Making Software FAIR: A machine-assisted workflow for the research software lifecycle

Petr Knoth¹, Laurent Romary², Patrice Lopez³, Roberto Di Cosmo², Pavel Smrz⁴, Tomasz Umerle⁵, Melissa Harrison⁶, Alain Monteil², Matteo Cancellieri¹, David Pride¹ 22nd October 2024

- 1: CORE, The Open University, United Kingdom;
- 2: Inria;
- 3: Science Miner;
- 4: Brno University of Technology;
- 5: Polish Academy of Sciences;
- 6: European Institute of Bioinformatics





CORE

ontochem

Qcypris

Fact checking

Finance Health

D turnitin

Plagiarism detection



Scientific output

Global scientific output **doubles every nine years** [Bornmann, 2015]







"Single occurrences that cannot be reproduced are of no significance to science" – Popper, <u>1935</u> –

S∂FAIR

Reproducibility crisis

More than **70%** of researchers have tried and failed to reproduce another scientist's experiments.

More than **50%** have failed to reproduce their own experiments.

The majority replied that there is a significant reproducibility crisis

IS THERE A REPRODUCIBILITY CRISIS?



Baker, M. 1,500 scientists lift the lid on reproducibility. Nature 533, 452–454 (2016). https://doi.org/10.1038/533452a



Reproducibility (according to Claerbout and Karrenbach, 1992)

"Reproducing"

means "running the same software on the same input data and obtaining the same results"

"Replicating"

means "writing and then running new software based on the description of a computational model or method provided in the original publication, and obtaining results that are similar enough ..."



Reproducibility (according to ACM, 2016)

Repeatability

same team | same experimental setup

The measurement can be obtained with stated precision by the same team using the same measurement procedure, the same measuring system, under the same operating conditions, in the same location on multiple trials. For computational experiments, this means that a researcher can reliably repeat her own computation.

Replicability

different team | same experimental setup

The measurement can be obtained with stated precision by a different team using the same measurement procedure, the same measuring system, under the same operating conditions, in the same or a different location on multiple trials. For computational experiments, this means that an independent group can obtain the same result using the author's own artifacts.

Reproducibility

different team | different experimental setup

The measurement can be obtained with stated precision by a different team using the same measurement procedure, the same measuring system, under the same operating conditions, in the same or a different location on multiple trials. For computational experiments, this means that an independent group can obtain the same result using the author's own artifacts.

S�FAIR

Reproducibility (according to Goodman, 2016)

Methods reproducibility: provide sufficient detail about procedures and data so that the same procedures could be exactly repeated.

Results reproducibility: obtain the same results from an independent study with procedures as closely matched to the original study as possible.

Inferential reproducibility: draw the same conclusions from either an independent replication of a study or a reanalysis of the original study.

Goodman	Claerbout	ACM
		Repeatability
Methods reproducibility	Reproducibility	Replicability
Results reproducibility Inferential reproducibility	Replicability	Reproducibility

Plesser HE (2018) **Reproducibility vs. Replicability: A Brief History of a Confused Terminology.** *Front. Neuroinform.* 11:76. doi: 10.3389/fninf.2017.00076



Reproducibility and SW

Unavailability of research software reported as the **6th** most significant reason for non-reproducibility.

S

Baker, M. 1,500 scientists lift the lid on reproducibility. *Nature* 533, 452–454 (2016). https://doi.org/10.1038/533452a

WHAT FACTORS CONTRIBUTE TO IRREPRODUCIBLE RESEARCH?

Many top-rated factors relate to intense competition and time pressure.



The SoFAIR research problem

A key issue hindering discoverability, attribution and reusability of **open research software** is that its **existence often remains hidden within the manuscript of research papers.**

For these resources to become **first-class bibliographic records**, they first need to be identified and subsequently registered with persistent identifiers (PIDs) to be made FAIR (Findable, Accessible, Interoperable and Reusable).

To this day, much open research software fails to meet FAIR principles and software resources are mostly not explicitly linked from the manuscripts that introduced them or used them.





Research software assets as first-class bibliographic records

Describe software assets using metadata Assign PIDs for software assets

Nake Software assets

Motivation:

Incentivise good practices of software assets curation:

- Facilitate correct attribution
- Credit researchers for the creation of research software
- Reward research software creation in institutional promotion processes

Contribute to an open scholarly

research graph connecting entities including papers, authors, institutions, data and software



Vision - 2/2

Scalable workflow for the software assets lifecycle for open repositories

Context

- Precious and limited time researchers have available
- Prevent re-typing of information
- Help researchers save time

Vision

- A workflow for the management of the entire lifecycle of research software assets, connecting and adapting existing open infrastructures and tools.
- Establish a machine-assisted workflow embedded into widely used open scholarly infrastructures to assist researchers in identifying, describing, registering, linking and archiving research software.

S**⊚**FAIR

Machine assisted workflow for software assets lifecycle

Embed this workflow into established scholarly infrastructures, making the solution available to the global network of open repositories





Approach





Infrastructures leveraged by the project

SoFAIR will extend	
Softcite with models	
for multidisciplinary	
identification of	
software mentions	
from research	
manuscripts,	
including their	
disambiguation and	
enrichment.	

GROBID / Softcite

CORE will enable the application of the developed MLassisted workflow on both pre-existing and new open access content from any open repository in the world.

CORE (core.ac.uk)

HAL will be used as a best practice example of a repository participating in the SoFAIR workflow, it will 1) participate in the routing of identified software mentions coming from CORE for validation by INRIA authors and 2) adapt its repository software to expose (over OAI-PMH) links between research manuscripts and software assets used in their creation.

HAL

Progress beyond the state-of-the-art:

Software Heritage will be embedded into the introduced workflow to support the registration of newly identified and validated software assets with PIDs and their subsequent archival.

Software Heritage

SPFAIR

Demonstrators and use cases

→ Demonstrator 1 (EMBL-EBI):

Linking research studies to software in life sciences for Europe PMC

→ Demonstrator 2 (INRIA):

Validating extracted software mentions within an institutional repository

→ Case study in the digital humanities (IBL-PAN)





A novel machine-assisted workflow for software assets lifecycle management

New machine learning models for software mentions extraction and disambiguation

Scalable application of the technology across open repositories and relevance to both pre-existing and new software assets

Some of the main challenges we are facing

 Coming up with an effective and efficient annotation schema Routing discovered software mentions back to authors via repository software and making them to act on them to register software PIDs

- → Performance (p/r) of our automatic software mention extraction and disambiguation models
- Scalability of our solution and demonstrating that it can be applied to both pre-existing and new articles.

→ Propagating registered software PIDs to research outputs metadata

→ Workflow integration

Expected impact

Increase the likelihood of both pre-existing and new research software assets being identified, registered and archived.

Contribute to equity and fairness in academia and increasing public trust in the research process.

Facilitate and contribute to the reproducibility of research software

S_PFAIR

A solution for both pre-existing and new manuscripts

Lower the barriers for making research software FAIR

Facilitate seamless access to, and management of, increasing volumes of research software.

Enable more researchers to cite and give credit to research software

Increase the ability of researchers to demonstrate their impact by quantifying the reuse of their research software

Reduce the barriers for entrepreneurs and enterprises to innovate

Incentivise researchers to develop better and more reusable software



Conclusions

- Recognising and archiving software assets mentioned in research manuscripts is one of the preconditions for solving the reproducibility crisis.
- → NLP / AI offers new opportunities to address and help semi-automate this
- → SoFAIR is developing a new workflow that will enable better management of SW assets leveraging CORE and Software Heritage



