

OPEN LETTER

REVISED The ESCAPE Open-source Software and Service

Repository [version 2; peer review: 2 approved, 1 not approved]

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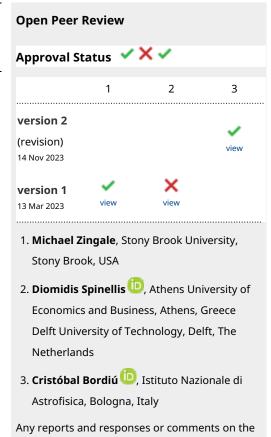
Abstract

Purpose

The purpose of the ESCAPE Open-source Software and Service Repository (OSSR) is to provide a central location for the dissemination and use of trusted open-source software in the fields of astronomy, astroparticle physics, and particle physics. The repository allows users to easily access and download tools and services developed within the community, and to contribute their own tools and services.

Methods

The ESCAPE project has set up a curated repository of software that provides tools and an environment to make it easy for users to find and download the software and services that they need. The repository is regularly updated and is maintained by a curation board, ensuring that the software and services are reliable and up-to-date. The curation and onboarding process makes the OSSR a trustworthy source of software that can be used for scientific analysis. The software included in the repository must include documentation and instructions and follow a set of modern best practices in software



article can be found at the end of the article.

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development. Training is provided to students and researchers to help them provide high-quality scientific software following modern software development practices.

Outcome

The OSSR currently contains a wide range of software and services, including those for data management, data analysis, and machine learning. These tools and services are used by researchers and other users around the world. The OSSR has proven to be an effective means for disseminating and providing open-source software and services developed by the ESCAPE project partners and welcomes contributions from the entire community.

Plain language summary

The ESCAPE (European Science Cluster of Astronomy & Particle physics ESFRI research infrastructures) Open-source Software and Service Repository (OSSR) is a place where scientists can find and download software and services they need for their work in astronomy, astroparticle physics, and particle physics. This repository is updated regularly and maintained by a group of experts to make sure that the software is reliable and open-source to maximize its reuse. The software available on the repository must come with instructions and follow good software development practices. The OSSR provides training to students, researchers, and software developers to help them create high-quality software. The OSSR includes a variety of tools and services for things like data management and analysis that are used by researchers worldwide.

Keywords

EOSC, open-source, software, repository, Zenodo, ESFRI



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REVISED Amendments from Version 1

The second version adresses various comments from the reviewers.

In particular:

- the missing acronyms definitions have been added;
- a section comparing the OSSR to similar initiatives, especially the ASCL, has been added (section 2.6);
- The OSSR is open to all community software and code bases, observational and theoretical, there are already entries of both in the repository. We added this OSSR aim to the text (section 2.1) as well as a the link to the always up-to-date list of entries (section 5.1);
- Software is added by the authors of the code themselves, it is not pulled by the ESCAPE community. This has been made clearer in the text (section 2.1) now.
- a section about the project organisation has been added
- there has been slight re-arrangements in the sections to improve readability
- several minor rephrasing and grammar/typo fixes

Any further responses from the reviewers can be found at the end of the article

1 Introduction

The ESCAPE project is a European H2020 project that brings together researchers and institutions from the European Strategy Forum on Research Infrastructures (ESFRI) and leading research infrastructures. Its goal is to develop new technologies and methods for dealing with the increasingly large and complex datasets that are generated in the fields of astronomy, astroparticle physics, and particle physics. The project also focuses on making these technologies and methods accessible to a wider audience, through the development of open-source software and services. The ESCAPE Open-source Software and Service Repository is a key component of this effort, providing a central and trusted location within the European Open Science Cloud (EOSC) for the dissemination of curated software and analysis tools. The OSSR follows a federated, community-driven approach, gathering from all researchers in the domains associated with the ESCAPE project.

In this open letter, we summarize the OSSR effort based on previously published,more technical material, and present its guidelines and views, while still giving an overview of the technical setup. In Section 2, we show how the OSSR has been built to provide software following the FAIR (Findable, Accessible, Interoperable and Reusable) principles¹ that are the core components of open science (based on the following OSSR publications: 2–5). Contributions to the OSSR are curated by a committee of domain experts following clear and published policies in order to build a trusted repository. Then in Section 3, we highlight the technical components of the OSSR which is built around a Zenodo (RRID:SCR_004129) community with enriched metadata and application programming interface (API) connection (based on 3,4,6–8). In Section 4, we show the importance of community building, and training

software developers to write and publish FAIR software, and our efforts in this regard (based on 9–15). Finally, we present the outcomes in Section 5 (based on 16,17).

