

European Science Cluster of Astronomy & Particle physics ESFRI research Infrastructures

### ESCAPE OSSR

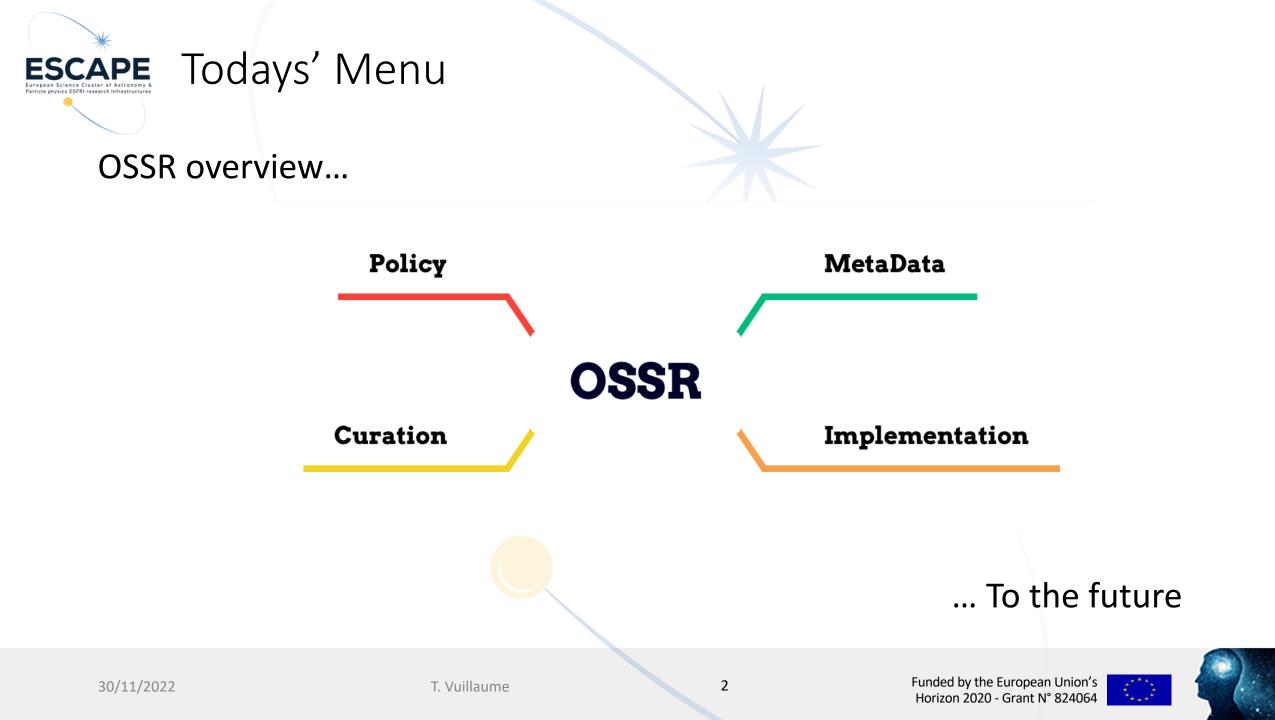
Thomas Vuillaume, on behalf of all contributors:

Enrique Garcia, Jutta Schnabel, Kay Graf, Tamas Gal, Mark Kettenis, Christian Tacke, Marjolein Verkouter ...

29-11-2022, ESCAPE OSSR workshop, Erlangen

ESCAPE - The European Science Cluster of Astronomy & Particle Physics ESFRI Research Infrastructures has received funding from the European Union's Horizon 2020 research and innovation programme under the Grant Agreement n° 824064.





#### A step back in time... Bruxelles, February 2020 **ESCAPE**

An example of open science project : The Crab bundle

The Crab multi-instrument gamma-ray analysis with MAGIC, VERITAS, FACT and H.E.S.S.

https://github.com/open-gamma-ray-astro/joint-crab/tree/v0.1 https://zenodo.org/record/2381863#.XkxcD5NKhhA

#### license ense (for files Software Open Acces 141 12 The joint-crab bundle ▲ download /ersions **OpenAIRE** 6.0 kB 100.8 kB 72.0 kB 65.4 kB Page size: 10 \$ 🗏 🔰 f 🗟 🕯 604 Byte: 1.5 kB 4.3 kB 2.9 kE 443 Byte: Cited 512 Bytes Pt 20131103 103 dl3 fits 25.9 kB 25.9 kB 23.0 kB P120131103 104 dl3.fits bv Cite as Source code and data Link to project and article

