Research software challenges and solutions

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Why do we care about research software?

- Funding
  - ~20% of NSF projects over 11 years topically discuss software in their abstracts ($10b)
  - 2 main DOE ECP areas were research software (~$2b)
  - $300m of FY2021 NIH projects include "software development"
  - 47% of 13,784 ARC grants between 2010 and 2019 produced software
- Publications
  - Software intensive projects are a majority of current publications
  - Most-cited papers are methods and software
- 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
- Hot areas depend on research software
  - AI (training & inference), quantum (research & modeling, programming)

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

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

Maxfield Brown & Weber, 10.5281/zenodo.10530616

Nangia and Katz; 10.1109/eScience.2017.78

"Top 100-cited papers of all time," Nature, 2014 10.1038/514550a

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
U. Nangia and D. S. Katz; 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/10.54900/9akm9y5-5ject5y

Photo by Markus Spiske on Unsplash

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. Hinsen, “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 (at least today, AI tomorrow?)
- 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

https://doi.org/10.5281/zenodo.10990391

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

https://doi.org/10.5281/zenodo.10990391

Potential research software sustainability solutions

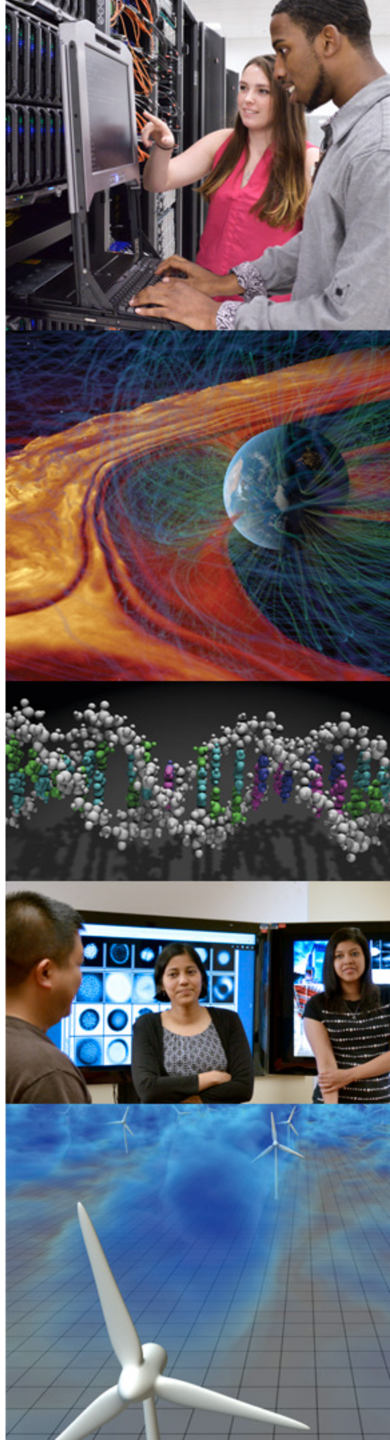
- Do things that reduce the amount of work needed: training, best practices
- Do things that increase the available resources
  - Create incentives so that people want to work on the software
    - Citations that help in existing career paths
    - New career paths
  - Increase available funding: make the role of software in research clear to research funders; then make the case for them to increase funding for new software, and to fund software maintenance
  - Seek institutional resources if the software is considered sufficiently important to the institution, operationally or reputationally
- Do things that both reduce the amount of work needed and increase the available resources
  - Encourage collaboration
    - Design software from start as modular and reusable, clearly documented and explained to all potential users
    - Put effort into engaging and working with the potential user and contributor community
  - Make the software findable, accessible, interoperable, reusable (FAIR)

More about citation coming: #1

More about new career paths coming: #2

More about FAIR coming: #3

#1(a): Software citation



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https://doi.org/10.5281/zenodo.10990391

FORCE11 Software Citation Working Group (2015-16)

