



# Developing Guidelines for Metadata Collection and Curation for Research Software

Morane Gruenpeter Software Heritage Inria, France





# Housekeeping

https://rb.gy/u5e04

Or

https://tinyurl.com/2023-05-23-RSMD-webinar

- Please be aware that the session is being recorded and will be made publicly available
- You can add yourself to the list of participants

#### Version 1.0

Lead Author (Org): **Morane Gruenpeter** (INRIA) Contributing Author(s) (Org):

- Sabrina Granger (INRIA),
- Alain Monteil (INRIA)
- Neil Chue Hong (UEDIN-SSI),
- Elena Breitmoser (UEDIN-SSI),
- Mario Antonioletti (UEDIN-SSI),
- Daniel Garijo (UPM),
- Esteban González Guardia (UPM),
- Alejandra Gonzalez Beltran (UKRI-STFC),
- Carole Goble (UNIMAN),
- Stian Soiland-Reves (UNIMAN),
- Gabriela Mejias (DataCite)

Contributions during the RDA-P20 Research Software workshop





# **Agenda**

- Research Software in the FAIR-IMPACT project
- Preparing the guidelines a large community effort
- The Research Software MetaData (RSMD) guidelines proposal
- How to contribute after this webinar?



Goal: Review and discuss the proposed RSMD guidelines



#### FAIR-IMPACT in a nutshell







Budget: 10 million EUR Time plan: 36 months Starting date: June 2022

6 Core Partners









Strategic cooperation with the EOSC Partnership, ESFRI Clusters, the FAIRCORE4EOSC project

...and many others





#### **Consortium Partners**















Science and Technology Facilities Council



Task 4.3

























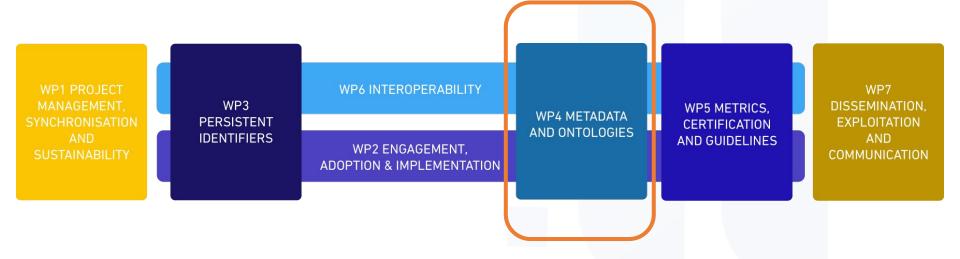






# **FAIR-IMPACT: Expanding FAIR solutions across EOSC**

FAIR-IMPACT will identify *practices*, *policies*, *tools* and *technical specifications* to guide researchers, repository managers, research performing organisations, policy makers and citizen scientists towards a FAIR data management cycle. The focus will be on **persistent identifiers (PIDs)**, **metadata**, **ontologies**, **metrics**, **certification** and **interoperability**,





# #RSMD guidelines timeline

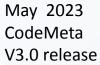
June 2022 **FAIR-IMPACT** 

March 2023 **#RS Workshop** Co-located **RDA P20** 



Research Software Metadata Guidelines

May 2023 #RSMD\_guidelines Community consultation



2024-2025 **Due:** June 2023 Dissemination D4.4 submission & adoption



October 2023 SSC IG session RDA P21

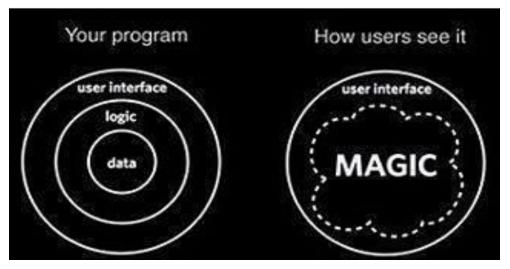
Sept. 2023 CodeMeta webinar

Launch



# **Clarifying the magic**





https://www.reddit.com/r/ProgrammerHumor/comments/70fuamp/programming\_is\_magic/

#### Software as a concept

- project or entity
- the community around the project
- the software idea / algorithms / solutions

