takes a huge amount of time. In addition to making the code better / more robust, making it public also requires a significant amount of documentation. There is little credit given for this effort, especially when the code is supporting a specific paper (rather than code for a tool that will be widely used by the community).”

Van den Eynden, Veerle; Knight, Gareth; Vlad, Anca; Radler, Barry; Tenopir, Carol; Leon, David; et al. (2016): Survey of Wellcome researchers and their attitudes to open research. figshare. Journal contribution. https://doi.org/10.6084/m9.figshare.4055448.v1

Benefits to sharing research software

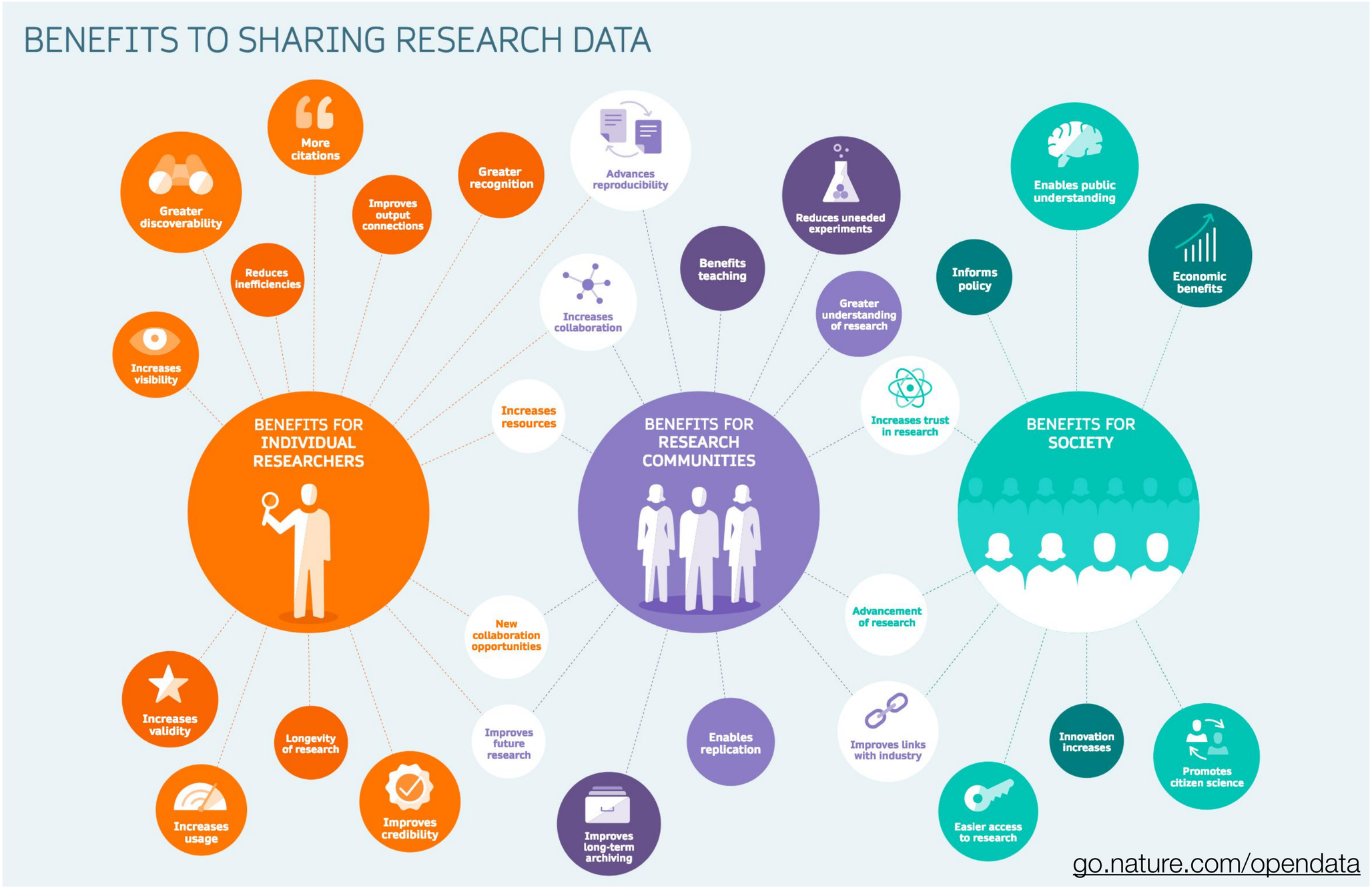
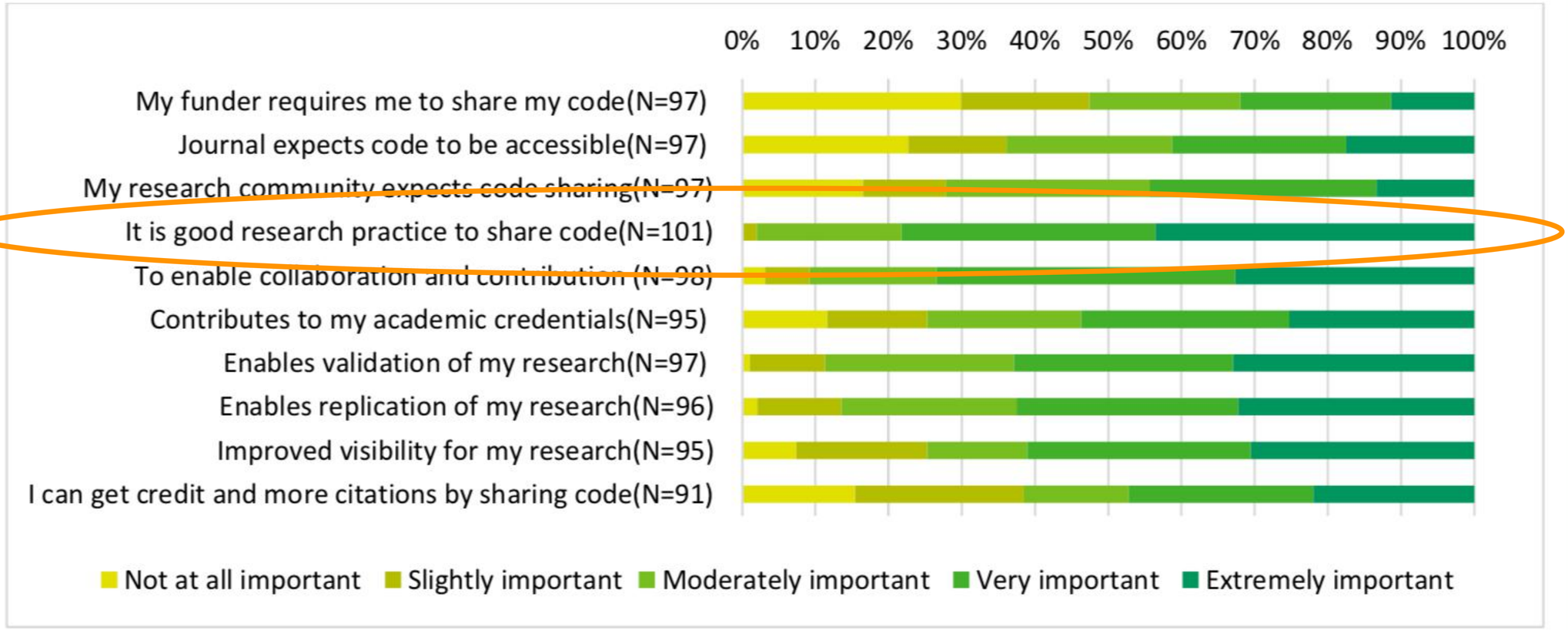
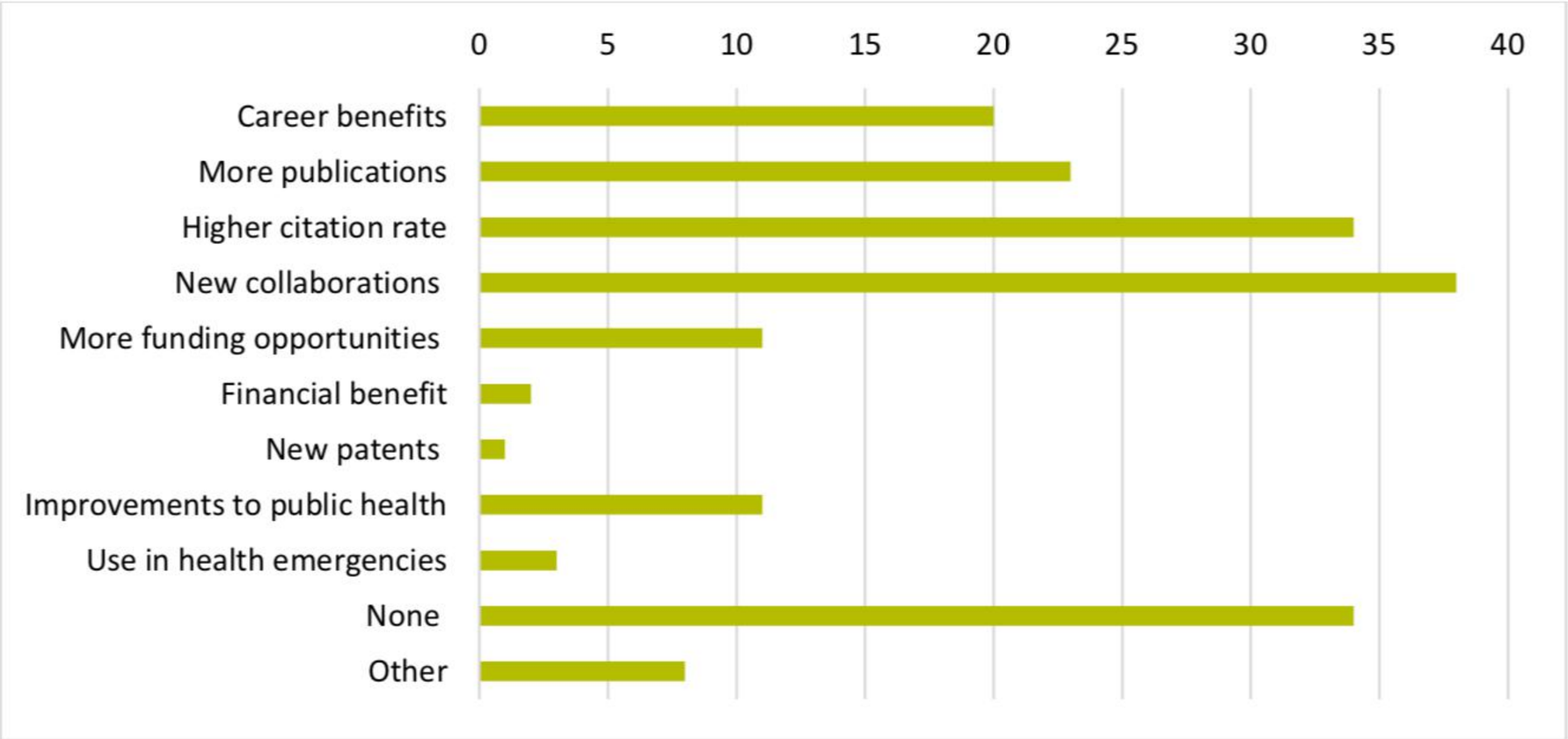

