Open Software in astro and particle physics - the *Open-source Software and Service Repository*

Journées Données Ouvertes IN2P3

December 2024, Thomas Vuillaume

Funded by the European Union

Who am I (to talk about software quality) ?

Astrophysics background
Turned data scientist
Research Engineer at LAPP since 2021
Interests: data analysis, machine learning & software development

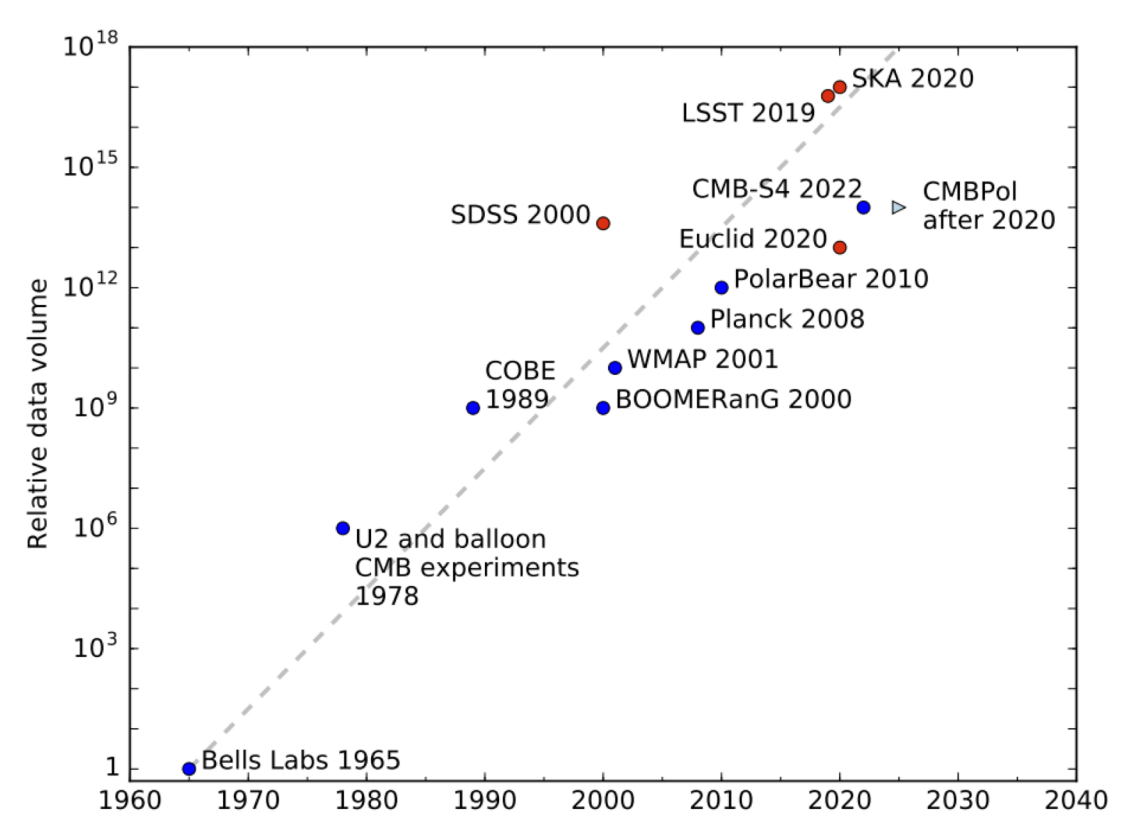
Who am I (to talk about software quality) ?

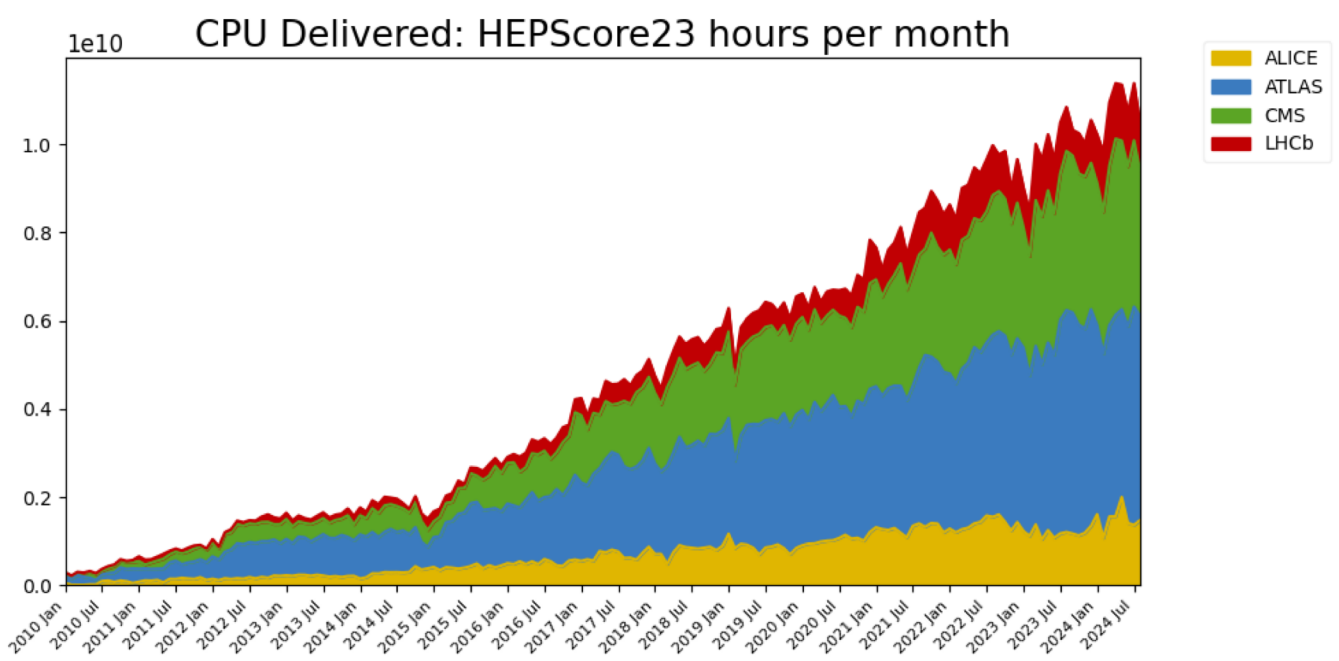
Astrophysics background
Turned data scientist
Research Engineer at LAPP since 2021