2 OSSR goals and governance

2.1 Goals

The OSSR acts as a central place to share curated open science software and services based on FAIR principles in the astronomy and particle physics communities with the ESFRIs in these communities at its core. It has been collaboratively developed by, for, and in alignment with the priorities and considerations of the ESFRIs after consultations with their members. The objectives of the repository are to facilitate and support the continuous development, deployment, exposure, and long-term preservation of partners' research software, tools, and the code base of services. Additionally, the repository aims to foster interoperability, research software re-use, and cross-fertilization between the members of the community. It offers an open innovation environment for open standards (e.g. workflows, data formats), common practices, and shared novel software (e.g. for multi-messenger and multi-probe data). The OSSR is built by and for the communities and follows an inclusive approach by federating available resources, with the goal of enabling open science and treating software as a central part of knowledge and science production. By highlighting software in research, the OSSR also emphasizes developer effort and helps to increase recognition of their contribution to science. This is possible in particular by facilitating software citation, promoting communication, collaboration, training, and recognition of developers. In addition, the OSSR onboarding procedure provides a mechanism to check the quality of the contributions, improving the trustability for end users.

The OSSR is open to all community contributions, including but not limited to research software, science workflows and specialized science services.

Entries to the OSSR are requested by the developers or maintainers of a possible contribution. This starts the onboarding procedure into the repository. Suitable candidate contributions will be actively approached by the OSSR community to submit an onboarding request.

2.2 Project organisation

Since January 2023, the ESCAPE project has been governed by a new Open Collaboration Agreement, unveiled at the "ESCAPE for the Future" event and endorsed by directors from all associated research infrastructures. The OSSR continues its collaborative efforts, welcoming new participants and convening monthly virtual board meetings, as well as biannual in-person gatherings that feature onboarding discussions. The OSSR is organized into three primary focus areas: Policy & Strategy, Technical, and Onboarding.

2.3 The FAIR principles

With the implementation of the OSSR, partners from the particle physics, astroparticle and astronomy communities are able to aggregate their software in a common place. This alone is not enough to ensure that the FAIR principles are respected, especially the ones for software¹⁸. Although used as guidelines throughout the development of the OSSR service, the FAIR principles for data are not fully valid in the regime of software and services, as the report from the EOSC Architecture Working Group on Scholarly Infrastructures for Research Software points out¹⁹. This is predominantly because software usually follows a more complex life cycle with elements such as development and maintenance which are not covered by the FAIR principles.

The choice of Zenodo²⁰ as the repository back-end (see Section 3.1) provides the basis for a FAIR and sustainable infrastructure¹. The OSSR policy furthers the adoption of the FAIR principles by imposing requirements on licensing and metadata before submissions are accepted into the OSSR (see Section 2.3). In particular, licensing ensures legal security for the user of the resources and is therefore considered an essential part of the "re-usability" requirement of FAIR resources. In addition, the usage of an extended and common metadata schema strengthens the "findability". Guidelines for license, provenance, and metadata have been developed². In order to meet the special demands for software, the OSSR linksdevelopment platforms, the repository itself, and additional information related to the software.

2.4 Policy

The OSSR policy³ provides the requirements, recommendations, guidelines, and user agreement to contribute to the repository and enforce its goals to create high-quality scientific products. The guidelines and rules of participation therefore contain as one of two obligatory clauses that the submission has a license, such that it is clear what use of the software or service is legal. However, the degree of openness of the license is not defined, although open licenses are recommended and various resources provided⁴ to help to choose a suitable license.

The aim to provide high-quality software and services leads to a number of requirements and recommendations. In particular, a minimum amount of provenance information needs to be provided together with the software, as well as a metadata file in a common human- and machine readable format (CodeMeta, see Section 3.4.1), enabling users and services to find it, understand the status, and integrate it in their respective environments. This metadata file must be provided as part of the archived record and must include a link to the software documentation, a versioning scheme, and author contact details. Compliance with these requirements is checked during the curation process described below.

Beyond these minimal requirements, the application of software quality standards such as the use of a testing scheme is encouraged. A software checklist is provided based on the outcomes of the Workshop on Open-Source Software Lifecycle organised by ESCAPE (see Section 4.2) which also includes external references³. The choice of the Zenodo platform to host the OSSR submissions results in an implicit requirement to agree with the Zenodo terms of use² before a submission can be included in the OSSR. To ensure quality and trustability, the integration of a new record in the OSSR is submitted to a curation process, validating its compliance with the guidelines and serving as a gatekeeper to the OSSR.

Apart from the quality standards described above, no strict restrictions are placed on the nature of the contribution, so entries might vary from installable software to analysis workflows to meta packages, including middleware. Beyond the contribution's quality, the relevance for the field of research serves as a selection criterion.

2.5 Curation

The curation process is overseen by a board of members of the ESCAPE open collaboration that meets monthly. This curation board initially consists of ESCAPE project members, but new members can join from the communities served by the OSSR in the future by joining the ESCAPE open collaboration. The board members, led by an assigned coordinator, are nominated from the open collaboration representatives. After the onboarding presentation and initial upload to Zenodo, new OSSR contributions are assigned to a board member. During curation, the items on the software checklist are checked based on the onboarding presentation, the software repository, the software documentation, and the provided metadata. The metadata itself is checked using a validator (see section 3.4.3) which signals missing required and recommended metadata. Curation is an iterative process: the curator will point the submitter of a new contribution to deficiencies and suggest improvements to meet the OSSR policy requirements. At the end of a (successful) curation process, the curator will make the Zenodo entry part of the ESCAPE community. At this point, the contribution is officially part of the OSSR.