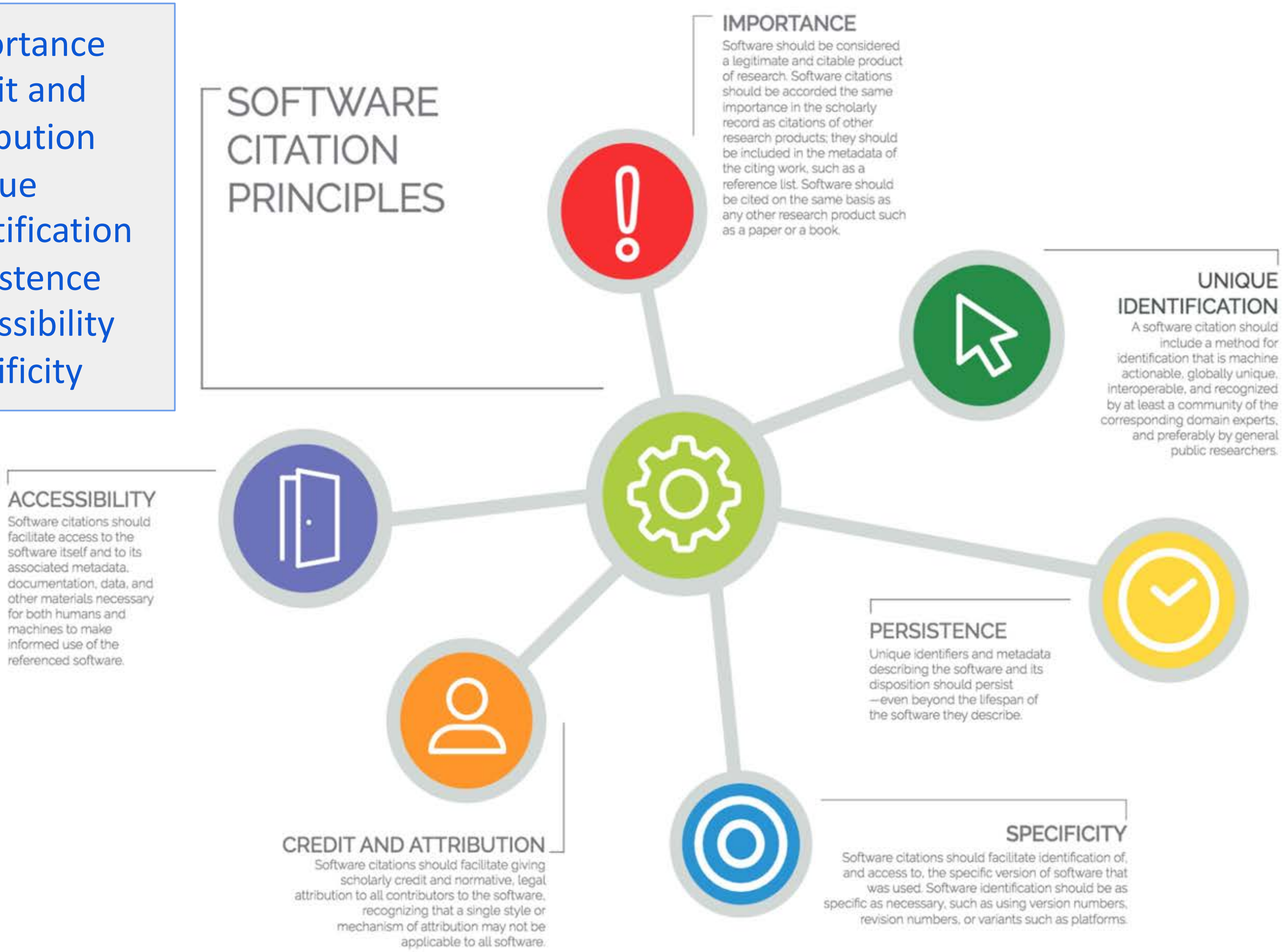
- Documented differences between software and data; defined software citation challenges
  - Katz DS, Niemeyer KE, et al. (2016) Software vs. data in the context of citation. PeerJ Preprints 4:e2630v1. DOI: 10.7287/peerj.preprints.2630v1
  - Niemeyer KE, Smith AM, Katz DS. (2016) The challenge and promise of software citation for credit, identification, discovery, and reuse. ACM Journal of Data and Information Quality, 7(4):16. DOI: 10.1145/2968452
- 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 and https://www.force11.org/software-citation-principles

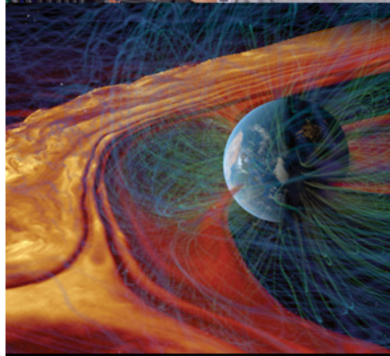
FORCE11
The Future of Research Communications and e-Scholarship

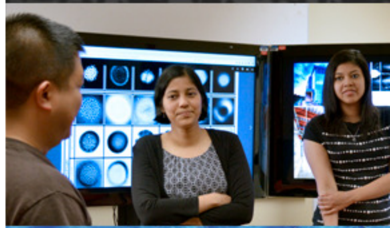
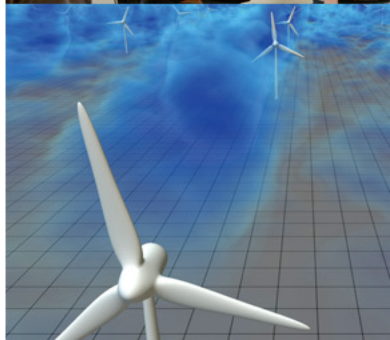
https://www.force11.org/group/software-citation-working-group
Co-Chairs: Arfon M. Smith, Daniel S. Katz, Kyle E. Niemeyer

Software is a critical part of modern research...