BENEFITS TO SHARING RESEARCH DATA
More citations
Greater discoverability
Improves output connections
Greater recognition
Advances reproducibility
Reduces uneeded experiments
Enables public understanding
Reduces inefficiencies
Benefits teaching
Informs policy
Economic benefits
Increases collaboration
Greater understanding of research
Increases visibility
Increases resources
BENEFITS FOR INDIVIDUAL RESEARCHERS
BENEFITS FOR RESEARCH COMMUNITIES
Increases trust in research
BENEFITS FOR SOCIETY
New collaboration opportunities
Advancement of research
Increases validity
Longevity of research
Improves future research
Enables replication
Improves links with industry
Innovation increases
Promotes citizen science
Increases usage
Improves credibility
Improves long-term archiving
Easier access to research
go.nature.com/opendata

FIGURE 23. REASONS FOR MAKING CODE AVAILABLE IN A REPOSITORY OR OTHER ONLINE FORM



Van den Eynden, Veerle; Knight, Gareth; Vlad, Anca; Radler, Barry; Tenopir, Carol; Leon, David; et al. (2016): Survey of Wellcome researchers and their attitudes to open research. figshare. Journal contribution. https://doi.org/10.6084/m9.figshare.4055448.v1

FIGURE 24. PERCENTAGE OF RESPONDENTS THAT HAVE GAINED PERSONAL BENEFITS BY CODE SHARING (N=100)



Van den Eynden, Veerle; Knight, Gareth; Vlad, Anca; Radler, Barry; Tenopir, Carol; Leon, David; et al. (2016): Survey of Wellcome researchers and their attitudes to open research. figshare. Journal contribution. https://doi.org/10.6084/m9.figshare.4055448.v1

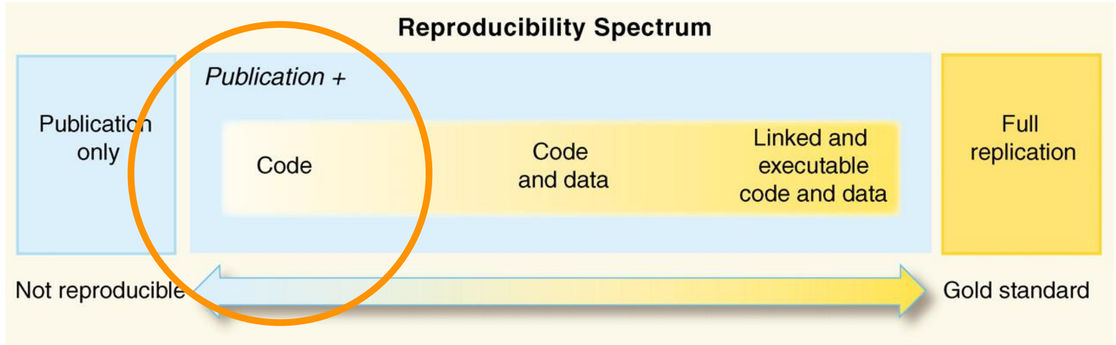
“It is about mind-sets and culture: An unsung part of open software are its communities that promote and enable a more inclusive, kinder culture.”

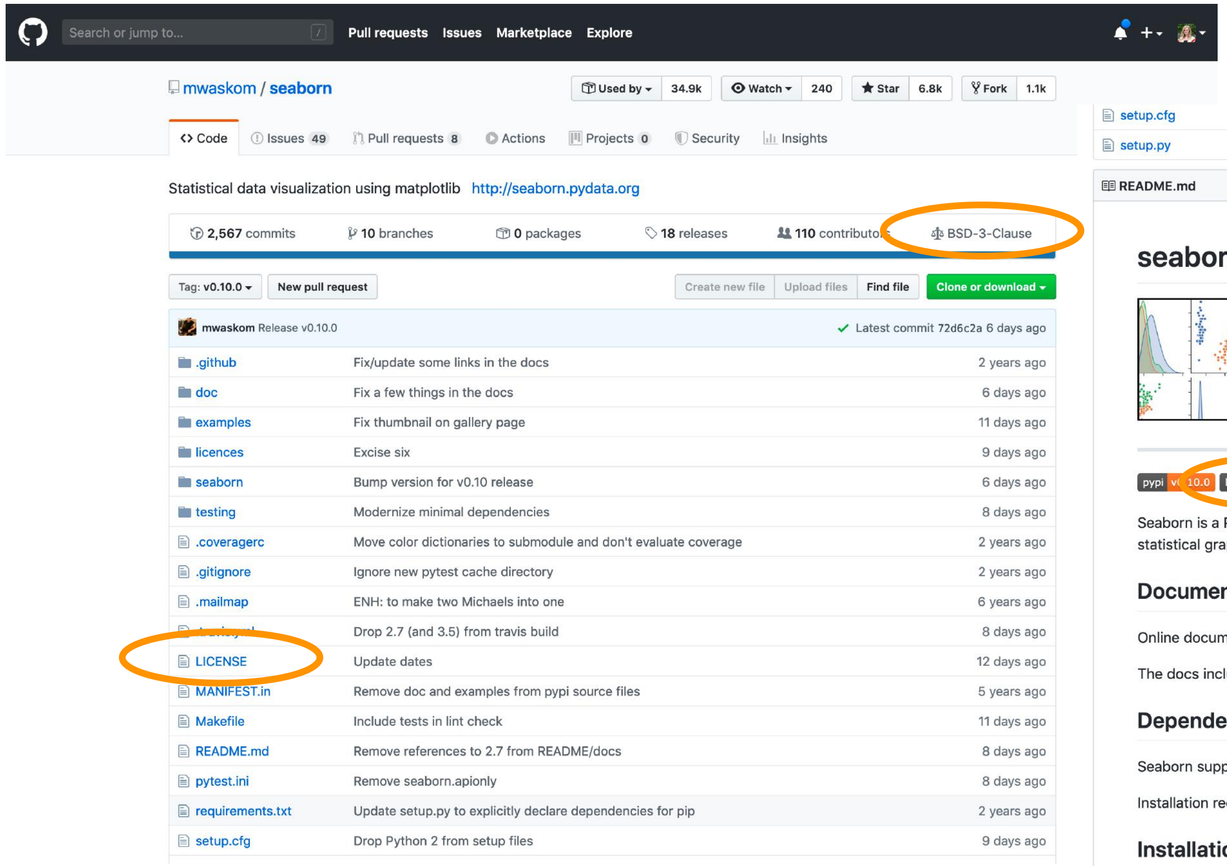
– Julia Stewart Lowndes, Open Software Means Kinder Science
https://blogs.scientificamerican.com/observations/open-software-means-kinder-science