I know what bad software is; I write it

Interests: data analysis, machine learning & software development

Context: A new paradigm - data-driven science



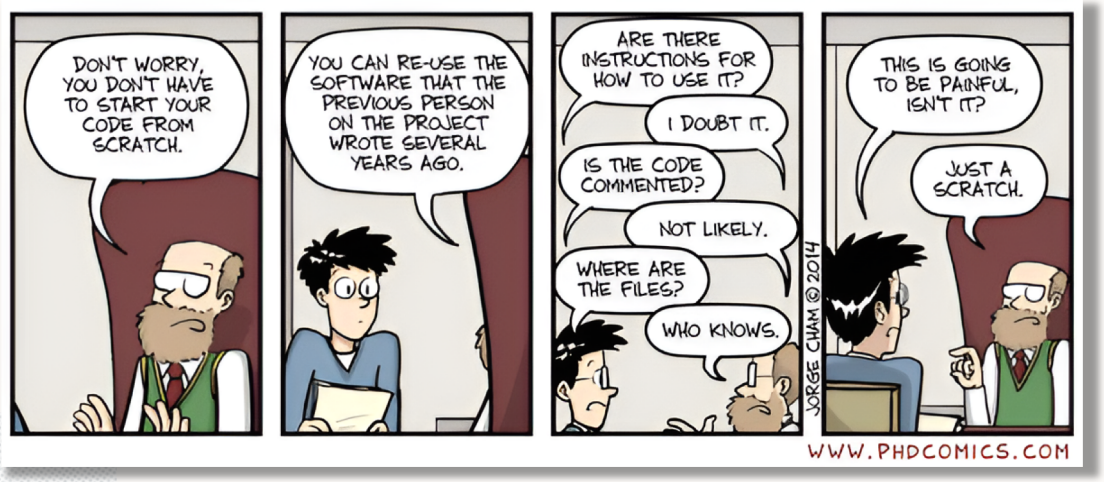


https://wlcg.web.cern.ch/using-wlcg/monitoring-visualisation/monthly-stats

DOI:10.3390/universe2040023

Software is not recognized as first-class output

1. Software is not shared and reused
   - waste of time, energy and resources
   - **reproducbility crisis**



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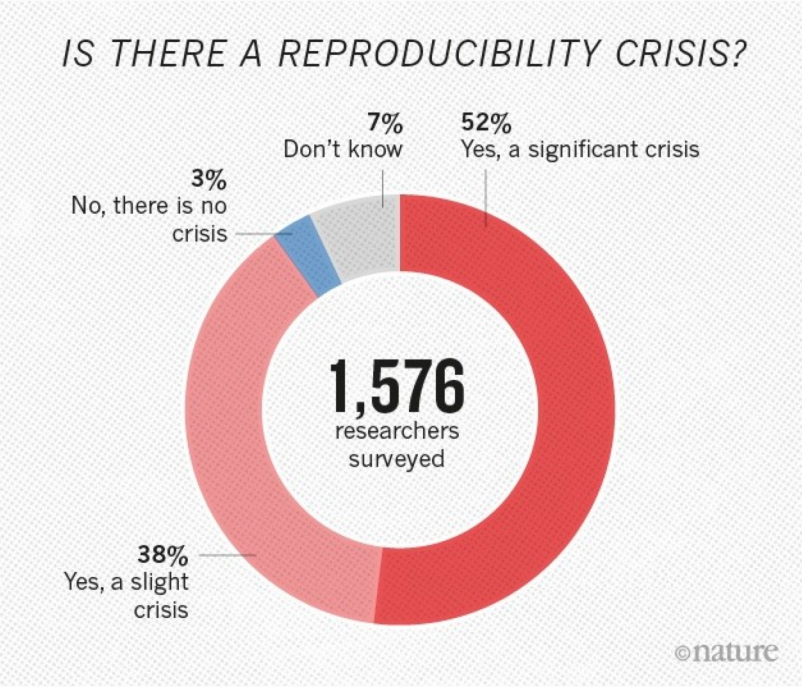
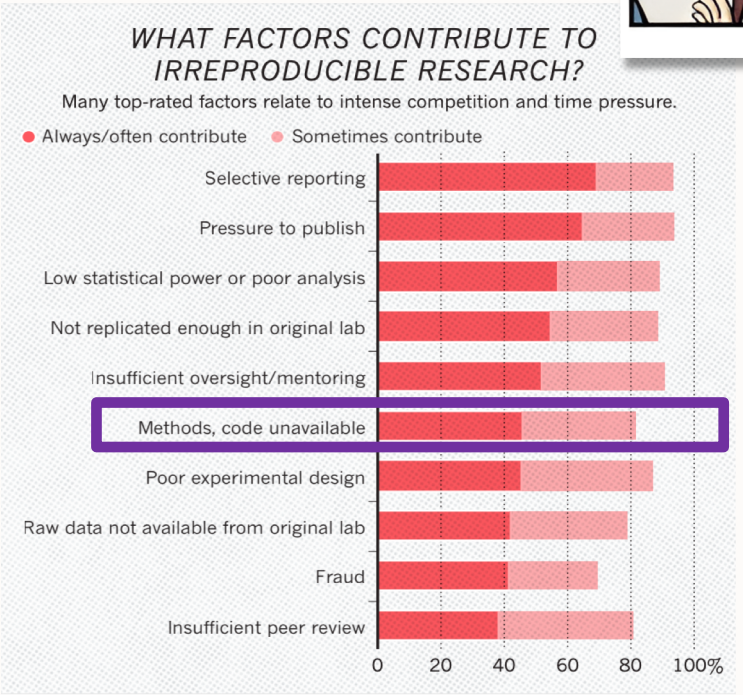




1,500 scientists lift the lid on reproducibility, https://doi.org/10.1038/533452a

Software is not recognized as first-class output

2. Research Software Engineers are not recognized
   - short-term contracts often related to specific projects
   - metrics mismatch (they don’t publish scientific papers)
   - talents loss to industry

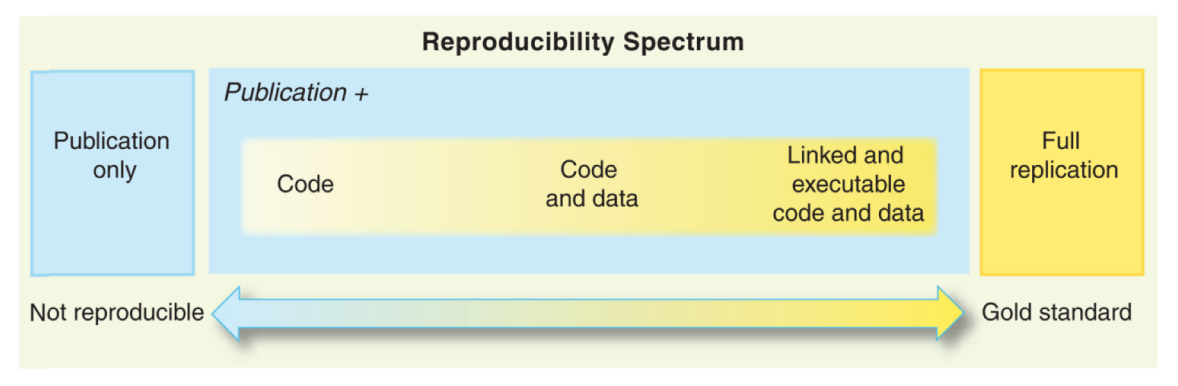
https://www.fz-juelich.de/en/rse/about/what-is-a-research-software-engineer
https://invenia.github.io/blog/2020/07/07/software-engineering/
https://researchcomputing.princeton.edu/news/2021/building-career-path-research-software-engineers
https://www.software.ac.uk/blog/why-research-software-engineers-should-have-permanent-contracts

So, we have two opposing considerations:

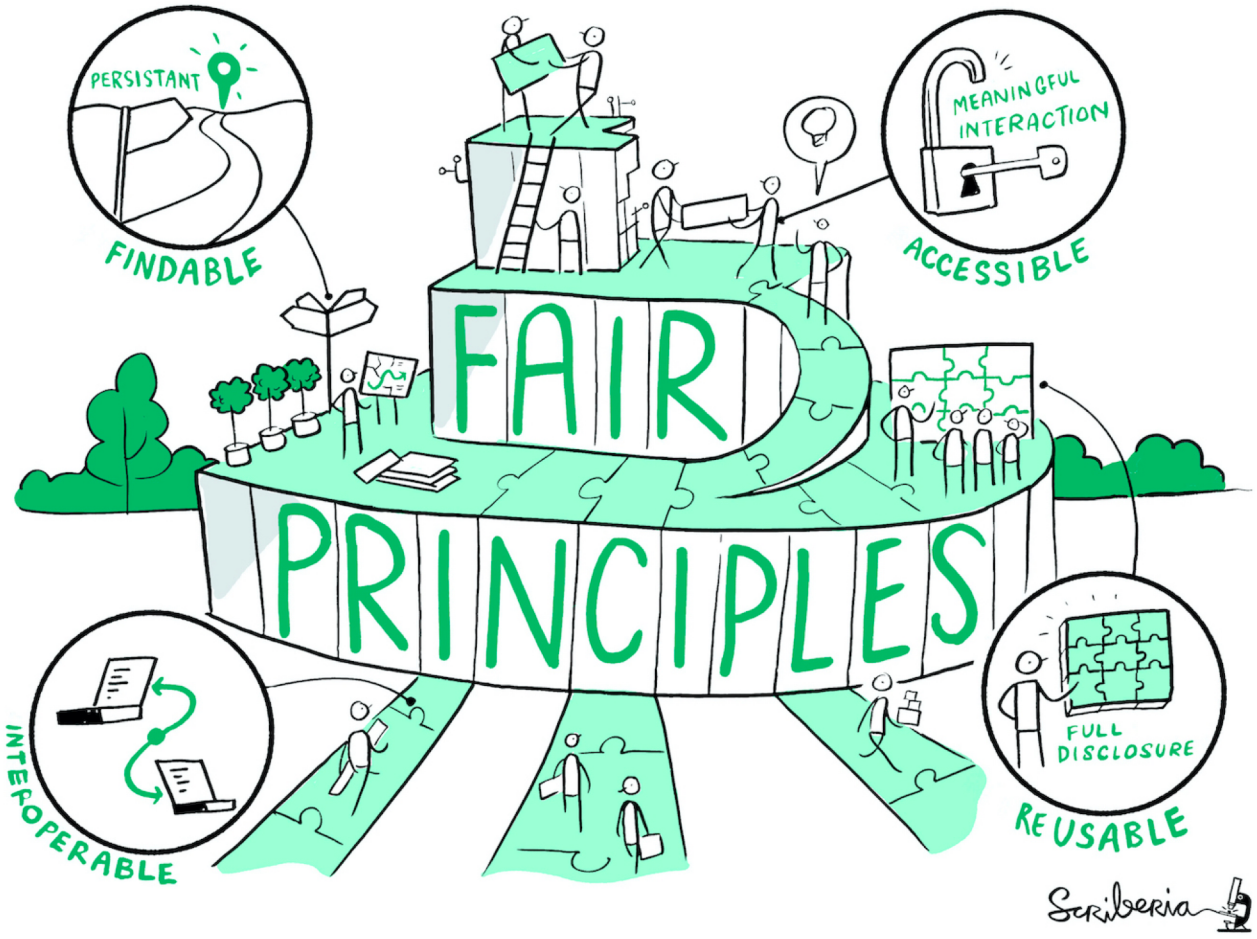
1. Software importance is increasing
2. Software importance is not recognized (enough)

What can we do about it ?