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



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 and https://www.force11.org/software-citation-principles

Image courtesy of DataCite

... yet there is little support for its acknowledgement and citation

FORCE11 Software Citation Implementation Working Group (2017-2023)

- 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 [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

FORCE11
The Future of Research Communications and e-Scholarship

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," Zenodo, 15-Oct-2019. 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," Zenodo, 15-Oct-2019. 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 to be a community group, with governance

Responses to challenges (2)

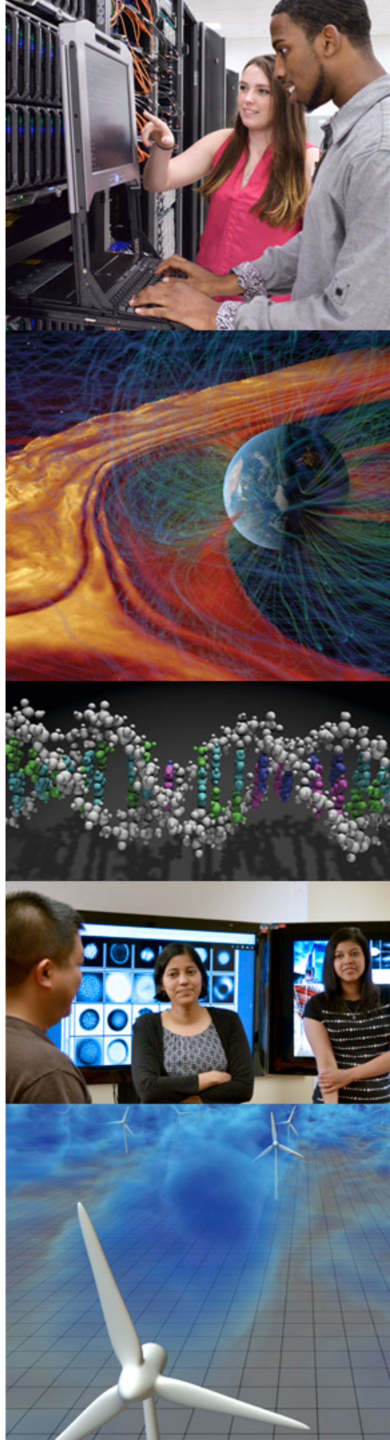
- Software Registries Task Force
  - Developed best practices document
    - Task Force on Best Practices for Software Registries, "Nine Best Practices for Research Software Registries and Repositories: A Concise Guide," 2020. arXiv 2012.13117
  - Community continuing in SciCodes: Consortium of scientific software registries and repositories, https://scicodes.net/
- Journals Task Force
  - Worked 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
    - Tracked by CHORUS in Software Citation Policy Index
  - Also worked 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", 10.1038/s41597-023-02491-7

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
- WG ended in May 2023, but community is interested in continued discussion
  - Currently writing a blog post to suggest topics and venues

https://doi.org/10.5281/zenodo.10990391

#1(b): Journal of Open Source Software (JOSS)