Not a digital artifact

#### **Software artifacts**

- Executables
- Source code

A very large collection of digital artifacts



# **Defining Research Software**

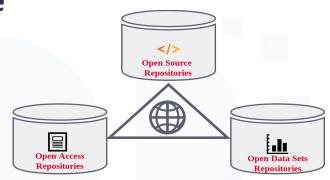
# Research Software

- → created
  - during the research process
  - o for a research purpose

# Software in research

used for research

FAIR4RS output: Gruenpeter et al. Defining Research Software: a controversial discussion (Version 1). Zenodo. <a href="https://doi.org/10.5281/zenodo.5504016">https://doi.org/10.5281/zenodo.5504016</a>



Three pillars of Open Science Software Heritage CC-By 4.0 2019

## Software has multiple facets:

- a tool
- a research outcome or result
- the object of research



# Why are we here? A plurality of needs

#### Researchers

- archive and reference software used and created in articles
- find useful software
- get credit for developed software
- verify/reproduce/improve results

#### Laboratories/teams

- track software contributions
- produce reports
- maintain web page

# **Research Organization**

#### know its software assets for:

- technology transfer,
- impact metrics,
- Strategy

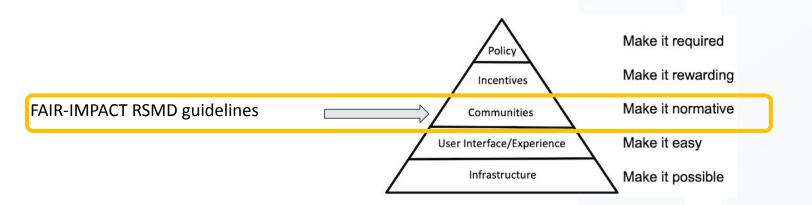
#### **Curators**

- verify and curate software metadata
- provide documentation on software curation
- monitor research teams' production



# The RSMD guidelines:

# Make it normative



Pyramid from Strategy for Culture Change: Brian Nosek (2019) https://www.cos.io/blog/strategy-for-culture-change



# The Research Software MetaData guidelines (RSMD)

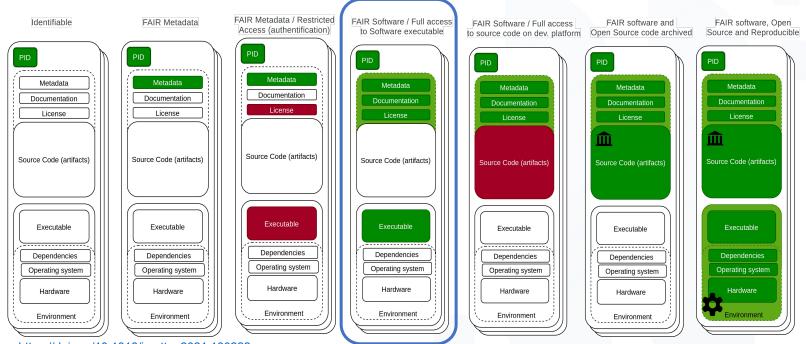
- Introduction
  - Scope & Goals
    - Why are we Here?
    - Who is the intended audience of this document?
  - Methodology
  - Use cases overview
- State of the art
  - Existing practices & guidelines
  - Metadata analysis
  - Curation workflows
- The **RSMD Guidelines** proposal for end-users
- Limitations & challenges
- Conclusion & next Steps
- Appendices
  - RSMD Checklist (only after the recommendations are stable)
  - Use cases collection
  - Infrastructure Using Codemeta



Zotero Library for software guidelines <a href="https://www.zotero.org/groups/5018631">https://www.zotero.org/groups/5018631</a> /fair-impact t4.3/library