To make sure the entries continue to meet the OSSR policy, the curation board will oversee the removal of the entries that no longer meet the requirements byreviewing all entries on a yearly basis. Examples of reasons for removal include the software no longer being maintained (defined by no new versions uploaded), or a change to an incompatible license. Zenodo entries will never be deleted, but will no longer be part of the OSSR by being removed from the Zenodo community (see section 3.1).

2.6. Related Work

Other significant domain-specific catalogues of software exist. In the communities covered by ESCAPE, the Astrophysics Source Code Library (ASCL)^{21,22} is worth noting. This is an extensive catalogue of codes used in astronomy/astrophysics research that has been around since 1999. The ASCL is curated by a small team of editors, but unlike the OSSR it does not really assess the quality and sustainability of the codes submitted for inclusion in the catalogue. In principle, all code

¹https://about.zenodo.org/principles/

²https://about.zenodo.org/terms/

that is used in a peer-reviewed paper or Ph.D. thesis is accepted in the catalogue. This includes code that is not open source. It also does not archive the software, but relies on links to the software instead. Although an effort is made by the community and editors to keep these links up to date, it is inevitable that some of the catalogue entries end up with dead links over time. A relatively new service is the Resource Software Directory3. This catalogue is not thematic and takes the different approach of harvesting information from source code repositories such as GitHub, GitLab and Zenodo and link those to a description of the software and to publications that cite the software. Like the ASCL it does not actually archive the software. It does not assess the quality and sustainability of the software, but the catalogue does provide some statistics about the software that makes it easy to establish whether the software is still actively maintained. Since the OSSR is built on top of Zenodo, including the complete OSSR into the Resource Software Directory would be possible. An effort is underway to achieve this goal.

There is active exchange between the academic discipline and institutional software registries and repositories within the SciCodes Consortium. https://scicodes.net/

3 OSSR technical implementation

3.1 A curated community of the Zenodo repository

The core of the OSSR is implemented as a curated community, named escape2020, of the Zenodo general-purpose repository20, of the Zenodo general-purpose as it is developed as an open-source project between CERN⁴ and the OpenAIRE project⁸, and is hosted by CERN, a partner of the ESCAPE project⁸. It is developed to respect the FAIR principles and is compliant with the recommendations from OpenAIRE as well as FAIR4RS¹⁸. Its main features are to provide a long-term, safe and secure archive. The service is able to deal with many kinds of content and implements publication versioning, providing a unique Digital Object Identifier (DOI) for each version, thus allowing precise citation of the used software, workflow, or dataset. Its long-term sustainability as well as machine- and

3.2 eOSSR library

A Python3 (RRID:SCR_008394) library called eOSSR^{6,7} has been developed as a central tool to interact with the OSSR. The library provides an API for exchanging information with the OSSR, such as pushing new contributions or searching and retrieving existing ones. It also includes the OSSR metadata definition and requirements based on CodeMeta and means to convert and validate the metadata associated to software records. Finally, it implements OSSR policies to allow automated validations and ease of the curation process.

The eOSSR library is open-source, it has been onboarded in the OSSR, so it can be found by the community and its documentation can be found online⁶.

3.3 API and GitLab to Zenodo

The eOSSR uses Zenodo's Application Programming Interface (API) to provide a set of high-level functionalities to programmatically communicate with the OSSR, as an alternative to the Zenodo web interface. Python functions or command-line tools allow for example to find software in the OSSR through full text searches, or specific searches using recognized metadata, e.g. keywords or file types. The API also provides several general purpose functions to query Zenodo content such as records, communities, licenses, grants, or funders. Using Zenodo tokens, the library can be used to programmatically modify existing metadata records, or to publish new ones. This functionality eases the publication of software from GitLab⁷ (RRID:SCR_013983) to Zenodo, offering a similar functionality to the Zenodo-GitHub integration8. eOSSR provides docker containers and code snippets that can be integrated in any GitLab continuous integration (CI) to automatically publish software in Zenodo when a new version is released (see workflow in Figure 1). More information can be found in the eOSSR documentation.

 $^{{}^{8}}https://docs.github.com/en/repositories/archiving-a-github-repository/referencing-and-citing-content\\$

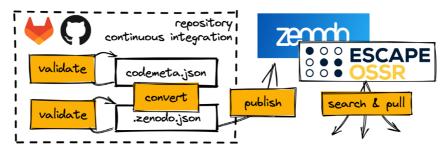


Figure 1. A typical software publication workflow in the Open-Source and Software Repository (OSSR) using the eOSSR library and repositories continuous integration.

human-interactionability are key aspects of the goals of the OSSR.

³https://research-software-directory.org/

⁴https://home.cern

⁵https://www.openaire.eu

⁶https://purl.org/escape/ossr/eossr-documentation

⁷https://about.gitlab.com/

3.4 Software Metadata

The purpose of metadata is to provide structured information about the entity it describes in order to improve its discoverability and reuse, as well as to provide information about its quality and reliability. A format like CITATION.cff⁹, developed for software citation, is therefore not sufficient to fully describe software. The OSSR metadata is based on CodeMeta to also include links to the software code repository, documentation, and CI environment. This format meets the OSSR requirements, is extensible, and has been created specifically to describe scientific software and analysis. The choice of CodeMeta makes software version and persistent identifiers part of the metadata and helps to fulfill the FAIR4RS principles¹⁸. The ASCL has also adopted codemeta as a standard to help populate the catalogue, but metadata here is limited to what is relevant for citation of the software.

