



# Towards FAIR Research Software

**Daniel Garijo, Ontology Engineering Group,  
Universidad Politécnica de Madrid, Spain**

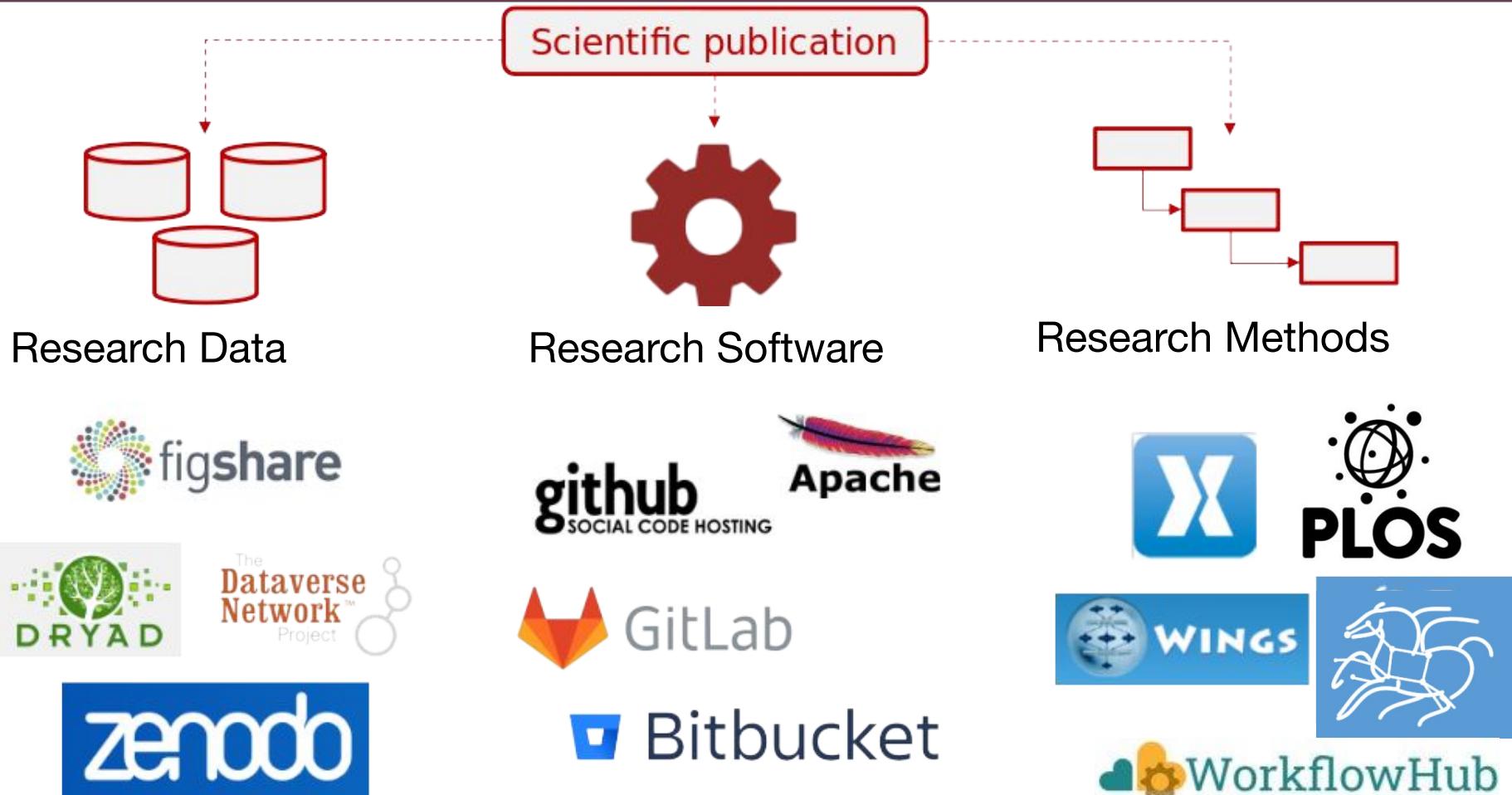
Assessing Best Research Software Practices  
through Metadata

✉ daniel.garijo@upm.es  
🐦 @dgarijov

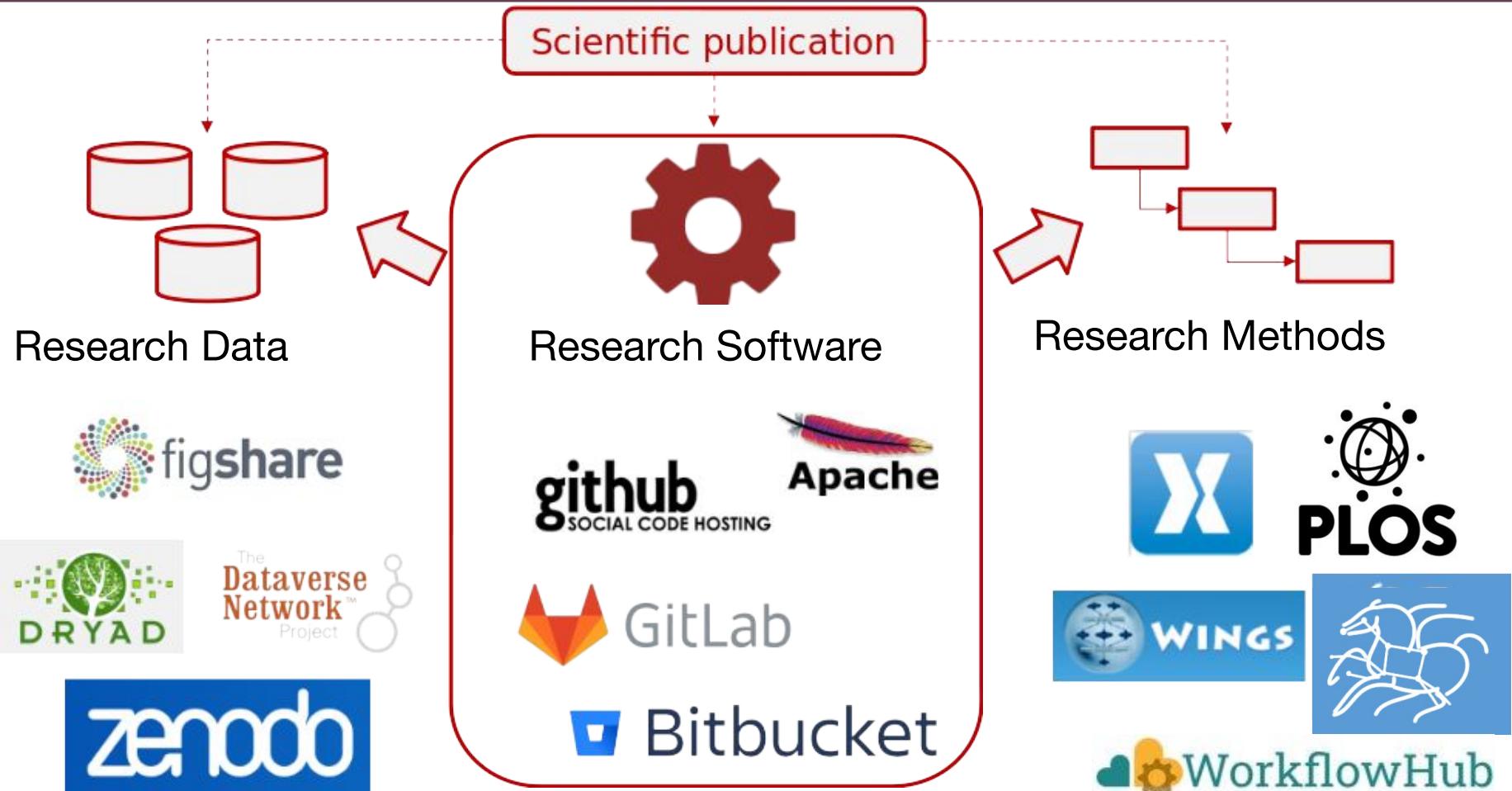
# Research Software is one of the pillars of Open Science