Now imagine this as a standard,

in an integrated environment - with a single

login,

allowing you to (re-)run (part of) any analysis,

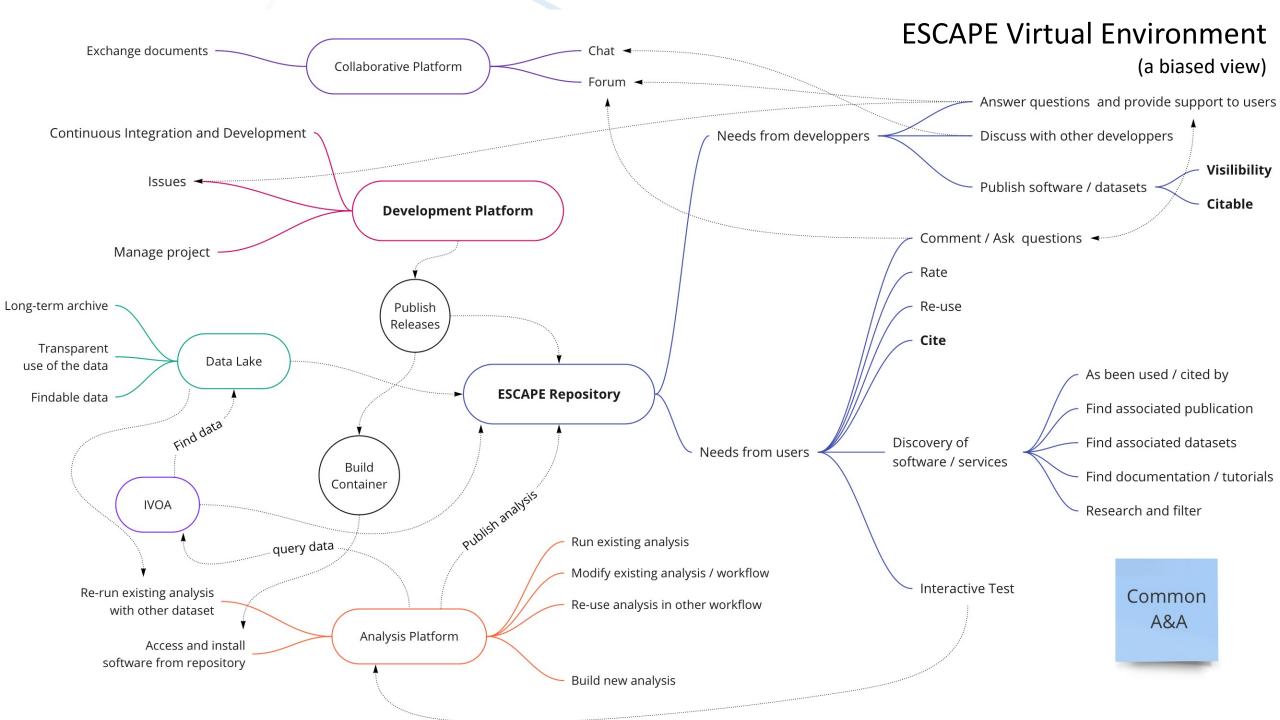
with another dataset,

and easily publish your new results,

automatically giving credit to original analysis, datasets, workflows...



cember 18, 2018





Community Driven Repository, Organised by Science Projects

- Starting a new Science projet (through validation) sets up a complete virtual environment
- Researchers / Institutes contribute to the science project by publishing software / workflow / data
- The contributions are validated by science project curators
- Users can search the repository or explore it through the science

projects





# Policy & recommendations







Find it... in the OSSR! <u>https://doi.org/10.5281/zenodo.6757113</u>

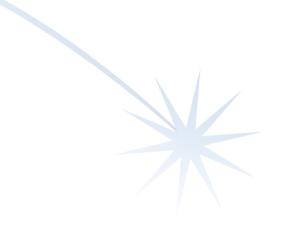
- TLDR
  - License !
    - Permissive and open-source if possible (MIT, BSD-3...)
  - Add metadata
    - As a CodeMeta file
    - The more (accurate) metadata, the better
  - Version
  - Follow modern development practices (git, environment files, dockerise...)

### Final/updated version before ESCAPE ends?





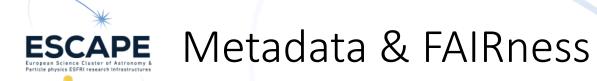




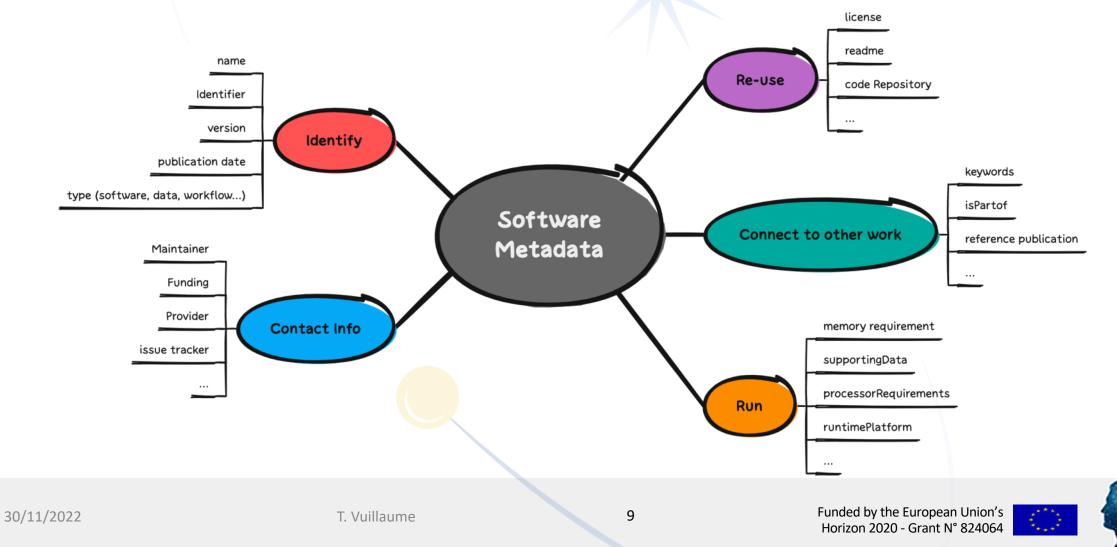
## MetaData & FAIRness

8





### MetaData are the heart of the FAIR principles





It also allows services to install a software or run an analysis

- by finding it: see e.g. the jupyter-notebook keyword in the OSSR allowing the ESAP to identify records that include and interative analysis
- by running it: e.g. knowing the CPU or memory requirements
- For FAIRness, MetaData must be included in a file included in each record.
- ESCAPE implementation choice for software: <u>CodeMeta</u> (as a codemeta.json file)
- CodeMeta generator and validator online





### An example of codemeta.json

	"@context": "https://doi.org/10.5063/schema/codemeta-2.0",
	"@type": "SoftwareSourceCode",
	"name": "eossr",
	<pre>"description": "<img src='\"docs/images/eossr_logo.png\"' width='\"400px\"'/><h1>The ESCAPE OSSR library</h1>T</pre>
	"license": "https://spdx.org/licenses/MIT",
	"version": "v0.6.2.dev34+g75395d9",
	"softwareVersion": "v0.6.2.dev34+g75395d9",
	<pre>"codeRepository": "https://gitlab.in2p3.fr/escape2020/wp3/eossr",</pre>
	"developmentStatus": "active",
	"isAccessibleForFree": true,
	"isPartOf": [
	"https://gitlab.in2p3.fr/escape2020",
	"https://projectescape.eu/"
	1,
	"contIntegration": "https://gitlab.in2p3.fr/escape2020/wp3/eossr/-/pipelines",
	"buildInstructions": "https://gitlab.in2p3.fr/escape2020/wp3/eossr/-/blob/master/README.md",
	"issueTracker": "https://gitlab.in2p3.fr/escape2020/wp3/eossr/-/issues",
	<pre>"readme": "https://gitlab.in2p3.fr/escape2020/wp3/eossr/-/blob/master/README.md",</pre>
	"programmingLanguage": [
	{           {{
	"@type": "ComputerLanguage",
	"name": "Python",
	"url": "https://www.python.org/"
	}
	"softwareRequirements": [
28 29	{
	"@type": "SoftwareApplication", "identifier": "requests",
30	"name": "requests",
32	"softwareVersion": ">=3.6"
33	},
34	
	"@type": "SoftwareApplication",
	"identifier": "pytest",
	"name": "pytest",
	"softwareVersion": ">=5.4.2"
	}
	"keywords": [
	"jupyter-notebook",
	"zenodo"
	1,
	"runtimePlatform": "Python 3",
	"downloadUrl": "https://gitlab.in2p3.fr/escape2020/wp3/eossr/-/archive/v0.6.2.dev34+g75395d9/eossr-v0.6.2.dev34+g75395d9.zip",
47	"releaseNotes": "",