The FAIR4RS principles emphasize metadata for software for the Findable, Accessible, and Interoperable parts of the FAIR acronym. To make software Findable they require that the software is described by rich metadata, that this metadata clearly and explicitly identifies the described software and that the metadata itself is FAIR, searchable and indexable. To make software accessible and interoperable, it is required that the metadata remains accessible and can be retrieved using a standardized protocol even if the software is no longer available. The OSSR meets this requirement by making the metadata part of the Zenodo record for the software. This allows the eOSSR software library to retrieve the CodeMeta file through the Zenodo API. The OSSR metadata also answers ESFRI's requirements to clearly identify the software providers, the affiliated packages and open-community versions while being available in the same repository. The interoperability is illustrated by the integration between the OSSR and the ESFRI Science Analysis Platform (ESAP) discussed later in this paper, see Section 5.2.

3.4.1 CodeMeta. CodeMeta²³, is a cross-platform and common standard metadata schema, has been selected by the OSSR to describe software. It is a metadata schema based on Schema.org¹⁰ (RRID:SCR_018291) and developed to describe software artifacts. It provides a standardized way to describe the software and its dependencies, as well as auxiliary information such as licenses, documentation, contact details, or development practices used to create it. It is based on the JSON-LD format, which allows the metadata to be easily embedded in the software's source code repository or distributed as a separate file named codemeta.json.

One of the main goals of CodeMeta is to facilitate the integration of software metadata with other research and discovery tools, such as search engines, citation indexing systems, and research data repositories. By providing a common metadata standard, CodeMeta aims to improve the interoperability and reuse of software within the research community, as well as to provide a means for researchers to properly acknowledge and cite the software they use in their work.

3.4.2 CodeMeta-Zenodo crosswalk. Zenodo has its own internal metadata schema for describing records such as software artifacts. CodeMeta is not yet supported natively by Zenodo, even though in the integration plan¹¹. Therefore, a converter, based on the CodeMeta official crosswalk¹², is provided in the eOSSR documentation to convert CodeMeta metadata into Zenodo metadata.

3.4.3 Metadata toolbox: generator, validator, and converter. Based on the metadata definition, three sets of tools have been developed to ease a software provider's life. All links and documentation to use these tools are available on the OSSR pages⁴.

Generator: The official CodeMeta online generator has been adapted to generate specifically ESCAPE metadata following the CodeMeta schema.

Converter: A CodeMeta-Zenodo metadata converter has been implemented in the eOSSR library. It is used internally in the library during software publication so that CodeMeta can be used as the source of metadata. It can also be used directly through a command line interface, or online.

Validator: A validator has also been developed. It can be used as a command line tool, *e.g.* during development or in continuous integration workflows to ensure that the CodeMeta file is always compliant with the up-to-date OSSR requirements, or with its online version to help creating a valid CodeMeta file.

3.5 Curation and onboarding process

The onboarding process³ serves two main purposes: on the one hand, the quality of the contributed software is ensured by checking the adherence to community standards, on the other hand, it offers a forum for discussion for the contributors to present their project and consider further enhancements and cooperation. The main steps in the process are:

- registration for the onboarding process, providing contact and software references,
- 2. giving an onboarding presentation introducing the software,
- 3. adding the software to Zenodo and applying for membership in the ESCAPE OSSR community, and
- 4. curation of the software and acceptance in the ESCAPE OSSR Zenodo community.

In the initial setup during the ESCAPE project, the various steps were organized on standard services setup for the ESCAPE

⁹https://citation-file-format.github.io/

¹⁰https://schema.org

¹¹https://github.com/inveniosoftware/invenio-swh/issues/4

¹²https://CodeMeta.github.io/crosswalk/

project (a Redmine platform¹³, an Indico platform¹⁴ and the GitLab (RRID:SCR_013983) IN2P3 platform¹⁵). After completion of the project in January 2023, the process is reorganized on gitlab.com¹⁶ ensuring centralized documentation and communication. Registration for the onboarding process (1) is managed by opening an issue, information on the contribution is collected there and, finally, the curation process is triggered (3 & 4) and managed by automatically created merge requests to a curation repository. The onboarding presentation (2), for which a template is provided, can be given at dedicated online meetings, during which presentations are recorded. The community is invited to discuss application of and cooperation for the presented software. This additional information is made available for each entry on the OSSR website⁴.

3.6 Reusability

The OSSR environment and tools use technologies that allow easy adoption by other institutes or communities. The setup answers the FAIR principles and can be reused by another domain that could create its own Zenodo community and configure the external tools (e.g. onboarding, eOSSR and specific metadata usage) to easily and rapidly set its own curated repository.