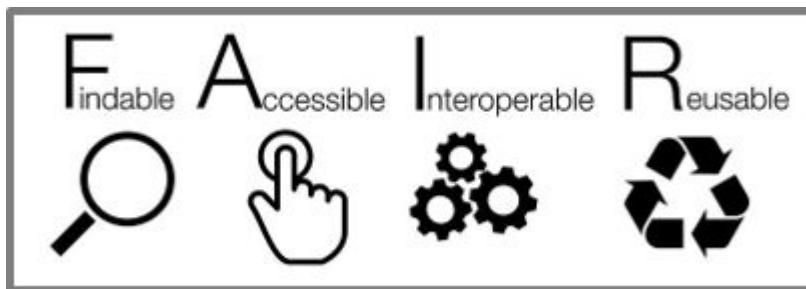


# Research Software is one of the pillars of Open Science



# Research Software is one of the pillars of Open Science





Data (initially) [1]



**Research Software**



Methods



Semantic artefacts

Other guidelines:

- Guidelines for Transparency and Openness Promotion (TOP) [2]
- Reproducibility Enhancement Principles (REP) [3]
- ...



[1] Wilkinson, M., Dumontier, M., Aalbersberg, I. et al. The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* 3, 160018 (2016). <https://doi.org/10.1038/sdata.2016.18>

[2] <https://www.cos.io/initiatives/top-guidelines>

[3] Stodden, V et al Enhancing reproducibility for computational methods  
<https://www.science.org/lookup/doi/10.1126/science.aah6168>

F 1 Create a description of your software  
 F 2 Register your software in a software registry  
 F 3 Use a Unique and Persistent Identifier for your software  
 A 4 Make sure that people can download your software  
 I 5 Explain the functionality of your software  
 I 6 Use standard (community agreed) formats for inputs and outputs  
 R 7 Document your software  
 R 8 Give your software a licence  
 R 9 State how to cite your software  
 R 10 Follow best practices for software development

<https://github.com/LibraryCarpentry/Top-10-FAIR>

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

- F1. Software is assigned a globally unique and persistent identifier.
- F1.1. Components of the software representing levels of granularity are assigned distinct identifiers.
  - F1.2. Different versions of the 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, searchable and indexable.

**A: 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.

**I: Software interoperates with other software by 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.

**R: Software is both usable (can be executed) and reusable (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.

FAIR4RS (RDA) [1]

[1] Chue Hong, Neil P., Katz, Daniel S., Barker, Michelle, Lamprecht, Anna-Lena, Martinez, Carlos, Psomopoulos, Fotis E., Harrow, Jen, Castro, Leyla Jael, Gruenpeter, Morane, Martinez, Paula Andrea, Honeyman, Tom, Struck, Alexander, Lee, Allen, Loewe, Axel, van Werkhoven, Ben, Jones, Catherine, Garijo, Daniel, Plomp, Esther, Genova, Francoise, ... RDA FAIR4RS WG. (2022). FAIR Principles for Research Software (FAIR4RS Principles) (1.0). <https://doi.org/10.15497/RDA00068>

# FAIR is highly related to metadata

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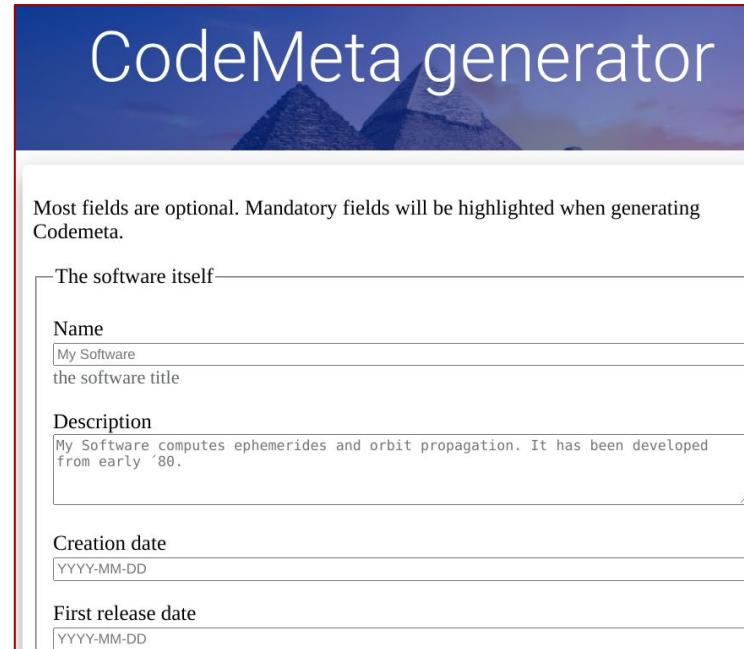
[1] Chue Hong, Neil P., Katz, Daniel S., Barker, Michelle, Lamprecht, Anna-Lena, Martinez, Carlos, Psomopoulos, Fotis E., Harrow, Jen, Castro, Leyla Jael, Gruenpeter, Morane, Martinez, Paula Andrea, Honeyman, Tom, Struck, Alexander, Lee, Allen, Loewe, Axel, van Werkhoven, Ben, Jones, Catherine, Garijo, Daniel, Plomp, Esther, Genova, Francoise, ... RDA FAIR4RS WG. (2022). FAIR Principles for Research Software (FAIR4RS Principles) (1.0). <https://doi.org/10.15497/RDA00068>

*“The goal of CodeMeta is to create a **concept vocabulary** that can be used to standardize the exchange of software metadata across repositories and organizations” - <https://github.com/codemeta/codemeta>*

Website: <https://codemeta.github.io/>

## The CodeMeta Project

JSON-LD representation  
Needs to be **filled by hand**



The screenshot shows a web application titled "CodeMeta generator" with a background image of the pyramids at Giza. The interface is a form for generating JSON-LD code. It includes fields for "The software itself" (Name and Description), "Creation date", and "First release date". Most fields are optional, as indicated by the text "Most fields are optional. Mandatory fields will be highlighted when generating Codemeta".