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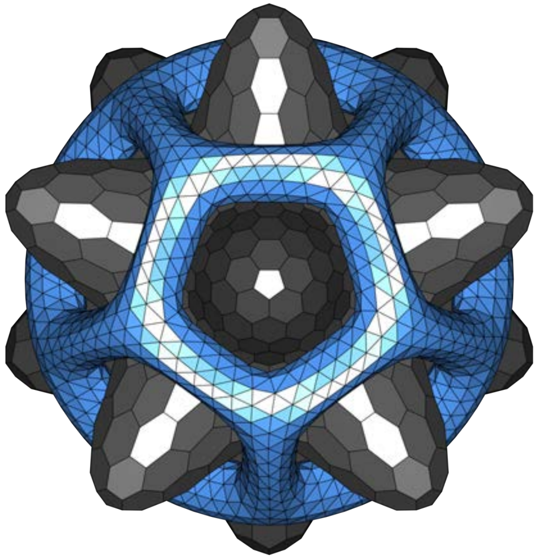
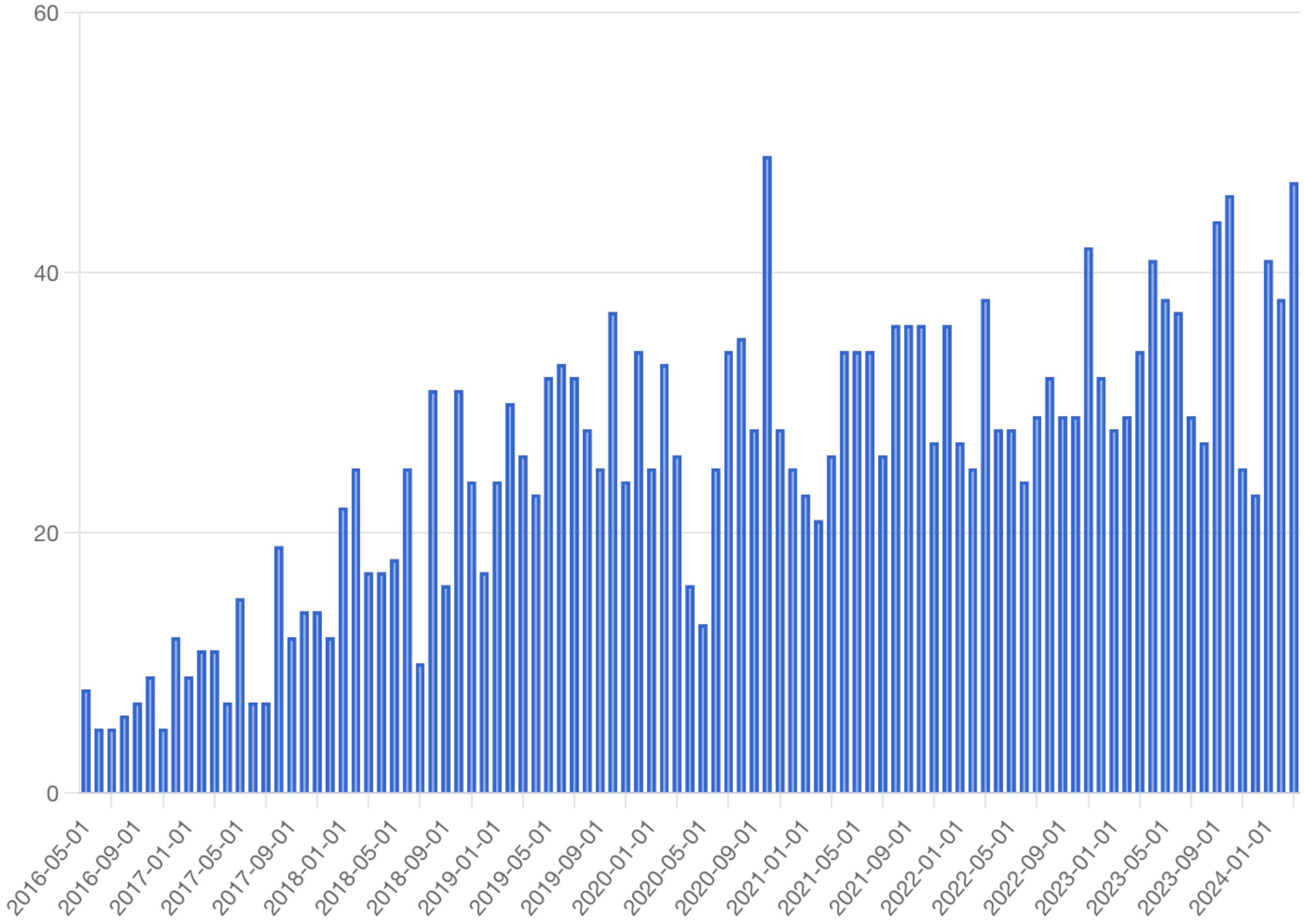
Journal of Open Source Software (JOSS)

- 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, increasingly indexed
- First paper submitted 4 May 2016
- 31 May 2017: 111 accepted papers, 56 under review and pre-review
- 10 Apr 2024: 2408 accepted papers, 326 under review and pre-review
- Current publication rate: ~1.1 paper/day (& slowly increasing)
- Editors:
  - 1 editor-in-chief and 11 editors at launch;
  - 1 EiC, 6 associate/track EiCs, 84 editors, 41 emeritus editors today