4 Community building

The OSSR mission includes the discussion and dissemination of best practices among the research community in order to improve the skills and knowledge of its researchers in building open science and therefore to grow its number of contributors. Training in the form of dedicated schools is an important part of this process, as it helps to ensure that research software developers and maintainers are able to effectively contribute. These schools provide an opportunity for participants to learn about the principles and practices of open-source software development, and to gain hands-on experience working on projects within the community. This helps to ensure that the repository is able to continue to grow and evolve over time, and that it remains a valuable resource for the ESFRIs and wider research community.

4.1 ESCAPE data science schools

The ESCAPE data science schools are the continuation of the three ASTERICS-OBELICS international schools⁹⁻¹¹ which were organized from 2017 to 2019 in Annecy (France) for PhD students, postdocs, and senior researchers working in the domain of astrophysics and astroparticle physics, as part of the ASTERICS H2020 project¹⁷.

During the ESCAPE project, two schools have been organized^{12,15}. The schools' program includes courses on machine learning, big data, organizing coding environments,

The first ESCAPE data science school¹² was organized online due to the COVID-19 pandemic restrictions. The lectures were live-broadcasted on YouTube and their recordings are still openly available on the platform¹⁹. The school took place in June 2021 with over a thousand registrants and seventeen tutors^{13,14} and a schedule spanned over 12 days.

In June 2022, the second ESCAPE data science school¹⁵ was held, this time in person, at the original location in Annecy, France, with a restricted audience.

Following the FAIR principles, the complete material of the courses including the presentations, exercises, and their solutions were put together in public GitHub repositories²⁰, allowing a collaborative and live construction of the material and knowledge by all tutors and participants. At the end of the schools, all the content was published on the OSSR, following a similar life-cycle as software.

4.2 Workshop WOSSL

As part of the community building effort, a workshop on open-source software life cycles²¹ was organized in July 2020. The objective of the workshop was to bring together the scientists' communities and ESFRIs of astrophysics, astroparticle physics, and particle physics who are supporting, leading, or financing the software development within their domain. Common and best practices in software development were discussed and shared, enabling cross-fertilization across the domains. During the workshop a wide range of topics were presented and discussed, ranging from software engineering techniques through software licensing best practices to concrete examples of software to be onboarded. The outcomes of this workshop -e.g. recommendations on containerization and the need for a GitLab-Zenodo integration - were used to further shape the OSSR guidelines as well as the repository's implementation. They form inputs for the ESCAPE Data Science schools for training young scientists to build and maintain the expertise in the field.

best practices in data management and collaborative research using state-of-the-art tools, continuous development and integration of software, and also low-level optimization including debugging and profiling. Python3 was chosen as the main programming language for most of the courses due to its popularity and rich ecosystem of scientific libraries and resources. The program includes theoretical and hands-on training such that participants can leave with new skills and ideas directly applicable to their own work. During the schools, participants were able to communicate with each other and the tutors *via* chat messages using Slack¹⁸ to raise issues, ask questions about the courses, as well as to socialize.

¹³https://projectescape.eu/

¹⁴https://indico.in2p3.fr/category/841/

¹⁵https://gitlab.in2p3.fr/escape2020/wp3

¹⁶https://gitlab.com/escape-ossr/

¹⁷https://www.asterics2020.eu/

¹⁸https://slack.com/intl/en-gb/

¹⁹https://www.youtube.com/live/TUrJ_IudVx8

²⁰https://github.com/escape2020/school2021,https://github.com/escape2020/school2022

²¹https://escape2020.pages.in2p3.fr/wp3/wossl/

5 Adoption and interactions

The OSSR is more than a simple software catalog as it provides a place for researchers and developers of ESFRIs to collaborate, share knowledge, and access a wide variety of tools and resources. As such, it can be used by other services and projects to provide a common platform.

5.1 Integration with EOSC Infrastructure

The OSSR was initiated within the EOSC environment and is fully embedded into the EOSC Infrastructure²² and thus its community uptake and usage statistics are openly accessible in the EOSC Explorer²³. It is registered as repository at re3data.org²⁴ and consequently its content is automatically harvested by the OpenAIRE Explore platform²⁵.

5.2 Integration with Matter and Technologies

Matter and Technologies (MT), a research program in the Helmholtz Association, combines development of both accelerators and detectors, and also focuses on the challenges of high-rate data ingestion from large-scale facilities, experiments, observatories, and accelerators. Data Management and Analysis (DMA) is one of three topics within MT, and focuses on and is driven by the data needs and challenges of the science within MT. The main goal of the Subtopic 2 of MT-DMA is to build an open-source repository with diverse software projects used for simulations and data analysis in Helmholtz institutes. Due to very similar objectives, requirements, and goals of OSSR and MT-DMA a decision towards a common effort was made and a cooperation was established. DMA software projects will be added to the OSSR repository as a sub-federation, profiting from well-established onboarding / curation processes, and metadata definition. In return, OSSR will gain more visibility and will be enriched by new entries from other fields such as gamma-and nuclear physics.

5.3 Integration with ESFRI Science Analysis Platform

The ESFRI Science Analysis Platform (ESAP)^{16,17} is a flexible toolkit designed to be used by ESCAPE project partners and others to easily deploy and customize their own platforms. The ESAP was created within a work package of the ESCAPE project and is able to connect together external services and other services developed by ESCAPE. To meet this goal, it is designed to be configurable, flexible, and extensible. This is achieved through the simplicity by which APIs can be integrated in the platform.