1. Publish Open & FAIR software



- Findable
- Accessible
- Interoperable
- Reusable

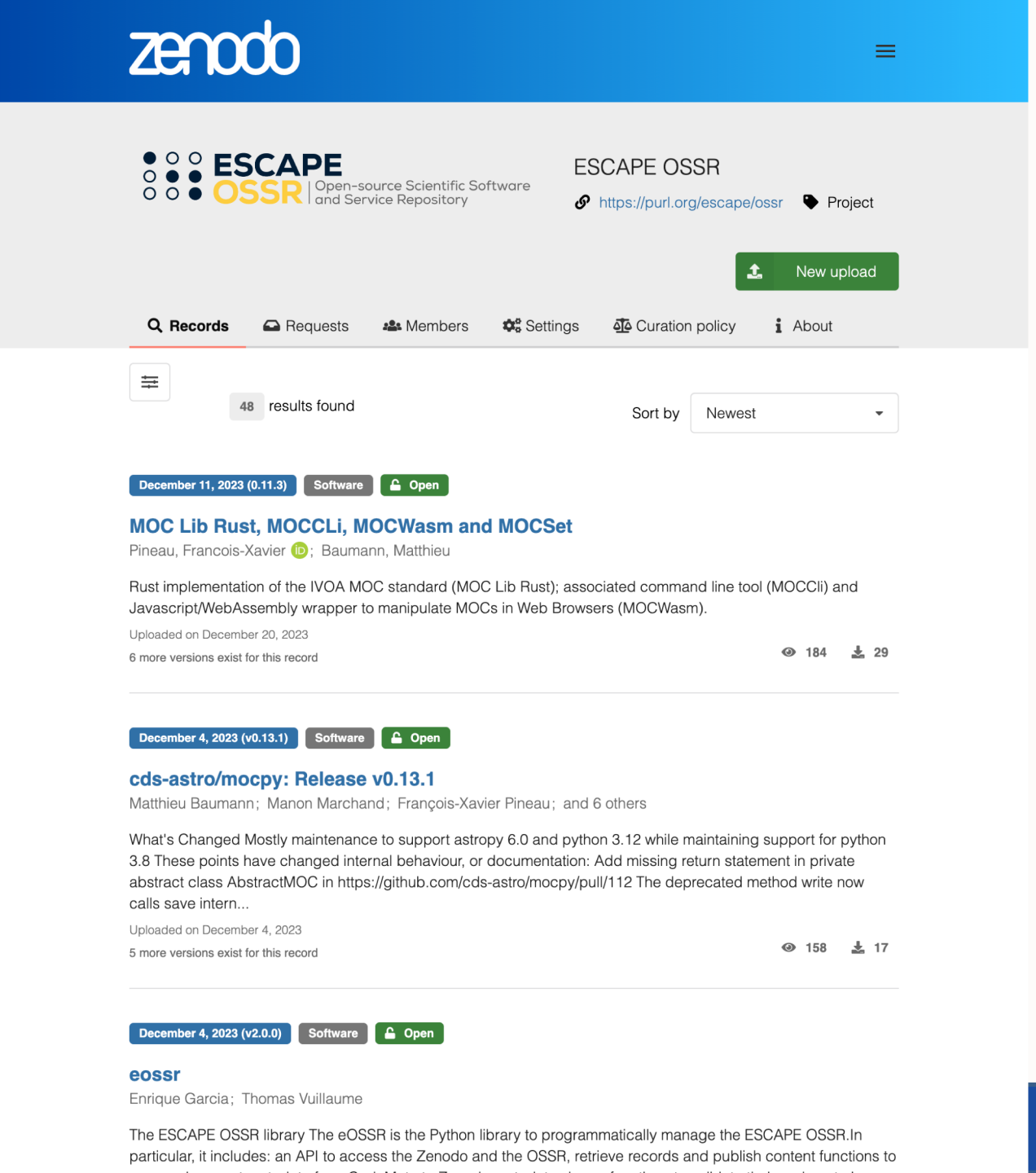


Barker, M., Chue Hong, N.P., Katz, D.S. *et al.* Introducing the FAIR Principles for research software. *Sci Data* 9, 622 (2022). https://doi.org/10.1038/s41597-022-01710-x

The Turing Way Community, & Scriberia. (2023). Illustrations from The Turing Way: Shared under CC-BY 4.0 for reuse. Zenodo. https://doi.org/10.5281/zenodo.8169292

Open-source Software and Service Repository

- A trusted software repository
- Community Centered
  ESCAPE = Particle Physics and Astronomy Cluster in EOSC
- FAIR
- Long-term
- Curated

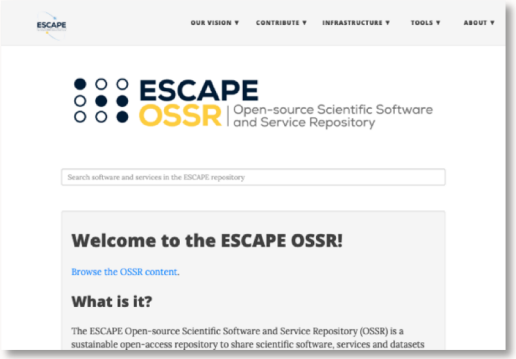


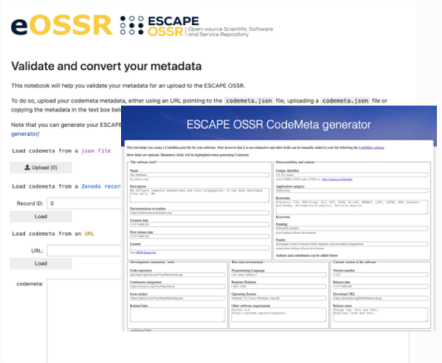
Zenodo as 💙

- FAIR centered
- long-term archive
- software citability (DOI)
- widely accepted and used
- don’t reinvent the ⚙️
- integrates with other services
- community management

❓ *escape2020* community

The OSSR galaxy

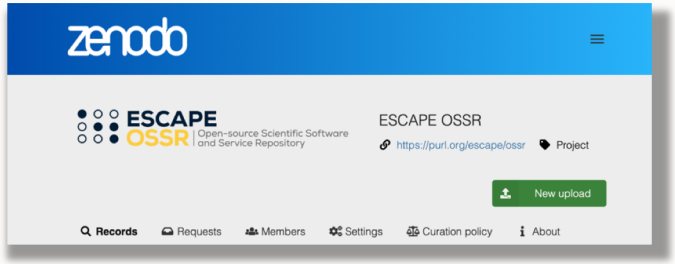




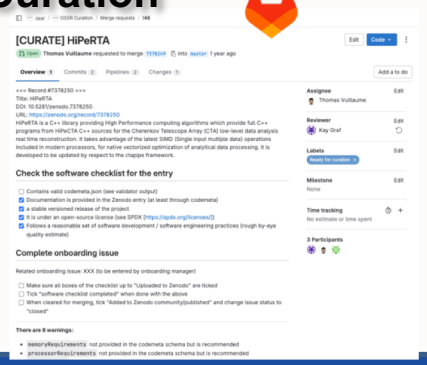
CodeMeta

ESCAPE ESAP | ESFRI Science Analysis Platform

OpenAIRE | EXPLORE



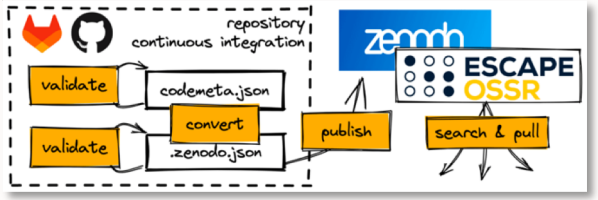
Curation



GitHub

GitLab

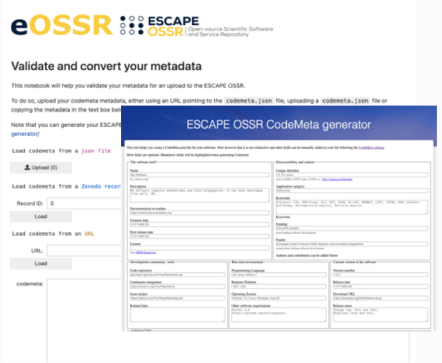
eOSSR



The OSSR galaxy - the software provider path

OSSR website
- Information
- Onboarding process

http://purl.org/escape/ossr



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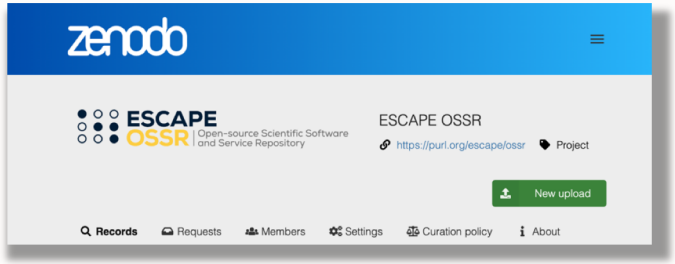