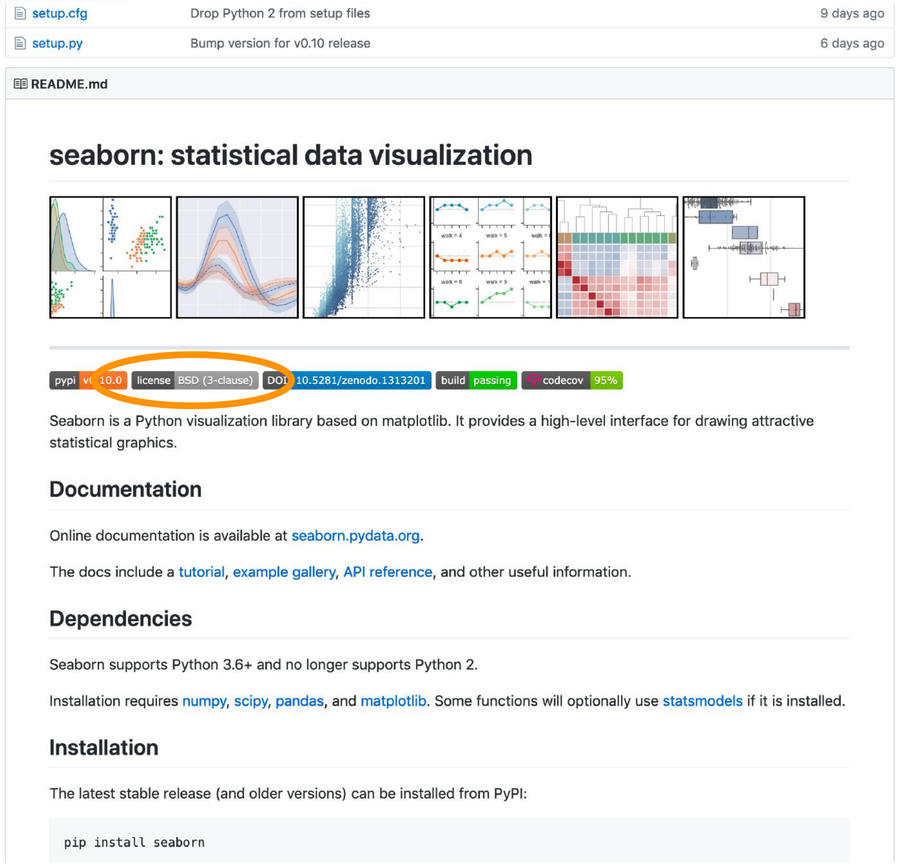
How to share your research software and get credit

Share software in repositories such as GitHub, Bitbucket & GitLab

- Version control
- Facilitates open, collaborative & reproducible science/code/ research
- Online portfolio & webpage for your work



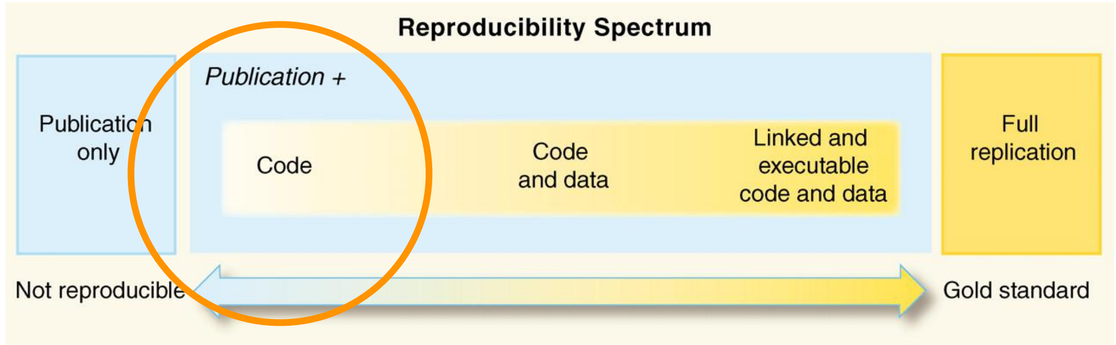




https://github.com/mwaskom/seaborn/tree/v0.10.0

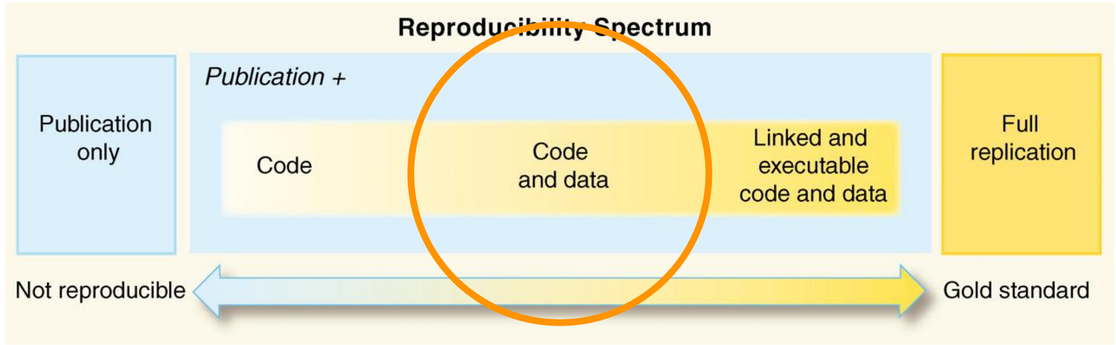
Choose an open source license to allow adoption & reuse

- GitHub guide on choosing an open source license: https://choosealicense.com/
- SSI Guide on Choosing an open-source licence: https://www.software.ac.uk/resources/guides/adopting-open-source-licence
- A Quick Guide to Software Licensing for the Scientist-Programmer: https://doi.org/10.1371/journal.pcbi.1002598
- tl;drLegal summarises software licenses in plain English and has developed a tool to help you manage your open source licenses: https://tldrlegal.com/

