

Towards sustainable research software through software citation, FAIR research software, and Research Software Engineer career paths

Daniel S. Katz (d.katz@ieee.org,  @danielskatz@fosstodon.org)

Chief Scientist, NCSA

Associate Research Professor, CS, ECE, iSchool

University of Illinois at Urbana Champaign



PyData Chicago Meetup

25 May 2023

 **ILLINOIS**

NCSA | National Center for
Supercomputing Applications

<https://doi.org/10.5281/zenodo.7951188>



We want to collaborate: Open Science

- The free sharing of scientific ideas, methods, and results
- But not just science, rather wissenschaft (knowledge, scholarship, ...)
- Initially via hand-written letters and books, mostly for other scientists
- Then more frequently via printed journals, expanding the audience
- Digitalization expanded opportunities for sharing, as well as what could be shared
- Democratization of research (public funding) and information sharing (BBS, WWW) expanded the community (at least the audience)
- Idea of knowledge as a common (societal) good
- “Open science” term documented in Science, July 1882, but having the sense of using the scientific method
- It seems to have become commonly used in the modern sense in the mid 1980s, perhaps when the AAAS Project on Secrecy and Openness in Science and Technology started in 1984

J. P. Tennant, ..., D. S. Katz, ..., "A tale of two 'opens': intersections between Free and Open Source Software and Open Scholarship," SocArXiv, 6 Mar. 2020. DOI: [10.31235/osf.io/2kxq8](https://doi.org/10.31235/osf.io/2kxq8)

We also compete: Economics drives our lives

- We live in a capitalistic society
- Economics drives our lives and careers
 - Where we work (hiring)
 - How we support ourselves (promotion)
 - How we get funding to do science (support, recognition)
 - Which science we do (what areas we think will lead to reward)
 - Which students we train or take advantage of (depending on your viewpoint)
- Economics: the science of allocating scarce resources to maximize the achievement of competing ends
 - Sometimes a false argument, some resources can be increased, e.g., digital

Paula Stephan, [How Economics Shapes Science](#), Harvard University Press, 2015.

Human behavior: Competition & Collaboration

- Engagement
 - Meaningful and valuable actions that produce a measurable result
 - Choosing when and where to come together to do something
- Engagement = Motivation + Support – Friction
 - Intrinsic motivation: self-fulfillment, altruism, satisfaction, accomplishment, pleasure of sharing, curiosity, real contribution to science
 - Extrinsic motivation: job, rewards, recognition, influence, knowledge, relationships, community membership
 - Support: ease, relevance, timeliness, value
 - Friction: technology, time, access, knowledge

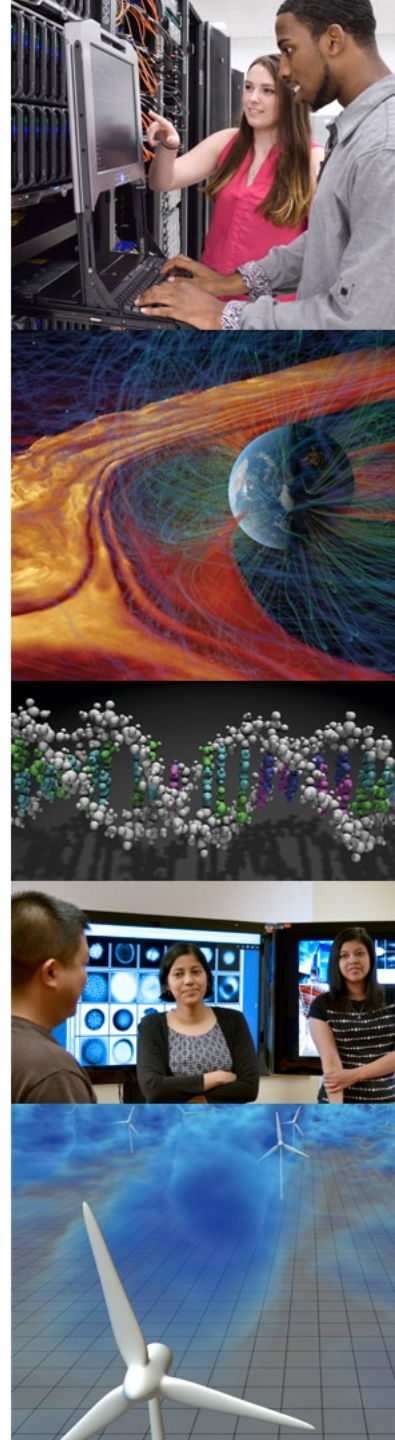
Adapted from Joseph Porcelli

Why we don't collaborate (Open Science)

- Sharing takes effort, immediate benefits go to others
- Embarrassment about details (e.g., coding practice)
- Don't want to have to support others
- Mechanisms of sharing are new, not the way we work
- Metrics for evaluating products that can be shared are underdeveloped
- Intellectual property laws
- Commercial entities profit from restricting access
- Non-profit scientific societies are dependent on journal subscription fees [to support themselves/work they do]

C. Titus Brown, "What is open science?," 24 October 2016. <http://ivory.idyll.org/blog/2016-what-is-open-science.html>

Research Software



Why do we care about research software?

- Funding

- ~20% of NSF projects over 11 years topically discuss software in their abstracts (\$10b)
- 2 of 3 main DOE ECP areas are research software (~\$4b)
- \$300m of FY2021 NIH projects include “software development”

Collected from <http://www.dia2.org> in 2017

Collected from <https://reporter.nih.gov> in 2022

- Publications

- Software intensive projects are a majority of current publications
- Most-cited papers are methods and software

Nangia and Katz; [10.1109/eScience.2017.78](https://doi.org/10.1109/eScience.2017.78)

“Top 100-cited papers of all time,” Nature, 2014
[10.1038/514550a](https://doi.org/10.1038/514550a)

- Researchers

- >90% of US/UK researchers use research software
- ~65% would not be able to do their research without it
- ~50% develop software as part of their research

S. Hettrick; <https://www.software.ac.uk/blog/2016-09-12-its-impossible-conduct-research-without-software-say-7-out-10-uk-researchers>

S.J. Hettrick, et al.; [10.5281/zenodo.14809](https://doi.org/10.5281/zenodo.14809)

U. Nangia and D. S. Katz; [10.6084/m9.figshare.5328442.v1](https://doi.org/10.6084/m9.figshare.5328442.v1)

What is research software?

- Research software is a component of our instruments
- Research software is the instrument
- Research software analyses research data
- Research software presents research results
- Research software assembles or integrates existing components into a working whole
- Research software is infrastructure or an underlying tool
- Research software facilitates distinctively research-oriented collaboration

R. van Nieuwpoort and D. S. Katz, “Defining the roles of research software,” <https://doi.org/10.54900/9akm9y5-5jlect5y>

A research and research software vision

- All research software that can be is open
- All research software is high-quality and robust
- All research software is findable, accessible, and usable & used by others (for their own research)
 - And is cited when it is used
- All contributors to research software are recognized for their work
 - With good careers
- All research software is sustained as long as it is useful
- All research is reproducible

Note overlaps in terms of incentives and policies; all start with recognition of research software

Software collapses

- Software stops working eventually if is not actively maintained
- Structure of computational science software stacks:
 1. Project-specific software (developed by researchers): software to do a computation using building blocks from the lower levels: scripts, workflows, computational notebooks, small special-purpose libraries & utilities
 2. Discipline-specific software (developed by developers & researchers): tools & libraries that implement disciplinary models & methods
 3. Scientific infrastructure (developed by developers): libraries & utilities used for research in many disciplines
 4. Non-scientific infrastructure (developed by developers): operating systems, compilers, and support code for I/O, user interfaces, etc.
- Software builds & depends on software in all layers below it; any change below may cause collapse

