Deliverable 8.2: Defining the needs for EOSC resources in ACTRIS

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1. Background and purpose of this document

ACTRIS is the European Research Infrastructure for short-lived atmospheric constituents, i.e. aerosol, clouds, and reactive trace gases. It covers services for observing concentration and properties of these constituents by surface in situ and ground-based remote sensing methods, as well as numerical modelling the same properties to assist data analysis. ACTRIS is currently in its implementation phase and has attained landmark status on the ESFRI roadmap in 2021. In providing its services, ACTRIS will meet the requirements of FAIRness (**F**indable, **A**ccessible, **I**nteroperable, **R**eusable) as defined by the FORCE11 group, and adopted by EU policies.

In this role, ACTRIS needs to have a well-defined relation to the European Open Science Cloud (EOSC). EOSC is an environment where any interested party can access, publish, analyse, or otherwise re-use research data of any type, where EOSC facilitates access to the data, data publishing services, or any types of tools and services to enable data analysis and re-use. Seamless interoperability of the services is to be achieved by means of consistent application of the FAIRness principles to both data and connected services. The idea of establishing EOSC was proposed by the EU commission in 2015 as a measure to make data available as resource for new services facilitating economic growth.

At the time of defining the ACTRIS-IMP project, structure and organization of EOSC were still under discussion. The options shifted between the poles of a monolithic organisation offering data access and analysis services to the scientific community, and a federation of entities offering data and pertaining data analysis services. This ambiguity is reflected in the title of this deliverable. The title implicitly assumes that it is EOSC itself as organisation that offers resources and services.

Since then, the structure of EOSC has been clarified, and the EOSC implementation has started. EOSC was formally established in 2020 as EOSC association, a federated framework connecting already existing data access and analysis services. This means, resources and services are not provided "by EOSC", but "through EOSC", where the service itself is provided by one or several of the federated contributors. EOSC provides the platform to list, find, and access these data services, called EOSC Marketplace. Nevertheless, the services of the European e-infrastructures connected to ESFRI such as EGI and EUDAT are available through the EOSC Marketplace.

The scope of this deliverable is adapted to the development of EOSC as described above. After a brief description of the structure and elements of EOSC, it will elaborate how ACTRIS could relate to the elements of EOSC, both from the data service user and the provider perspective.

2. Organisation of EOSC services & resources

The EOSC core consists of 2 elements:

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1. **The EOSC Catalogue and Marketplace (EOSC Marketplace)**
   "Serves as a universal entry point to the EOSC services and EOSC research products, offering: publications, software and data along with distributed cloud computing resources enabling researchers and other users to process and analyse data in a distributed computing environment, access and order public and commercial e-infrastructure services supplied at national, regional and institutional levels."[1]
2. **The EOSC Interoperability Framework**
   "Set of policies and guidelines that enable interoperability of resources and services and will facilitate service composability. The guidelines could be documents, procedures, workflows, scripts, code, datasets, formats, and guidelines used in science."[1]

2.1 EOSC Marketplace Structure

The EOSC Marketplace organises services alternatively by scientific domain or by the following, partly overlapping categories. The categories are explained by examples since a proper definition of the vocabulary is lacking. The examples give an overview over the intended and anticipated use of the EOSC Marketplace:

- **Discover Research Outputs**
  Access services to primary or secondary research data. Examples of access services to primary research data (unfiltered, but FAIR annotated data as measured) are the data portals and machine access points of Research Infrastructures. An example for an access service to secondary data, i.e. data that has been filtered and analysed for a specific purpose, e.g. a publication, is Zenodo. It is important to note that the listing comprises access points, not individual datasets.
- **Publish Research Outputs**
  Services for publishing primary or secondary research data following FAIR data principles. Examples include again Zenodo, but also domain specific data curation services offered by Research Infrastructures.
- **Access Computing and Storage Resources**
  Classical e-infrastructure services such as high-performance computing, data staging, virtual private cloud services.
- **Process and Analyse**
  Data analysis services such as Jupyter notebook, transcription of historical documents, or gene sequencing.
- **Access Research Infrastructures**
  Co-lists many of the services mentioned above since these contain the core services of e-infrastructures, but also services for Research Infrastructure Management, Authentication /

[1] https://eosc-portal.eu/services-resources

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Authorisation management, or user-driven scientific workflow management for data analysis.

- **Manage Research Data**
  Example for services managing research data include the EGI Workload Manager for decentrally distributing computation workload, a service for creating data management plans, or an API for accessing the OpenAire research graph mapping the links between DOI identified objects.
- **Access Training Material**
  Contains training material packages on data management and analysis topics.
- **Find Instruments & Equipment**
  Currently only one entry, a service for accessing a numerical simulator for a cosmic ray detector.