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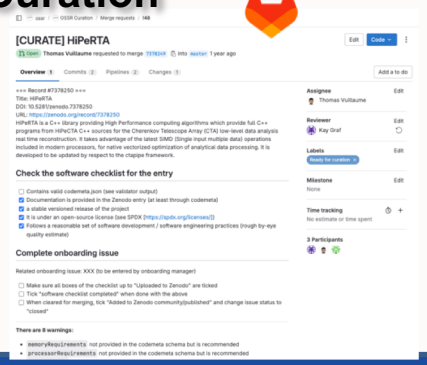

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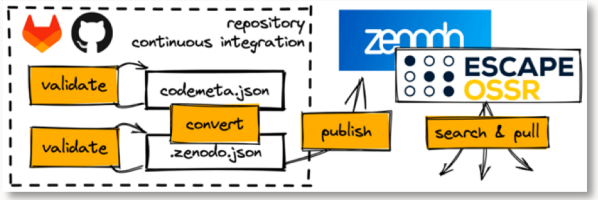

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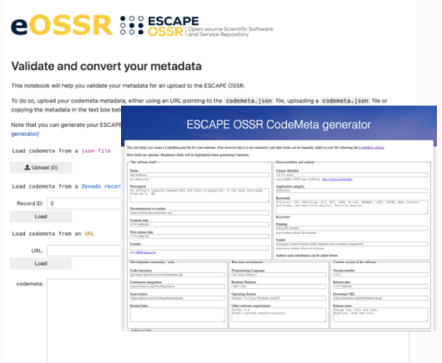

Tools to help RSEs generate the right metadata for their software

CodeMeta

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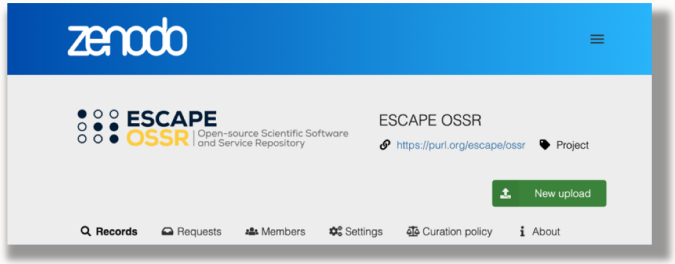

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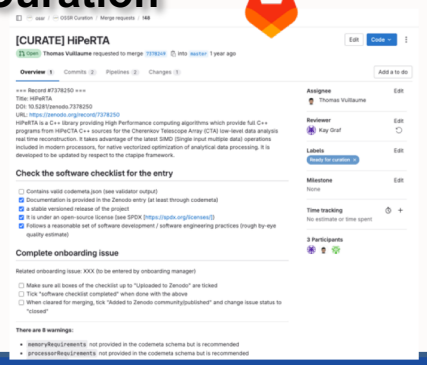

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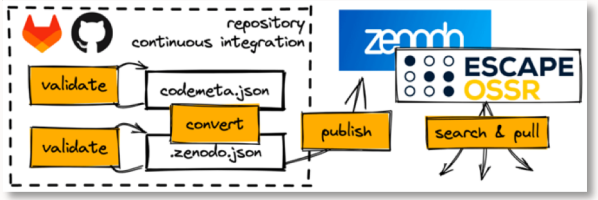

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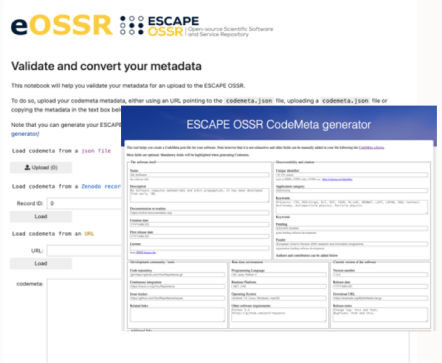

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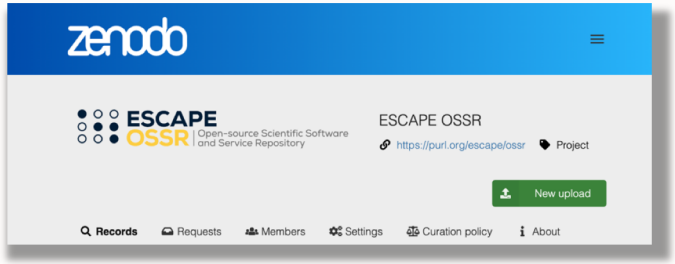

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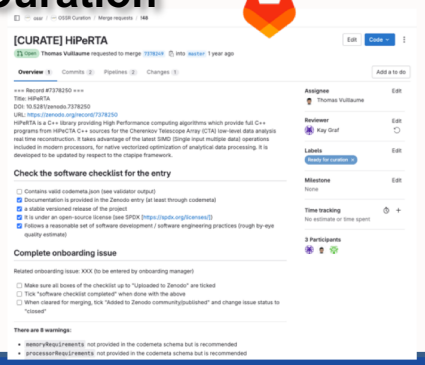
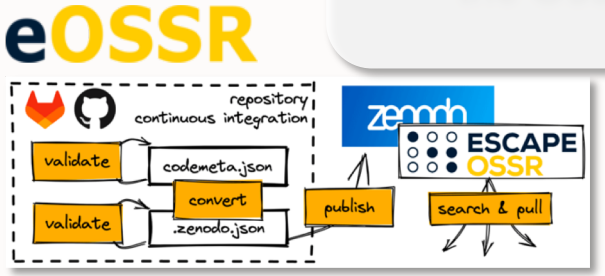


GitHub

GitLab

A python library to communicate with the OSSR



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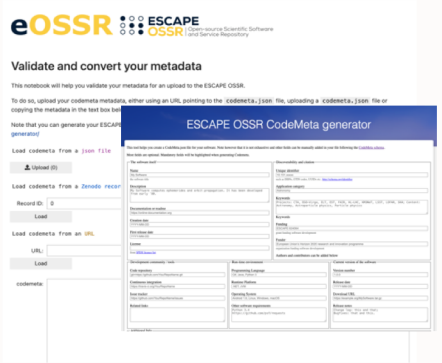

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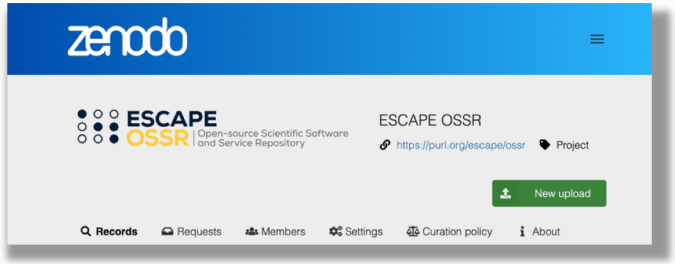

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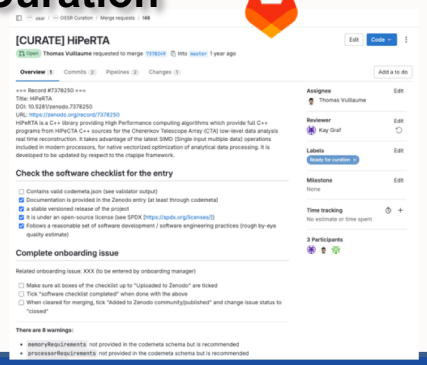

GitHub

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Tools to automatically publish software from GitHub or GitLab

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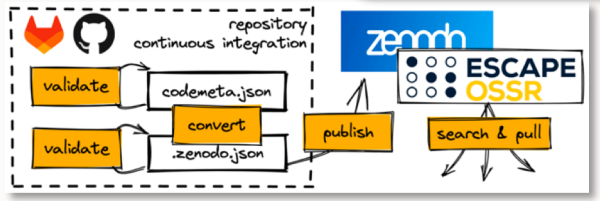

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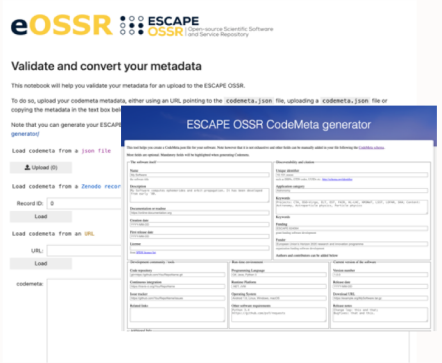

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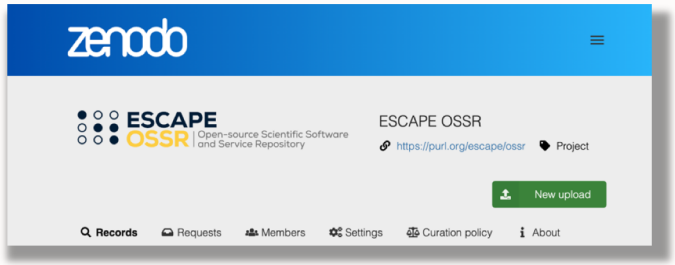
OpenAIRE EXPLORE