K. Hinsien, "Dealing With Software Collapse," 2019.
<https://doi.org/10.1109/MCSE.2019.2900945>

Challenges

- Research software: developed and used for the purpose of research - to generate, process, analyze results within the scholarly process
- Increasingly essential in the overall research process
- But there are research software challenges:
 - Software will collapse if not maintained
 - Software bugs are found, new features are needed, new platforms arise
 - Software development and maintenance is human-intensive
- And human challenges:
 - Much software developed specifically for research, by researchers
 - Researchers know their disciplines, but often not software best practices
 - Researchers are not rewarded for software development and maintenance in academia
 - Developers don't match the diversity of overall society or of user communities

Software sustainability

- Software sustainability \equiv the software endures
 - Will the software will continue to be available in the future, on new platforms, meeting new needs?
 - Can only be measured in hindsight – looking forward is only a prediction
- Software development and maintenance requires active human effort
- Human effort \Leftrightarrow \$
 - All human effort works (community open source)
 - All \$ (salary) works (commercial software, grant funded projects)
 - Combined is hard: effort \neq \$; humans are not purely rational

Research software sustainability defined

Research software sustainability is the process of developing and maintaining software that continues to meet its purpose over time, which includes that the software adds new capabilities as needed by its users, responds to bugs and other problems that are discovered, and is ported to work with new versions of the underlying layers, including software as well as new hardware

Potential solutions

- In order to sustain research software, we can
 - Do things that reduce the amount of work needed
 - Do things that increase the available resources
 - Do things that both reduce the amount of work needed and increase the available resources

Methods to sustain research software (1)

- To reduce the amount of work needed
 - Train its developers, which involves finding or developing training material
 - Carpentries, discipline-specific materials, language-specific materials
 - Use best practices, which involves finding or developing best practices
 - Software Carpentry, incubators (e.g. ESIP, Apache)

Methods to sustain research software (2)

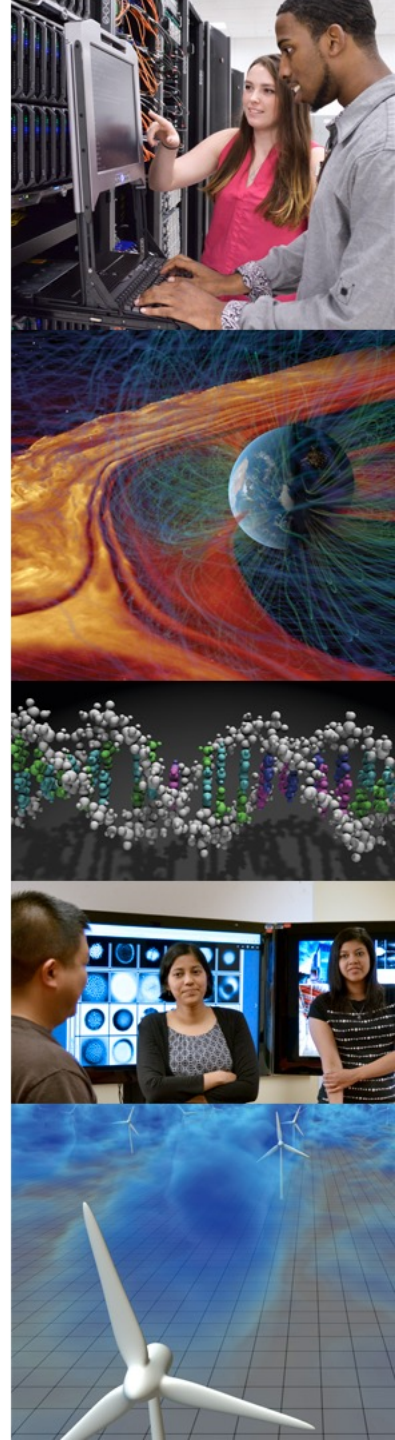
- To increase the available resources
 - Create incentives so that people want to work on the software
 - Citations that help in existing career paths [More about citation coming: #1](#)
 - Adjusted existing career paths that reward software work
 - New career paths [More about new career paths coming: #2](#)
 - Increase available funding by first making the role of software in research clear to research funders, and then by clearly making the case for them to increase funding for new software, and to provide funding for software maintenance
 - Seek institutional resources if the software is considered sufficiently important to the institution, operationally or reputationally

Methods to sustain research software (3)

- To both reduce work and bring in new resources, encourage collaboration
 - Using the work of others rather than reimplementing a function or package reduces what a software team (or its developers) needs to do themselves, even without assuming that the collaborators contribute to the software, which also may happen
 - Similarly, if others use a team's software and contribute to maintaining it, the team has less they need to do
 - To make this work, software has to be designed from the start to be modular and reusable, and it must also be clearly documented and explained to potential users, even those in fields other than the developer's
 - And the team has to put effort into engaging and working with the potential user and contributor community
 - Summary: Make the software findable, accessible, interoperable, reusable (FAIR)

More about FAIR coming: #3

#1: Software citation & Journal of Open Source Software (JOSS)



FORCE11 Software Citation Working Group (2015-16)

- Documented differences between software and data; defined software citation challenges
 - Katz DS, Niemeyer KE, et al. (2016) Software vs. data in the context of citation. PeerJ Preprints 4:e2630v1. DOI: [10.7287/peerj.preprints.2630v1](https://doi.org/10.7287/peerj.preprints.2630v1)
 - Niemeyer KE, Smith AM, Katz DS. (2016) The challenge and promise of software citation for credit, identification, discovery, and reuse. ACM Journal of Data and Information Quality, 7(4):16. DOI: [10.1145/2968452](https://doi.org/10.1145/2968452)
- Created software citation principles
 - Smith AM, Katz DS, Niemeyer KE, FORCE11 Software Citation Working Group. (2016) Software Citation Principles. PeerJ Computer Science 2:e86. DOI: [10.7717/peerj-cs.86](https://doi.org/10.7717/peerj-cs.86) and <https://www.force11.org/software-citation-principles>



<https://www.force11.org/group/software-citation-working-group>
Co-Chairs: Arfon M. Smith, Daniel S. Katz, Kyle E. Niemeyer

Software is a critical part of modern research...

1. Importance
2. Credit and Attribution
3. Unique Identification
4. Persistence
5. Accessibility
6. Specificity

SOFTWARE CITATION PRINCIPLES

IMPORTANCE

Software should be considered a legitimate and citable product of research. Software citations should be accorded the same importance in the scholarly record as citations of other research products; they should be included in the metadata of the citing work, such as a reference list. Software should be cited on the same basis as any other research product such as a paper or a book.

UNIQUE IDENTIFICATION

A software citation should include a method for identification that is machine actionable, globally unique, interoperable, and recognized by at least a community of the corresponding domain experts, and preferably by general public researchers.

PERSISTENCE

Unique identifiers and metadata describing the software and its disposition should persist—even beyond the lifespan of the software they describe.