Most fields are optional. Mandatory fields will be highlighted when generating Codemeta.

The software itself

Name

My Software  
the software title

Description

My Software computes ephemerides and orbit propagation. It has been developed from early '80.

Creation date

YYYY-MM-DD

First release date

YYYY-MM-DD

Research Software metadata is not ~~abundant~~ machine readable

Can you please describe your software component with metadata?

I already did! Did you read the project readme?

Did you see the online documentation?

Perhaps the you saw the paper?



Many domain-specific registries are **curated by hand by experts**

## ▪ Documentation

- Text classification
- Named entity recognition and relation extraction

## ▪ Code

- Static code analysis

 docs	update doc	13 days ago
 experiments	Added pipeline missed in previous version of create_models	8 months ago
 notebook	Fix #180	15 months ago
 src/somef	update version	13 days ago
 .gitignore	Fix test and added env to gitignore	29 days ago
 .readthedocs.yml	documentation	2 years ago
 CITATION.cff	Add citation file	4 months ago
 Dockerfile	updating Docker image	4 months ago
 LICENSE	initial cleanup	2 years ago
 README.md	update doc	13 days ago
 config.json	Created script to generate models and updated python version to 3.9	8 months ago
 mkdocs.yml	Fix #178	15 months ago
 pyproject.toml	minor package changes	4 months ago
 setup.py	Fix #437	28 days ago

# Text classification: Software Metadata Extraction Framework

<https://github.com/KnowledgeCaptureAndDiscovery/somef/>



Repository



Results (Metadata)

dgarijo Merge pull request #174 from KnowledgeCaptureAndDiscovery/dev	
docs	Typos
experiments	Improved header analysis. Fix #166
notebook	Fix #96
src	Typos
.gitignore	Fix #147 and working towards automatic corpus va
.readthedocs.yml	documentation
Dockerfile	Fix #113 creating a Dockerfile
LICENSE	initial cleanup
README.md	Typos
config.json	Provide Fix for issues - 12, 35,36
mkdocs.yml	typos and reorganization
setup.py	Fix #113 creating a Dockerfile

- **Readme Analysis**

- Supervised classification
- Regular expressions
- Header analysis

- **File exploration**

- Notebooks
- Dockerfiles
- Documentation

- **GitHub API**



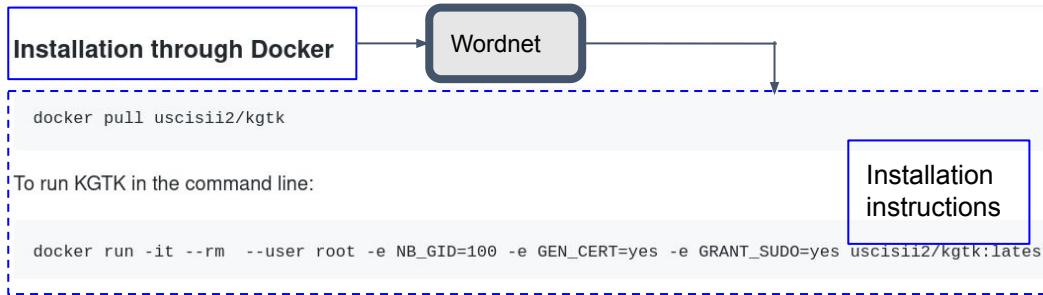
CodeMeta



Kelley, A., & Garijo, D. (2021). A framework for creating knowledge graphs of scientific software metadata. *Quantitative Science Studies*, 1-37.

- Extraction based on frequent header analysis
  - Fuzzy matching based on synsets

## Installation



## KGTK: Knowledge Graph Toolkit

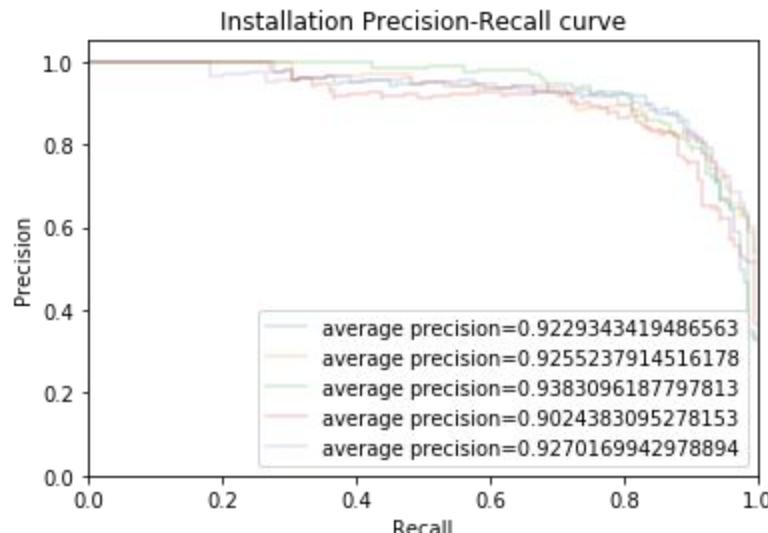
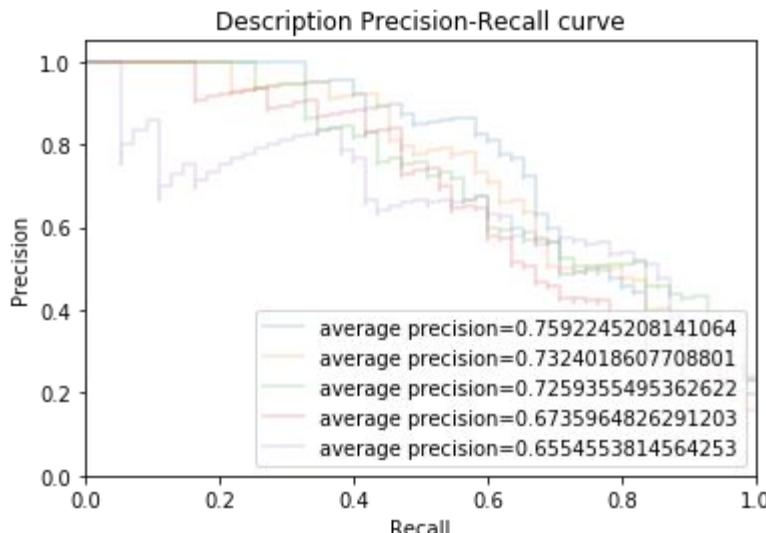


Regular expressions, based on common practices (e.g., DOI, .bib, etc.)