# **Technical Implementation**







### OSSR entry point: <a href="https://purl.org/escape/ossr">https://purl.org/escape/ossr</a>

ESCAPE
energy a

FIND SOFTWARE V CONTRIBUTE V INFRASTRUCTURE V ABOUT V

	0	0	ESCAPE OSSR   Open-source Scientific Software and Service Repository
ŏ	õ	ĕ	OSSR Open-source Scientific Software and Service Repository

#### Welcome to the ESCAPE OSSR!

Browse the OSSR content.

What is it?

The ESCAPE Open-source Scientific Software and Service Repository (OSSR) is a sustainable open-access repository to share scientific software, services and datasets to the astro-particle-physics-related communities and enable open science. It is built as a curated Zenodo community integrated with several tools to enable a complete software and service projects in the OSSR such as user-support documentation, tutorials, presentations and training activities. It also encourage at gratual of documents and material that disseminate and support the goals of SCAPE.

#### How to contribute to the ESCAPE OSSR?

You can onboard your project right now - see here how.

Learn more about our projects in this website or contact us!

#### Research infrastructures and Science Projects in the OSSR

Directly find software and dataset related to our scientific partners in the OSSR:



### Browse the OSSR

### Guidelines & policy

Tutorials





## **ESCAPE** OSSR core: Zenodo & the *escape2020* community

ESCAPE 2020	
P All versions Access Right	Found 33 results.
🗆 Open (33)	November 21, 2022 (00.18.02) Software Open Access View gLike
File Type	Rico, Javier, Nigro, Cosimo, Kerszberg, Daniel, Miener, Tjark; gLike is a general-purpose R00T-based code framework for the numerical maximization of joint likelihood functions. The joint likelihood
□ Zip (16)	function has one free parameter (named g) and as many nuisance parameters as wanted, which will be profiled in the maximization process.
Pdf (13)     Json (4)	upposed on November 21, 2022 7 more version(s) exist for this record
Gz (3)	Nevember 17, 2022 (3.1.0) Software Open Access. View
□ Tar (2)	agnpy Naro, Cosimo,  Starek, Juliar,  Gliwny, Pawel; Sanchez, David;  Craig, Matthew;  Vuillaume, Thomas; Viale, Ilaria; Maniadakis,  Dimitrice
Keywords	Dimitros, agryp is a python package focusing on the computation of the radiative processes of relativistic particles accelerated in the jets of Active Galactic Nuclei (AGN), It includes classes describing the galaxy components responsible for line and thermal emission and calculates the
ESCAPE (7)	absorption due to gamm Uploaded on November 17, 2022
Jupyter-Notebook (5) CTA (3)	operation of the method of the second
Astronomy (2)	November 10, 2022 (1.0) Software Open Access View
Analysis (2)	Gammapy: Python toolbox for gamma-ray astronomy
ATLAS (1)  Astronomy And Astrophysics (1)  Compact Groups (1)  Data Analysis (1)  EOSC (1)	Aeror, Fabio, Aguasca-Cabot, Arnau, © Buchner, Johannes, © Carreto Fidajo, David, © Chrei, Andrew, Chromey, Allaha, Contreras Gonzalez, José Luis, de Boyd ed Laverpin, Mahriu, ed Marinda Cardoso, José Vinicius, Ed, Christoph, Donath, Aek, © Giunti, Luca; © Hinton, James, Jourin, Lé, © Khélifi, Bruno, King, Johannes, Lefaucheur, Julien, © Lenain, Jean-Philippe, © Linhoff, Maxomillari G Jopez- Coto, Rukén, Mohrman, Lusa, Com, Kong, Johannes, Lefaucheur, Julien, © Lenain, Jean-Philippe, © Linhoff, Maxomillari G Jopez- Coto, Rukén, Mohrman, Luca; Shinta, Artiyee, © Spotz, Brigtita M Saylani, Kakon Lindon, Ponner, Benzy, Quentin, @ Ruki, Joné Erringue, © Selvioxeki, Huber, E Sinha, Artiyee, © Spotz, Brigtita M Sayla-Liacho, Mainon, © Terrier, Röjs; © Tibaido, Luigi; © Unbehaun, Tim, © van Eldik, Christopher; © Vuillaume, Thomas, © Weinstein, Amanda, Wood, Matthew; Gammaray analyzes gamma-ray data and creates sky images, spectra and lightcurves, from event lists and instrument response Information; Lina alos determine the position, monphology and spectra of gamma-ray source, It is used to analyze data from H.E.S.s.,
Туре	millimitation, it can also been time the position, morphology and spectra or gammenay sources, it is used to analyze tata from H.E.S.S., FermiLAT, HANC, and the Cherenkov Telesco Uploaded on November 10, 2022
Software (19)	7 more version(s) exist for this record
Publication (11) +     Poster (2)     Lesson (1)	November 4, 2022 (r) 1.3.1         Software         Open Access           IndexedConv/IndexedConv: v1.3.2         Mikei Jacquemont Thomas Vullaume;
	minder Jacquerindin, Inninias Yuliauzii Polygi Maria (1990) What's Charled Uddate test badge by @ivuillaut in https://github.com/indexedCom/indexedCom/pull/33 Create codemeta json by @ivuillaut in https://github.com/indexedCom/indexedCom/pull/34 Version 1.3.2 by @ivuillaut in https://github.com/indexedCom/indexedCom/pull/35 Full Changelog: https://githu Updaddo in Novmber 4. 2022.