SPECIFICITY

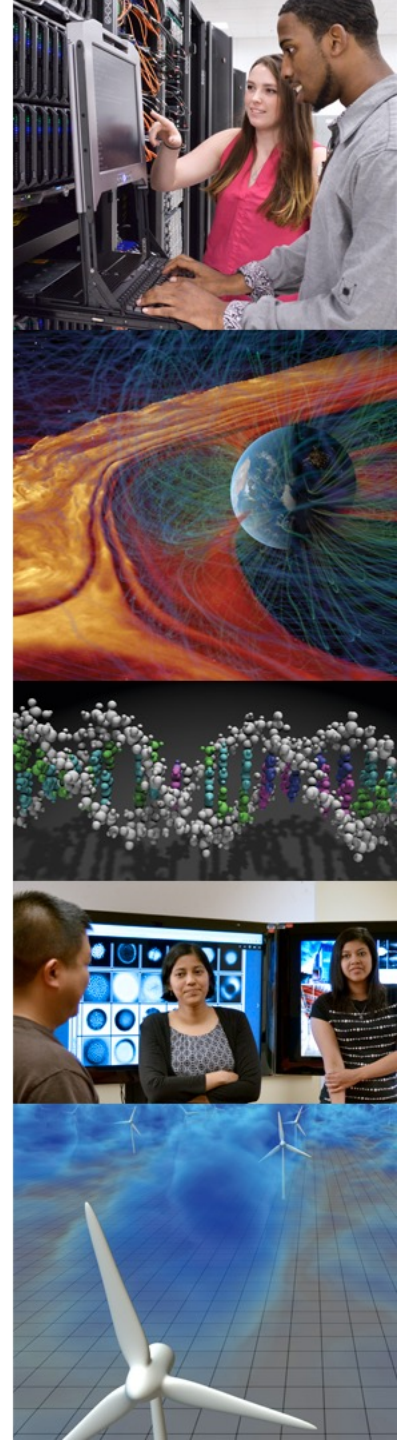
Software citations should facilitate identification of, and access to, the specific version of software that was used. Software identification should be as specific as necessary, such as using version numbers, revision numbers, or variants such as platforms.

CREDIT AND ATTRIBUTION

Software citations should facilitate giving scholarly credit and normative, legal attribution to all contributors to the software, recognizing that a single style or mechanism of attribution may not be applicable to all software.

ACCESSIBILITY

Software citations should facilitate access to the software itself and to its associated metadata, documentation, data, and other materials necessary for both humans and machines to make informed use of the referenced software.



Smith AM, Katz DS, Niemeyer KE, FORCE11 Software Citation Working Group.(2016) Software Citation Principles. PeerJ Computer Science 2:e86.
DOI: [10.7717/peerj-cs.86](https://doi.org/10.7717/peerj-cs.86) and <https://www.force11.org/software-citation-principles>

FORCE11 Software Citation Implementation Working Group (2017-present)

- Initial goals:
 - Write out the “small amount” of detail needed to implement the principles
 - Coordinate research & other work going on in many areas
 - Work with communities to actually implement the principles
- Quickly realized “small amount” of detail wasn’t small, scattered progress wasn't sufficient, underlying challenges not being addressed
 - D. S. Katz, et al., "Software Citation Implementation Challenges", [arXiv 1905.08674](https://arxiv.org/abs/1905.08674) [cs.CY], 2019.
 - Technical challenges include complexity of software types and identifiers, where to store metadata, ...
 - Social challenges need groups that work on implementation in context (disciplinary communities, publishers, repositories & registries, indexers, funders, institutions) to come together and run pilots to establish norms



<https://www.force11.org/group/software-citation-implementation-working-group>

Co-Chairs: Neil Chue Hong, Martin Fenner, Daniel S. Katz

Responses to challenges (1)

- Guidance task force
 - For paper authors who want to cite software
 - N. P. Chue Hong, et al., “[Software Citation Checklist for Authors](https://doi.org/10.5281/zenodo.3479198),” Zenodo, 15-Oct-2019. [10.5281/zenodo.3479198](https://doi.org/10.5281/zenodo.3479198)
 - For software developers who want to make their software citable
 - N. P. Chue Hong, et al., “[Software Citation Checklist for Developers](https://doi.org/10.5281/zenodo.3482768),” Zenodo, 15-Oct-2019. [10.5281/zenodo.3482768](https://doi.org/10.5281/zenodo.3482768)
- CodeMeta task force
 - Following CodeMeta project
 - Aiming to understand metadata for software, not just for use in citation
 - Built a crosswalk of existing metadata standards for software
 - Then developed a CodeMeta standard to describe software based on these crosswalks
 - Updating the CodeMeta standard
 - Describing everything in CodeMeta using schema.org properties
 - Moving CodeMeta into a community group, with governance

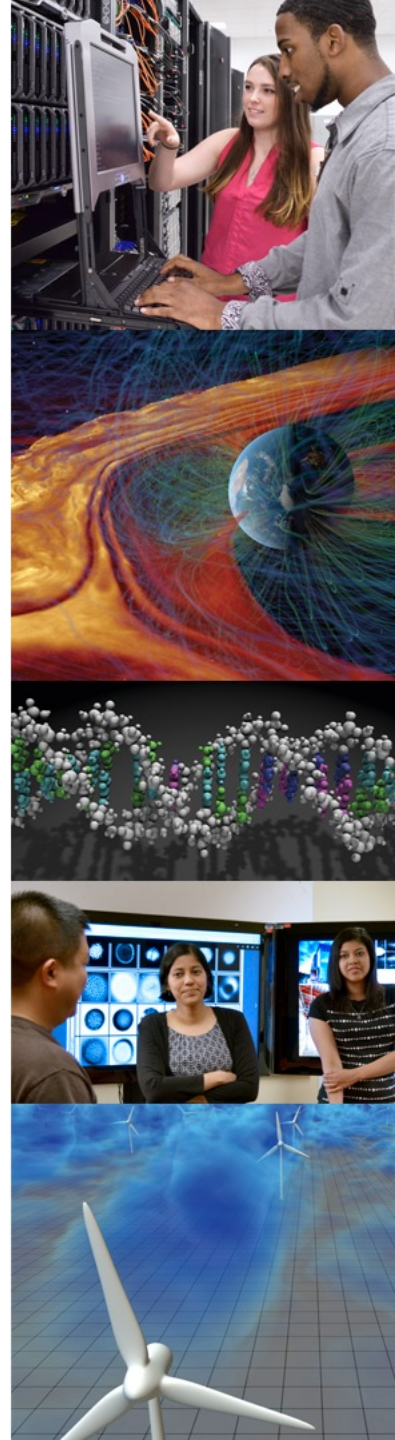
Responses to challenges (2)

- Software Registries Task Force
 - Developed best practices document
 - Task Force on Best Practices for Software Registries, "Nine Best Practices for Research Software Registries and Repositories: A Concise Guide," 2020. [arXiv 2012.13117](https://arxiv.org/abs/2012.13117)
 - Community continuing in SciCodes: Consortium of scientific software registries and repositories, <https://scicodes.net/>
- Journals Task Force
 - Working with publishers to provide generic guidelines for journals and conferences to provide to authors
 - They then provide specific guidelines, with community-accepted language and examples
 - D. S. Katz, et al., "Recognizing the value of software: a software citation guide [version 2; peer review: 2 approved]," F1000Research 9:1257, 2021. [10.12688/f1000research.26932.2](https://doi.org/10.12688/f1000research.26932.2)
 - Tracked by CHORUS in [Software Citation Policy Index](#)
 - Also working on publication processing
 - How citation information moves from author provides to internal publisher/contractor systems and then to indices
 - S. Stall, et al., "Journal Production Guidance for Data and Software Citations", under review

Responses to challenges (3)

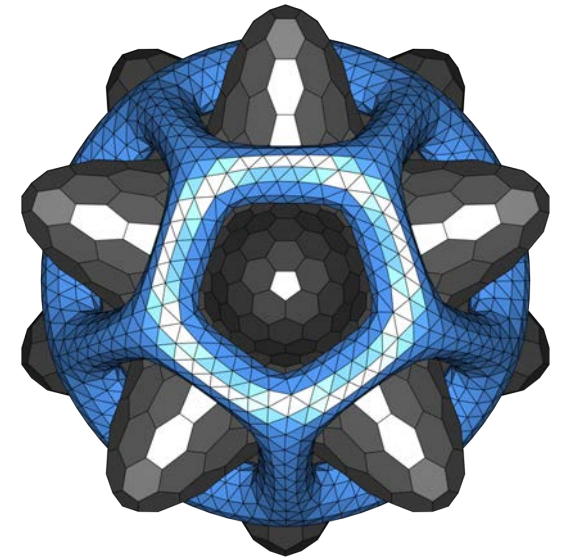
- Considered institutions task force
 - Institutions: places where people work
 - Universities, laboratories, industry, government, etc.
 - Want to affect policies and practices
 - How do they encourage software citation
 - How do they use software citation information in hiring & promotion
 - Collect and share examples
 - Help form communities
 - But insufficient interest from FORCE11 WG members
- Given progress to date, what else makes sense to do, and who can do it?
 - Software citation workshop summer 2022 addressed this; report [available](#)
- As of May 2023, WG has completed, but community is interested in continued discussion
 - Currently writing a blog post to suggest topics and venues