# **FAIR4RS** principles published in 2021



https://doi.org/10.1016/j.patter.2021.100222

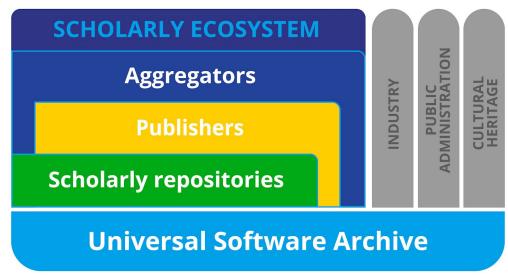


# **EOSC SIRS report published in 2020**

# Scholarly Infrastructures for Research Software

- Four Pillars
  - Archive, Reference, Describe, Credit
- State of the Art
  - Best Practices & Open Problems
  - Cross Cutting Concerns
- Participants
  - Representatives from 9 infrastructures:
  - Archives
    - **■** HAL, Software Heritage, Zenodo
  - Publishers
    - Dagstuhl, eLife, IPOL
  - Aggregators
    - OpenAIRE, scanR, swMATH

FAIRCORE4EOSC is turning the SIRS report into a reality
WP6 creating the component called RSAC - EOSC Research Software APIs
and Connectors



SIRS report: European Commission, Directorate-General for Research and Innovation, Scholarly infrastructures for research software: report from the EOSC Executive Board Working Group (WG) Architecture Task Force (TF) SIRS, Publications Office, 2020, https://data.europa.eu/doi/10.2777/28598

Video: EOSC Software Infrastructures for Research Software: J. B. Gonzalez Lopez (CERN)



# The guidelines for software archival



# Software Heritage

- Prepare your public repository README, AUTHORS & LICENSE files
- Save your code http://save.softwareheritage.org/
- Reference your work (full repository, specific version or code fragment)

https://www.softwareheritage.org/save-and-reference-research-software/

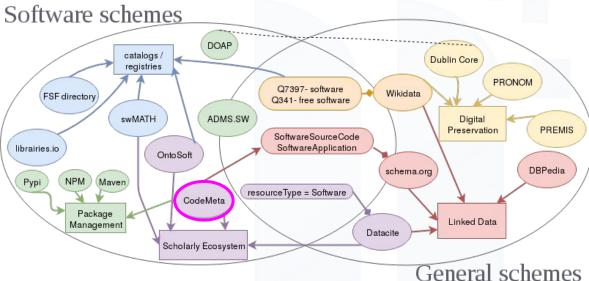


# CodeMeta initiative - V1.0 released in 2017

- A subset of schema.org
- An academic community discussing software metadata
- A crosswalk table mapping the metadata landscape

V2.0 released in 2020,

V3.0 is expected soon!!



Gruenpeter M. and Thornton K. (2018) Pathways for Discovery of Free Software (slide deck from LibrePlanet 2018). <a href="https://en.wikipedia.org/wiki/File:Pathways-discovery-free.pdf">https://en.wikipedia.org/wiki/File:Pathways-discovery-free.pdf</a>



#### #RSMD\_guidelines

# The Research Software MetaData guidelines

The RSMD seven Aspects

1. General Metadata Requirements

2. Accessibility & preservation

3. Reference & identification

4. Description & classification

5. Attribution & credit

6. Reuse, licensing & legal aspects

7. Re-execute: Dependencies & execution environment

SIRS report

FAIR4RS

A = Archive

A = Accessible

R = Reference

D = Describe

I = Interoperable

F = Findable

C = Cite

R = Reusable



# Each aspect has a high-level objective with a series of recommendations

Description & classification

High-level objective

Actionable, detailed recommendations

#### Objective

#### Objective:

Software is properly described with name, purpose and functionalities alongside other software specific metadata properties (programming language, domain, etc.) to ensure software findability.

ID	Recommendation	Priority		
RSMD-4.1	Add <b>software name</b> and <b>description</b> of the software's functionality and purpose, using a README file in the root directory of the source code or other intrinsic metadata file (e.g codemeta.json with the properties <i>name</i> and <i>description</i> ).	Essential ☆☆☆		
RSMD-4.2	Add descriptive metadata for classification purposes on metadata record (extrinsic metadata), which can be available in a scholarly infrastructure. This includes, but is not limited to:  Name Description Domain	Essential		
	Programming language     Date created			



# Validating the guidelines

We'll answer these questions by writing in parallel in the document. Please comment on others' answers by using the Google Doc commenting function.