### Current stats:

1:	OSSR statistics generated the 2022-11-30
4]:	md(text)
4]:	There are 19 records in the OSSR.
	downloads: 4806
	unique downloads: 2042
	views: 19073
	unique views: 6964
5]:	md(text)
	Note that there are also 14 records in the ``escape2020`` community that are not software or datasets.

#### You may find them directly on Zenodo

-







- eOSSR library
  - Dev: <u>https://gitlab.in2p3.fr/escape2020/wp3/eossr</u>
  - Doc: <u>https://escape2020.pages.in2p3.fr/wp3/eossr/</u>
  - OSSR: <u>https://doi.org/10.5281/zenodo.6826881</u>
  - Gathers all OSSR developments and technical definitions







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    - **CI**: automated upload / update using gitlab CI

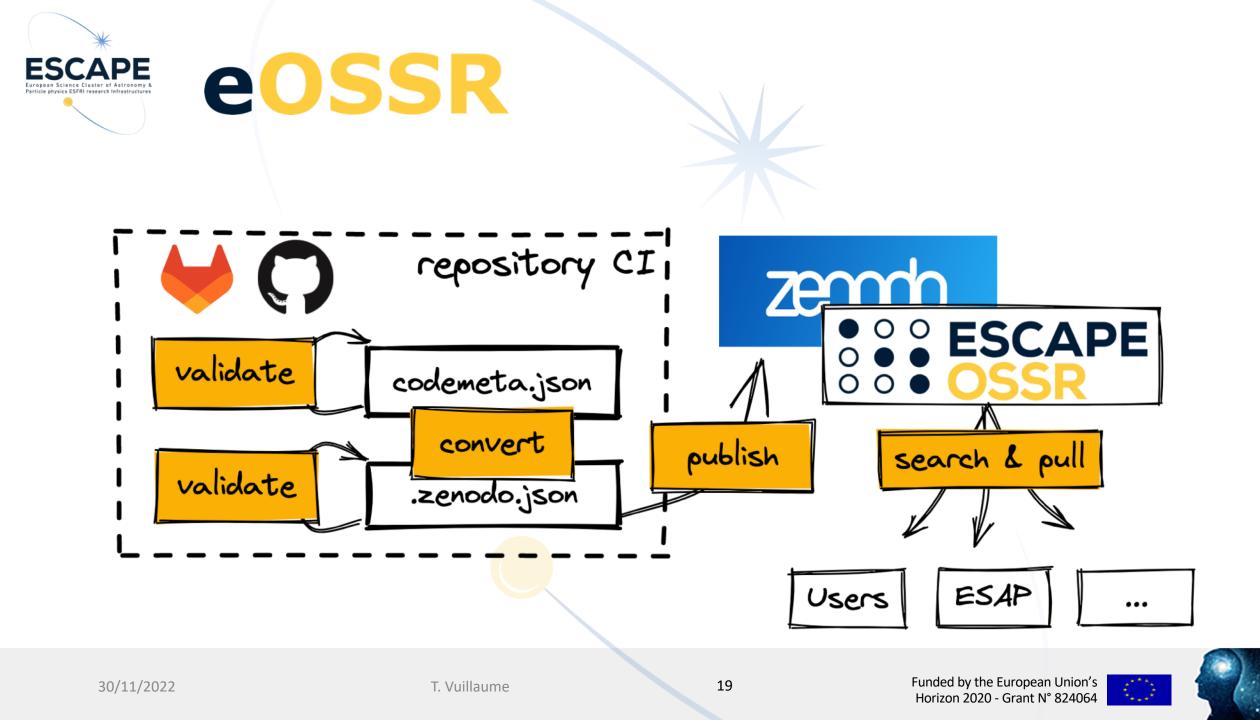






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    - **CI**: automated upload / update using gitlab CI
    - Metadata: schema definition, crosswalk between CodeMeta and Zenodo, validation







### eOSSR presented as ADASS 2022 poster

proceedings: https://hal.archivesouvertes.fr/hal-03876630v1



ESCAPE brings together the astronomy astroparticle and particle physics ESFRI and pan-European communities with aligned challenges of data-driven research and demonstrated capabilities in addressing various stages of data workflow and concerned with fundamental research through complementary approaches.

**eoss** 

Authors: Thomas Vuillaume\*, Enrique Garcia, Christiar Tacke, Tamas Gal, for the ESCAPE project \*thomas.Vuillaume@lapp.in2p3.fr

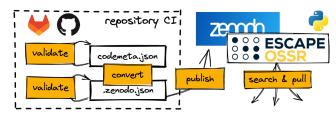
The aim of the ESCAPE WP3-OSSR (Open-source Scientific Software and Service Repository) is to provide the tools necessary for the communities to share their science products in a harmonized way respecting the FAIR principles, promoting open science and maximizing cros tilization by s and c One of the key components to achieve this goal is the software and service repository.

For its concept implementation, the ESCAPE repository is using Zenodo web service through the curated escape2020 community integrated with several tools to enable a complete software life-cycle. The ESCAPE Zenodo community welcomes entries that support the software and service projects in the OSSR such as usersupport documentation, tutorials, presentations and training activities. It also encourages the archival of documents and material that disseminate and support the goals of ESCAPE.

We developed a Python library called eOSSR in order to allow an automated integration of Zenodo with other tools and platforms forming the OSSR as well as providing an integrated environment to external users. The library is open-source and has been published in the OSSR itself.

You may find it at htt

You may find documentation and running examples online: https://escape2020.pages.in2p3.fr/wp3/eossr/



Metadata: The OSSR has chosen codemeta ison as schema and format for its software metadata. The definition of this schema has been integrated within the eOSSR, thus allowing: - A converter between Zenodo metadata schema

and the OSSR metadata

JOIN OUR COMMUNITY REGISTER ON THE WEBSITE! () www.projectescape.eu

@ESCAPE\_EU Inlinkedin.com/in/escape-eu

ESCAPE - The European Science Cluster of Astronomy & Particle Physics ESFRI Research Infrastructures has received funding from the European Union's Horizon 2020 research and innovation programme under the Grant Agreement No. 824064.