Journal of Open Source Software (JOSS)



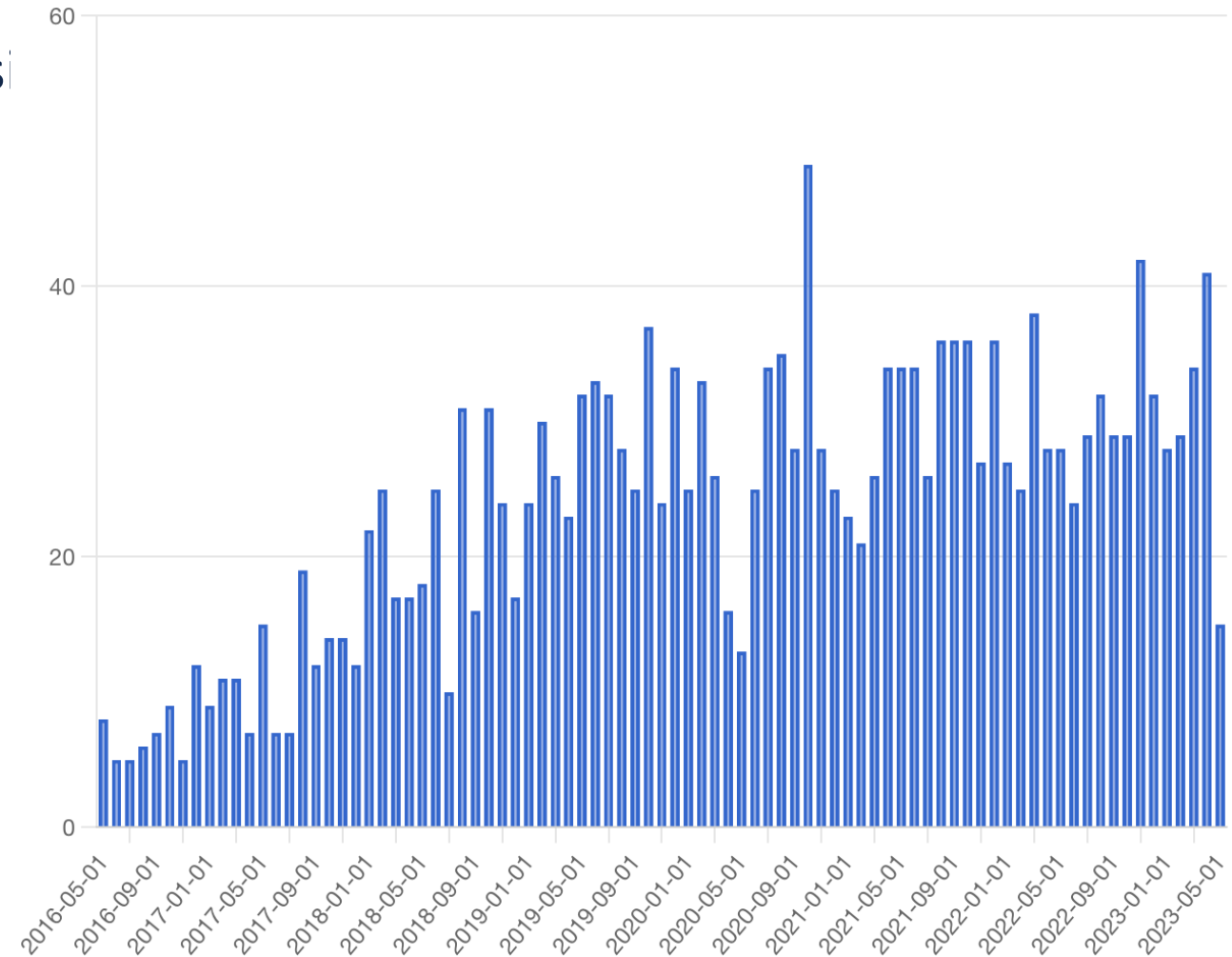
Journal of Open Source Software (JOSS)

- A developer friendly journal for research software packages
 - “If you've already licensed your code and have good documentation then we expect that it should take less than an hour to prepare and submit your paper”
- Everything is open:
 - Submitted/published paper: <https://joss.theoj.org>
 - Code itself: where is up to the author(s)
 - Reviews & process:
<https://github.com/openjournals/joss-reviews>
 - Adapted from rOpenSci
 - Expedited process for software already reviewed by rOpenSci & pyOpenSci
 - Code for the journal itself: <https://github.com/openjournals/joss>
 - Reused for Journal of Open Source Education (JOSE) and Proceedings of the JuliaCon Conferences



Journal of Open Source Software (JOSS)

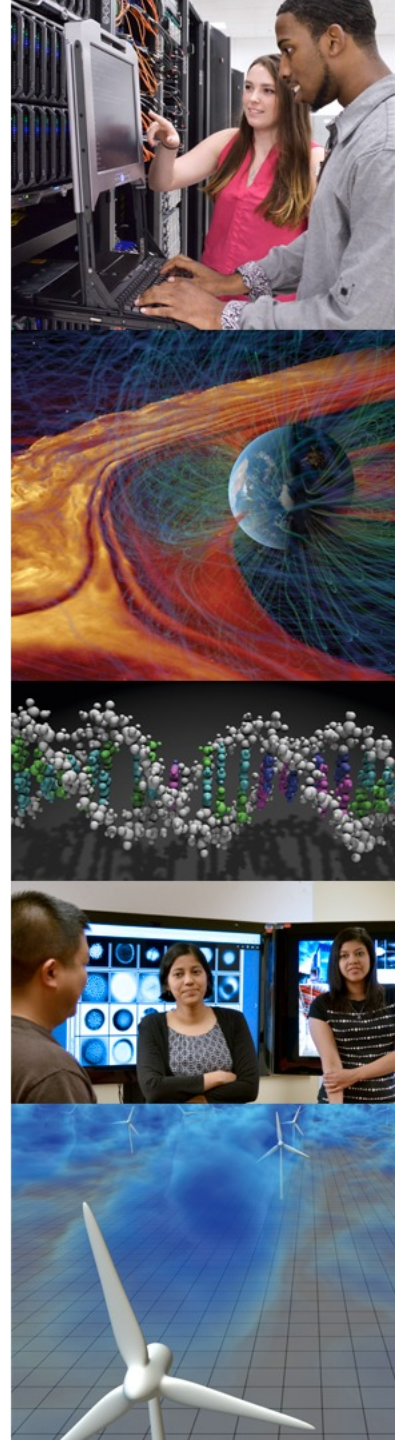
- JOSS papers archived, have DOIs, increasing
- First paper submitted 4 May 2016
- 31 May 2017: 111 accepted papers, 56 under review and pre-review
- 11 May 2023: 2012 accepted papers, 232 under review and pre-review
- Current publication rate:
~1 paper/day (& slowly increasing)
- Editors:
 - 1 editor-in-chief and 11 editors at launch;
 - 1 EiC, 7 associate/track EiCs, 69 editors, 35 emeritus editors today



JOSS as a community

- Culture changes based on rules and incentives
- JOSS practices have influenced reviewers and developers in terms of what's good and what's minimally acceptable
 - Similar to rOpenSci's influence in the R community
 - Minimum criteria for successful review change over time as community best practices develop
 - E.g., packaging, testing/CI, documentation
- JOSS applies open source software practices to reviews: openness & collaboration
- JOSS provides rules, and at a high-level, tries to nudge incentives
 - Accepted software = accepted paper
- If software was cited directly, JOSS papers wouldn't be needed, but JOSS reviews and JOSS community would still have great value

#2: Research Software Engineers



Where does research software come from?