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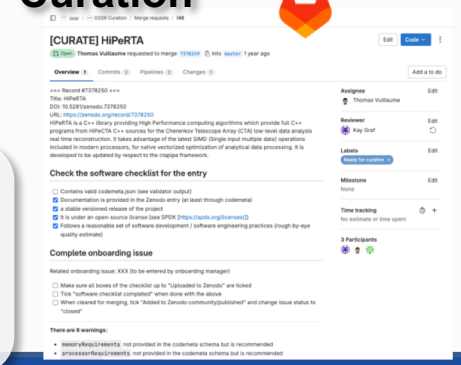


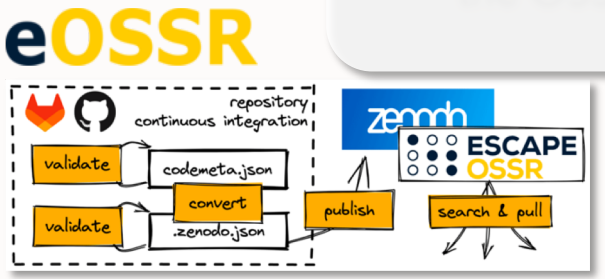
A curation platform to review the requests

OSSR accepted

GitHub

GitLab

Tools to automatically publish software from GitHub or GitLab



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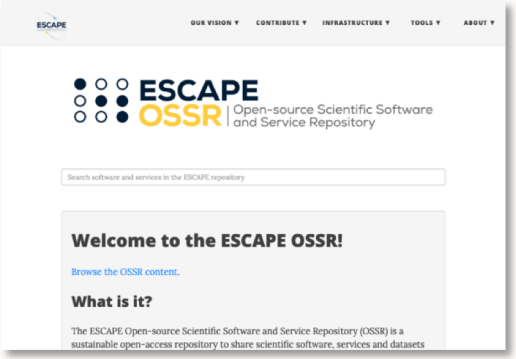
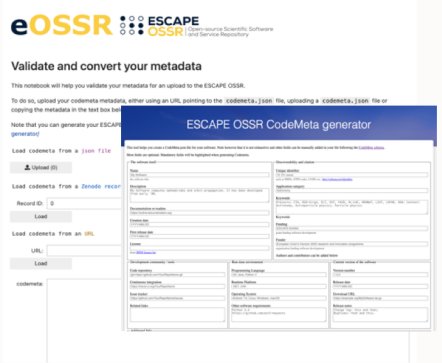
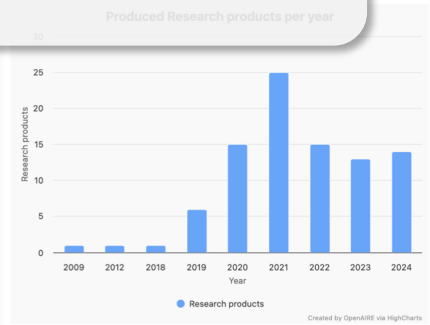




Tools to help RSEs generate the right metadata for their software

CodeMeta

A connection to other services



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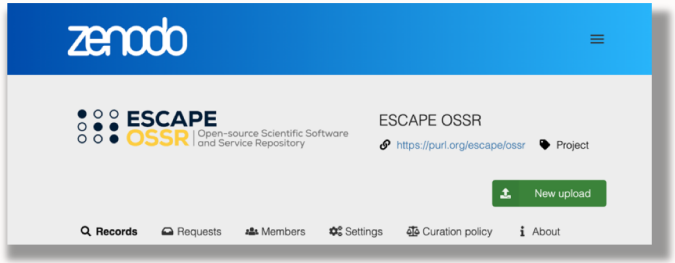

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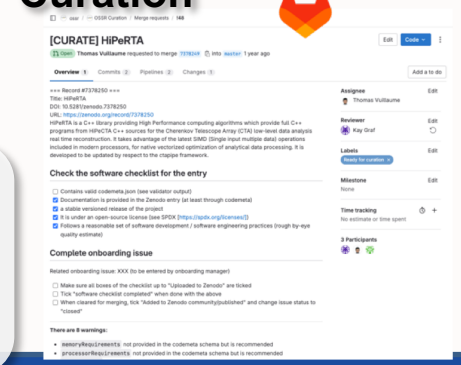

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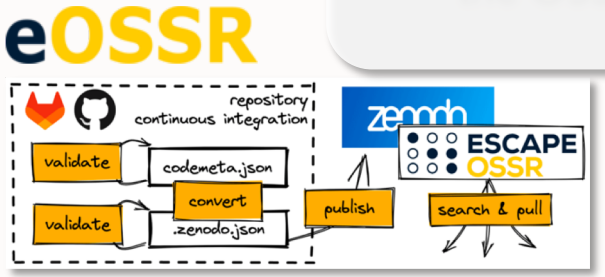
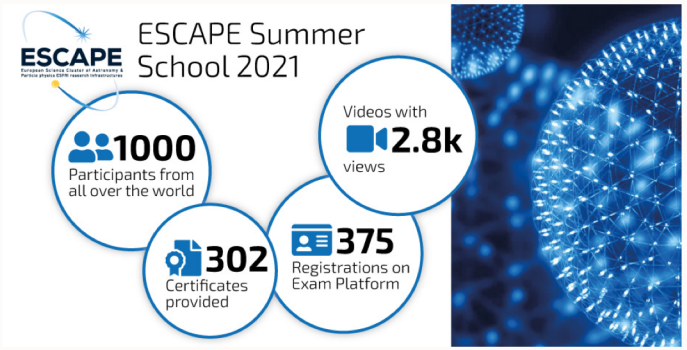


2. Improve software quality

- Programming schools at LAPP since 2017



Code development for physicists:

- Coding environment and good code practices
- Version control and collaborative development
- Debugging and profiling
- Python packaging
- Scientific libraries for data science and analysis
- Machine learning

All courses open-source, recorded and available online DOI 10.5281/zenodo.5093909

- HPC
- Heteregeneous architectures
- Code optimisation
- 12 satellite sites

https://indico.in2p3.fr/event/14227/
https://indico.in2p3.fr/event/16864/
https://indico.in2p3.fr/event/18333/

https://escape2020.github.io/school2021/
https://escape2020.github.io/school2022/

https://indico.in2p3.fr/event/30939/

2. Improve software quality

EVERSE

Paving the way towards a

European Virtual Institute for Research Software Excellence

Pilots & Drivers

Environmental Sciences: *Integration of Science Cluster ENVRI through ENVRI-HUB*

- Integrate EVERSE framework into the ENVRI-HUB Knowledge base and Virtual Research Environment
- Apply to the development of the Essential Climate Variable computing program and cloud workflows

Life Sciences: *Integration of Science Cluster EOSC-Life through ELIXIR*

- Make RO-Crate actionable by incorporating the five safes concept into WfExS for secure and federated workflow orchestration
- Use of community-led standards for materialising research software packaged using container technologies and mobilising encrypted data whenever needed

Astronomy and particle physics: *Integration of Science Cluster ESCAPE through the Dark Matter Test Science Project*

- ML for scientific data compression (standalone code, python)
- A Common Tracking Software
- Choose an ATLAS trigger algorithm as an option for the collaboration

Proton and neutron science: *Integration of Science Cluster PaNOSC through LEAPS/LENS*
Transition software to high performance computing (HPC) and heterogeneous computing architectures

Social sciences: *Integration of Science Cluster SSHOC*
Develop a multilanguage textual analysis pipeline of tools that use a combination of open source tools and own code to create an integrated SotA tool capable of deploying locally or as a service

Paving the way towards a **E**uropean **V**irtual Institut**e** for **R**esearch **S**oftware **E**xcellence

EVERSE aims to create a framework for research software and code excellence, collaboratively designed and championed by the research communities, in pursuit of building a European network of Research Software Quality and setting the foundations of a future Virtual Institute for Research Software Excellence

ensure **research software curation, quality, preservation and adoption of best practices**, by the Communities, for the Communities, build on collaboration with the five EOSC Science Clusters

adopt a **three-tier model for research software**, i.e., analysis code, prototype tools and research software infrastructure, which captures the varying complexity of research software and its development, and can be used as a basis for research software excellence

credit and recognition for both developers and software are essential components of our strategy to promote sustainable software practices

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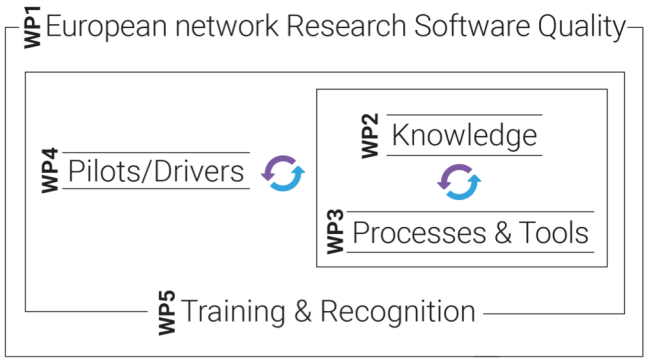
Mar/2024 → Feb/2027 (36 months)

15 Beneficiaries, 1 Associated partner & 2 Affiliated entities

Coordinated by CERTH

Project objectives



Provide a **framework** that will ensure appropriate **recognition, reward, and career development** for researchers and RSEs who implement research software and code quality assurance practices and policies

Leverage existing tools and resources to support the evaluation, verification and improvement of research software and code quality, based on **existing practices and standards** across research communities represented by the five EOSC Science Clusters.