The Knowledge Graph Toolkit (KGTK) is a comprehensive framework for the creation and exploitation of large hyper-relational knowledge graphs (KGs), designed for ease of use, scalability, and speed. KGTK represents KGs in tab-separated (TSV) files with four columns: edge-identifier, head, edge-label, and tail. All KGTK commands consume and produce KGs represented in this simple format, so they can be composed into pipelines to perform complex transformations on KGs. KGTK provides:

- Paragraph-based text classification
- Four main categories:
  - Installation, citation, description, invocation.
- Binary classification problem

Truth Value	Category	Apprx. Ratio	Count
True	Description	0.5	275
False	Installation	0.125	68
	Invocation	0.125	68
	Citation	0.125	68
	Treebank	0.125	68
Total		1.0	547



- Name (GA)
- Full title (RE)
- Description (SC, HA)
- Citation (SC, RE, HA)
- Installation instructions (SC, HA)
- Invocation (SC)
- Usage examples (HA)
- Documentation (HA, FE)
- Requirements (HA)
- Contributors (HA)
- FAQ (HA)
- Support (HA)
- License (GA, HA, FE)
- Stars (GA)
- Contact (HA)
- Download URL (HA, GA)
- DOI (RE)
- DockerFile (FE)
- Notebooks (FE)
- Executable notebooks (Binder, Collab) (RE)
- Owner: (GA)
- Keywords (GA)
- Source code (GA)
- Releases (GA)
- Changelog (GA)
- Issue tracker (GA)
- Programming languages (GA)
- Acknowledgements (HA)
- Logos (RE)
- Images (RE)
- Shell scripts (FE)
- Code of conduct (FE)
- Repository status (RE)
- Arxiv links (RE)
- Support channels (RE)
- Software category (SC) (Work in progress)
- ...

## Method used (provenance):

- Supervised Classification (SC)
- Header Analysis and Synset comparison (HA)
- File Exploration (FE)
- Regular Expressions (RE)
- GitHub API (GA)

## Static code analysis in Python

- Extraction of available classes and functions
  - Documentation
- Requirements (reusing existing libraries)
- Call list
- File hierarchy
- Control flow (reusing existing libraries)
- Software invocation
  - Service? Package? Library? & invocation command
- Metadata export in JSON



Rosa Filgueira



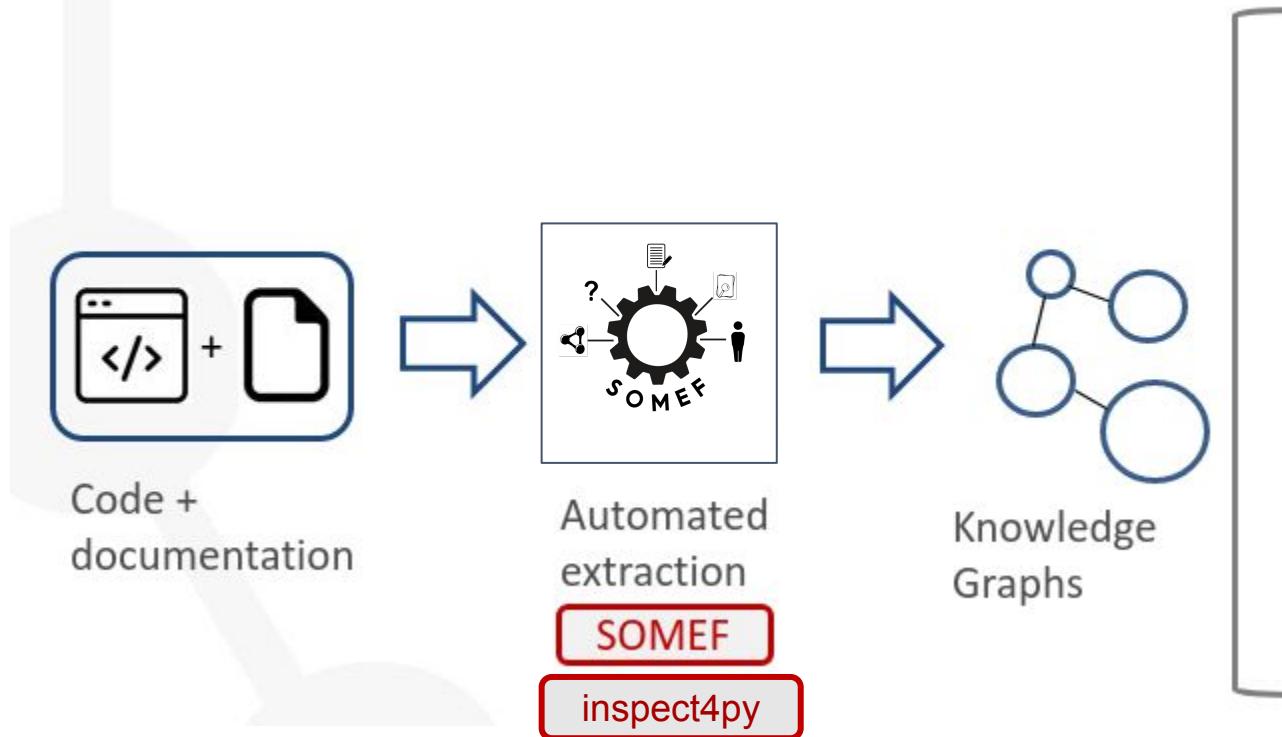
University of  
St Andrews

## Benefits

- Understanding, reuse, ML featurization, similarity, best practices

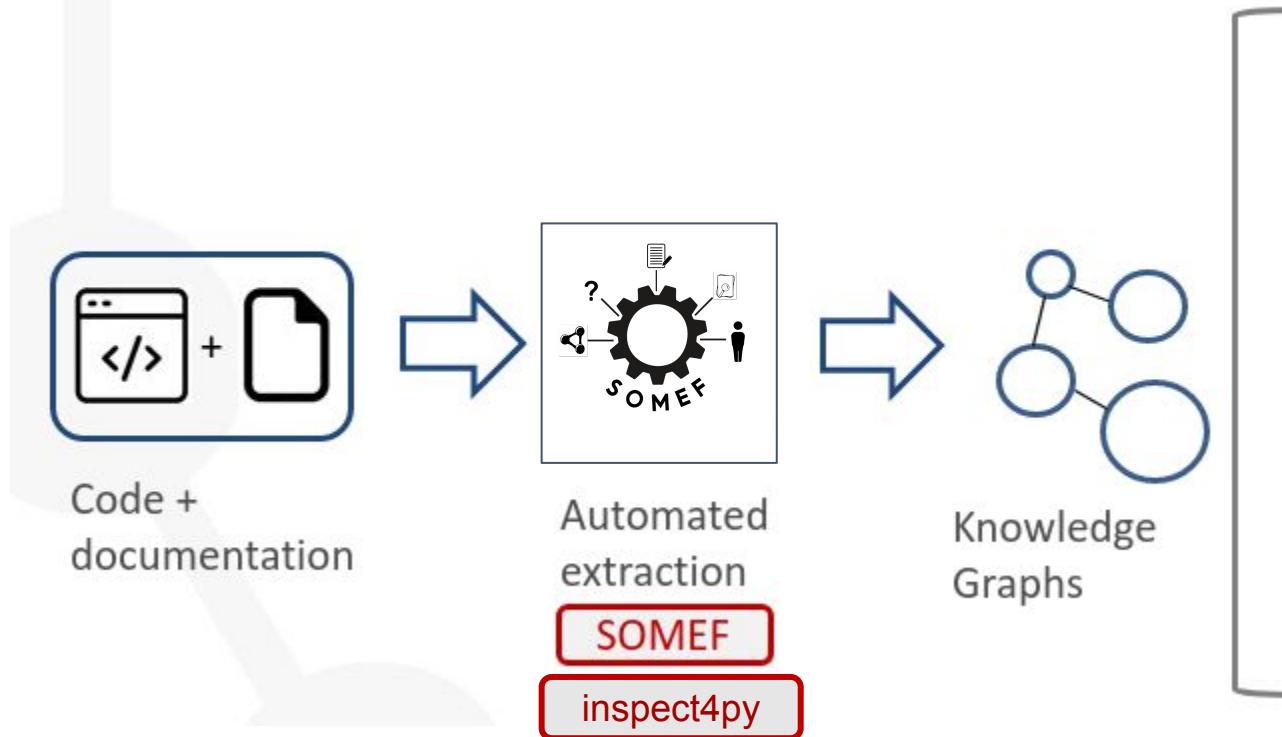
<https://github.com/SoftwareUnderstanding/inspect4py>