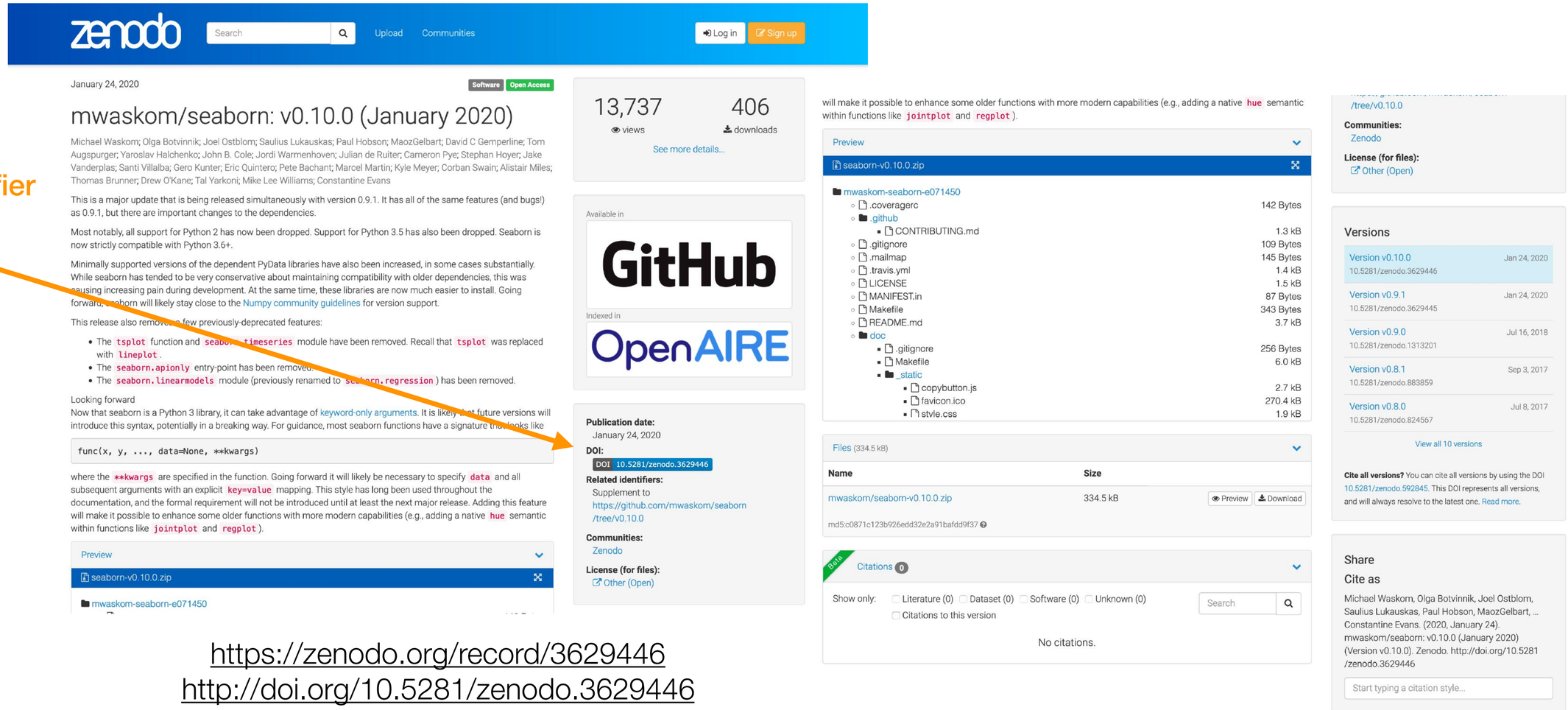


https://choosealicense.com/

Make software citable by archiving in repositories such as Zenodo & Figshare

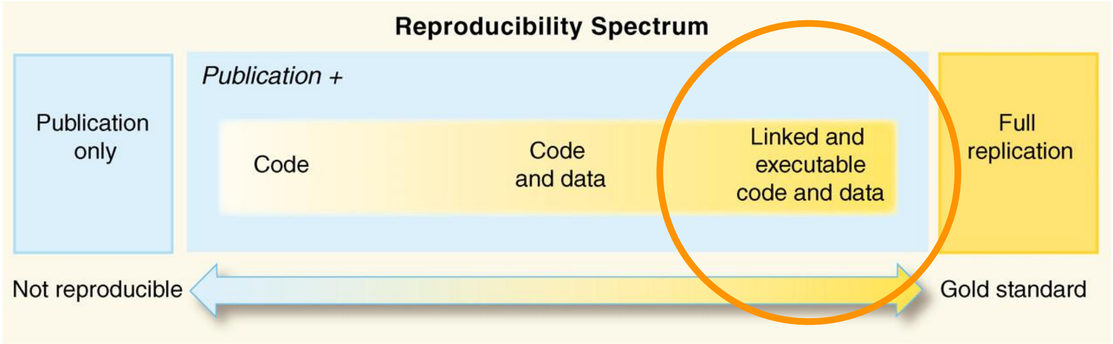


Assigns a distinct persistent identifier: Digital Object Identifier (DOI)



https://zenodo.org/record/3629446
http://doi.org/10.5281/zenodo.3629446

Make it as easy as possible for others to use your software



- Open Notebooks display code that can be executed independently and interactively, facilitating transparency in the analysis of data, reproducibility, and documentation of the entire workflow
  - Jupyter and RStudio
- Containers can be used to package entire scientific workflows, software and libraries, and even data, eliminating the pain of having to install missing dependencies
  - Docker and Singularity
- Binder launches a Git repository containing open notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere

Publish your Research Software

- Full article in peer reviewed domain specific journals (example: Astropy article in *Astronomy & Astrophysics*, https://doi.org/10.1051/0004-6361/201322068)
- *Journal of Open Research Software* (JORS) features peer reviewed Software Metapapers describing research software with high reuse potential
- *Journal of Open Source Software* (JOSS) is a developer friendly academic journal with a formal peer review process that is designed to improve the quality of the software submitted


