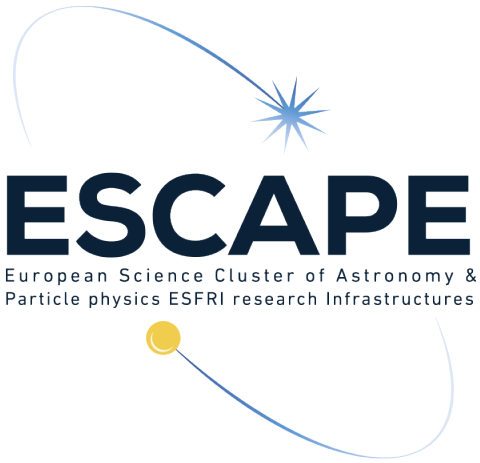

Project Title	European Science Cluster of Astronomy & Particle physics ESFRI research Infrastructure
Project Acronym	ESCAPE
Grant Agreement No	824064
Instrument	Research and Innovation Action (RIA)
Topic	Connecting ESFRI infrastructures through Cluster projects (INFRA-EOSC-4-2018)
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MS14: LIST OF SOFTWARE AND SERVICES

Work Package	WP3, OSSR - Open Science Software and Service Repository
Lead Author (Org)	Kay Graf (FAU)
Contributing Author(s) (Org)	
Due Date	30.04.2020, M15
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Version	1.1

Dissemination Level

X	PU: Public
	PP: Restricted to other programme participants (including the Commission)
	RE: Restricted to a group specified by the consortium (including the Commission)
	CO: Confidential, only for members of the consortium (including the Commission)

Versioning and contribution history

Version	Date	Authors	Notes
1.1	29.04.2020	Kay Graf (FAU)	Add final remarks and cosmetics
1.0	20.04.2020	Kay Graf (FAU)	Implementing return of review session
0.1	02.04.2020	Kay Graf (FAU)	Start of drafting

Disclaimer

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Executive Summary

This document constitutes MS14 of the ESCAPE project, the review of the D3.2, the *Software and Service List and Integration Plan.* ESCAPE partners will contribute the listed software and services to the *ESCAPE Work Package 3* and especially to the *OSSR (Open source Software and Service Repository)*.
The review contains general considerations and recommendations towards the establishment of a collection of community software and services within the OSSR.

Project Summary

ESCAPE (European Science Cluster of Astronomy & Particle physics ESFRI research infrastructures) addresses the Open Science challenges shared by ESFRI facilities (SKA, CTA, KM3NeT, EST, ELT, HL-LHC, FAIR) as well as other pan-European research infrastructures (CERN, ESO, JIVE) in astronomy and particle physics. ESCAPE actions are focused on developing solutions for the large data sets handled by the ESFRI facilities. These solutions shall: i) connect ESFRI projects to EOSC ensuring integration of data and tools; ii) foster common approaches to implement open-data stewardship; iii) establish interoperability within EOSC as an integrated multi-messenger facility for fundamental science. To accomplish these objectives, ESCAPE aims to unite astrophysics and particle physics communities with proven expertise in computing and data management by setting up a data infrastructure beyond the current state-of-the-art in support of the FAIR principles. These joint efforts are expected to result into a data-lake infrastructure as cloud open-science analysis facility linked with the EOSC. ESCAPE supports already existing infrastructures such as astronomy Virtual Observatory to connect with the EOSC. With the commitment from various ESFRI projects in the cluster, ESCAPE will develop and integrate the EOSC catalogue with a dedicated catalogue of open-source analysis software. This catalogue will provide researchers across the disciplines with new software tools and services developed by astronomy and particle physics community. Through this catalogue, ESCAPE will strive to provide researchers with consistent access to an integrated open-science platform for data-analysis workflows. As a result, a large community "foundation" approach for cross-fertilisation and continuous development will be strengthened. ESCAPE has the ambition to be a flagship for scientific and societal impact that the EOSC can deliver.

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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.