Filgueira, R. and Garijo, D. (2022). Inspect4py: A Knowledge Extraction Framework for Python Code Repositories. To appear in Mining Software Repositories, 2022 (demo)



## What can we do now?

- Assist
  - Ease descriptions
  - Ease reuse
  - Augment impact
- Assess (measure practices)



## What can we do now?

- **Assist**
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## SOMEF Vider

<https://somef.linkeddata.es/>

GitHub URL

Threshold  SUBMIT

Description  

Citation    

**APA Style**  
Mao, A., Garijo, D., & Fakhraei, S. (2019). SoMEF: A Framework for Capturing Scientific Software Metadata from its Documentation. 2019 IEEE International Conference on Big Data (Big Data), 3032–3037. <https://doi.org/10.1109/BigData47090.2019.9006447>

**Bibtex**  
@INPROCEEDINGS{9006447, author={A. {Mao} and D. {Garijo} and S. {Fakhraei}}, booktitle={(2019 IEEE International Conference on Big Data (Big Data)}}, title={SoMEF: A Framework for Capturing Scientific Software Metadata from its Documentation}, doi={10.1109/BigData47090.2019.9006447}, url={http://dgarijo.com/papers/SoMEF.pdf}, pages={3032-3037}, year={2019}}

...

Victor, F. A., & Daniel, G. (2021). SOMEF VIDER (Version 0.0.1) [Computer software]. <https://github.com/SoftwareUnderstanding/SOMEF-Vider>

Get Codemeta files automatically!

 JSON

 CodeMeta

Turtle

# Easing reuse and explore: Automated software catalogs



## Software Catalog

Search for repositories...

Title Stars Releases Last updated



**Morph-OME** Online Mapping Editor



6 ★  
v.2.1 3 ↗

**gtfs-bench** GTFS-Madrid-Bench: A Benchmark for Knowledge Graph Construction Engines



11 ★  
v1.2.2 5 ↗

**morph-csv** Enhancing virtual KG access over tabular data with RML and CSVW



8 ★  
v1.1.0 3 ↗

**pytada-hdt-entity** A python library binding of the c++ library tada-hdt-entity



0 ★  
v1.8 3 ↗

**tada-web** This is a web API project using tada-hdt-entity and the pytada-hdt-entity libraries



0 ★  
v1.0 1 ↗

**Widoco** Wizard for documenting ontologies. WIDOCO is a step by step generator of HTML templates with the documentation of your ontology. It uses the LODE environment to create part of the template.

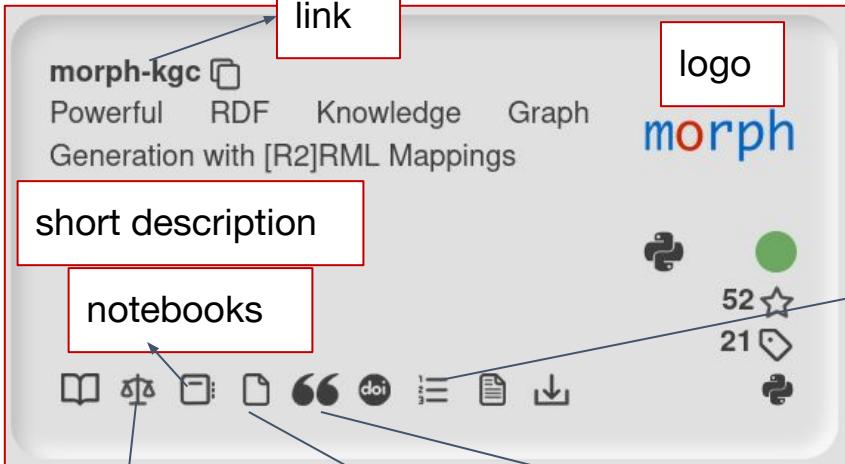


0 ★  
0 ↗

Alpha available at: <https://software.oeg.fi.upm.es/> GitHub: <https://github.com/oeg-upm/soca>

Work by Daniel Rodriguez

**link**



The screenshot shows the GitHub repository page for 'morph-kgc'. It features a logo with the word 'morph' in blue and red, a Python icon, and statistics: 52 stars, 21 forks, and 13 issues. Below the logo are icons for code, issues, pull requests, and a PDF file. A 'short description' box highlights 'Powerful RDF Knowledge Graph Generation with [R2]RML Mappings'. A 'notebooks' box contains links to Jupyter notebooks. A 'License' box indicates the Apache License 2.0. A 'Citation' box contains the BibTeX entry for the paper.

**Usage**

Learn quickly with the tutorial in [Google Colaboratory!](#)  
**PyPi** is the fastest way to install Morph-KGC:  
`pip install morph-kgc`  
 We recommend to use [virtual environments](#) to install Morph-KGC.  
 To run the engine via [command line](#) you just need to execute the following:  
`python3 -m morph_kgc config.ini`  
 Check the [documentation](#) to can see how to generate the configuration INI file.  
[Here](#) you can also see an example INI file.  
 It is also possible to run Morph-KGC as a [library](#) with [RDFLib](#) and [Oxigraph](#):

```

import morph_kgc

# generate the triples and load them to an RDFLib graph
g_rdflib = morph_kgc.materialize('/path/to/config.ini')
# work with the RDFLib graph
q_res = g_rdflib.query(' SELECT DISTINCT ?classes WHERE { ?s a ?classes } ')

# generate the triples and load them to Oxigraph
g_oxigraph = morph_kgc.materialize_oxigraph('/path/to/config.ini')
# work with Oxigraph
q_res = graph.query(' SELECT DISTINCT ?classes WHERE { ?s a ?classes } ')

# the methods above also accept the config as a string
config = """
[DataSource1]
mappings: /path/to/mapping/mapping_file.rml.ttl
db_url: mysql+pymysql://user:password@localhost
"""
g_rdflib = morph_kgc.materialize(config)

How to use it
python /morph-kgc/oeg-upm_morph-kgc/morph-kgc-main/src/morph_kgc/main.py
    
```