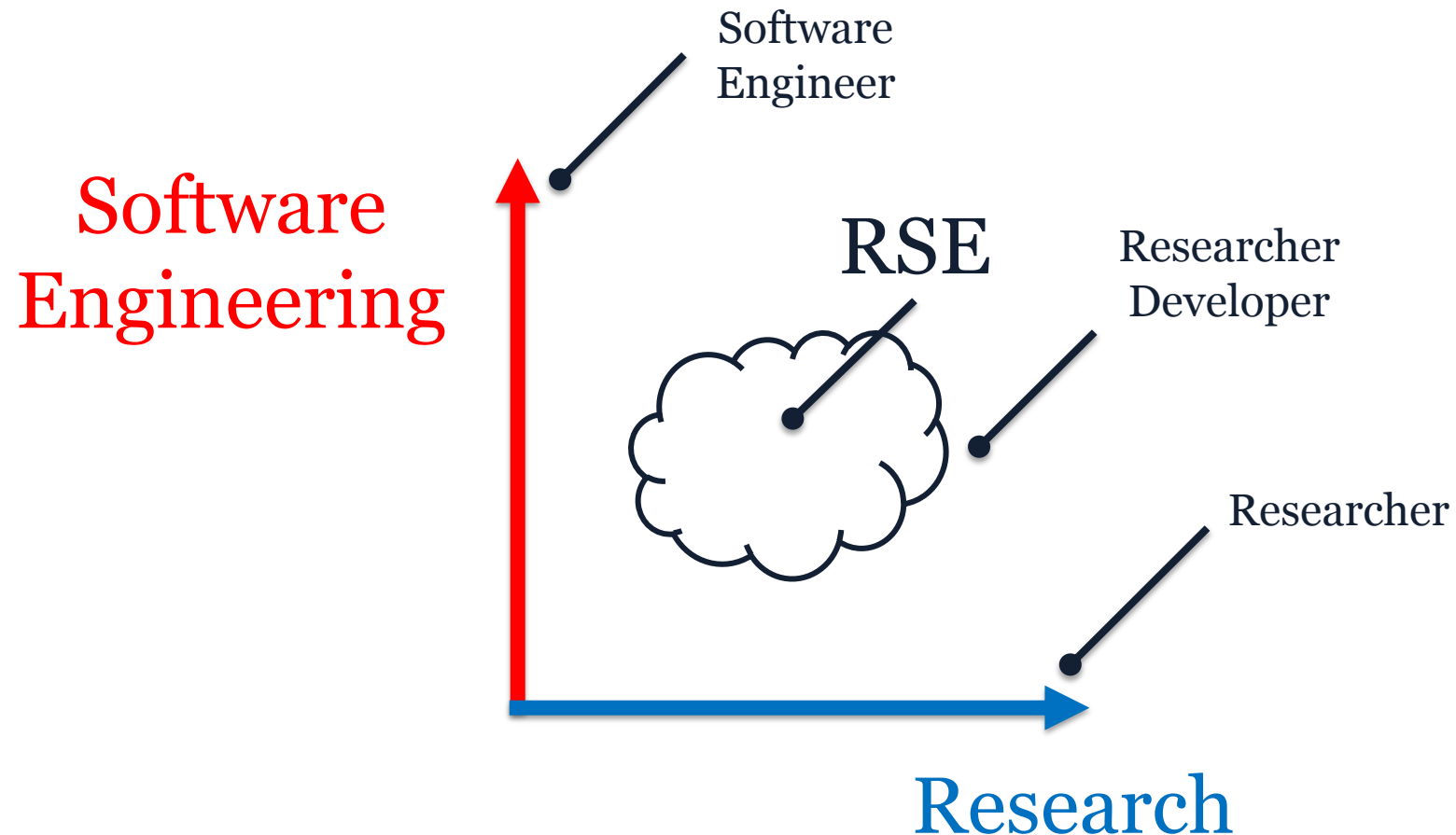
- Significant fraction developed in research
- From the start of computing
 - Software appears around 1948
 - Research software (weather) in early 1950s
 - Software engineering starting in late 1960s, mostly initially applied to operational software (operating system, NASA flights, etc.)
- Researchers (faculty) generally don't know good software practices
- Software engineers generally don't understand research context
- Students & postdocs generally don't know good software practices and don't stick around
- Some postdocs do stay, join staff (perhaps unofficially)
- Staff with research understanding and software engineering skills develop

The Craftsperson and the Scholar

- Scholar: archetypical researcher driven to understand things to their fullest capability
 - Find intellectually-demanding problems
 - Curiosity-driven, work on a topic until understanding has been acquired, pass on that understanding through teaching
- Craftsperson: driven to create and leave behind an artifact that reifies their efforts in a field
 - Feels pain when things they make are fragile or ugly
 - Prefer to make things that explain themselves
 - Work requires patience, and pride in doing a job well
- Scientific software requires individuals who combine the best of both roles



What is a Research Software Engineer?



<https://danielskatzblog.wordpress.com/2019/07/12/super-rses-combining-research-and-service-in-three-dimensions-of-research-software-engineering/>

Collaborations Workshop 2012

- Lots of people already doing this work
- No common title
 - ✓ Research Software Engineer (RSE)
- No community
 - ✓ Associations/societies
- Not a profession
 - ✓ Career paths, structure