The eOSSR library

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<sup>2</sup>IT Department, CERN - 1211 Geneva 23 - Switzerland

<sup>3</sup>GSI Helmholtz Centre for Heavy Ion Research GmbH, Darmstadt, Germany

<sup>4</sup>IT Erlangen Centre for Astroparticle Physics, Erlangen, Germany

#### Abstract.

The astronomy, astroparticle and particle physics communities are brought together through the ESCAPE (European Science Cluster of Astronomy and Particle Physics ESFRI research infrastructures) project to create a cluster focused on common issues in data-driven research. Among the ESCAPE work packages, the OSSR (ESCAPE Open-source Scientific Software and Service Repository) is a curated, longterm, open-access repository that makes it possible for scientists to exchange software and services and promote open science. It has been developed on top of a Zenodo community, connected to other services. A Python library, the eOSSR, has been developed to take care of the interactivity between Zenodo, services and OSSR users, allowing an automated handling of the OSSR records. In this work, we present the eOSSR, its main functionalities and how it's been used in the ESCAPE context to ease the publication of scientific software, analysis, and datasets by researchers.

#### 1. The ESCAPE OSSR

The aim of the ESCAPE OSSR (Open-source Scientific Software and Service Repository) is to provide the tools necessary for the communities to share their science products in a harmonized way respecting the FAIR principles, promoting open science and maximizing cross-fertilization by software re-use and co-development. One of the key components to achieve this goal is the software and service repository. For its concept implementation, the ESCAPE repository is using Zenodo web service through the curated escape2020 community integrated with several tools to enable a complete software life-cycle. The ESCAPE Zenodo community welcomes entries that support the software and service projects in the OSSR such as user-support documentation, tutorials, presentations, and training activities. It also encourages the archival of documents and material that disseminate and support the goals of ESCAPE.



API: For other tool to communicate with the OSSR,

an API was necessary. The eOSSR takes

advantage of Zenodo's API to propose a set of

high-level functionalities through Python functions

specific searches, using plain text or recognized

metadata such as keywords or file type.

Search for Zenodo's communities, and

supported licenses, funders and grants,

ftware in the OSSR via wide or

ware to the OSSR (or Zenodo) via

or command-lines, such as:

the CLI.

### **ESCAPE** MetaData generator and validator

#### https://escape2020.pages.in2p3.fr/wp3/codemeta-generator/

#### ESCAPE OSSR CodeMeta generator

The software itself	Discoverability and citation		- Development community / tools
ame	Unique identifier		Code repository
eat-software	10.151.xxxxx	I	git+https://github.com/You/RepoName.git
software title	such as ISBNs, GTIN codes, UUIDs etc., http://schema.org/identifier		gr-mps/gards.com/rounteportante.gr
			Continuous integration
scription	Application category		https://travis-ci.org/You/RepoName
great	Astronomy		Issue tracker
0	Keywords		https://github.com/You/RepoName/issues
	Projects: CTA, EGO-Virgo, ELT, EST, FAIR, HL-LHC, KM3NeT, LSST, SKA; Content: Astronomy, Astroparticle physics, Particle physics	LOFAR,	
cumentation or readme	SKA; Content: Astronomy, Astroparticle physics, Particle physics		Related links
ps://great.doc.com			
	Keywords		
ation date			
22-11-30	Funding		
st release date	ESCAPE 824064 grant funding software development		
12-11-30	grant funding software development		
	Funder		
ense	European Union's Horizon 2020 research and innovation programme		
T	organization funding software development		
a SPDX licence list	Authors and contributors can be added below		
n-time environment	Current version of the software	Addition	nal Info
			P. 1.1
gramming Language , Java, Python 3	Version number		bi.org/10.1000/xyz123
Java, Fylion J	1.0.0	[Inche-viol	3.01g-10.1000/Xy2123
ntime Platform	Release date	Develop	ment Status
ET, JVM	2022-11-30		
	Download URL	see www.	repostatus.org for details
erating System droid 1.8, Linux, Windows, macOS	https://example.org/MySoftware.tar.gz	Is part o	ſ
diola 1.0, Ellan, Wildows, Historia	Indease of the continue of the	http://Th	e.Bigger.Framework.org
her software requirements	Release notes		
ython 3.4	Change log: this and that;		
	change rog, chis and chac,		
ttps://github.com/psf/requests	Bugfixes: that and this.		
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#### Validate and convert your metadata

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/codemeta-generator/

Load codemeta from a json file

1 Upload (0)

Load codemeta from an URL

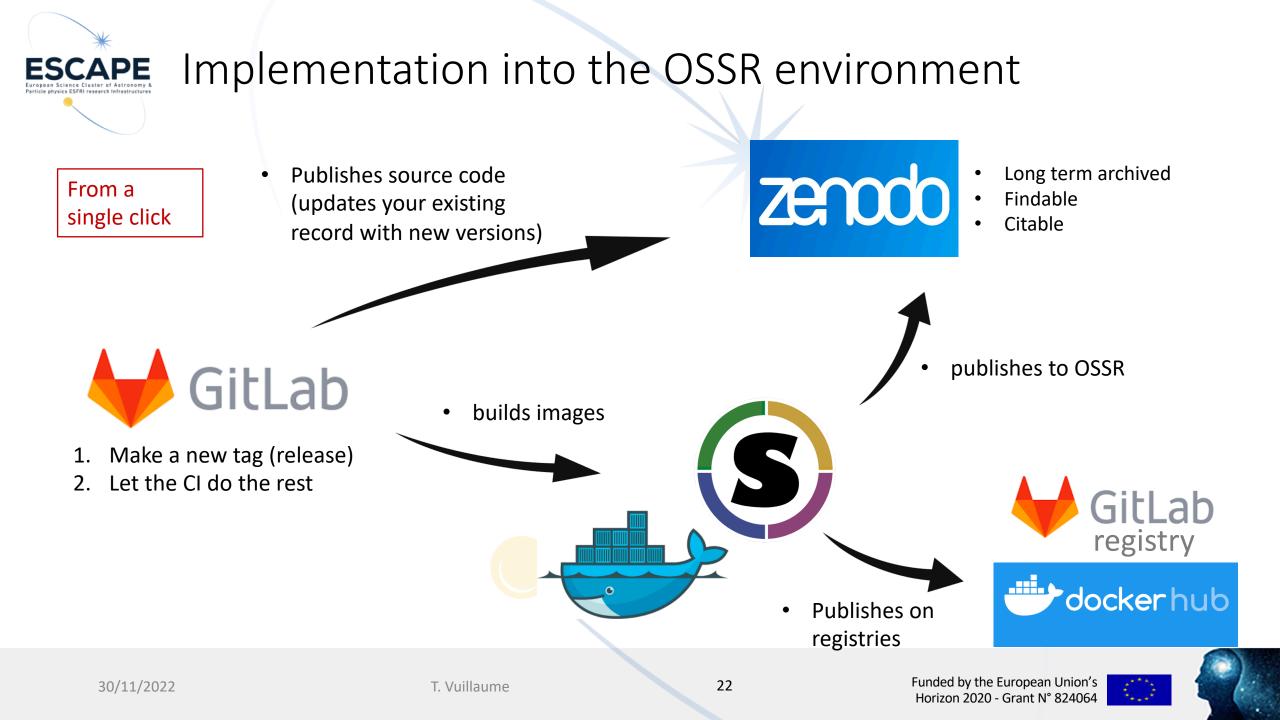
URL:

codemeta:

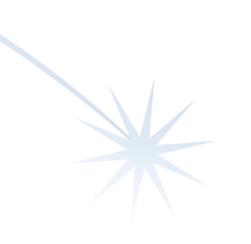
Validate !

Convert to .zenodo.json 🗹 Add ESCAPE metadata

Note that you can validate your generated codemeta.json with the eOSSR CLI tool eossr-metadata-validator







# Curation





### Each entry in the OSSR is reviewed to:

- Ensure that it matches our policy and requirements
- Make recommendations
- Help implement them

### It happens through:

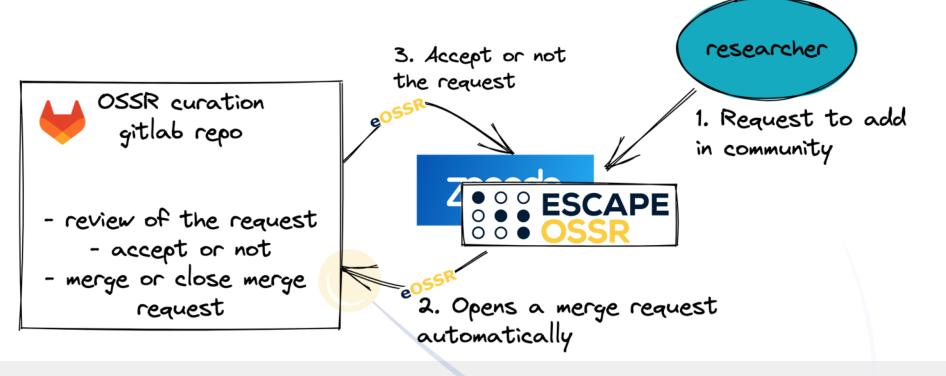
- A recorded presentation of the software, analysis or service
- A formal final review and acceptance through ossr-curation



#### **ESCAPE** United physics ESFRI research laffastructure Curration: ossr-curation

Issue: Zenodo currently supports a single community maintainer and reviewer

OSSR curation: a solution to collaboratively and openly review requests in a Zenodo community. Note that it might become obsolete in a future version of Zenodo built on Invenio RDM







### **ESCAPE** Curation: ossr-curation

#### https://gitlab.in2p3.fr/escape2020/wp3/ossr-curation

ESCAPE2020 > 🕐 WP3 > 🕐 ossr-curation > Merge requests		
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[CURATE] JColl88/sdc1-solution-binder: SDC1 Solution 1.0.0 0 of 8 tasks completed 129 · created 3 months ago by Vuillaume In curation		🛕 💿 🗗 1 updated 1 week ago
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30/11/2022 T. Y	Vuillaume	

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Ø	Vuillaume @vuillaume added (Ready for curation) label 3 months ago		
	Vuillaume @vuillaume changed the description 3 months ago		
0	Jutta Schnabel @jschnabel removed (Ready for curation) label 3 months ago		
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۲	Jutta Schnabel @jschnabel - 3 months ago Owner ③ □ 2 : @vullaume Same question as with ctapipe - part of another project or separate onboarding?		
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26

Open Created 3 months ago by 👩 Vuillaume 0 of 8 tasks completed Edit Mark as draft 🗸





# How to publish in the OSSR





Instructions online: <u>https://escape2020.pages.in2p3.fr/wp3/ossr-pages/page/contribute/onboarding/</u>

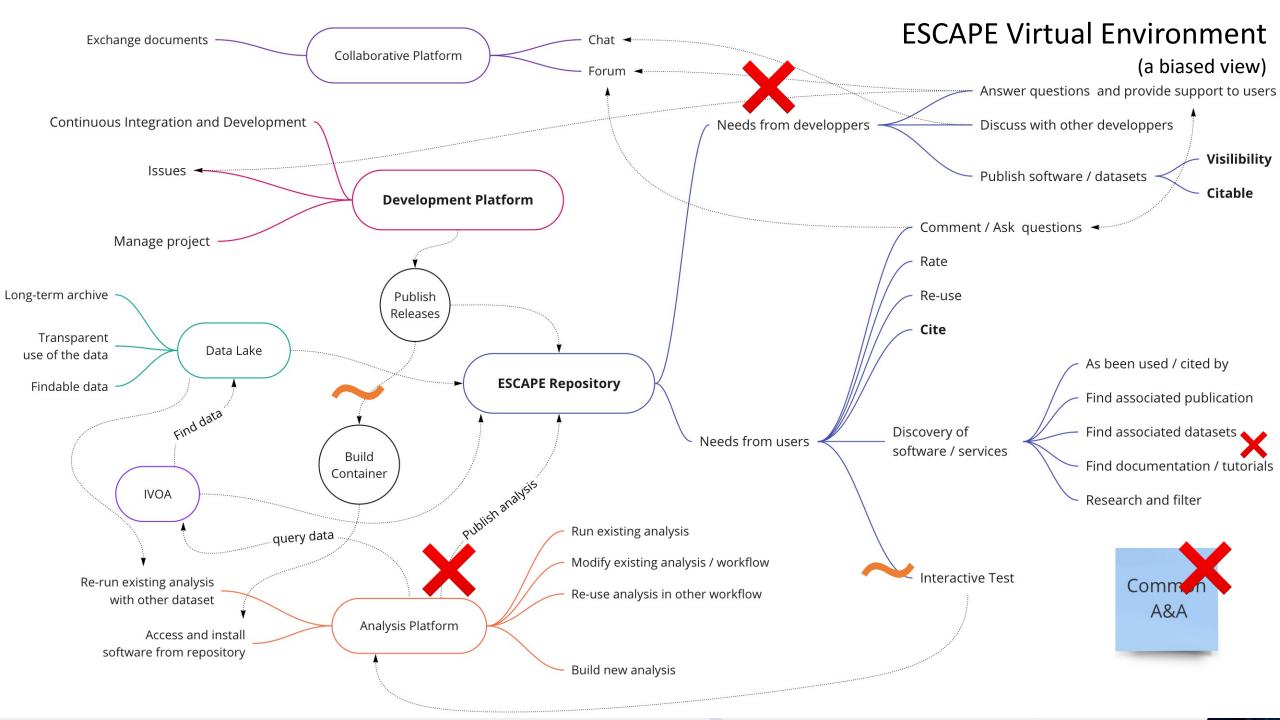
- 1. Fill a form to request a presentation
- 2. Prepare your repository: see requirements and metadata
  - Validate your codemeta.json using the eOSSR in your Cl
- 3. Publish to Zenodo: ease your life <u>using the eOSSR</u>
- 4. Add escape2020 as a community (this comes for free if you use the eOSSR)
  - If your software was already in Zenodo, you can edit the metadata and add the escape2020 community through the web portal
- 5. Final review and acceptance  $\rightarrow$  ossr-curation





