

# **Better Software, Better Science**

#### LAPP contribution to Software in EOSC

September 2024, Journées Informatiques IN2P3 Thomas Vuillaume







JI IN2P3, 19/09/2024

**Thomas Vuillaume** 

## 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



## 1. New paradigm: data-driven science



DOI:10.3390/universe2040023



# 2. Software is not recognized as first-class output



JI IN2P3, 19/09/2024



# 2. Software is not recognized as first-class output

- 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:

Software importance is increasing
 Software importance is not recognized (enough)

What can we do about it ?



# 1. Publish Open & FAIR software

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



- 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). <u>https://doi.org/10.1038/s41597-022-01710-x</u>





## **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

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Pineau, Francois-Xavier 🝺; Baumann, Matthieu

Rust implementation of the IVOA MOC standard (MOC Lib Rust); associated command line tool (MOCCli) and Javascript/WebAssembly wrapper to manipulate MOCs in Web Browsers (MOCWasm).

Uploaded on December 20, 2023 6 more versions exist for this record

③ 184 4 29

#### December 4, 2023 (v0.13.1) Software 🕒 Open

#### cds-astro/mocpy: Release v0.13.1

Matthieu Baumann; Manon Marchand; François-Xavier Pineau; and 6 others

What's Changed Mostly maintenance to support astropy 6.0 and python 3.12 while maintaining support for python 3.8 These points have changed internal behaviour, or documentation: Add missing return statement in private abstract class AbstractMOC in https://github.com/cds-astro/mocpy/pull/112 The deprecated method write now calls save intern...

Uploaded on December 4, 2023 5 more versions exist for this record



#### eossr

Enrique Garcia; Thomas Vuillaume

The ESCAPE OSSR library The eOSSR is the Python library to programmatically manage the ESCAPE OSSR.In particular, it includes: an API to access the Zenodo and the OSSR, retrieve records and publish content functions to



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

## → *escape2020* community



**OSSR** website

Information

Onboarding process http://purl.org/escape/ossr

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repository continuous integration

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search & pull





#### OSSR website

- Information
- Onboarding process <u>http://purl.org/escape/ossr</u>

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Tools to help RSEs generate the right metadata for their software













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Tools to help RSEs generate the right metadata for their software







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Tools to help RSEs generate the right metadata for their software







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repository, continuous integration

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Tools to help RSEs generate the right metadata for their software





A curation platform to review the requests

publish software from GitHub or GitLab

GitLab

A python library to communicate with the OSSR

Zemr

• • • • **ESCAPE** • • • **OSSR** 

search & pul





<u>http://purl.org/escape/oss</u>r

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

## 2. Improve software quality

Programming schools at LAPP since 2017



SCAPE

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/

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# EVERSE

Paving the way towards a European Virtual Institute for Research Software Excellence



Funded by the European Union







# **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



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**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 European Virtual Institute for Research Software Excellence

**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

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.



# WP1: Network

• Establish the EVERSE Network of Research Software Quality (T1.1)

- A meeting point for a Community of Practice for software quality
  - Open to individuals and organisations internationally
- Will be an EOSC Expert Group on software
- Help to shape best practices and get help and advice from like minded partners
- · Will host seminars, webinars and other events to promote and recognise software quality
- The network is forming now, so we are very interested to work with any *early adopters*
- Reaching out to **Science Communities** (T1.2)
  - Showing the benefits of the EVERSE network and matching specific domain needs
  - Organisation of events such as hackathons to promote best practive and network involvement
- Links to European, international organisations and industry (T1.3)
  - Benefit from and reinforce existing policies and practice regarding software quality
  - Align and co-develop shared solutions and host common events



# WP2: Best practices

Community-led best practices for developing high-quality research software

Each research community has its own techniques for computing-based research. Work package 2 works towards assessing all these approaches and developing common grounds for best practices applicable to all developers. The Research Software Quality kit will be a knowledge hub that collects existing expertise while ensuring improvement.

The curated best practices are gathered across four pillars: technical quality, FAIR principles, Openness and Software Sustainability. They are used to find a common framework and act as measurables for indicators of software quality. Woven into the RSQkit, these practices will be incorporated into the future Virtual Institute driven by WP1.