194 different job titles

Casebooks Project Editor (Research Assistant/ Associate) Climate Researcher (Research Associate) Clinical Study Programmer CoMPLEX Research Associate Computational Biologist / Bioinformatician Computational Scientist Computational Scientist in Computational Fluid Dynamics & Industrial Applications Computational Scientist in Structural Mechanics and Industrial Applications Computer Scientist Computer Vision Researcher Content Developer / Programmer Control Engineer-IMG - 3 posts CREATE Data Specialist Data Analyst Data Integration Coordinator Data Manager x3 Database and Software Engineer Database Manager / Researcher Database Programmer Digital Media Technician E-Learning Portal Manager (KTP Associate) e-Learning Systems Development Analyst e-Learning Systems Development Analyst (Moodle, SQL) E-Learning Web Developer E-Portfolio Learning Technology Embedded Systems Engineer Engineering Technician Environmental Scientist EPSRC Studentship on Algorithmic Construction of Finsler-Lyapunov Functions Experimental Officer in Bioinformatics Experimental Psychologist Finance Assistant Gaia Alerts Software Developer Gaia Software Developer (Gaia UK Team) GIS Applications Specialist Graduate Programmer / Software Developer Graphics Programmer Health Data Manager / Scientist High Throughput Bioinformatician High Throughput Sequencing Bioinformatician (Two posts) HIVE Manager / HIVE Co-ordinator HIVE Senior Researcher and Technical Lead Hydroinformatics Scientific Software Developer Image Analysis Software Engineer Information Systems Developer Instrumentation Engineer Investigator Statistician IT Developer / Support Engineer IT Support Technician (Unix / Windows Systems) Knowledge Transfer Partnerships (KTP) Knowledge Transfer Partnerships (KTP) Knowledge Transfer Partnerships (KTP) Associate - Software Developer KTP Associate - Robot Vision Scientist (Research Fellow) KTP Associate (Fixed Term Contract for 24 months) KTP Associate (Precision Agriculture Data Analyst) KTP Associate â€œ Graduate Web Developer KTP Associate: Electronics / Robotics Engineer Learning Technologist Leicester Respiratory BRIT Developer Linguist / Psycholinguist Maker Space Technician Marie Curie Early Stage Researcher Marie Curie Early Stage Researcher in Rail Researcher in Rail for Integrated Web Community Modelling Marine Earth Observation Scientists Medical Statistician Medical Statistician / Senior Medical Statistician Meteorologist Mobile Application Developer NASC IT Support - Programmer and Systems Administrator (Fixed Term) NERC Research Fellow on the PDRA on EU Project on Automated Multisensor Surveillance Planning Officer Policy Modeller 2011 Post - Doctoral Research Assistant INSTRON Post Doctoral Research Worker Post Doctoral Researcher in the application of Digital Technology Post-Doctoral Research Assistant in Simulation and Visualization Post-Doctoral Research Associate Post-Doctoral Research Associate (Pathogen Genomics) Post-Doctoral Research Fellow Postdoctoral Fellow - population genetics / evolutionary genetic Postdoctoral Fellow in Bioinformatics Postdoctoral Fellow in Cancer Therapeutics Postdoctoral Research Assistant Postdoctoral Research Associate Postdoctoral Research Fellow Postdoctoral Research Scientist Postdoctoral Researcher in Declarative (Logic and Functional) Programming Postdoctoral Researcher Postdoctoral Scientist Postdoctoral statistician Postdoctoral Training Fellow - Statistical and Computational Genetics of Autism Principal / Senior Bioinformatician Principal Bioinformatician Product Development Engineer (Rail) Publishing Portal Web Developer Radio Frequency Engineer Reader in Computer Science Reporting Analyst Research (Software) Engineer Research Assistant Research Associate Research Fellow Research Image Data Manager, Biomedical Engineering Research Officer Research Officer â€œ Social Protection Research postgraduate Research Programmer Research Scientist Research Scientist / Senior Research Scientist Research Scientist in Machine Learning and Computer Vision Research Software Developer Research Software Developer for the Herchel Smith Professor of Organic Chemistry Research Software Engineer Research Studentship Research Worker Researcher SAP Trainee Technical Analyst Scientific Officer with Michela Garofalo Scientist SEAHA Studentship: Extracting epidemiological data from collections SEEG Data Archive Manager Senior / Research Associate in Clinical Integration and Image Analysis for Fetal Surgery Senior Analyst Programmer (Business Analysis) Senior Analyst / Programmer Senior Bioinformatician Senior Bioinformatician / Bioinformatician Senior Computational Statistician - Spatial Models Senior Data Acquisition Scientist / Data Acquisition Scientist Senior Data Manager Senior Database Administrator Senior IT Developer Analyst Senior Mathematical Modeller Senior Media Developer Senior Postdoctoral Researcher - Evolutionary and Computational Analysis of Infectious Disease (Phylogenetics) Senior Research Assistant Senior Research Associate Senior Research Associate â€œ Molecular Modelling & Simulation Senior Research Associate in Quantitative Clinical MRI Senior Research Fellow Senior Research Fellow / Research Fellow in Vibration Diagnostics and Prognostics / Digital Signal Processing Senior Research Laboratory Technician Senior Research Technician Senior Software Developer in Bioinformatics Senior Software Engineer / Software Engineer Senior Statistical Epidemiologist Senior Systems

Credit: Simon Hettrick

10+ years of RSEs

- Movement and term: Born in the UK
 - Late 2013 UKRSE Association forms with ~50 members
 - Now society, ~700 dues-paying members, ~4600-member community
- Also: Belgium, Germany, Netherlands, Nordic, Australia/New Zealand
- And US-RSE (<https://us-rse.org>), ~1700 members across universities, national labs, industry
- New associations now forming
 - Africa & Asia
- Associations work on local issues collectively, and can coordinate

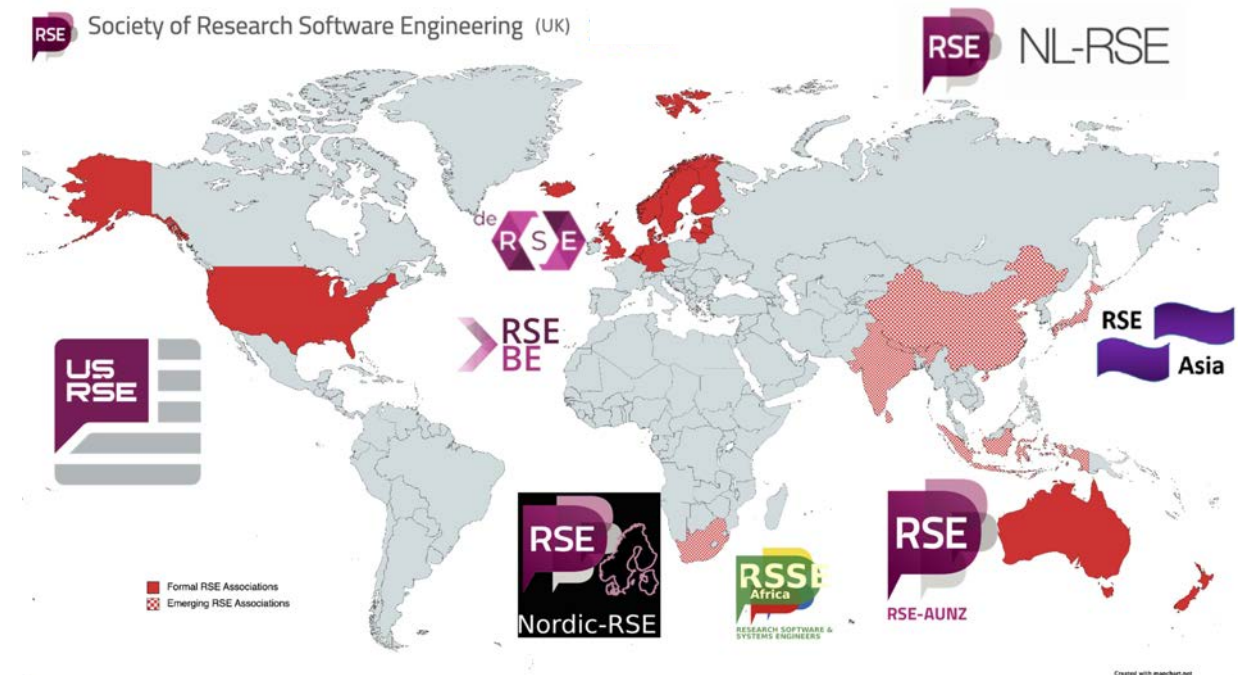
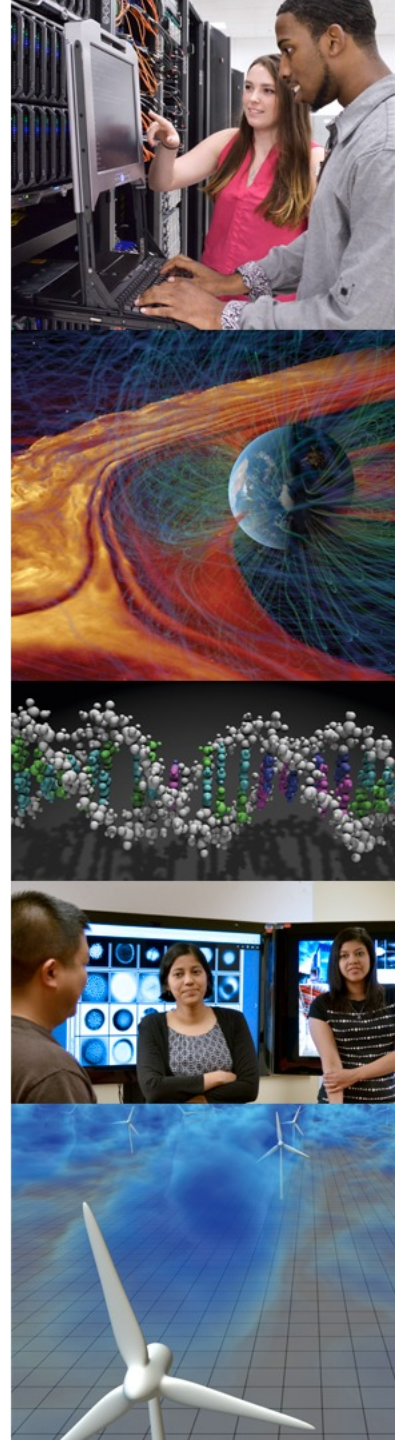