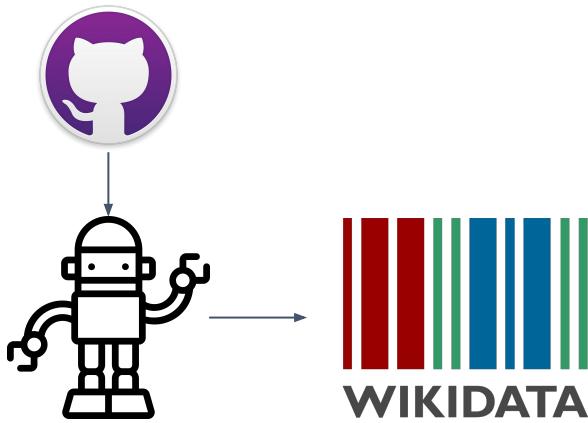
**invocation**

Towards FAIR Research Software FAIR ZB\_MED Colloquium, June, 2023

20

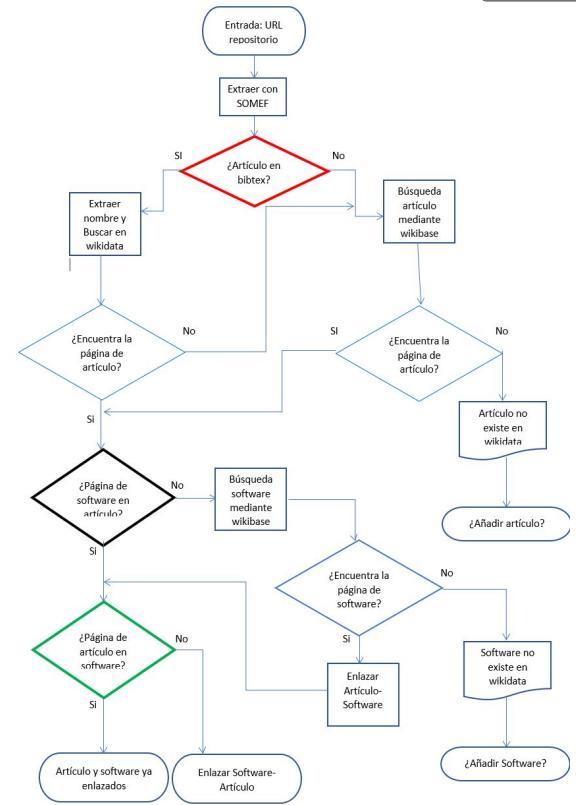


Wikidata bot to link code repositories with Wikidata articles



Does the repository have a link to a paper?  
Does the paper exist in Wikidata?  
**Connect them!** Create a software entry if it does  
not exist

Jorge Bolinches (work in progress)



(included by Saltbot, from a CFF file)

Created by SALTBot

Widoco (Q118564029)

Wizard for documenting ontologies. WIDOCO is a step by step generator of HTML templates with the documentation of your ontology. It uses the LODE environment to create part of the template.

In more languages

Language	Label	Description	Also known as
English	Widoco	Wizard for documenting ontologies. WIDOCO is a step by step generator of HTML templates with the documentation of your ontology. It uses the LODE environment to create part of the template.	

described by source

WIDOCO: A Wizard for Documenting Ontologies

0 references

Created by SALTBot

+ add reference

+ add value

Existing WD knowledge

Statements

instance of

scholarly article

WIDOCO: A Wizard for Documenting Ontologies

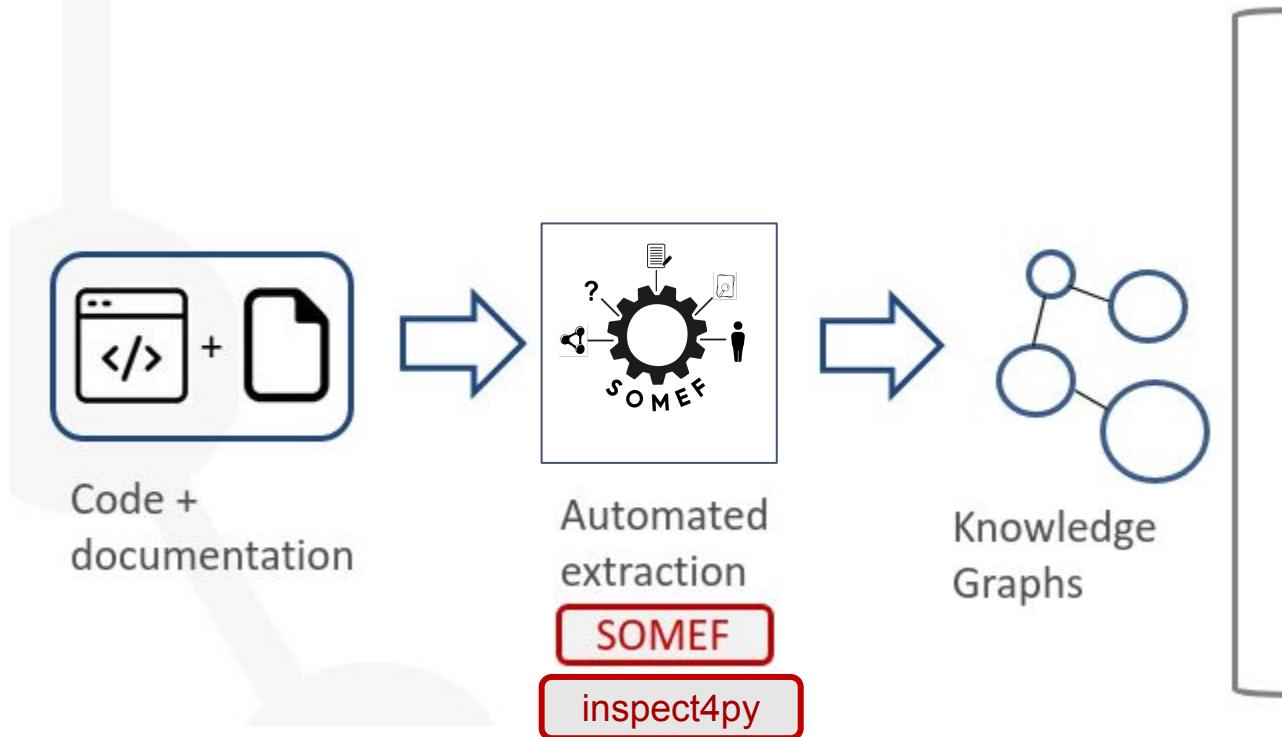
article published in 2017

In more languages

Language	Label	Description
English	WIDOCO: A Wizard for Documenting Ontologies	article published in 2017
Spanish	No label defined	No description defined
Traditional Chinese	No label defined	No description defined
Chinese	No label defined	No description defined

All entered languages

Many articles are not in WD. Can we include them?