2.2 EOSC Interoperability Framework Structure

The EOSC Interoperability Framework (EOSC-IF) consists again of 2 parts:

- EOSC-Core, which defines the specifications for interacting with the EOSC core resources such as the Marketplace and computing resources. A list of standards and technologies defined to implement EOSC-Core can be found in Appendix I in section 6. Central elements of EOSC-Core include:
  - Metadata standards.
  - PIDs and identification
  - Authentication and Authorisation (AAI)
  - Accounting of service use
  - Monitoring of service use
  - Order management
  - Accounting for research products, including accounting of data use, but only across EOSC attached repositories.
  - Helpdesk
- EOSC-exchange, which defines interoperability guidelines of services among each other, for example inside a research community. This allows room for community-driven for organisation of FAIRness by choosing community specific FAIR Enabling Resources (vocabularies, metadata standards, data formats, …) while keeping the EOSC core elements intact.

EOSC-IF is governed by formally open, topic specific bodies. EOSC users can file petitions and requests to these bodies, who decide on acceptance or rejection. In practice, these bodies are dominated by the major e-infrastructures (OpenAIRE, EGI, EUDAT, …).

The following section analyses how ACTRIS should relate to the EOSC Marketplace, both from the provider and the user perspective, but also how to relate to the EOSC Interoperability Framework.

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3. ACTRIS' Relation to the EOSC Marketplace, Provider Perspective

Simply because of the amount of funding invested, the EOSC Marketplace will develop into a major forum for offering research data products and services around them, e.g. for analysing, transforming them, and publishing the result, but also services around collecting the data. Most services offered by ACTRIS can be listed and offered through the EOSC Marketplace to reach the widest possible user audience, while at the same time ensuring appropriate branding of ACTRIS. A non-exhaustive list of ACTRIS services that could be listed in the EOSC Marketplace includes:

- ACTRIS Data Portal (under "Discover Research Outputs")
- ACTRIS machine-to-machine interfaces for metadata listing, metadata search (under "Discover Research Outputs")
- ACTRIS data machine-to-machine interfaces for data listing, data search, and data access (under "Discover Research Outputs")
- ACTRIS secondary data product archive (under "Discover Research Outputs")
- ACTRIS vocabulary server (under "Discover Research Outputs" and "Access Research Infrastructures")
- Homeless data curation services for all ACTRIS branches, available through the ATMO-ACCESS homeless data portal (under "Publish Research Outputs" and "Access Research Infrastructures").
- Realtime data production and dissemination services for those ACTRIS branches offering this service (under "Publish Research Outputs" and "Access Research Infrastructures").
- ACTRIS instrument calibration services through SAMU (under "Access Research Infrastructures"). SAMU is the Service and Access Management Unit, managing access to all resource limited ACTRIS services for users outside ACTRIS.
- Access to ACTRIS National Facilities and exploratory platform service through SAMU (under "Access Research Infrastructures"). National Facilities can be observation platforms such as observation stations, but also exploratory platforms such as simulation chambers.
- Access to ACTRIS training resources (courses and e-learning material on instrument operation, data quality control, research infrastructure management) service (under "Access Research Infrastructures" and "Access Training Material").

4. ACTRIS' Relation to the EOSC Marketplace, User Perspective

Since services around data use and re-use are at the centre of EOSC, the services available through EOSC were assessed by the needs of the ACTRIS Data Centre. Due to the steadily shifting content of the EOSC Marketplace while being established, the evaluation focusses on the services of the established e-infrastructures EUDAT and EGI, which were known to be available through the EOSC Marketplace.

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The evaluation of the services offered through the EOSC Marketplace should be repeated periodically (e.g. yearly) since new services might become available which can be useful not only to the ACTRIS Data Centre, but also other Central Facilities (European level ACTRIS component, e.g. Head Office or Data Centre).

4.1 EUDAT Collaborative Data Infrastructure

The following EUDAT services were evaluated for use in ACTRIS. For services https://www.egi.eu/that will or might be used, the assessment is stated in **bold face**.

- **B2ACCESS**
  Authorisation and authentication proxy for user identification and community-defined access control enforcement.
  B2ACCESS can be a possible solution for single-sign-on (SSO) to ACTRIS services where authentication is needed. This will depend on pricing, as compared to running a corresponding solution inside ACTRIS.

- **B2DROP**
  Low-barrier storage environment which allows users to synchronise their active data across different desktops and to easily share this data with peers.
  ACTRIS has decided to take its own hosted intranet solution into use for internal document and data sharing.

- **B2FIND**
  Interdisciplinary discovery portal for research output that allows free term search, results may be narrowed down using several facets, including spatial and temporal search options.
  ACTRIS will focus on domain-specific data discovery portals which are more likely to be used by ACTRIS data users.