Image credit: Ian Cosden

Advantages of RSEs

- Better software & more mature project management aspect/structure
 - Team organization, work organization, software organization, coding practices
 - better, more sustainable code & more efficient group coordination
- Institutional memory
 - Research software is becoming more important, complex, and costly, expertise is valuable
 - RSEs have longevity beyond individual projects and students
 - RSEs often mobile across domains, can translate knowledge/artifacts across communities
- Build community expertise
 - RSEs typically work on series of grant-funded (typically less than 1 RSE FTE) projects
 - Shorter duration than staff careers
 - RSE groups tend towards a form of “Matrix Management”
 - Principle Investigator axis: changes over time, funded by projects
 - RSE group manager axis: fixed, funded by overhead, tax on projects, institution, ...
 - pool of experts/expertise, welcomes others with shared interests

#3: FAIR for Research Software



The FAIR Principles

The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson, Michel Dumontier, [...] Barend Mons 

Scientific Data **3**, Article number: 160018 (2016) | [Cite this article](#)

194k Accesses | **2450** Citations | **1852** Altmetric | [Metrics](#)

A set of principles, to ensure that data are shared in a way that enables and enhances reuse by humans and machines

Findable

- F1. (Meta)data are assigned a globally unique and eternally persistent identifier.
- F2. Data are described with rich metadata.
- F3. (Meta)data are registered or indexed in a searchable resource.
- F4. Metadata specify the data identifier.

Accessible

- A1. (Meta)data are retrievable by their identifier using a standardized communications protocol.
 - A1.1. The protocol is open, free, and universally implementable.
 - A1.2. The protocol allows for an authentication and authorization procedure, where necessary.
- A2. Metadata are accessible, even when the data are no longer available.

Interoperable

- I1. (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (Meta)data use vocabularies that follow FAIR principles.
- I3. (Meta)data include qualified references to other (meta)data.

Reusable

- R1. (Meta)data have a plurality of accurate and relevant attributes.
 - R1.1. (Meta)data are released with a clear and accessible data usage license.
 - R1.2. (Meta)data are associated with their provenance.
 - R1.3. (Meta)data meet domain-relevant community standards.

FAIR for non-data objects: some context

- FAIR Principles, at a high level, are intended to apply to all research objects; both those used in research and those that are research outputs
- Text in principles often includes "(Meta)data ..."
 - Shorthand for "metadata and data ..."
- Principles applied via dataset creators and repositories, collectively responsible for creating, annotating, indexing, preserving, sharing the datasets and their metadata
 - Assumes separate and sequential creator/publisher (repository) roles
- What about non-data objects?
 - While they can often be stored as data, they are not just data
- While high level goals (F, A, I, R) are mostly the same, the details and how they are implemented depend on
 - How objects are created and used
 - How/where the objects are stored and shared
 - How/where metadata is stored and indexed
- Work needed to define, then implement, then adopt principles

Need for FAIR for non-data objects

- FAIR Principles are intended to apply to all digital objects (Wilkinson et al. 2016)

Recommendation 5:

*Recognise that FAIR guidelines will require **translation for other digital objects** and support such efforts.*

2020: ‘Six Recommendations for Implementation of FAIR Practice’
(FAIR Practice Task Force EOSC, 2020)

Recommendation 2:

*Make sure **the specific nature of software** is recognized and not considered as “just data” particularly in the context of discussion about the notion of FAIR data.*

2019: Opportunity Note by French national Committee for Open Science's Free Software and Open Source Project Group
(Clément-Fontaine, 2019)

- We focused on **adaptation and adoption** of the FAIR principles to research software

Software vs. data

- Software is data, but it's not just data
 - Software is executable, data is not
 - Data provides evidence, software provides a tool
 - Software is a creative work, scientific data are facts or observations
 - Different licensing and copyright practices
 - Software suffers from a different type of bit rot (collapse) than data
 - The lifetime of software is generally not as long as that of data
 - For open source, no natural sequential creator/publisher process & no natural publisher (repository)

D. S. Katz et al., "Software vs. data in the context of citation," PeerJ Preprints 4:e2630v1, 2016. <https://doi.org/10.7287/peerj.preprints.2630v1>

FAIR for Research Software (FAIR4RS)

- Working group defined consensus FAIR principles for research software
 - Led by Michelle Barker, Neil Chue Hong, Leyla Garcia, Morane Gruenpeter, Jennifer Harrow, Daniel S. Katz, Carlos Martinez, Paula A. Martinez, Fotis Psomopoulos



Defining Research Software

- **Research Software** includes source code files, algorithms, scripts, computational workflows and executables that were **created during the research process or for a research purpose**
- Additional software components (e.g., operating systems, libraries, dependencies, packages, scripts, etc.) that are used for research but were **not created during or with a clear research intent should be considered software in research** and not Research Software
- This differentiation may vary between disciplines

“Defining Research Software: a controversial discussion,” <https://doi.org/10.5281/zenodo.5504016>

FAIR4RS principles

Chue Hong, N. P., Katz, D. S., Barker, M., Lamprecht, A-L, Martinez, C., Psomopoulos, F. E., Harrow, J., Castro, L. J., Gruenpeter, M., Martinez, P. A., Honeyman, T., et al. (2022). FAIR Principles for Research Software version 1.0. (FAIR4RS Principles v1.0). Research Data Alliance. DOI: [10.15497/RDA00068](https://doi.org/10.15497/RDA00068)

Findable: Software, and its associated metadata, is easy to find for both humans and machines.

F1. Software is assigned a globally unique and persistent identifier

- F1.1. Different components of the software are assigned distinct identifiers representing different levels of granularity
- F1.2. Different versions of the same software are assigned distinct identifiers

F2. Software is described with rich metadata

F3. Metadata clearly and explicitly include the identifier of the software they describe

F4. Metadata are FAIR and are searchable and indexable

Accessible: Software, and its metadata, is retrievable via standardized protocols.

A1. Software is retrievable by its identifier using a standardized communications protocol

- A1.1. The protocol is open, free, and universally implementable
- A1.2. The protocol allows for an authentication and authorization procedure, where necessary

A2. Metadata are accessible, even when the software is no longer available

Interoperable: Software interoperates with other software through exchanging data and/or metadata, and/or through interaction via application programming interfaces (APIs), described through standards.

I1. Software reads, writes and exchanges data in a way that meets domain-relevant community standards

I2. Software includes qualified references to other objects

Reusable: Software is both usable (it can be executed) and reusable (it can be understood, modified, built upon, or incorporated into other software).