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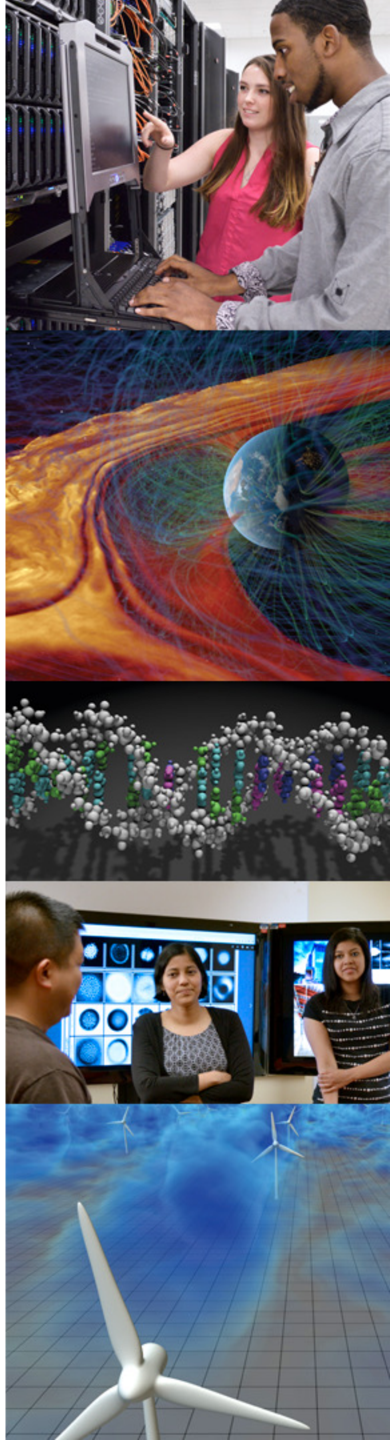
#2: Research Software Engineers



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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

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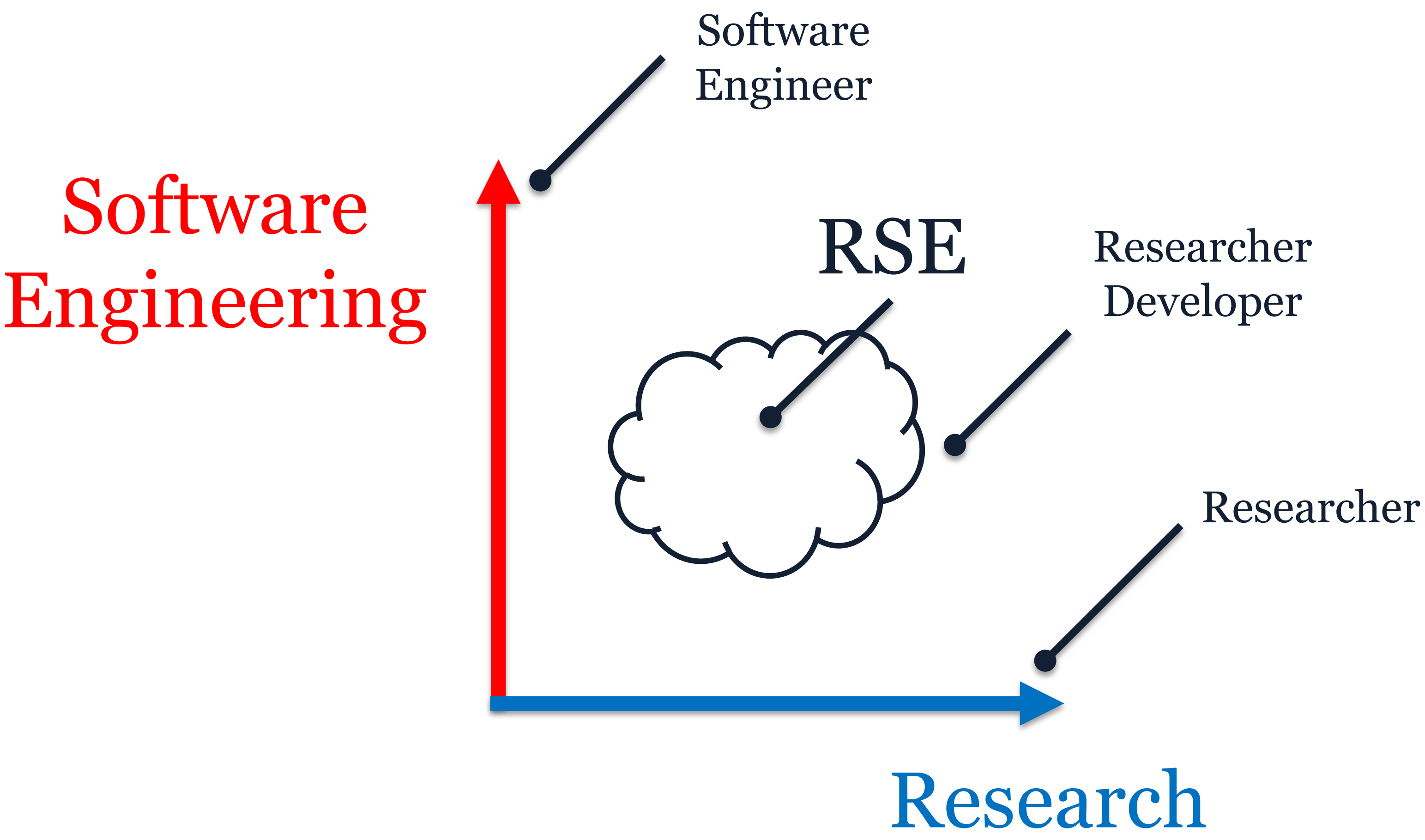
The Craftsperson and the Scholar