Services currently integrated into the ESAP include elements of International Virtual Observatory Alliance (IVOA) tools²⁴, various archives of ESFRIs and other observatories, a batch

data processing framework and the possibility to search the ESCAPE data lake. For example, integrating IVOA tools gives the ESAP the ability to locate and access data for processing using Virtual Observatory (VO) systems, and use the IVOA-SAMP²⁵ standard.

A key feature of the ESAP is interactive analysis, which enables scientists to perform an analysis in real-time. Through the platform, users can search for and deploy software using JupyterLab²⁶ on binderhub-like²⁶ services²⁷. The list of available software includes eligible packages from the OSSR repository. The ESAP utilizes the eOSSR library (see Section 3.2) to search Zenodo for ESCAPE-community software. If the metadata of a software package contains the correct metadata entry, it will automatically be detected by the platform and be presented to users for deployment.

Additionally, from the ESAP-archive page, Zenodo can be accessed directly, also taking advantage of the eOSSR library. Users are able to search for entries of all types across all communities. The ESAP software stack was onboarded as an entry to the OSSR.

6 Conclusion and outlook

In conclusion, the ESCAPE Open-source Software and Service Repository (OSSR) serves as a central location for the dissemination and use of trusted open-source software in the fields of astronomy, astroparticle physics, and particle physics. Based on the general-purpose repository Zenodo, the OSSR is designed to make it easy for researchers, developers, and ESFRIs to find, access and download the software and services in their community, and to contribute their own tools and services. The curation process happening during the onboarding of software improves the quality of contributions, ensuring they comply to the FAIR principles, and makes the OSSR a source of trusted software that can be used for scientific analysis. The tools developed by the project, such as metadata generator, converter, and validator can ease the developers' life by streamlining the software life cycle and could increase the number of contributions by lowering the barrier to sustainable open-science. The OSSR is also a place to share the know-how and best-practices of the community. By providing training on scientific software and analysis development and championing the FAIR principles, it accelerates their implementation within the community and ESFRIs. The OSSR is integrated in the EOSC infrastructure and will continue to grow and is supported by the ESCAPE Open Collaboration Agreement²⁷.

Disclaimer

The views expressed in this article are those of the authors. Publication in Open Research Europe does not imply endorsement of the European Commission.

²²https://marketplace.eosc-portal.eu/

²³https://explore.eosc-portal.eu/search/dataprovider?datasourceId=re3data___::c19518b015a3941a3e0675d398ca33f6

²⁴https://www.re3data.org/repository/r3d100013827

²⁵https://explore.openaire.eu/search/dataprovider?datasourceId=re3data____:: c19518b015a3941a3e0675d398ca33f6

²⁶https://binderhub.readthedocs.io/en/latest/index.html

²⁷https://indico.in2p3.fr/event/27202/

Ethics and consent

Ethical approval and consent were not required

Data availability

No data are associated with this article

Acknowledgments

We would like to thank all partners of the ESCAPE WP3 group that participated in shaping and building the OSSR: the Leibniz-Institut für Astrophysik Postdam (AIP), the European Organization for Nuclear Research (CERN), the Centre National de la Recherche Scientifique (CNRS-CPPM, CNRS-LAPP), the Cherenkov Telescope Array Observatory

(CTAO), the European Gravitational Observatory (EGO), the Friedrich-Alexander-Universität Erlangen Nürnberg (FAU), the GSI Helmholtzzentrum für Schwerionenforschung GmbH (GSI), the HITS gGmbH, the Instituto de Fisica de Altas Energias (IFAE), the Istituto Nazionale di Fisica Nucleare (INFN), the Joint Institute for Very Long Baseline Interferometry as a European Research Infrastructure Consortium (JIVE), the Max-Planck-Gesellschaft zur Förderung der Wissenschaften (MPG-MPIK), the Centrum Wiskunde & Informatica, part of NWO-I, OROBIX, the SKA Organisation (SKAO), the Universidad Complutense de Madrid (UCM) and the Universita Degli Studi di Roma Torvergata (UNITOV).

We also thank Carsten Denker and Meetu Verma (AIP) for their feedback on the first draft of this article.

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Open Peer Review

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Version 2

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Cristóbal Bordiú 🗓



Istituto Nazionale di Astrofisica, Bologna, Italy

This article nicely outlines the Open Source Software and Service Repository (OSSR) developed in the context of the ESCAPE project. Promoting Open Science practices, not only for data but also for software and services, is definitely crucial to maximise scientific exploitation and ensure reproducibility in this age of massive and increasingly complex datasets. Moreover, the emphasis on acknowledging developers' effort and contribution is much needed. The significance of having such a software repository is thus evident.

The article is well written and organised, providing sufficient context and a comprehensive overview of the project-specific goals before diving into the technical details of the OSSR implementation. In particular, the authors make a good effort in explaining the different assets that compose the OSSR from a high-level perspective. They also clearly underline what makes the OSSR different from other solutions like the ASCL.