# Things we could improve (a.k.a. I wished we did better)







Find associated software / dataset / analysis...

- Possible in metadata but still not clearly defined and in the hands of developers
- In Zenodo, related identifiers (continues this upload, is cited by this upload, etc...)

Publish analysis from analysis platform

 Possible using eOSSR but requires an integration between ESAP and the development platforms

### CodeMeta

- Not automated enough
- Not integrated enough => some hope with InvenioRDM ?
- Still too much a burden for developers





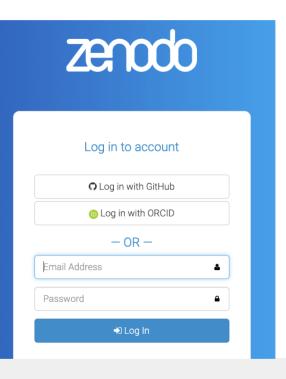
### Containers and registry

Some attempts: <u>https://gitlab.in2p3.fr/escape2020/wp3/ossr-registry</u>

We rely on developers to do their job

### Common A&A

Not entirely in our hands for the OSSRWill improve with InvenioRDM?







# The future of the OSSR ?





eOSSR v1.0 release – see milestone in GitLab

make clear recommendations on how to maintain codemeta.json in a repository

Based on the work done recently for gammapy and other repositories

Finish all on-going curations

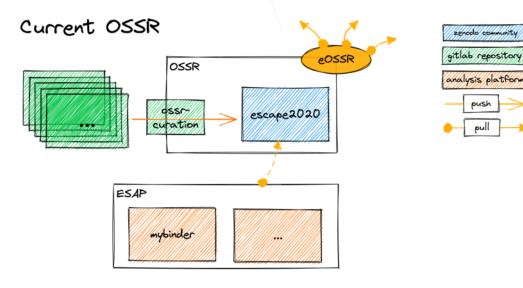
OSSR paper gathering these technical developments and recommendations

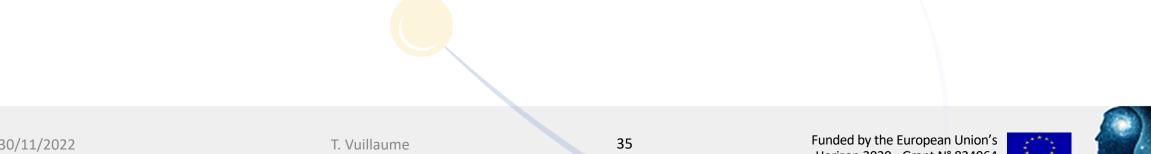




### The future of the OSSR: federating the decentralized? ESCAPE

ESCAPE as a funded project is ending, but the OSSR can stay (though in different forms)