For each aspect we will review its objective and each recommendation by answering the following questions in the table:

- Is this recommendation clear.
- Is this objective/recommendation relevant for research software?
  - <u>4</u>/ or +1/-1

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment



#### **Objective:**

To ensure the collection, curation, and maintenance of research software metadata, the following general requirements are recommended for end users, including researchers, software engineers, curators, and institution staff.

- Is this objective/recommendation <u>clear</u>.
- Is this objective/recommendation relevant for research software?

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment



# Where is the metadata available? Extrinsic

#### **Catalogs and registries**

- ASCL
- swMath
- OpenAire
- libraries.io
- Research Software Directory escience center
- ...

# Software development platforms (on platform page)

- GitHub
- Bitbucket
- SourceForge
- ...

# Scholarly repositories

- Zenodo (InvenioRDM)
- HAL
- ...

# Package manager platform (not intrinsic file)

- NPM
- PyPI
- ...

#### Scholarly publishers

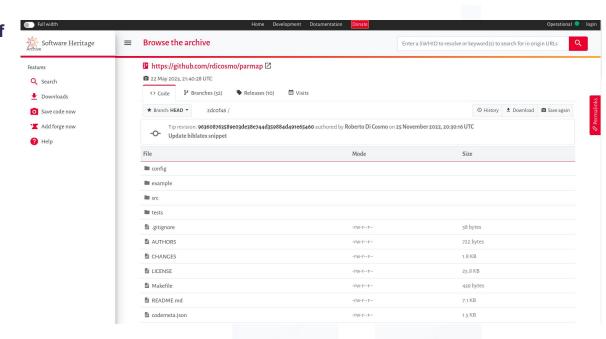
- IPOL
- eLife
- Dagstuhl
- Episciences
- ...



# The case of intrinsic metadata

#### In the software source code itself

- README
- LICENSE
- AUTHORS
- codemeta.json
- package management
  - pom.xml
  - o package.json
  - 0 ...
- CITATION.cff
- About
- ..

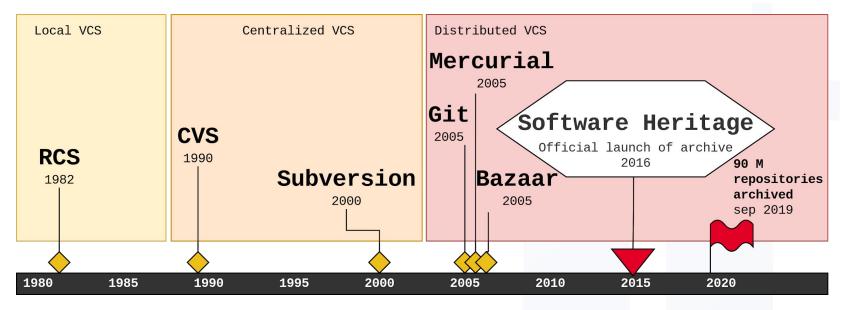


**Human readable (e.g README)** 

Machine actionable (e.g codemeta.json)



# Version control system (VCS) history



- records changes made to a (set of) source code file (s)
- allows to operate on versions: diff/merge/fork/recover etc.
- essential tool for software development



#### **Objective:**

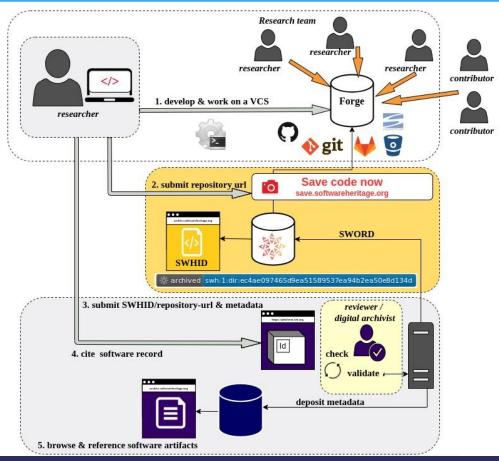
To ensure accessibility and preservation, researchers and software engineers are strongly recommended to follow the archival and sharing recommendations below.

- Is this objective/recommendation <u>clear</u>.
- Is this objective/recommendation relevant for research software?