I only have a few minor comments/questions:

- 1. Sec. 1: "...published,more..." [missing whitespace]
- 2. Sec. 2.1: "...suitable candidate contributions will be actively approached by the OSSR community ..." [How does the OSSR community monitor the "software ecosystem" to find those "suitable candidate contributions" in order to approach them?]
- 3. Sec 2.3: "...the OSSR linksdevelopment platforms"... [missing whitespace]
- 4. Sec 2.4: "...the relevance for the field of research serves as a selection criterion" [how is the relevance evaluated? this may be a source of bias]
- 5. Sec 2.5: "byreviewing" [missing whitespace] // "...Examples of reasons for removal... no new versions uploaded..." [This could be dangerous. What period of time without new updates is needed to consider the software is no longer maintained? Anyway, well-built codes can still be useful even if they're no longer maintained.]
- 6. Sec 3.1: "FAIR4RS" [expand the acronym on 1st appearance]
- 7. Sec 3.3: "The eOSSR uses Zenodo's Application Programming Interface (API) to..." [change to Zenodo's API, as API has been already expanded in Section 1]

- 8. Sec 3.4.2: "even though (it is present) in the integration plan"
- 9. Sec 3.5: "...the process is reorganized on gitlab.com" [it would be better to refer to Gitlab (the platform) instead of the webpage (gitlab.com), especially since you put the URL in the footnote.]

Is the rationale for the Open Letter provided in sufficient detail? (Please consider whether existing challenges in the field are outlined clearly and whether the purpose of the letter is explained)

Yes

Does the article adequately reference differing views and opinions?

Are all factual statements correct, and are statements and arguments made adequately supported by citations?

Yes

Is the Open Letter written in accessible language? (Please consider whether all subjectspecific terms, concepts and abbreviations are explained)

Yes

Where applicable, are recommendations and next steps explained clearly for others to follow? (Please consider whether others in the research community would be able to implement guidelines or recommendations and/or constructively engage in the debate) Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Astrophysics & Software engineering

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Version 1

Reviewer Report 19 July 2023

https://doi.org/10.21956/openreseurope.16954.r33278

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Diomidis Spinellis 🗓

- ¹ Athens University of Economics and Business, Athens, Greece
- ² Department of Software Technology, Delft University of Technology, Delft, South Holland, The Netherlands

This paper describes the goals and high-level implementation of a repository to host software in the fields of astronomy, astroparticle physics, and particle physics. This is interesting work, which however requires many improvements and considerable refinement.

Regarding soundness, the study's contributions seem to address its goals, but in some cases the applied research methods lack the required rigor. It is unclear what specific requirements drove the development of the platform and how these were collected. At no point does the text clarify how services (as mentioned in the title) are supported by the repository. The library's API is neither described nor referenced. Importantly no attempt is made to evaluate the platform. Threats to validity and their effect on the results' soundness are not explicitly presented.

Regarding significance, no motivation is provided for performing the research. The work's potential impact to the field is clear, but not substantiated.

Regarding novelty, there is no systematic presentation of existing work in the area. It is not apparent how the work's contributions offer an improvement over to the state-of-the-art. Many other repositories that can, in theory, satisfy the described goals exist. No empirical evidence is offered to show that ESCAPE improves upon the state of the art. A table listing similar repositories and the quantitative and qualitative attributes of each one would help in this direction.

Regarding verifiability and transparency, the method's description and the provided data allow the independent verification of the outlined findings. The study's verifiability would benefit by providing additional materials to support independent verification or replication of the paper's claimed contributions. In particular the study would benefit from a quantitative analysis of the repository's and the library's usage in terms of uploads, downloads, citations, and content and the extent to which the stated goals have been satisfied.

Regarding presentation, the paper's structure can be improved. In a number of places (see below) terms are used before they are introduced. The paper does not follow a typical research study structure. This would not be a problem, if the corresponding material (methods, results, related work) was present and easily identifiable, which however is not the case. The writing is clear and easy to understand. The paper is mostly well-written, though some typos and grammar errors can distract the reader. Careful copy-editing is required. Some minor issues are identified below. The formatting follows the provided instructions. Note that superscripts are commonly set after commas and periods. The abstract is self-standing and summarizes succinctly the paper's essence. The paper could benefit from the addition of figures in particular ones visualizing quantitative attributes of the repository's use.

Minor comments

- Section -1: Please start with a short description of the problem and current solutions, followed by your contribution. The project can be described later on as an enabler for your work or part of your methods.
- Section -Summary: Consider changing "is reliable and open-source" into "is reliable and

distributed under an open-source license".

- o Please expand all initials FAIR ,SIRS, WOSSL) on their first use
- Section -2.1: Please rephrase the content to reflect the research's goals rather than outcomes.
- Section -2.2: Please start by introducing the FAIR principles and their importance to scientific research
- Section -2.3: Consider changing "such that" into "so that".
- Section -2.3: Consider changing "trustability" into "trustworthiness".
- Section -2.4: Please specify, how often does the board meet? How is the board governed?
 How are outdated entries detected and reviewed?
- Section -3.2: Please specify which specific policies are validated through the library. What prevents a cloned library that skips validation to push a contribution to OSSR?
- Section -3.3: Consider changing "docker" into "Docker".
- Section -3.4: Please introduce CodeMeta before referring to it.
- Section -3.4.3: Please clarify how these tools are used. Are they accessed through the command line, do they offer a graphical interface?