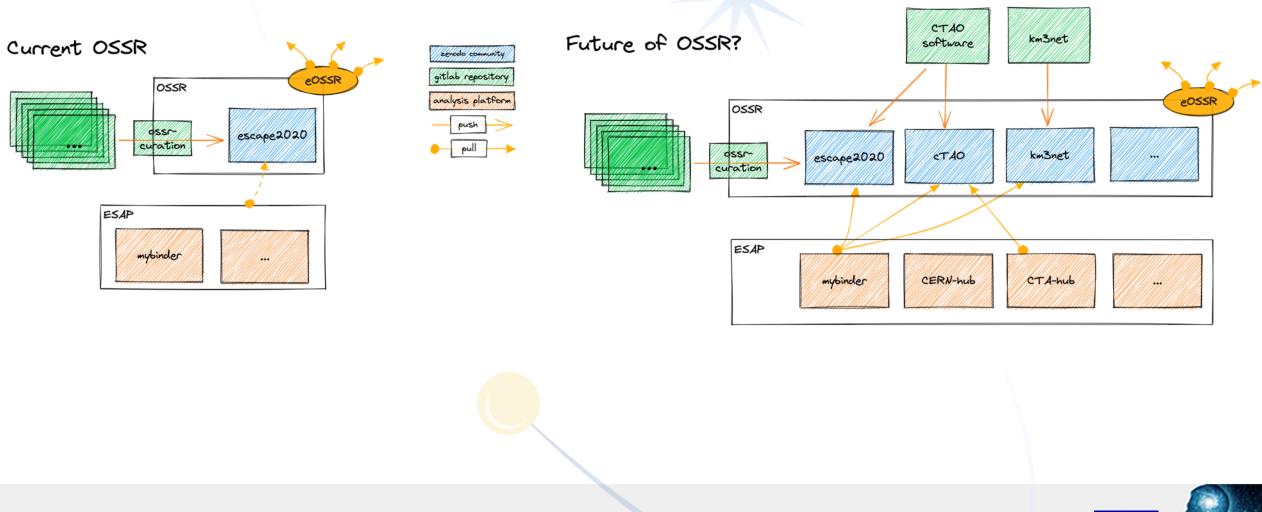






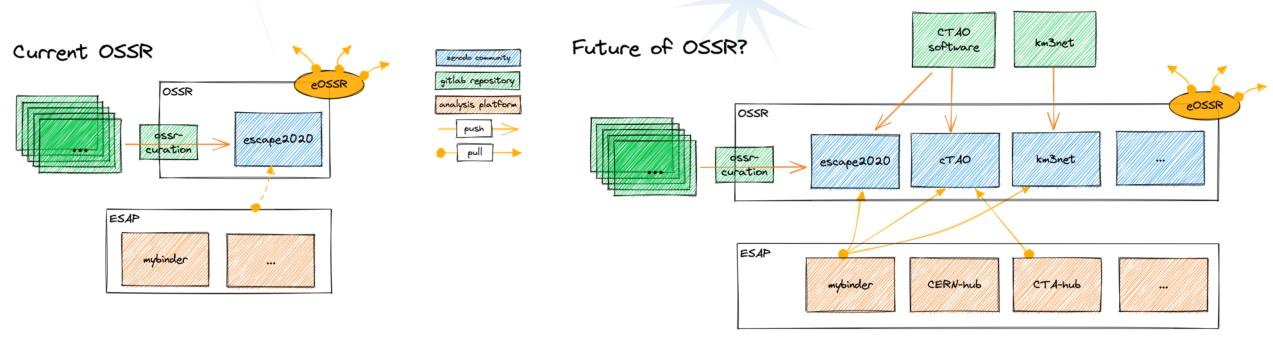
# **ESCAPE** The future of the OSSR: federating the decentralized?

ESCAPE as a funded project is ending, but the OSSR can stay (though in different forms)



# **ESCAPE** The future of the OSSR: federating the decentralized?

ESCAPE as a funded project is ending, but the OSSR can stay (though in different forms)



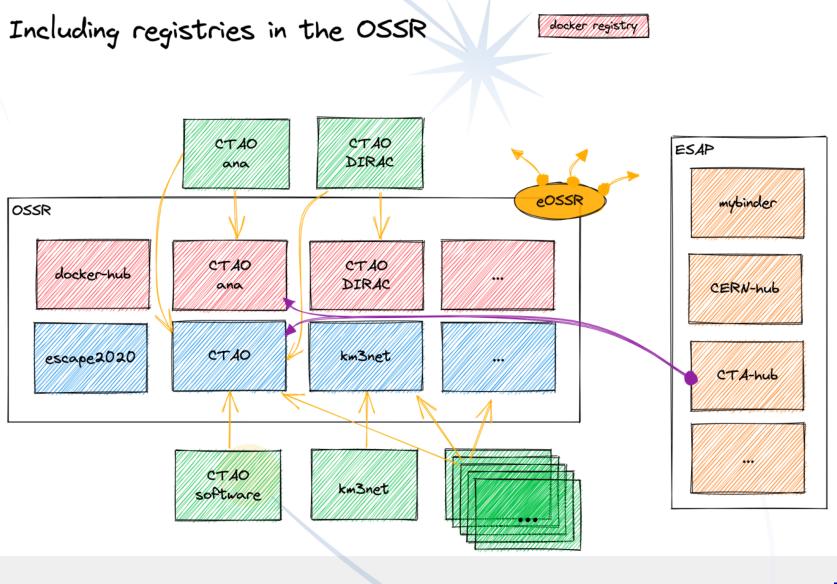
- Decentralization powered by the eOSSR, serving the API to fetch the federated OSSR
- Each community has to commit to follow a minimal set of requirements to be part of the OSSR
- Domain specific platforms will have different requirements, that can be requirements of each Zenodo community







The extra mile: community specific **registries** could also be integrated the same way in the OSSR







### The curation is a central part of a trusted repository

- part of it is automated (e.g. checking for correct metadata)
- but human curation is essential
- Ouration is (sometimes) domain specific
- For the OSSR to keep growing after ESCAPE ending, we need curators
- ⇒ A commitment from the research infrastructure is needed to assign experts able to do software curation in their domain
- ⇒ In the decentralized version, RI commit to maintain and follow a common base of requirements, and do the curation internally (with potentially more requirements)





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- ⇒ In the decentralized version, RI commit to maintain and follow a common base of requirements, and do the curation internally (with potentially more requirement)
  ⇒ In line with the Open Collaboration agreement signed in Brussels





- A clear set of guidelines and requirements to publish any software and analysis in collaborations
  - Following OSSR requirements
- A curation team dedicated to software and analysis code
- A software/analysis publication process for analysers
- A software/analysis review process for curators
- A set of templates for software and analysis for members to use



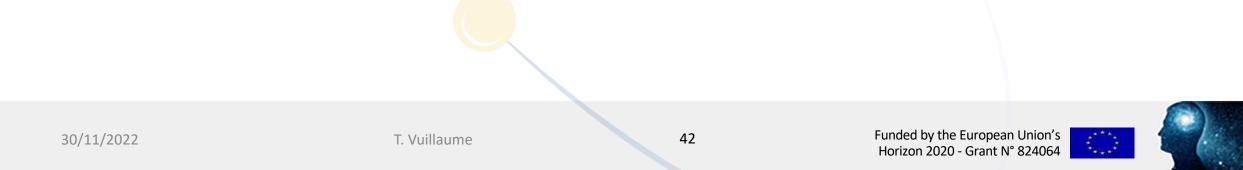


**E** Conclusion: mission accomplished!

There are still things to improve

We did a good job and achieved our goals and more

Let's make sure it does not all disappear with ESCAPE ending





# Thank you for your attention

# Questions?



# **ESCAPE** Finally, some inspiring projects

### A list of conference publications:

- ESCAPE Open-source Scientific Software and Service Repository
- The ESCAPE Data Science Summer School 2021 ADASS XXXI Poster
  The eOSSR library

### Some inspiring projects:

- <u>https://deepnote.com/</u> collaborative analysis platform
- <u>https://codeocean.com/</u> an analysis platform with and integration publication process
  - eOSSR demo: https://codeocean.com/capsule/6789403/tree
- https://biocontainers.pro/ an example of workflows registry in the bio community