Acronym list

Partners

AIP	Leibnitz-Institut für Astrophysik Potsdam
CERN	European Organization for Nuclear Research
CNRS-LAPP:	Laboratoire d'Annecy de Physique des Particules (CNRS)
CNRS-CPPM:	Centre de Physique des Particules de Marseille (CNRS)
NWO-I-CWI:	Centrum Wiskunde & Informatica (NWO-I)
CTA:	Cherenkov Telescope Array
CTAO:	Cherenkov Telescope Array Observatory
EGO-Virgo:	European Gravitational Observatory
CERN:	European Organization for Nuclear Research
EST:	European Solar Telescope
ESO:	European Southern Observatory
ELT:	Extremely Large Telescope (was E-ELT)
FAIR:	Facility for Antiproton and Ion Research
FAU:	Friedrich-Alexander University Erlangen-Nuremberg
GSI:	GSI Helmholtzzentrum für Schwerionenforschung
HITS:	Heidelberg Institute for Theoretical Studies
HL-LHC:	High-Luminosity Large Hardon Collider
IFAE:	Institut de Fisica d'Altes Energies
INFN:	Istituto Nazionale di Fisica Nucleare
JIVE:	Joint Institute for VLBI ERIC
AIP:	Leibnitz-Institut für Astrophysik Potsdam
MPG-MPIK:	Max-Planck-Institut für Kernphysik (MPG)
KM3NeT:	multi-km3 sized Neutrino Telescope
NWO-I-Nikhef:	Nationaal instituut voor subatomaire fysica (NWO-I)
OROBIX:	OROBIX SRL
SKA:	Square Kilometre Array
SKAO:	Square Kilometre Array Organisation
UCM:	Universidad Complutense de Madrid
UNITOV:	Universita degli Studi di Roma Torvergata

General

ASTERICS:	Astronomy ESFRI & Research Infrastructure Cluster
E-EAB	ESCAPE External Advisory Board
E-EB	ESCAPE Executive Board
EOSC:	European Open Science Cloud
EOSC-Hub:	Integrating and managing services for the European Open Science Cloud
ESCAPE:	European Science Cluster of Astronomy & Particle physics ESFRI research infrastructures
ESFRI:	European Strategy Forum on Research Infrastructures

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ESF/RI:	ESFRIs and major RIs as projects within ESCAPE
FAIR:	Findable, Accessible, Interoperable, Reusable
IVOA:	International Virtual Observatory Alliance
KPI:	Key Performance Indicator
OSSR:	Open Science Software and Service Repository (ESCAPE WP3 itself and the final product within the EOSC catalogue of services)
RDA:	Research Data Alliance
RI:	Research Infrastructure
TSP:	Test Science Project
VO:	Virtual Observatory
WP:	Work Package

Reference Documents, Deliverables and Milestones

D3.1	Deliverable D3.1: Detailed project plan for ESCAPE WP3
D3.2	Deliverable D3.2: Software and service list and integration plan
D3.3	Deliverable D3.3: Conceptual design report on the software and service repository, demonstrator
MS14	Milestone 14: List of software and services (review of D3.2)
MS17	Milestone 17: Progress of common software and service proposition

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1. Introduction and Background

A review of the *D3.2: Software and Service List and Integration Plan* was performed in a review session and a collection of feedback by all partners.

The deliverable was reviewed along the following guidelines:

- General content;
- Extent and completeness of the software and service list, especially with the objective of enabling open science involving the ESCAPE communities;
- Solidity of the implementation scheme;
- Missing steps towards OSSR (from the software/service collection perspective).

Also, feedback from the E-EAB review of M1-M12 of the project was received and taken into consideration:

"Annex A of D3.2 is really helpful in understanding what could be the content of the OSSR. It would be useful to expand further the software integration requirements to understand the real system and technical requirements that will need to be defined and implemented."

2. Review Summary

The review conclusions and recommendations can be summarised as follows:

General content:

The general content of the deliverable D3.2 is complete in the sense that all the necessary points for the software and service list and the integration plan have been addressed, however not always completely, i.e. not for all components of the final OSSR. As D3.2 is an intermediate report, it is important to identify and follow up the missing points which will be done below. The key performance indicator for the OSSR will be the coverage of software packages and services provided by the partners and ESF/RIs and included in the OSSR, so this KPI is the main guiding principle for the follow up actions, see in Section 3.

Extent and completeness of the software and service list, especially with the objective of enabling open science involving the ESCAPE communities:

The extent and completeness were reviewed against the objectives, that are (see D3.1):

- Support a community-based approach for continuous development, deployment, exposure and preservation of domain-specific open-source scientific software and services in the global context of the EOSC catalogue of services;
- Enable open science interoperability and software re-use for the data analysis of the ESCAPE ESF/RI projects based on FAIR principles;
- Create an open innovation environment for establishing open standards, common regulations and shared software libraries for multi-messenger/multi-probe data.