R1. Software is described with a plurality of accurate and relevant attributes

- R1.1. Software is given a clear and accessible license
- R1.2. Software is associated with detailed provenance

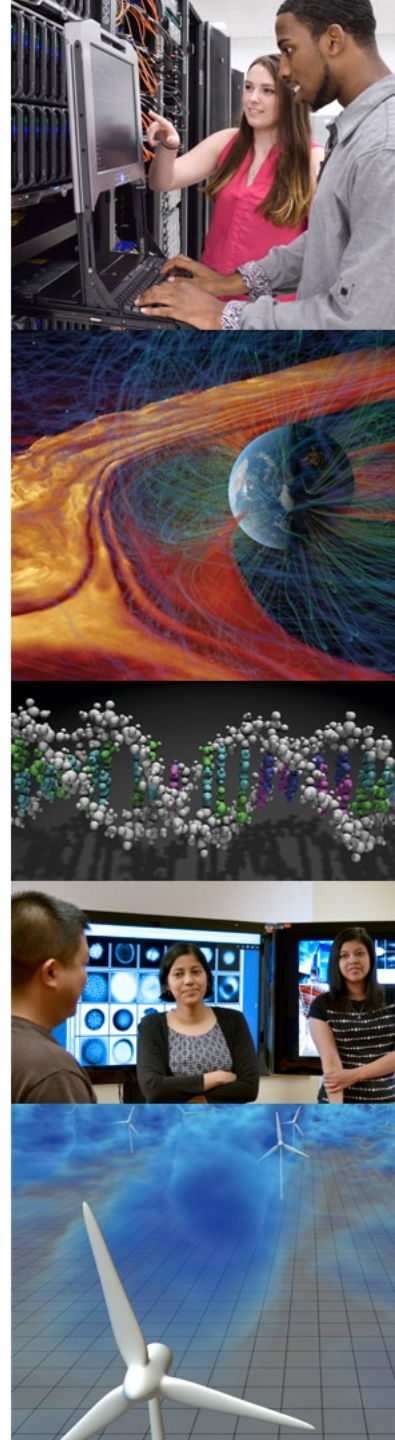
R2. Software includes qualified references to other software

R3. Software meets domain-relevant community standards

Using FAIR4RS and what's next

- Governance (interpretation, future revisions) turned over to RDA Software Source Code Interest Group
- Survey of adoption guidelines: <https://doi.org/10.5281/zenodo.6374598>
- Study of adopting organizations: <https://doi.org/10.5281/zenodo.6258366>
- FAIR4RS exposes ecosystem gaps, particularly related to metadata, archiving, versions
 - Creator/publisher sequence doesn't typically apply
 - Where is metadata stored? (in code repository for open source?, for closed source?, in archival repository?, in registry?)
 - Where is code archived? (GitHub/Gitlab are not archival, registries are not archival, repositories? Software Heritage?)
 - Different use cases need specific version, latest version, all versions
- Lots of work beyond FAIR: quality, correctness, reproducibility, openness, ...

Context: ReSA



Research Software Alliance (ReSA)



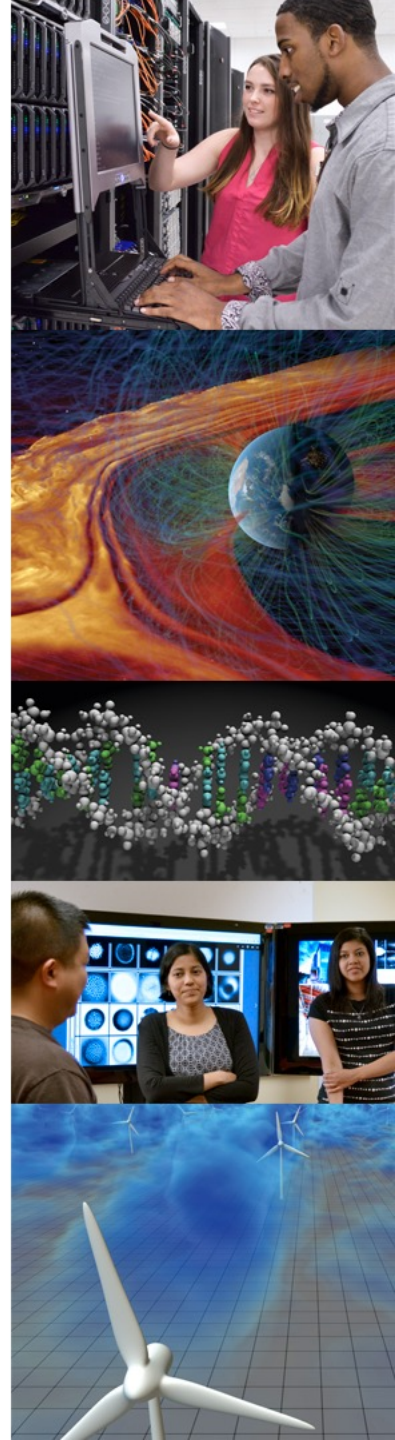
- Vision: Research software and those who develop and maintain it are recognized and valued as fundamental and vital to research worldwide
- Mission: to advance the research software ecosystem by collaborating with key influencers and decision makers
- Founded in 2019, fiscally sponsored by Code for Science & Society
- ReSA has recently
 - Co-developed the FAIR for research software principles
 - Shared diversity, equity, and inclusion best practices at Vive la difference - research software engineers workshop
 - Expanded its global mapping of the international research software community landscape
 - Gathered global research software funders to set the agenda for sustainable research software
 - Leading to the draft ADORE.software (Amsterdam Declaration on Funding Research Software Sustainability)
 - Collaborated in task forces on specific issues affecting the global research software community

- Individual Participation
 - Receive our newsletter
 - Join the ReSA Slack
 - Add to our funding call database
 - Join task forces focused on specific activities

<https://www.researchsoft.org>

<https://doi.org/10.5281/zenodo.7951188>

Summary



You are here

- Research software is increasingly important to research
- Citation is the accepted mechanism for scholarly credit in academia
 - Software citation starting to become accepted, w/ uptake from researchers, publishers, librarians, etc.
 - Software papers are partially a placeholder for software citation, but also have an important community function
- Research software Engineers (RSEs)
 - Recently recognized as a role, but a long history
 - Now building community & making case for formal career paths
- FAIR (data) principles set out good goal: share data to enable and enhance reuse
 - Work is needed to apply this goal to research software, both open source and not, to fulfil the open science concepts
 - Principles have been created, with ~500 people involved & ~60 events
 - Chue Hong, et al. (2022). FAIR Principles for Research Software version 1.0. (FAIR4RS Principles v1.0). DOI: 10.15497/RDA00068
 - Work underway to create guidance, adopt principles, define governance
 - Next steps will be to create metrics and widen adoption

What you can do

- Promote software sharing and credit
 - When you are an author, cite the software you use
 - When you develop software, make it easy to cite
 - When you review, demand software be cited
 - Work to make your own software FAIR – follow the principles
- Support RSEs
 - Support software developers and maintainers
 - Consider how your organization does this, and if you can change it
 - See <http://us-rse.org> or <https://society-rse.org>
- Work to make sure software work is included in hiring and promotion for everyone
- Open science, open software, FAIR4RS, Citation, RSE, ReSA are open communities
 - Join one!
- Overall, raise awareness of research software as a key element of research
 - Understand that research software is not business software, w/ different goals, incentives, methods, practices, workforce, education

Credits

- Thanks to Arfon Smith and Kyle Niemeyer for co-leadership in FORCE11 Software Citation WG
- And Arfon Smith for JOSS leadership
- And Neil Chue Hong & Martin Fenner for co-leadership in FORCE11 Software Citation Implementation WG
- And Neil Chue Hong, Simon Hettrick, James Hetherington, Rob Haines, Ian Cosden, Kenton McHenry for RSE discussions
- And Morane Gruenpeter, Carlos Martinez, Neil Chue Hong, Paula A. Martinez, Michelle Barker, Leyla Jael Castro, Jennifer Harrow, Fotis Psomopoulos for co-leadership in RDA/ReSA/FORCE11 FAIR4RS
- And colleagues Gabrielle Allen, C. Titus Brown, Kyle Chard, Ian Foster, Melissa Haendel, Christie Koehler, Bill Miller, Tom Honeyman, Anna-Lena Lamprecht
- And to the BSSw project (<http://bssw.io>) for a fellowship to pursue some parts of the citation work
- More of Dan's thinking
 - Blog: <http://danielskatzblog.wordpress.com>
 - Mastodon: [@danielskatz@fosstodon.org](https://fosstodon.org/@danielskatz)