A&A 558, A33 (2013)
DOI: 10.1051/0004-6361/201322068
© ESO 2013

Astronomy & Astrophysics

Astropy: A community Python package for astronomy

The Astropy Collaboration, Thomas P. Robitaille[1], Erik J. Tollerud[2,3], Perry Greenfield[4], Michael Droettboom[4], Erik Bray[4], Tom Aldcroft[5], Matt Davis[4], Adam Ginsburg[6], Adrian M. Price-Whelan[7], Wolfgang E. Kerzendorf[8], Alexander Conley[8], Neil Crighton[1], Kyle Barbary[9], Demitri Muna[10], Henry Ferguson[4], Frédéric Grollier[12], Madhura M. Parikh[11], Prasanth H. Nair[12], Hans M. Günther[5], Christoph Deil[13], Julien Woillez[14], Simon Conseil[15], Roban Kramer[16], James E. H. Turner[17], Leo Singer[18], Ryan Fox[12], Benjamin A. Weaver[19], Victor Zabalza[13], Zachary I. Edwards[20], K. Azalee Bostroem[4], D. J. Burke[5], Andrew R. Casey[21], Steven M. Crawford[22], Nadia Dencheva[4], Justin Ely[4], Tim Jenness[23,24], Kathleen Labrie[25], Pey Lian Lim[4], Francesco Pierfederici[4], Andrew Pontzen[26,27], Andy Ptak[28], Brian Refsdal[5], Mathieu Servillat[29,5], and Ole Streicher[30]

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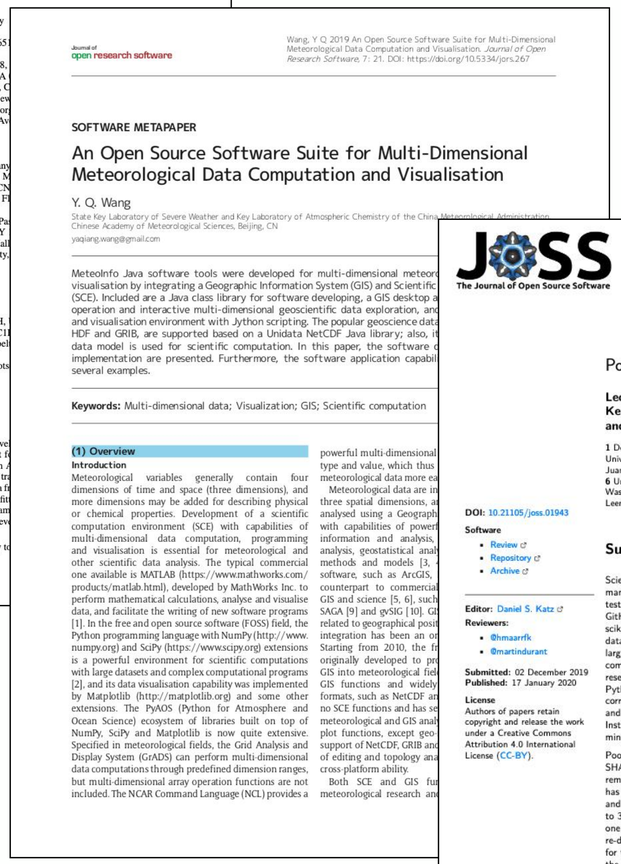
Received 12 June 2013 / Accepted 23 July 2013

ABSTRACT

We present the first public version (v0.2) of the open-source and community-deve
provides core astronomy-related functionality to the community, including support f
image transport system (FITS) files, Virtual Observatory (VO) tables, and common A
conversions, physical constants specific to astronomy, celestial coordinate and time tr
support, generalized containers for representing gridded as well as tabular data, and a fr
conversions. Significant functionality is under active development, such as a model fit
aperture and point spread function (PSF) photometry tools. The core development team
to the current code base, and we encourage anyone interested to participate in the deve

Key words. methods: data analysis – methods: miscellaneous – virtual observatory t

Article published by EDP Sciences


Journal of open research software

Wang, Y Q 2019 An Open Source Software Suite for Multi-Dimensional Meteorological Data Computation and Visualisation. *Journal of Open Research Software*, 7: 21. DOI: https://doi.org/10.5334/jors.267

SOFTWARE METAPAPER

An Open Source Software Suite for Multi-Dimensional Meteorological Data Computation and Visualisation

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State Key Laboratory of Severe Weather and Key Laboratory of Atmospheric Chemistry of the China Meteorological Administration, Chinese Academy of Meteorological Sciences, Beijing, CN
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MeteoInfo Java software tools were developed for multi-dimensional meteoro
visualisation by integrating a Geographic Information System (GIS) and Scientific
(SCE). Included are a Java class library for software developing, a GIS desktop a
operation and interactive multi-dimensional geoscientific data exploration, and
and visualisation environment with Jython scripting. The popular geoscience data
HDF and GRIB, are supported based on a Unidata NetCDF Java library; also, it
data model is used for scientific computation. In this paper, the software c
implementation are presented. Furthermore, the software application capabil
several examples.

Keywords: Multi-dimensional data; Visualization; GIS; Scientific computation

(1) Overview

Introduction

Meteorological variables generally contain four dimensions of time and space (three dimensions), and more dimensions may be added for describing physical or chemical properties. Development of a scientific computation environment (SCE) with capabilities of multi-dimensional data computation, programming and visualisation is essential for meteorological and other scientific data analysis. The typical commercial one available is MATLAB (https://www.mathworks.com/products/matlab.html), developed by MathWorks Inc. to perform mathematical calculations, analyse and visualise data, and facilitate the writing of new software programs [1]. In the free and open source software (FOSS) field, the Python programming language with NumPy (http://www.numpy.org) and SciPy (https://www.scipy.org) extensions is a powerful environment for scientific computations with large datasets and complex computational programs [2], and its data visualisation capability was implemented by Matplotlib (http://matplotlib.org) and some other extensions. The PyAOS (Python for Atmosphere and Ocean Science) ecosystem of libraries built on top of NumPy, SciPy and Matplotlib is now quite extensive. Specified in meteorological fields, the Grid Analysis and Display System (GrADS) can perform multi-dimensional data computations through predefined dimension ranges, but multi-dimensional array operation functions are not included. The NCAR Command Language (NCL) provides a powerful multi-dimensional type and value, which thus meteorological data more ea

Meteorological data are in three spatial dimensions, a analysed using a Geograph with capabilities of powerf information and analysis, analysis, geostatistical anal methods and models [3, software, such as ArcGIS, counterpart to commercial GIS and science [5, 6], such SAGA [9] and gvSIG [10]. GI related to geographical posit integration has been an or Starting from 2010, the fr originally developed to pr GIS into meteorological fiel GIS functions and widely formats, such as NetCDF ar no SCE functions and has se meteorological and GIS anal plot functions, except geo- support of NetCDF, GRIB an of editing and topology ana cross-platform ability.