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The objectives have been satisfactorily addressed both in content and in the follow-up procedures. The current list of software and services is compiled in a bottom-up approach from the partners and can be grouped in the categories:

- Common developments:
  - Templates for services and meta data;
  - CORSIKA enhancements.
- Innovative approaches:
  - Machine Learning Software and Libraries.
- Data processing software:
  - For low level data (on- and offline);
  - Process distribution and handling;
  - Workflow handling;
  - Post processing.
- Data analysis software:
  - Instrument response function generation;
  - Likelihood maximisation;
  - Extraction of observables from data;
  - Generation of derived science data products;
  - General purpose science tools.
- Data Models:
  - Version control;
  - Data format generation.

The categories comprise all functionality to ensure the utilisation of open access data from the perspective of Task 3.2. The content of the categories, however is lacking software for some ESF/RIs (EGO-Virgo, ELT, EST, HL-LHC/CERN, SKA). The list is incomplete for others that are currently in the process of selecting their respective central software stacks (CTA, KM3NeT). All ESF/RIs are in contact in Task 3.2. The missing entries are not from a general lack of the intended entries of software and services, but rather from ESF/RI-internal decision and publication processes. A more direct involvement of the ESF/RIs should be sought to ensure that the objectives can be reached by a complete set of open-science-relevant software packages and services.

A categorised approach for the implementation of OSSR is proposed to cover the full extent and diversity of proposed software and services and to ensure inclusiveness of the repository. The latter could be structured as follows:

a) software and services of general interest to show best or common practices with stand-alone use cases (provided by partners);
b) software and services from the central service stacks of the research projects with project-internal use cases (provided by the ESF/RIs themselves);
c) interoperable software and services across the community with open science use cases, in the largest scope: the test science projects of ESCAPE (provided by several ESF/RIs)
d) services provided by ESCAPE, especially also of the WP2 (Data Infrastructure for Open Science), WP4 (Virtual Observatory) and WP5 (Science Analysis Platform)

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Also, the further collection of software and services should be structured along the categories above.

Concerning d), the - sometimes ambiguous - relationship between the available e-infrastructures (e.g. the registry-of-registries in the IVOA), the deployment of services developed in ESCAPE to be picked up by the ESF/RIs themselves (e.g. the data lake and science analysis platform), and the OSSR needs to be clarified and implemented accordingly. The interaction between work packages toward this goal has intensified during and after the ESCAPE progress meeting in February 2020, this development should continue and be strengthened.

The providers need to ensure that documentation, CI/CD services and evaluation data sets are provided - this will be fostered by the common service template and by the rules of participation to the OSSR. The implementation - especially with respect to versioning - needs to be addressed further. Also, the providers will be encouraged to indicate if the contributions were developed along certain best practices/guidelines, and if so, along which. Those best practises should be collected and disseminated.

Solidity of the implementation scheme:

The implementation scheme is driven by the deliverables and milestones of WP3, which currently seem adequate to ensure reaching the objectives. Task 3.1 is in charge to steer the work package resources that the steps defined are reached in time. The structuring of OSSR, as suggested above, needs to be taken into account.

Missing steps towards OSSR (from the software/service collection perspective):

There are some missing steps towards OSSR already defined in D3.1 and D3.2, those need to be followed, see Section 3. In addition to those, the procedure for handling the entries in the ASTERICS/OBELICS repository, and generally the inclusiveness of the OSSR to all relevant software and services in the ESCAPE science communities - also beyond direct ESCAPE partners - needs to be defined more clearly.

The definition and implementation of WP3-internal use cases (from the category cases a) and b) above) are needed to check the completeness of the collection and to finalise requirements to the OSSR. Further, tests via the foreseen ESCAPE TSPs (Test Science Projects case c) above) will be essential to uncover further missing steps and open a new perspective by a top-down approach starting from the scientific needs. This should drive the collection of software and service to be added to the list during the rest of the project.

To further the interoperability between entries in the OSSR, machine readable, and better actionable, meta-data shall be added such that higher-level services (e.g. the ESCAPE Science Analysis Platform) can link OSSR entries based on, e.g. supported input/output data formats or on a computing platform based on technical requirements.

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3. Follow Up Actions

Based on the review, the follow up actions formulated below will be stimulated by the working group leaders and via Task 3.1. The further progress will be re-evaluated in MS17:

- Following the procedures, deliverables and milestones as described in D3.1; to be followed up in Task 3.1.
- Update and complete the software and service list by re-current surveys and partner input, involve the ESF/RIs to ensure an OSSR with a maximal impact towards the defined objectives; to be followed up in Task 3.2.
- Expand the software integration requirements in the survey and understand the technical requirements to be implemented, including use cases as means of verification; to be followed up in Task 3.5 towards D3.3.
- Define the structure of OSSR as part of the catalogue of services; followed up by Task 3.1 in co-operation with all WG leads.

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