Establish a **sustainable and collaborative ecosystem of stakeholders** across the research communities associated with the five **EOSC Science Clusters** to ensure research software and code quality assurance and support the advancement of reliable and reproducible research.

Build a **collaborative, community-led structure** for evaluating, verifying, and improving the quality of research software and code, by **actively involving** researchers, software developers, and other stakeholders in the research community.

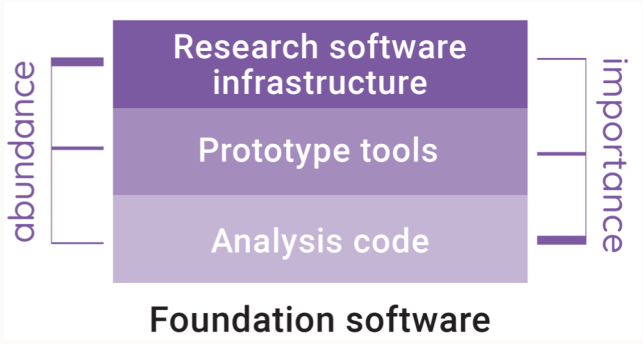
eosc | EVERSE

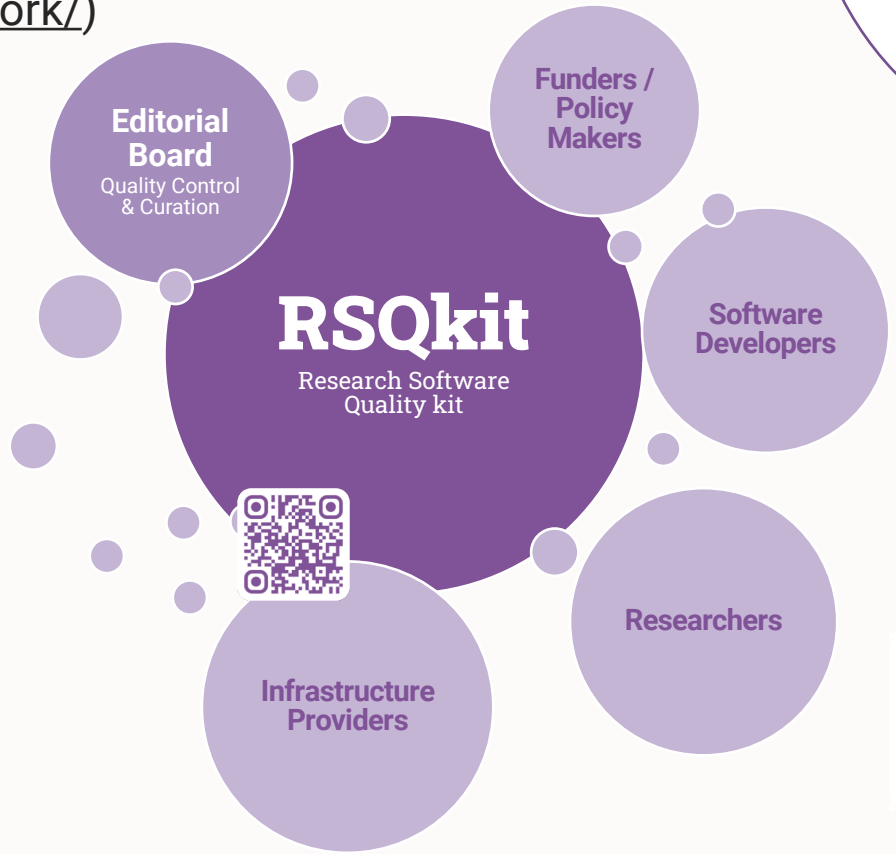
Establishing a Community

How to contribute to, and engage with EVERSE

Elements of EVERSE

- The Network (https://everse.software/network/)
- RSQkit (https://everse.software/RSQKit/)
- Software Reference model
- Training
- Recognition framework



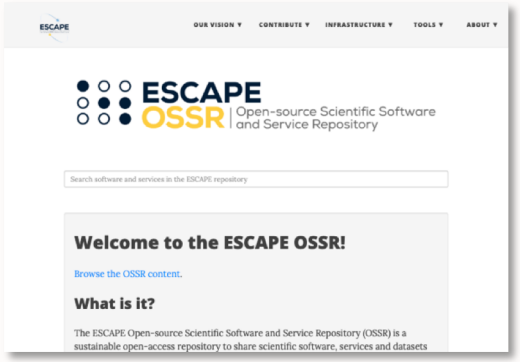


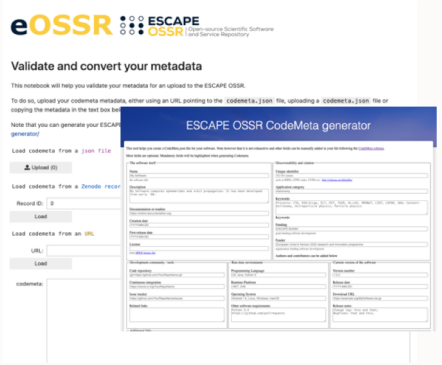
Join Us

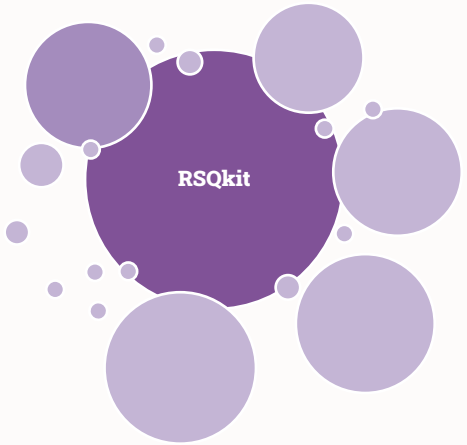
Any individual or organization that agrees with our vision statement is welcome to join the network

eosc | EVERSE

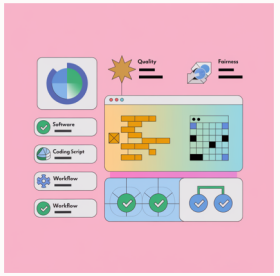
Recognition for software providers







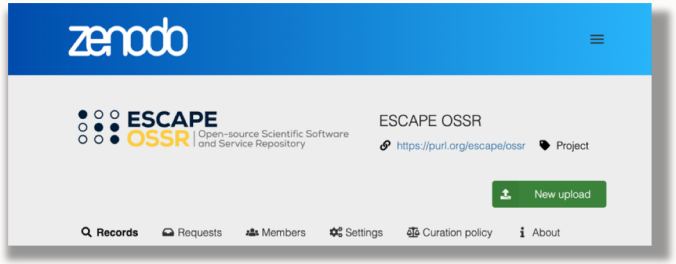
CodeMeta



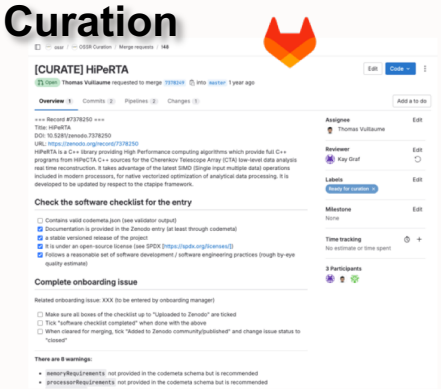
Dashboards to measure globally the software quality and its evolution

ESCAPE ESAP | ESFRI Science Analysis Platform

OpenAIRE | EXPLORE



Curation

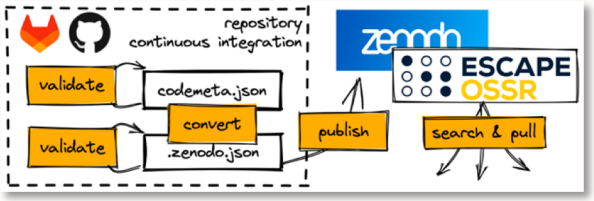


Integrated pipelines to measure and improve software quality

GitHub

GitLab

eOSSR



CONCLUSION

- OSSR establishes a community-based approach to publish **curated** software
- With EVERSE, it provides a **framework** to improve **software quality and recognition**
- **Contribute** your software now!

http://purl.org/escape/ossr

Vuillaume T, Al-Turany M, Füßling M et al. The ESCAPE Open-source Software and Service Repository, Open Res Europe 2023, https://doi.org/10.12688/openreseurope.15692.2

BACK-UP SLIDES

Software metadata

Software metadata are the implementation of FAIR principles

- Findable, Interoperable
- They should be part of the software and not defined or retained by an external service