Both SCE and GIS fu meteorological research an


JOSS The Journal of Open Source Software

Pooch: A friend to fetch your data files

Leonardo Uieda[1], Santiago Rubén Soler[2,3], Rémi Rampin[4], Hugo van Kemenade[5], Matthew Turk[6], Daniel Shapero[7], Anderson Banihirwe[8], and John Leeman[9]

1 Department of Earth, Ocean and Ecological Sciences, School of Environmental Sciences, University of Liverpool, UK **2** Instituto Geofísico Sismológico Volponi, Universidad Nacional de San Juan, Argentina **3** CONICET, Argentina **4** New York University, USA **5** Independent (Non-affiliated) **6** University of Illinois at Urbana-Champaign, USA **7** Polar Science Center, University of Washington Applied Physics Lab, USA **8** The US National Center for Atmospheric Research, USA **9** Leeman Geophysical, USA

DOI: 10.21105/joss.01943

Software
- Review
- Repository
- Archive

Editor: Daniel S. Katz
Reviewers:
- @hmaarrfk
- @martindurant

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Published: 17 January 2020

Summary

Scientific software is usually created to acquire, analyze, model, and visualize data. As such, many software libraries include sample datasets in their distributions for use in documentation, tests, benchmarks, and workshops. A common approach is to include smaller datasets in the GitHub repository directly and package them with the source and binary distributions (e.g., scikit-learn (Pedregosa et al., 2011) and scikit-image (Van der Walt et al., 2014) do this). As data files increase in size, it becomes unfeasible to store them in GitHub repositories. Thus, larger datasets require writing code to download the files from a remote server to the user's computer. The same problem is faced by scientists using version control to manage their research projects. While downloading a data file over HTTPS can be done easily with modern Python libraries, it is not trivial to manage a set of files, keep them updated, and check for corruption. For example, scikit-learn (Pedregosa et al., 2011), Cartopy (Met Office, n.d.), and PyVista (Sullivan & Kaszynski, 2019) all include code dedicated to this particular task. Instead of scientists and library authors recreating the same code, it would be best to have a minimalistic and easy to set up tool for fetching and maintaining data files.

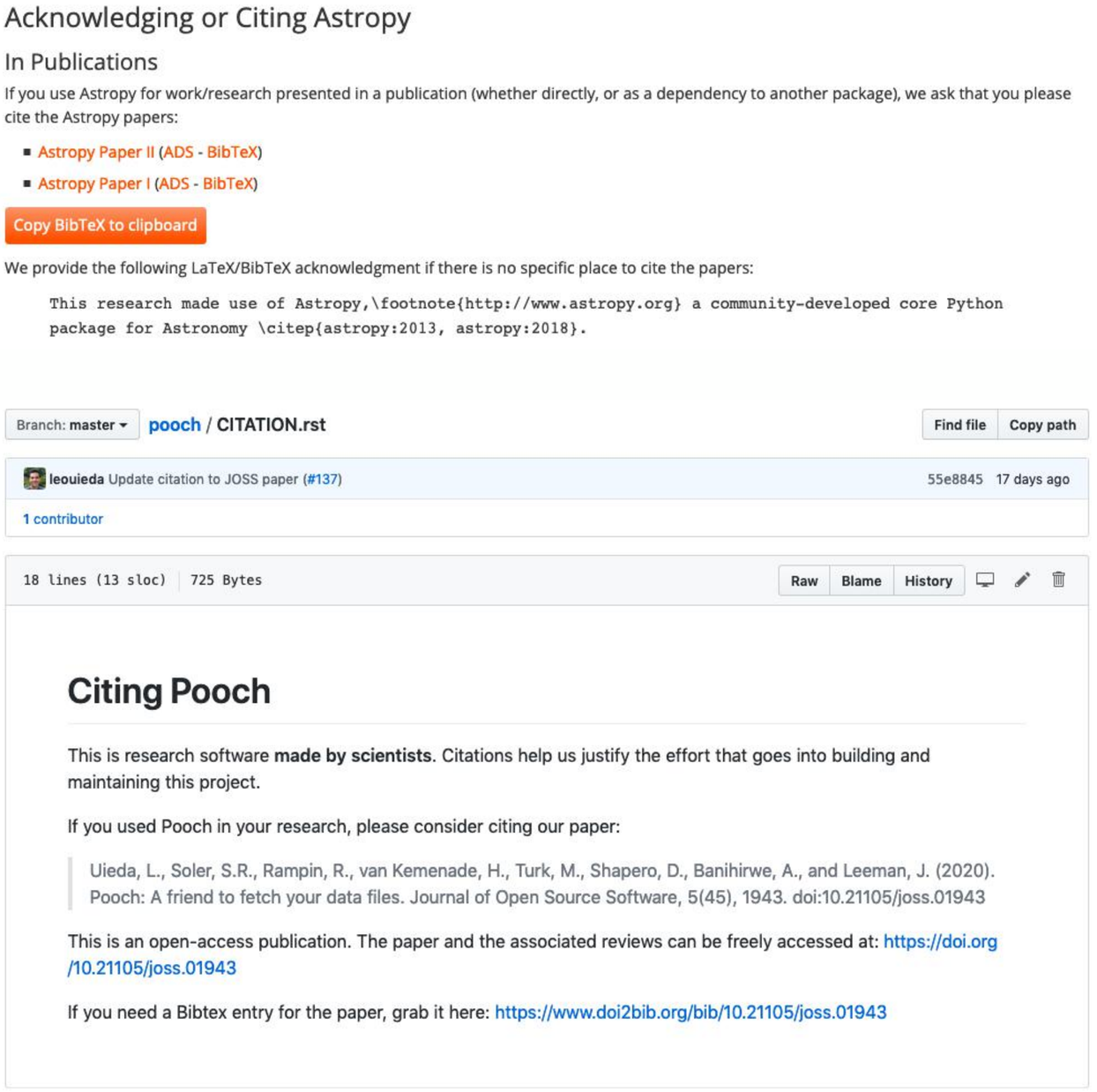
Pooch is a Python library that fills this gap. It manages a data *registry* (containing file names, SHA-256 cryptographic hashes, and download URLs) by downloading files from one or more remote servers and storing them in a local data cache. Pooch is written in pure Python and has minimal dependencies. It can be easily installed from the Python Package Index (PyPI) and conda-forge on a wide range of Python versions: 2.7 (up to Pooch 0.6.0) and from 3.5 to 3.8. The integrity of downloads is verified by comparing the file's SHA-256 hash with the one stored in the data registry. This is also the mechanism used to detect if a file needs to be re-downloaded due to an update in the registry. Pooch is meant to be a drop-in replacement for the custom download code that users have already written (or are planning to write). In the ideal scenario, the end-user of a software package should not need to know that Pooch is being used. Setup is as easy as calling a single function (`pooch.create`), including setting up an environment variable for overwriting the data cache path and versioning the downloads so that multiple versions of the same package can coexist in the same machine. For example, this is the code required to set up a module `datasets.py` that uses Pooch to manage data downloads:

```
import pooch

# Get the version string from the project
```