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment



#### #RSMD\_quidelines



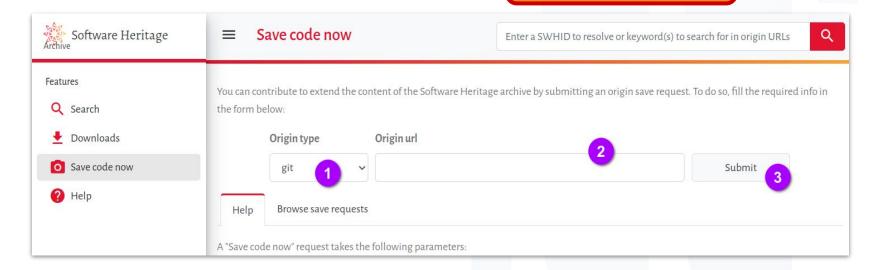


# Save any your code now!



## https://save.softwareheritage.org/

#### Save code now





#### **Objective:**

To ensure that research software projects, modules, versions and source code artifacts can be precisely identified and referenced.

- Is this objective/recommendation <u>clear</u>.
- Is this objective/recommendation relevant for research software?

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment



# Software source code identification

#### Software concept / project / collection

Description in registry, a homepage or any other form of metadata record

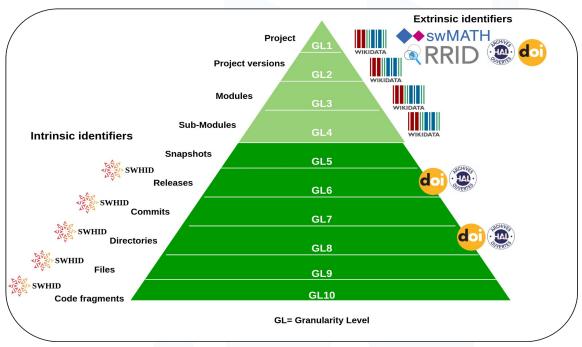
- Project versions (for example Python2 and Python3)
- Modules
- Sub-modules

#### Software artifact

- Executable (download link)
- Software source code
  - Dynamic artifact current development code
  - Archived copy
    - Snapshot (all branches, all dev history)
    - Release / Package
    - Commit- a specific point in development history
    - Directory
    - File
    - Algorithm

#### Software context

- Complementary artifacts Software artifacts that are external to the source code
  - the software environment, tutorial (Jupyter notebook),
     Data (input/output data), etc.
- Articles
- Documentation



Research Data Alliance/FORCE11 Software Source Code Identification WG et al. (2020). Use cases and identifier schemes for persistent software source code identification (V1.1). Research Data Alliance. https://doi.org/10.15497/RDA00053



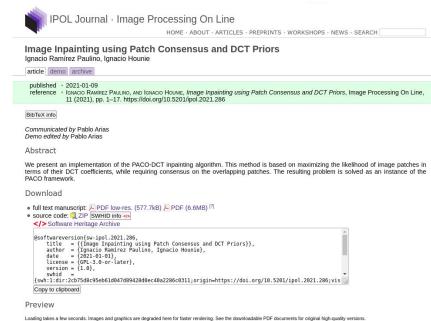
# **Granularity level summary (SCID output, 2020)**

Gran ularit y level (GL)	ID target	Extrinsic identifiers								Intrinsic identifiers		
		ASCL	SCL ARK	DOI	HAL	URL	RRID	SwMath	Wikidata		Hash	swn
(OL)									entity	property		
GL1	project	Х	х	Х	Х	х	х	Х	Х			
GL2	project version		х						Х			
GL3	module		Х						Х			
GL4	repository		Х			Х				Х		
GL5	repository snapshot		х							Х		Х
GL6	release		х	X**						Х	Х	х
GL7	commit		х							Х	Х	Х
GL8	directory		Х	X**	X*					Х	Х	Х
GL9	file		х	X**							Х	Х
GL10	Code fragment		Х									Х