- 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

http://www.software.ac.uk/blog/2012-11-09-craftsperson-and-scholar

https://doi.org/10.5281/zenodo.10990391

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/

https://doi.org/10.5281/zenodo.10990391

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

Credit: Simon Hettrick

11 years of RSEs

- Movement and term: Born in the UK
  - Late 2013 UKRSE Association forms with ~50 members
  - Now society, ~700 dues-paying members, ~5300-member community
- Also: Belgium, Germany, Netherlands, Nordic, Australia/New Zealand
- And US-RSE (https://us-rse.org), ~2400 members across universities, national labs, industry
- New associations now forming
  - Africa & Asia
- Associations work on local issues collectively, and can coordinate

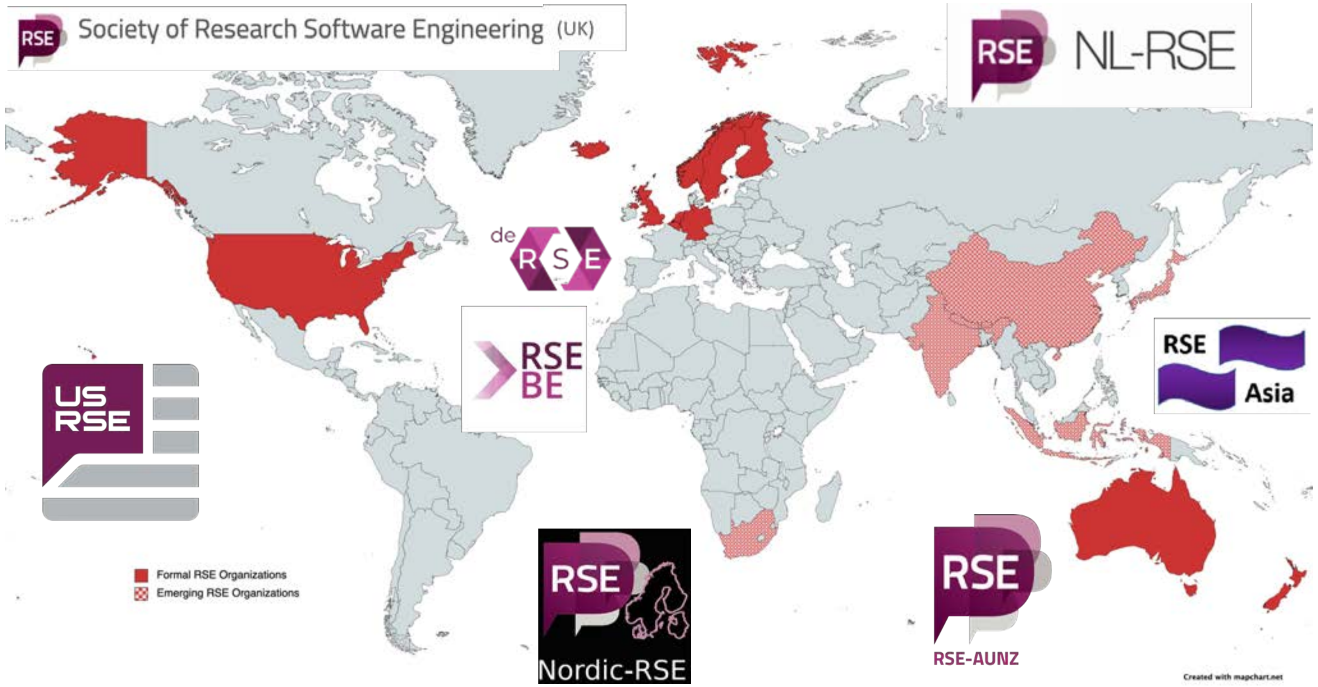
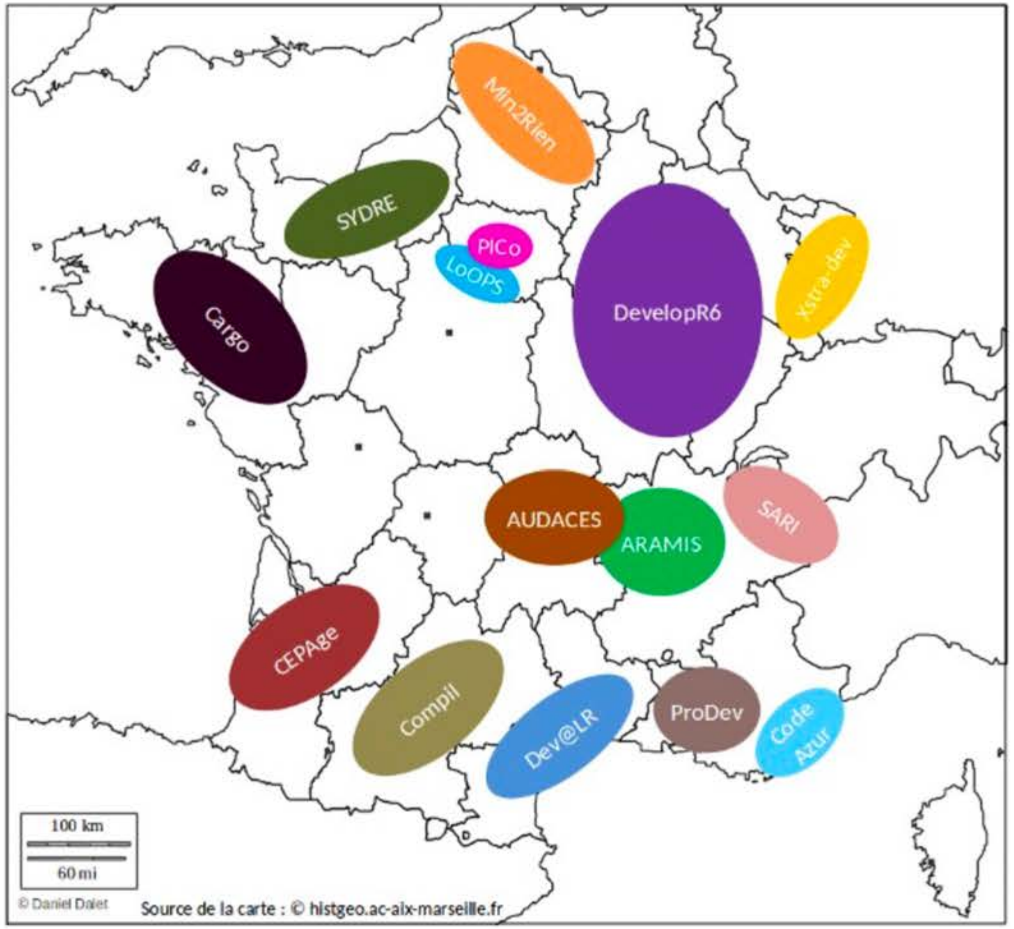