Make it easy for people to cite you

Include instructions in your software documentation (README or CITATION file), whether that includes citing a published article about your software or an archived version of your software in a digital repository like Zenodo or Figshare



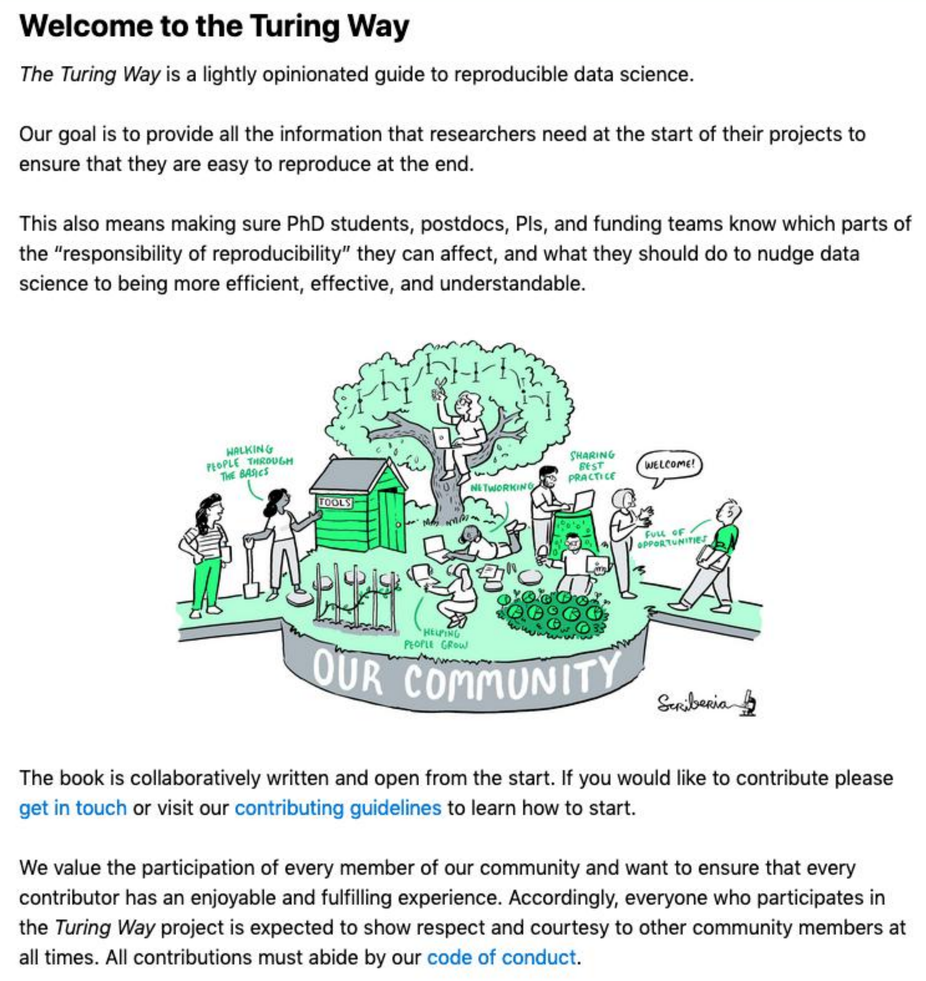
The Turing Way Project

- Project led by Kirstie Whitaker at The Alan Turing Institute to make reproducible research "too easy not to do"
- In short: *The Turing Way* encompasses a handbook, community, collaboration, workshops and training
- Team of researchers, research software engineers, librarians and YOU!
- Demonstrates open and transparent project management and communication with future users, as it is openly developed at our GitHub repository: https://github.com/alan-turing-institute/the-turing-way

The Turing Way

1. Introduction
2. Reproducibility
3. Open Research
4. Version Control
5. Collaborating on GitHub/GitLab
6. Credit for reproducible research
7. Research Data Management
8. Reproducible Environments
9. Testing
10. Reviewing
11. Continuous Integration
12. Reproducible Research with Make
13. Risk Assessment
14. BinderHub
15. Glossary

Powered by Jupyter Book



Welcome to the Turing Way

The Turing Way is a lightly opinionated guide to reproducible data science.

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

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

The book is collaboratively written and open from the start. If you would like to contribute please get in touch or visit our contributing guidelines to learn how to start.

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

Handbook at: https://the-turing-way.netlify.com

Takeaways

1. Make your software available in a stable, version-controlled repository
2. Choose an open source license to allow adoption and reuse
3. Assign a distinct persistent identifier (DOI) for each version release
4. Include instructions and examples of how to cite your software in its documentation

- Check out *The Turing Way* - a handbook on reproducible research/data science openly developed at https://github.com/alan-turing-institute/the-turing-way/
- TEDx talk: Research Culture is Broken; Open Science can [help] fix it https://youtu.be/c-bemNZ-IqA
- More of my slide decks on Open Research can be found on Figshare: https://figshare.com/authors/Rachael_Ainsworth/4824354