# DOI and SWHID on IPOL articles

- Journal Image Processing On Line (IPOL, <a href="https://www.ipol.im/">https://www.ipol.im/</a>)
- Research software packages are identified with:
  - The article DOI: (https://doi.org/10.5201/ipol.2021.286)
  - The software SWHID: The publisher deposits the software in Software Heritage with the DOI as an origin (https://archive.softwareheritage.org/swh:1:dir:2cb75d8c95eb61d047d89428d0ec40a2286c0311;origin=https://doi.org/10.5201/ipol.2021.286;visit=swh:1:snp:23a5f7ee209b593e9b3e60ebe2bc42f1e6b76ff3;anchor=swh:1:rel:2de235c8fc3dd527cfaaba5cbf1d8144fee14f40)
- Links from the paper and metadata DOI to:
  - the software deposit and its SWHID,
  - the live demo of the software (in the demo tab)



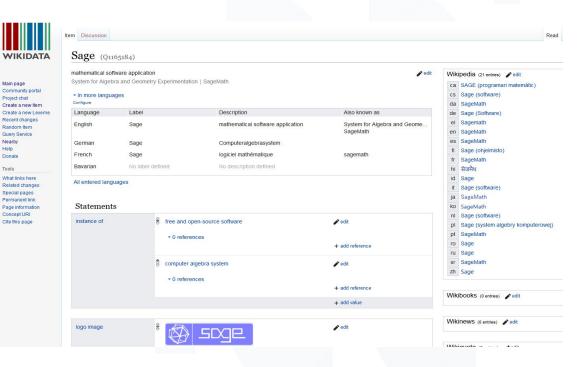


# Wikidata entities (Qxxx) - an extrinsic identifier

Q1165184=SageMath.

A few examples of external identifiers properties of used on software entities:

- Arch package <u>sagemath</u>
- Debian stable package sagemath
- Fedora package
- Free Software Directory entry
- Freebase
- Gentoo package
- Open Hub ID <u>sage</u>
- Quora topic
- Ubuntu Package
- swMATH work ID <u>825</u>
- SWHID snapshot (15.11.2020)
- and many more





# The SoftWare Heritage ID - a.k.a SWHID

SWH provides a Persistent IDentifier (PID) that can identify each and every source code artifact with integrity, called a SWHID.

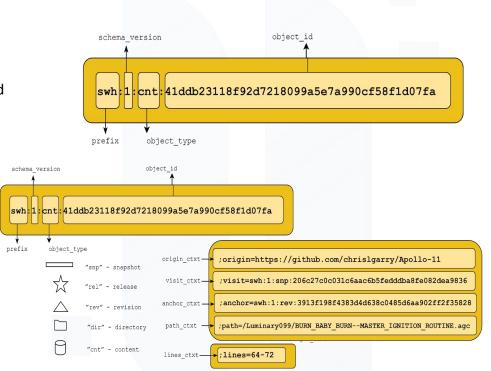
SWHIDs are intrinsic identifiers which are intimately bound to the designated object, they do not need a register, only agreement on a standard.

Intrinsic vs. extrinsic blog post

Go to API endpoint











#### **Objective:**

To ensure software findability and comprehensibility, provide descriptive metadata (software's name, purpose, functionalities, programming language, domain, etc.). These metadata facilitate accurate representation of the software and enable users to easily discover and understand its capabilities.

- Is this objective/recommendation <u>clear</u>.
- Is this objective/recommendation relevant for research software?

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment



# **Describe: What's a good README**

- ★ MUST include:
  - Name and a description of the software.
- **★** SHOULD include:
  - how to run and use the source code
  - build environment, installation, requirements
- ★ CAN include:
  - project website or documentation pointer and recent news
  - visuals

extracted from Eric Steven Raymond and Make a README



# **CodeMeta properties**

## Identify

- identifier
- name
- author
- version, softwareVersion

#### **Execute**

- codeRepository
- operatingSystem
- softwareRequirements
- buildInstructions
- Not in CodeMeta:
  - a. Examples
  - b. Compiler
  - c. Executable link
  - d. Other documentation

#### Classify

- description
- releaseNotes
- keywords
- supportingData (in/out data)
- fileFormat
- programmingLanguage
- Not in CodeMeta:
  - a. references
  - b. algorithms

#### **Administrate**

- maintainer
- copyrightHolder
- funder
- license
- editor
- publisher
- dateCreated
- dateModified
- datePublished
- developmentStatus



#### **Objective:**

To ensure proper crediting and acknowledgment of software creators, authors, and contributors, it is important to follow citation recommendations.