Image credit: Ian Cosden

But also, in France…



DEVLOG
RÉSEAU DU DEVELOPPEMENT LOGICIEL
Recherche et Enseignement Supérieur

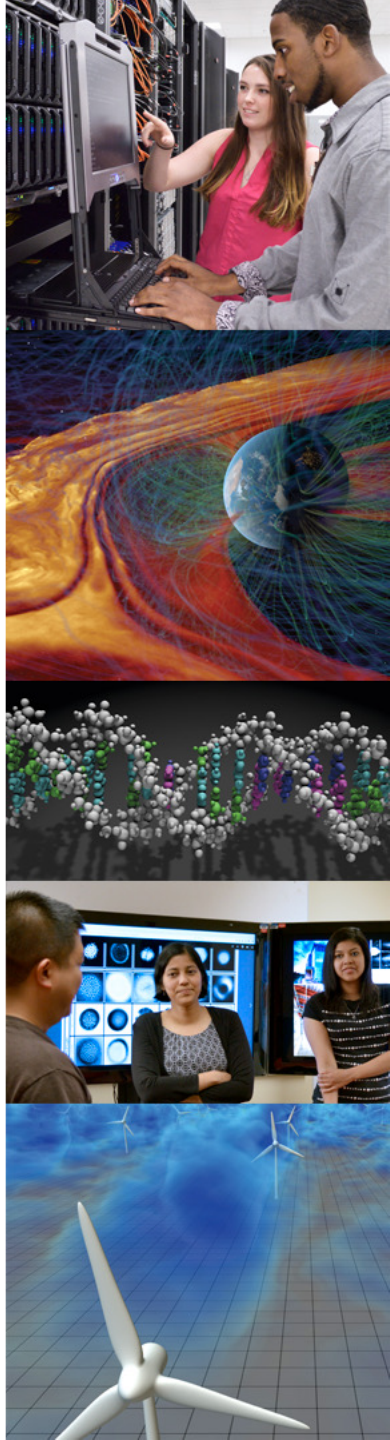
National network of Research Software Engineers created in 2011

15 local networks (sometimes older)

Current challenge: Join French and English RSE worlds!

https://doi.org/10.5281/zenodo.10990391

#3: FAIR for Research Software



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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

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

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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