CURRENT ACTION: conducting survey among communities => landscaping of best practices (T2.1)

**UPCOMING: consolidate/curate** best practices in RSQkit





## WP3: Tools and services for software quality and FAIRness

## **O3.1 (on-going):** To establish a **technology watch** identifying and **gathering tools and services** targeting scientific software, code, and workflows **quality and FAIRness**

O3.2 (2<sup>nd</sup> phase): To assist the Science Clusters in measuring and improving software, code, and workflows quality and FAIRness globally by combining existing tools and services into common frameworks



Technology Watch for tools and services for softwarequality







**Dashboards** to measure globally the software quality and its evolution



# WP5: Capacity Building and Recognition

- Collect, curate and enhance training resources
  - Align training material with best practices in the science clusters
  - Conduct a landscape analysis of existing material and fill the gaps as needed
  - Make training resources available via tools developed by EVERSE partners (e.g. <u>TeSS</u>) and connect those to the RSQKit
- Build a framework for recognition of trainers and RSEs
  - Start from tools developed within EVERSE (e.g. <u>Bip!Scholar</u>, <u>Apicuron</u>) and extend as needed
  - Align with EOSC "Research careers, recognition and credit" task force
- Establish long-term training activities
  - Incorporate training into existing curricula and make those available (e.g. via a "monthly discovery series")
  - Develop a network of trainers and establish a process to keep them engaged
  - Provide feedback to universities and schools on needed training for research software engineering

# What's next?

- Improve OSSR with EVERSE outcomes
  - improve curation and automated code review
  - provide high-level software quality metrics to developers, reviewers, instances
  - better recognition of software developers
- Extend or bring OSSR framework to other communities
- Continue training scientists (not only in physics) to modern software development
- Think about LLMs and code assistants impact on software development in research
  - Software development will drastically change in the coming years months
  - Software quality ? Up or down ?
  - Code generation ? Code reviews ?



# CONCLUSION

- LAPP is working to improve research software quality and to promote its importance to instances as well as to individuals that produce it.
- We are involved in several EU projects to reach that goal.
  - ASTERICS (2016-2019)
  - ESCAPE (2019-...) <u>https://projectescape.eu/</u>
  - EVERSE (2024-...) <u>https://everse.software/</u>
  - OSCARS (2024-2027) <u>https://oscars-project.eu/</u>
  - CodeMetaSoft (2025-2027)
- Contact me if you are interested or want to participate.



# **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.









- 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



#### Validate and convert your metadata

OSSR metadata tool binder

This notebook will help you validate your metadata for an upload to the ESCAPE OSSR.

To do so, upload your codemeta metadata, either using an URL pointing to the codemeta.json file, uploading a codemeta.json file or copying the metadata in the text box below.

Note that you can generate your ESCAPE codemeta file using the online generator: https://escape2020.pages.in2p3.fr/wp3/codemetagenerator/

Load codemeta from a json file

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ESCAPE OSSR	CodeMeta	generator
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Projects: CTA, EGO-Virgo, ELT, EST, FAIR, HL-LHC, KM3NeT, LSST, LOFAR, SKA; Content Astronomy. Astroparticle physics. Particle physics

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Record ID: 0		Name		Unique identifier	
		My Software		10.151.xxxxx	
Load		the software title		such as ISBNs, GTIN codes, UUIDs etc., http://schema.org/identifier	
		Description		Application category	
		My Software computes ephemerides and orbit propagation. It has been developed		Astronomy	
		Trom early 80.		V	
Load codemeta from an URL				Projects: CTA EGO_Virgo_ELT_EST_EATR_HI_IHC_KM2NoT_LSST	
				Astronomy, Astroparticle physics, Particle physics	
		Documentation or readme			
		https://online-documentation.org			
URL:		Counting data		Keywords	
		VVVVAM DD		Funding	
Load		TTTT-MM-DD		ESCAPE 824064	
		First release date		grant funding software development	
		YYYY-MM-DD			
				Funder	
		License		European Union's Horizon 2020 research and innovation programme	
codemeta:				organization funding software development	
		from SPDX licence list		Authors and contributors can be added below	
		Development community / tools	Run-time environment		Current version of the software
		Code repository	Programming Language		Version number
		ait+https://aithub.com/You/RepoName.git	C# Java. Python 3		1.0.0
		8	[		
		Continuous integration	Runtime Platform		Release date
		https://travis-ci.org/You/RepoName	.NET, JVM		YYYY-MM-DD
		Issue tracker	Operating System		Download URL
		https://github.com/You/RepoName/issues	Android 1.6, Linux, Windows, n	nacOS	https://example.org/MySoftware.tar.gz
		Palatad links	Other software requirements		Palassa notas
		INCLAUCU HIINS	Python 3.4		Change log: this and that:
			https://github.com/psf/	requests	Bugfixes: that and this.

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

Gitlab to 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



- The OSSR is a curated software repository
  - implementation of the FAIR principles
  - good code practices
  - software quality
  - do not review scientific results  $\rightarrow$  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



- memoryRequirements not provided in the codemeta schema but is recommended
- processorRequirements not provided in the codemeta schema but is recommended





#### connects to other services

analyze data

ESCAPE

search and pull software from the OSSR





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



Research Software as a first class citizen for the scientific endeavours

# abundance

2

# 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.

#### 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.

#### 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.

#### **Foundational Software**



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