- Is this objective/recommendation clear.
- Is this objective/recommendation relevant for research software?

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment



mechanism of attribution may not be applicable to all software.

# Software citation principles - published in 2016

Software is a critical part of modern research... 2021: Github & CFF -**IMPORTANCE** Software should be considered of research. Software citations Citation File Format: SOFTWARE importance in the scholarly record as citations of other BibTeX export with type CITATION be included in the metadata of the citing work, such as a **PRINCIPLES** be cited on the same basis as @software any other research product such as a paper or a book. UNIQUE IDENTIFICATION A software citation should actionable, globally unique RESEARCHERS by at least a community of the **ACCESSIBILITY** Software citations should facilitate access to the software itself and to its associated metadata, documentation, data, and other materials necessary machines to make **PERSISTENCE** informed use of the referenced software. disposition should persist even beyond the lifespan of the software they describe. SPECIFICITY CREDIT AND ATTRIBUTION . Software citations should facilitate identification of Scriberia Software citations should facilitate giving and access to the specific version of software that scholarly credit and normative, legal was used. Software identification should be as attribution to all contributors to the software, pecific as necessary, such as using version numbers recognizing that a single style or

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

revision numbers, or variants such as platforms

*Fig.* 69 Research software developers get recognition by making software citable. *The Turing Way* project illustration by Scriberia. Zenodo. http://doi.org/10.5281/zenodo.3332807



#### **Objective:**

To ensure proper software reuse and license compliance, it is essential to accurately describe software licensing and legal aspects. This includes providing clear guidance on proper usage and distribution rights, clarifying the terms and conditions under which the software can be used and shared.

- Is this objective/recommendation <u>clear</u>.
- Is this objective/recommendation relevant for research software?

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment





Get Started

AQ Developers

Specification

Resources

Supporters

API

# REUSE SOFTWARE



Inofficial translations are available in: Deutsch, Česky, Українська

We make licensing easy for humans and machines alike. We solve a fundamental issue that Free Software licensing has at the very source: what license is a file licensed under, and who owns the copyright? Adopting our recommendations is as easy as one-two-three!



- 1. Choose and provide licenses
  - Add copyright and licensing information to each file
    - 3. Confirm REUSE compliance



#### **Objective:**

To ensure the usability of software and the ability to reproduce the same results in experiments, it is important that the software can be easily rebuilt and executed. This ensures that others can use the software effectively and achieve consistent outcomes.

- Is this objective/recommendation <u>clear</u>.
- Is this objective/recommendation relevant for research software?

- 1. General Metadata Requirements
- 2. Accessibility & preservation
- 3. Reference & identification
- 4. Description & classification
- 5. Attribution & credit
- 6. Reuse, licensing & legal aspects
- 7. Re-execute: Dependencies & execution environment



# **Conclusion and next steps**

D4.4 Research Software Metadata guidelines - deadline for the review (May 29th at 12.00 UTC)

- Our How to review and comment the deliverables?
  - Comment in the live notes
    - open until <u>May 25th at 12.00 UTC</u>
    - https://tinyurl.com/2023-05-23-RSMD-webinar
  - Review first draft of the deliverable V1.0 (which includes state of the art):
    - open until May 29th at 12.00 UTC
    - https://tinyurl.com/RSMD-quidelines-v1
- Contribute to <u>CodeMeta!</u> (participate in the community discussion)
  - V3.0 of the vocabulary is expected at the end of the month
  - A dedicated webinar will be scheduled for September 2023



# Making the RSMD guidelines useful

How can we make the RSMD guidelines format of most value to you?

Keep in touch: <a href="mailto:morane@softwareheritage.org">morane@softwareheritage.org</a>
@moraneottilia, @SWHeritage

https://www.softwareheritage.org/newsletter/







@fairimpact\_eu /company/fair-impact-eu-projectt