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RDA
RESEARCH DATA ALLIANCE

<ReSA>
Research Software Alliance

https://doi.org/10.5281/zenodo.10990391

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

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

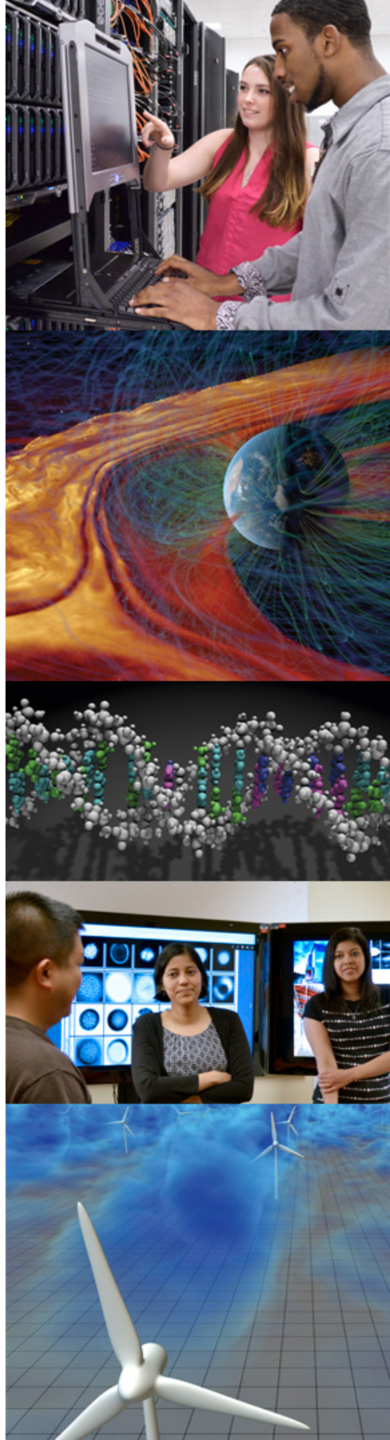
R3. Software meets domain-relevant community standards

Using FAIR4RS and what's next

- Governance (interpretation, future revisions) turned over to RDA Software Source Code Interest Group
- Initial survey of adoption guidelines: https://doi.org/10.5281/zenodo.6374598
- Initial study of adopting organizations: https://doi.org/10.5281/zenodo.6258366
- 2-year adoption report: https://doi.org/10.5281/zenodo.10816032
- 2-year principles review happening this year

- 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



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Research Software Alliance (ReSA)

<ReSA>
Research Software Alliance

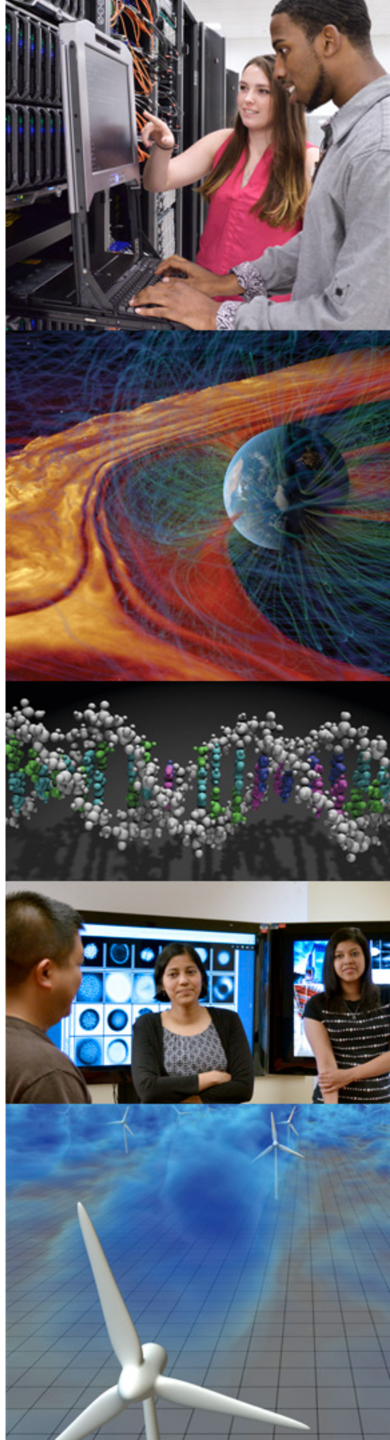
- Vision: Research software and those who develop and maintain it are recognized and valued as fundamental and vital to research worldwide
- Mission: to advance the research software ecosystem by collaborating with key influencers and decision makers
- Founded in 2019, fiscally sponsored by Code for 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 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.10990391

Summary



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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
  - And have guidance, adoption examples, governance, initial 2 years of progress
  - Next steps will be to widen adoption and review

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!
  - Submit/come to Research Software Engineers in HPC workshop at SC24: RSE-HPC-2024
- 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

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- More of Dan's thinking
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