OSSR uses CodeMeta

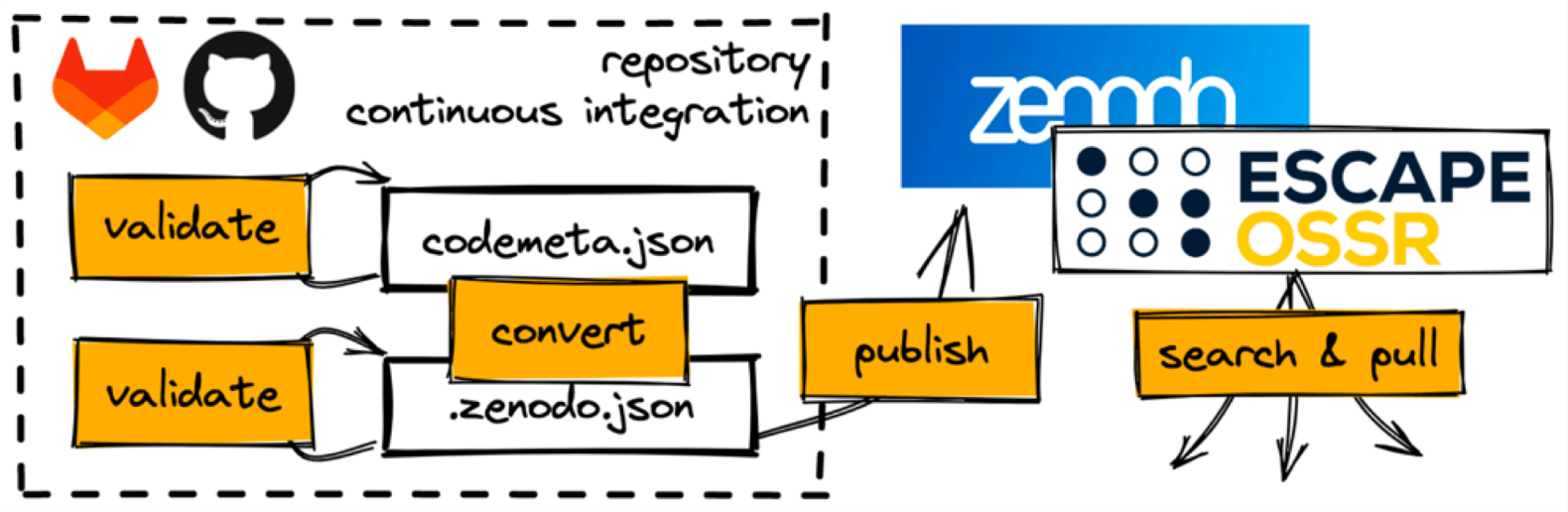
- Universal metadata schema to describe software
- Not limited or linked to a specific service
- Increasing adoption
- Integration with other services

➢ A ***codemeta.json*** file with a number of required keys is mandatory to submit software to the OSSR. The file comes with the source code, at the root of the repository.

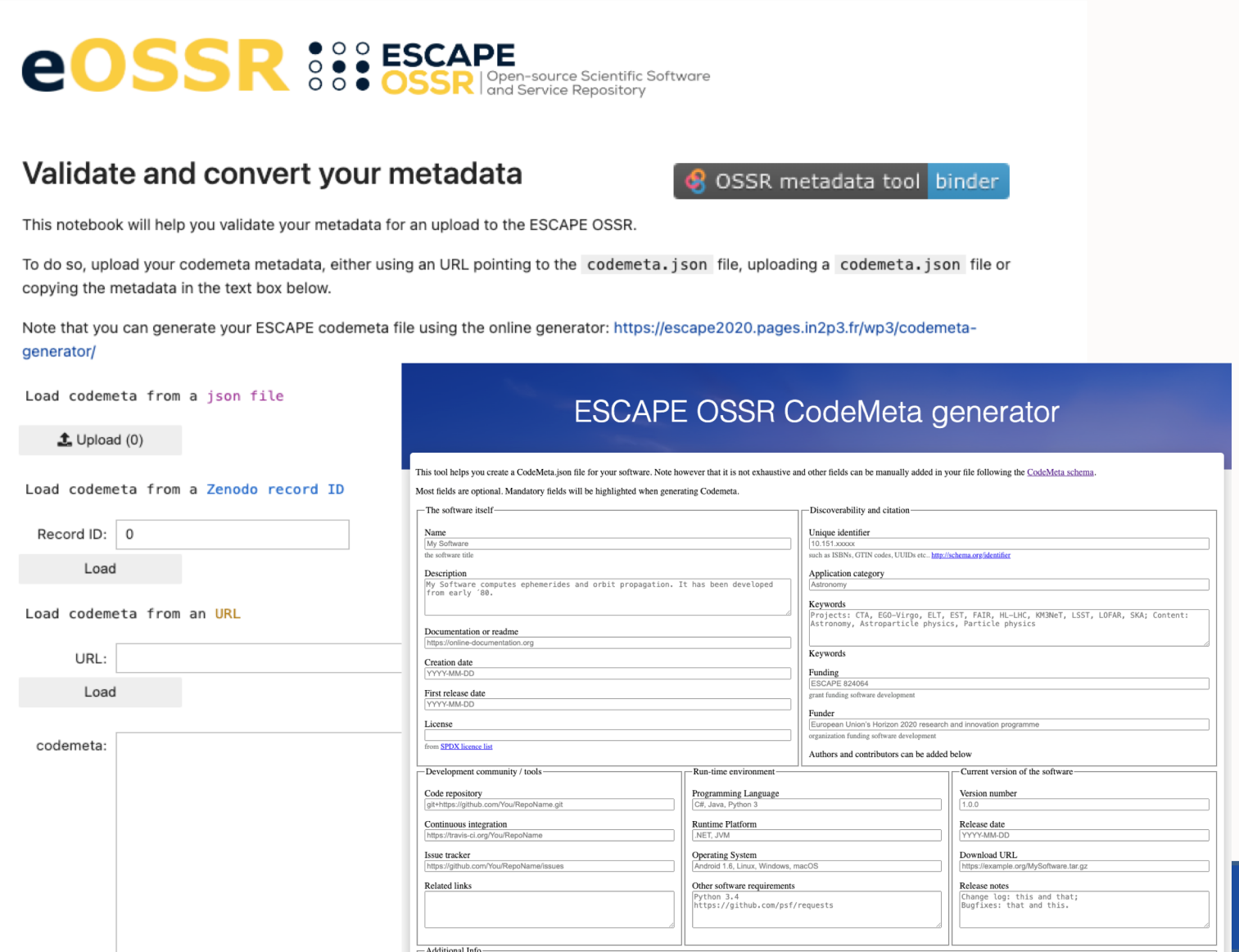
eOSSR

DOI 10.5281/zenodo.5524912 License MIT gitlab eossr

- The eOSSR is the OSSR Python library
  - Connects to Zenodo API to handle:
    - records: search, download, upload, publish, submit…
    - communities: list records, list and handle submissions
  - Handles OSSR metadata:
    - Defines required one
    - Converts from CodeMeta to Zenodo schema
    - Validates ***codemeta.json*** file



Online tools: metadata generator, converter & validator



- Help software developers to provide valid and complete metadata
- Get that first working version of ***codemeta.json***
- Test things out

Gitlab to Zenodo

GitLab → zenodo

- Zenodo has an efficient GitHub integration, but no GitLab integration
- Many ESFRIs use their own Gitlab instance

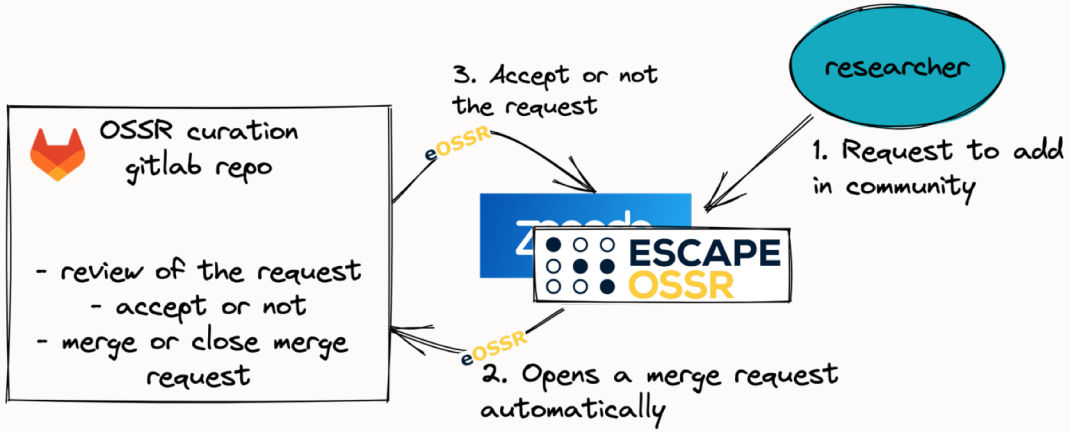
➢ We provide a simple gitlab-ci snippet
  - to publish your software to Zenodo / OSSR, e.g. when making a release in gitlab
  - using metadata provided in ***codemeta.json***