## What can we do now?

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  - Augment impact
- **Assess (measure practices)**

# Which best practices are followed in an organization?

## Software Catalog

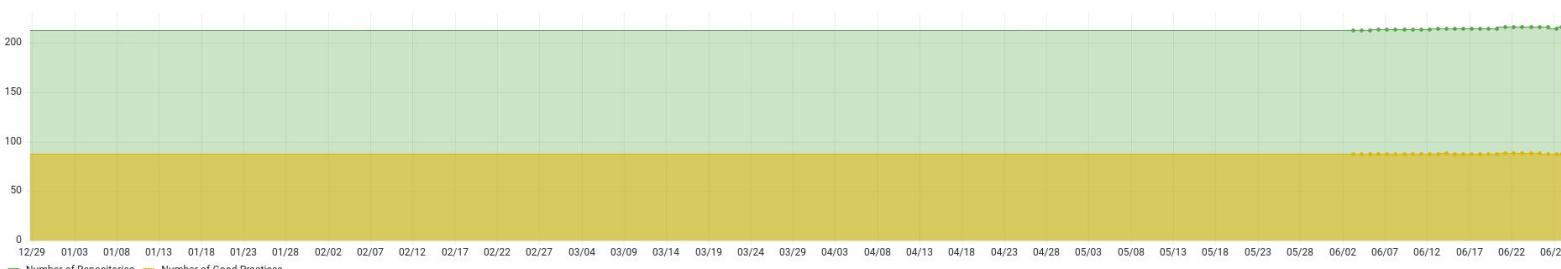
Search for repositories...



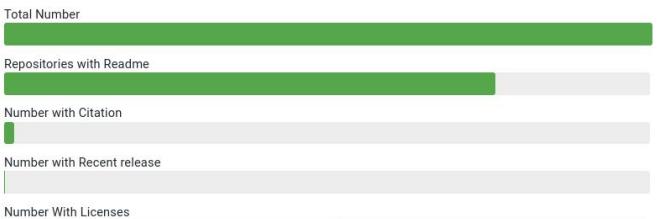
Title Stars Releases Last updated



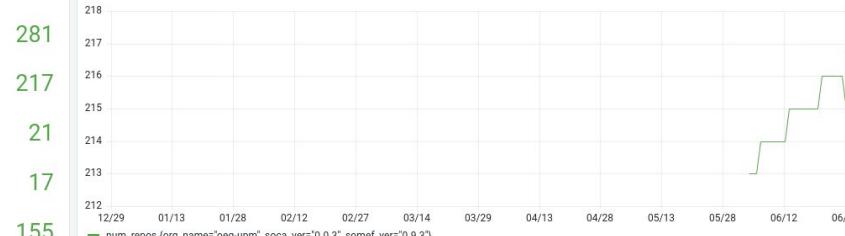
Number of Repositories vs Number of Good Practices



Number of Repositories per best practice

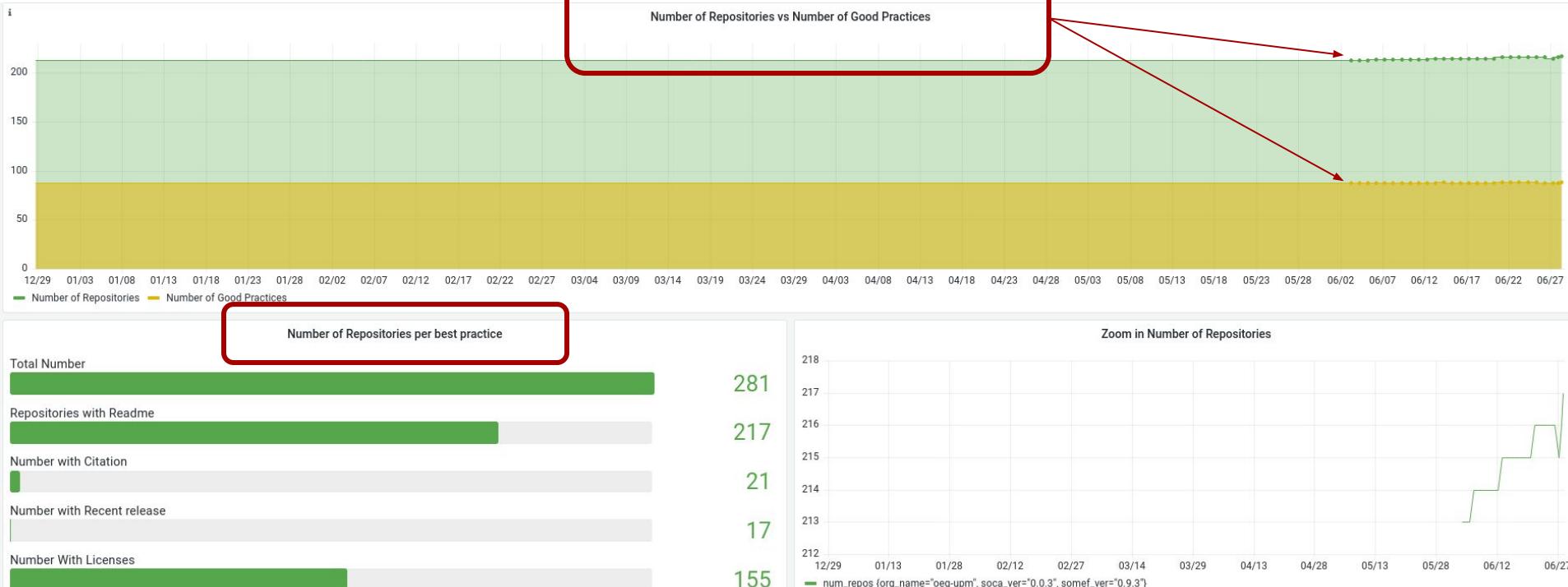


Zoom in Number of Repositories



Tracking number of best practices across time

Work by Miguel Arroyo





Number of Repositories per Readme Best Practice

217

58

19

36

requirement section?

Readthedocs?  
External doc? Wiki?