Is the rationale for the Open Letter provided in sufficient detail? (Please consider whether existing challenges in the field are outlined clearly and whether the purpose of the letter is explained)

No

Does the article adequately reference differing views and opinions? No

Are all factual statements correct, and are statements and arguments made adequately supported by citations?

Partly

Is the Open Letter written in accessible language? (Please consider whether all subject-specific terms, concepts and abbreviations are explained)

Partly

Where applicable, are recommendations and next steps explained clearly for others to follow? (Please consider whether others in the research community would be able to implement guidelines or recommendations and/or constructively engage in the debate)

Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Software engineering

I confirm that I have read this submission and believe that I have an appropriate level of expertise to state that I do not consider it to be of an acceptable scientific standard, for reasons outlined above.

Author Response 27 Oct 2023

Thomas Vuillaume

We thank the reviewer for their time and effort in reviewing our work. Their comments and feedback were essential to improve the paper and we have taken them into consideration to better explain the genesis and goals of the ESCAPE OSSR. Upon careful consideration of their comments, we recognize that there appears to be a difference in perception regarding the scope and purpose of the article, as well as the thematic focus of the journal to which we are submitting. Specifically, it seems that the main point of contention is whether the paper is intended to function as an overview or a technical paper. As an open letter, our intent here is not to be technically exhaustive but to present the views and ideas behind the ESCAPE OSSR. Previous works, cited here, present these technical details more thoroughly. We have revised the manuscript to better reflect its purpose. In addition, the ESCAPE project deliverables (https://projectescape.eu/deliverables-and-reports) deliver a more in-depth technical view of the OSSR, in particular https://projectescape.eu/deliverables-andreports/d33-conceptual-design-report-software-and-service-repository and https://projectescape.eu/deliverables-and-reports/milestone-17-status-common-softwareand-services-proposal-and-integration. All the minor comments have been corrected in the second version of the manuscript and we would like to provide some answers to your valid questions: Regarding the API, it appears that there might be a misunderstanding of its goal as it does not provide an interface to the hosted services but to the OSSR itself, allowing automated management of its content. The technical description of the API is done in 10.48550/arXiv.2212.00499 and in the online, up-to-date, documentation (https://escapeossr.gitlab.io/eossr/), we believe it was not the purpose of this paper to present it. The services are not provided through the OSSR, they are recorded via their software or documentation in the OSSR. The OSSR API is therefore not designed to access these services directly.

Competing Interests: No competing interests were disclosed.

Reviewer Report 12 July 2023

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Michael Zingale

Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York, USA

This article describes an open source software repository, ESCAPE. This is a very nice project and the authors are clearly excited about promoting open source scientific software. Overall, I only have minor comments.

There are a lot of acronyms in the article, which makes it very difficult to read. For example FAIR is used 4 times before it is actually defined. SIRS is never defined. These acronyms should be defined when they are first used. Even better would be to include a table of abbreviations. It is a little unclear what type of software is welcomed in the ESCAPE repository. The authors should list some of the packages (and their uses) that are already in ESCAPE. My read of this article suggests that ESCAPE is primarily for experimental/observational codes, but what about simulation/theoretical codes?

More discussion about the relation to other repositories would be useful. For example, how does this differ from the goals of the Astronomy Source Code Library (ASCL)?

The procedure by which a package is added to ESCAPE should be expanded. Can the author of a package ask to be included? And what if ESCAPE wants to add a package but the authors of that package don't want to be included – is there a procedure for that?

Overall this is a nice resource, and my comments above are primarily meant to help readers more clearly understand the goal and how they will benefit from ESCAPE.

Is the rationale for the Open Letter provided in sufficient detail? (Please consider whether existing challenges in the field are outlined clearly and whether the purpose of the letter is explained)

Yes

Does the article adequately reference differing views and opinions?

Yes

Are all factual statements correct, and are statements and arguments made adequately supported by citations?

Yes

Is the Open Letter written in accessible language? (Please consider whether all subject-specific terms, concepts and abbreviations are explained)

Yes

Where applicable, are recommendations and next steps explained clearly for others to

follow? (Please consider whether others in the research community would be able to implement guidelines or recommendations and/or constructively engage in the debate) Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Computational astrophysics

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Author Response 27 Oct 2023

Thomas Vuillaume

We thank the referee for their time and effort reviewing our work. We believe all comments have been addressed in the version 2, in particular:

- the missing acronyms definitions have been added;
- a section comparing the OSSR to similar initiatives, especially the ASCL, has been added (section 2.6);
- The OSSR is open to all community software and code bases, observational and theoretical, there are already entries of both in the repository. Wwe added this OSSR aim to the text (section 2.1) as well as a the link to the always up-to-date list of entries (section 5.1);
- Software is added by the authors of the code themselves, it is not pulled by the ESCAPE community. This has been made clearer in the text (section 2.1) now.

Competing Interests: No competing interests were disclosed.