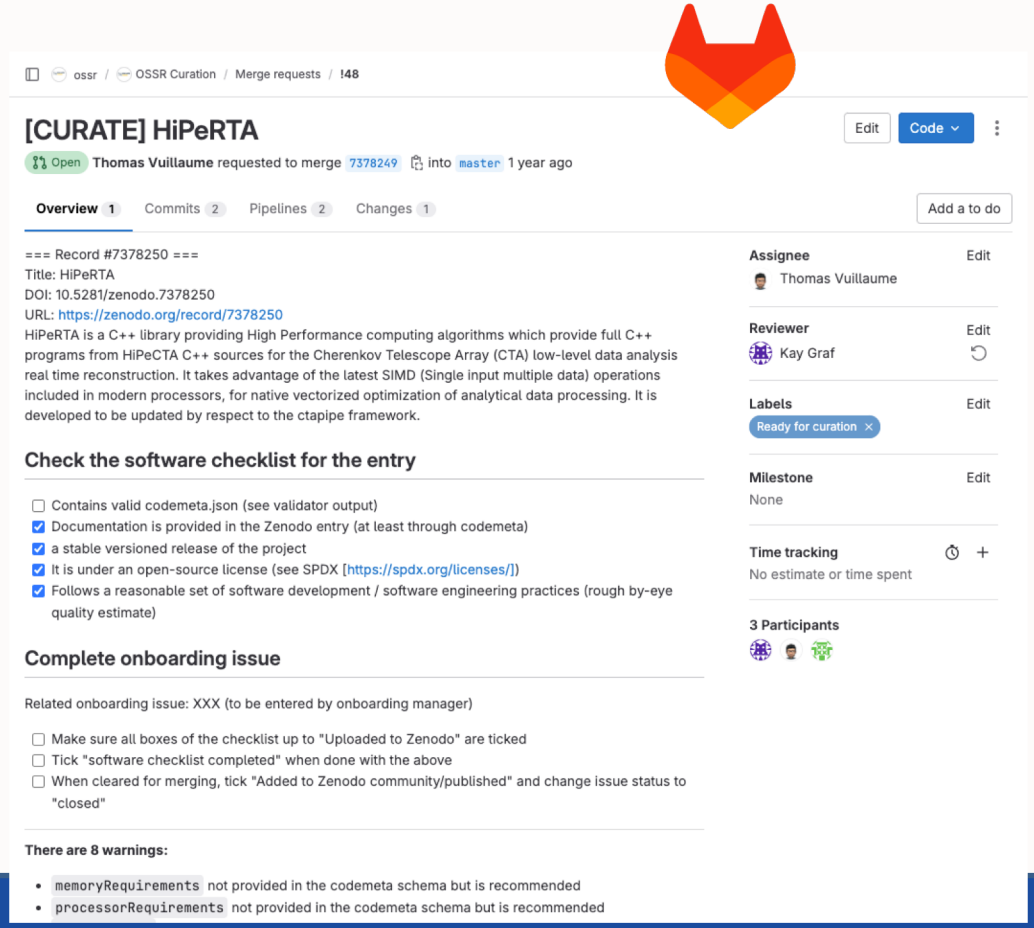
Software curation

- The OSSR is a curated software repository
  - implementation of the FAIR principles
  - good code practices
  - software quality
  - do not review scientific results ⇒ science paper

- Curation happens in a dedicated gitlab repository
  - completely open
  - automated checks
  - discussion between reviewers and providers

- Curation provides
  - Trust in the repository and provided content
  - Recognition for software providers

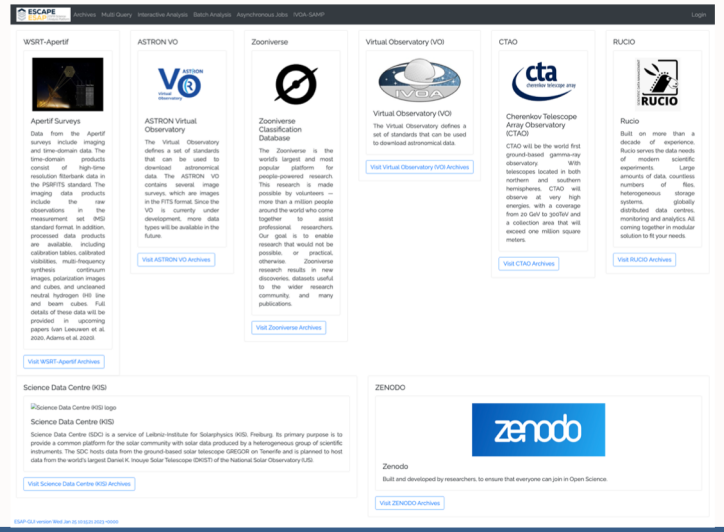




Integration with other services

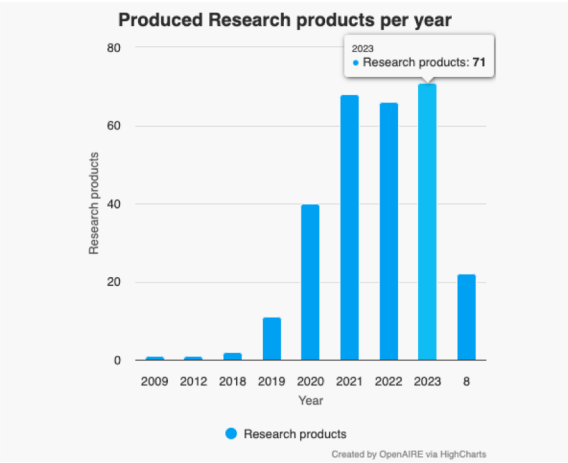
ESCAPE ESAP | ESFRI Science Analysis Platform

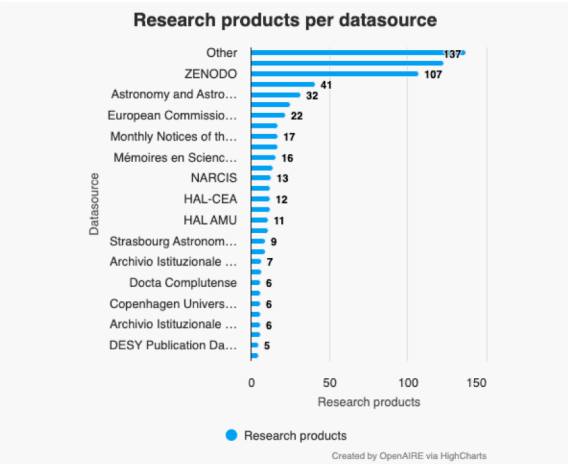
- connects to other services
- analyze data
- search and pull software from the OSSR



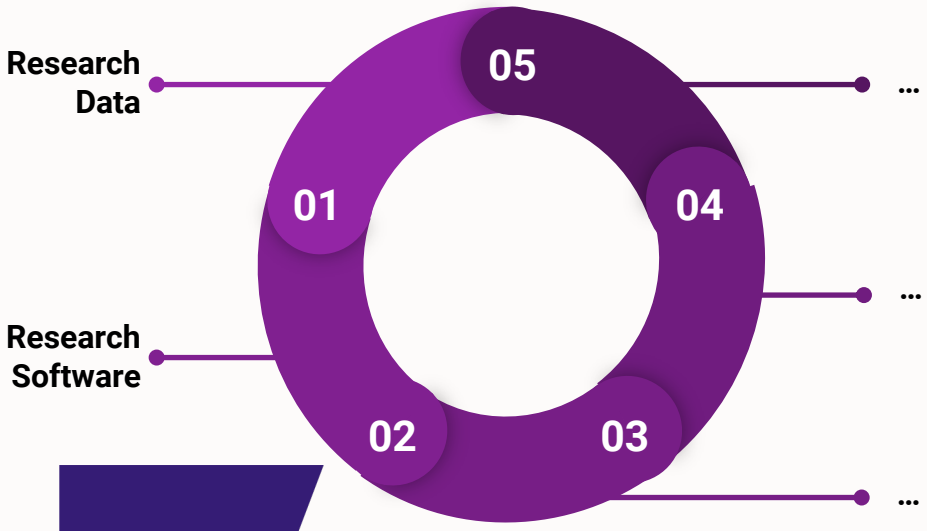
OpenAIRE | EXPLORE

- EOSC integration
- Provides integrated statistics
- Connects with other data sources





Research Software as a first class citizen for the scientific endeavours



abundance

1. **Research software infrastructure**
   It involves research software that captures more broadly accepted and used ideas, methods and models for use in research, and warrants close researcher involvement in their development.
2. **Prototype tools**
   It refers to research software that demonstrates a new idea, method or model for use by others outside the project within which it originated, often as a substantive intellectual contribution in its own right and often in the form of a proof of concept.
3. **Analysis code**
   It includes research software that captures computational research processes and methodology, and often occurs in the context of simulation, data generation, preparation, analysis and visualisation.

Importance

Foundational Software

Not all software has the same level of importance