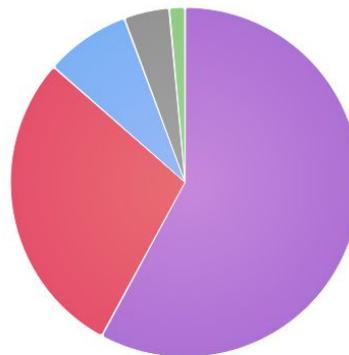
Number with Readme

Number with Installation

Number with Requirement

Number with Documentation

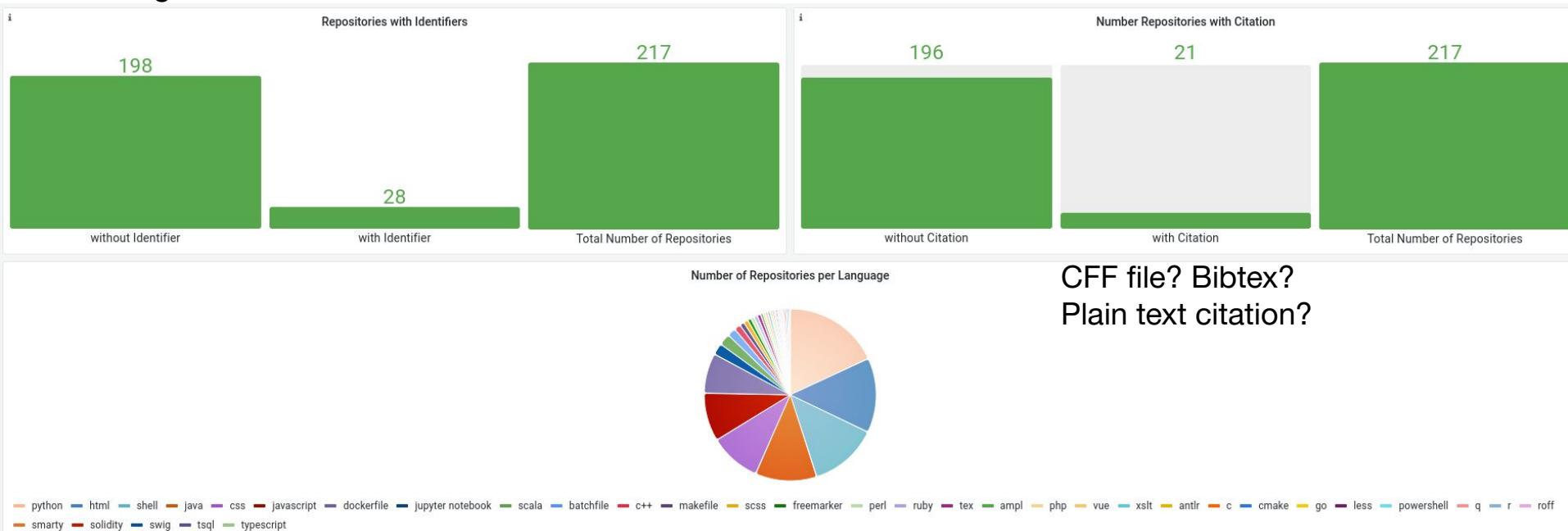
Licenses



Additional insight on licenses used

— Apache — Missing — MIT — Other — GPL

## Zenodo DOI? Paper DOI? Software heritage?



This is **work in progress!** We are including Containerization, package managers, individual repository assessment, etc.

## Current life cycle requires researchers to:

- Create separate metadata files
- Curate them and maintain them
- Re-introduce metadata manually in different registries

## Current aim:

- Improve and maintain **high quality readme files**
- Let the extraction tools do the work
- Maximize benefits from metadata extraction
  - Move **towards assisting researchers** produce FAIR software



Research software is a **critical asset for Open Science**

Software metadata **is key**:

- Reusability, Comparison, Search
- FAIR research software
- **Propagate** impact of research



From **ASSESSing**, we are working towards **ASSISTing** using metadata

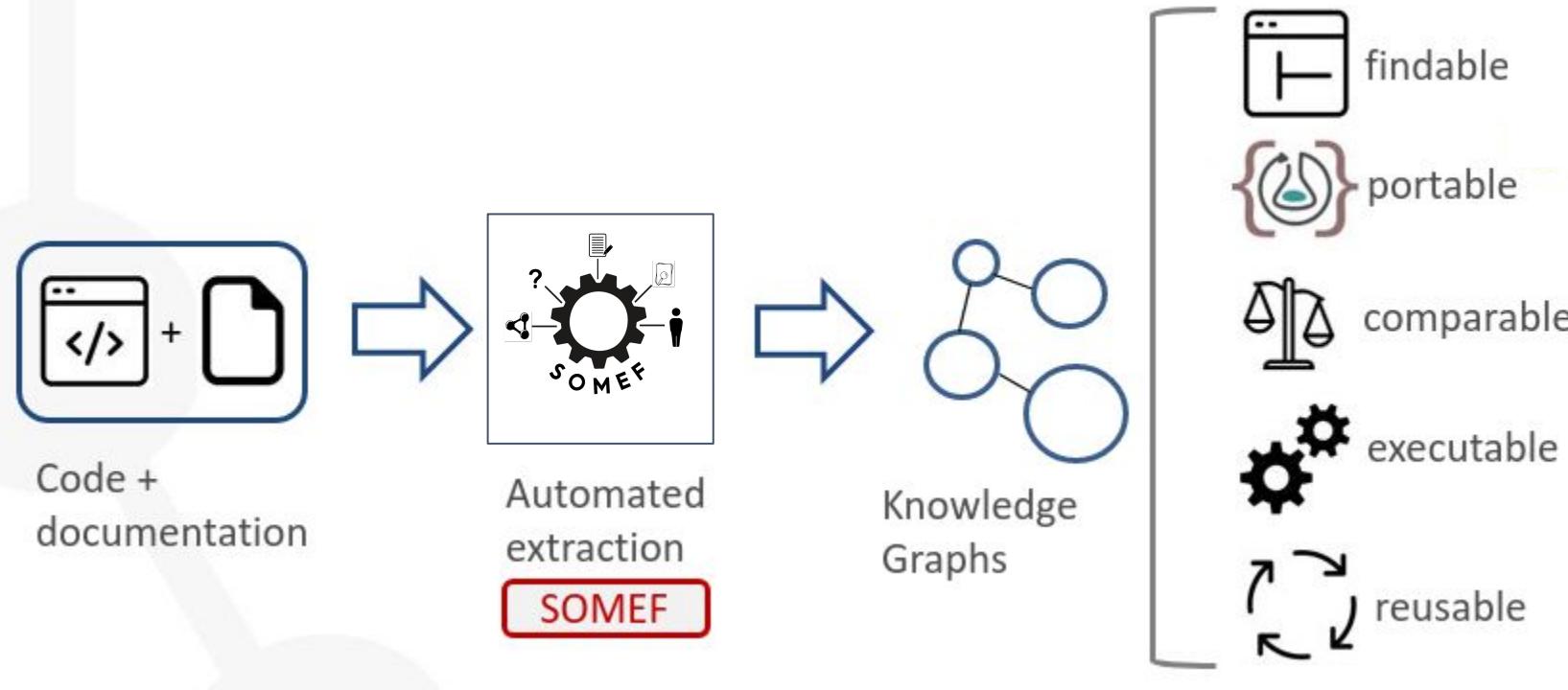
- Highlight the **added benefit** to researchers and developers

# Acknowledgements



Thanks to Yolanda Gil, Varun Ratnakar, Maximiliano Osorio, Hernán Vargas, Deborah Khider, Allen Mao, Aidan Kelley, Haripriya Dharmala, Jiajing Wang, Rosa Filgueira, Pablo Calleja, Oscar Corcho, Laura Camacho, Jhon Toledo, Miguel Angel García, Esteban Gonzalez & all the students at UPM and USC who participated in the initiatives mentioned in this presentation

This work has been supported by the Madrid Government (Comunidad de Madrid-Spain) under the Multiannual Agreement with Universidad Politécnica de Madrid in the line Support for R&D projects for Beatriz Galindo researchers, in the context of the V PRICIT (Regional Programme of Research and Technological Innovation)



Let's create **machine-actionable** software metadata