- **B2HANDLE**
  Distributed service for storing, managing and accessing persistent identifiers (PIDs) and essential metadata (PID records) as well as managing PID namespaces. Includes ePIC PIDs.
  ACTRIS will follow the ENVRI-FAIR recommendation of using ePIC PIDs, e.g. for identification of data pre-products and instruments. EPIC PIDs are in practice identical with the B2HANDLE service.

- **B2SAFE**
  High-availability service which allows community and departmental repositories to implement data management policies on their research data across multiple administrative domains in a trustworthy manner.

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ACTRIS Data Centre units will take own, domain-specific solutions into use since data provision and the control over data access is at the core of ACTRIS services.

- **B2SHARE**
  Data sharing service. for researchers, scientific communities and citizen scientists to store, publish and share research data in a FAIR way.
  It is the ambition of ACTRIS Data Centre to give access to ACTRIS data with sufficient performance to make a dedicated data sharing service unnecessary.

- **B2STAGE**
  Service to transfer research data sets between EUDAT storage resources and high-performance computing (HPC) workspaces.
  A staging service is meaningful only in connection with HPC applications. Use cases involving HPC with ACTRIS data aren't currently foreseen. The need for data staging will be re-evaluated if HPC use cases with ACTRIS data should occur.

4.2 EGI - advanced computing for research

The following EGI services were evaluated for use in ACTRIS. For services https://www.egi.eu/that will or might be used, the assessment is stated in **bold face**.

- **Compute: Cloud Compute**
  Run virtual machines on demand with complete control over computing resources
  This service is easier accessible through the IT departments of the ACTRIS host organisations.

- **Compute: Cloud Container Compute**
  Run Docker containers in a lightweight virtualised environment.
  This service is easier accessible through the IT departments of the ACTRIS host organisations.

- **Compute: High-Throughput Compute**
  Execute thousands of computational tasks to analyse large datasets.
  This service is easier accessible through the IT departments of the ACTRIS host organisations.

- **Compute: Workload Manager**
  Manage computing workloads in an efficient way.
  This service is easier accessible through the IT departments of the ACTRIS host organisations.

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- **Storage and Data: Online Storage**
  Store, share and access your files and their metadata on a global scale.
  This service is easier accessible through the IT departments of the ACTRIS host organisations.

- **Storage and Data: Data Transfer**
  Transfer large sets of data from one place to another.
  This service is easier accessible through the IT departments of the ACTRIS host organisations. With few exceptions, data volume is not an issue with ACTRIS data. For the exception cases, dedicated solutions are already in place.

- **Storage and Data: DataHub**
  Access key scientific datasets in a scalable way.
  Data access is a core service of ACTRIS Data Centre, which ACTRIS likes to keep complete control over.

- **Security: Check-in**
  Login with your own credentials.
  See assessment of EUDAT's B2ACCESS service.

- **Applications: Applications on Demand**
  Share online applications for your data and compute-intensive research.
  Applications are domain specific and require domain knowledge. ACTRIS would like to host these on its own platforms for strategic reasons.

- **Applications: Notebooks**
  Create interactive documents with live code, visualisations and text.
  User-driven data analysis with virtual research environments (VREs) and notebooks will grow in volume over the upcoming years. ACTRIS intends to offer these services on its own servers in the start, but will re-evaluate needs once use of these services increases.

- **Training: FitSM Training**
  Learn how to manage IT services with a pragmatic and lightweight standard.
  Solved in collaboration with host institutions IT departments.

- **Training: ISO 27001 Training**
  Learn how to manage and secure information assets.
  Solved in collaboration with host institutions IT departments.

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- **Training: Training Infrastructure**
  Dedicated computing and storage for training and education.
  Solved in collaboration with host institutions IT departments.

5. ACTRIS' Relation to the EOSC Interoperability Framework

ACTRIS' objectives concerning its relation to the EOSC-IF could be:

- To ensure visibility of ACTRIS in relevant EOSC channels, certainly the EOSC Marketplace.
- To ensure attribution of ACTRIS for services provided.
- To make implementation and maintenance of the link to EOSC core services easy and cost efficient for ACTRIS.
- To make interoperability of ACTRIS services with services offered by other providers in the same domain (EOSC-exchange) easy and cost efficient.
- Have an influence on the ongoing processes in establishing EOSC governance to ensure influence in the future.

At least from today's perspective, visibility of service providers in EOSC seems to be ensured. The listing of services in the EOSC Marketplace always refers to the service provider, and the list of EOSC-Core functionalities (see Appendix I in section 6) includes functions such as "Accounting for services" and "Accounting for Research Products". As a result, the first 2 objectives seem to be met already with the existing state of EOSC.

Even though formally possible, it will be rather difficult to influence choices of standards and technologies used to implement the EOSC-Core part of the EOSC-IF due to the dominating role of the e-infrastructures. However, this isn't necessarily a problem for meeting the third objective. With few exceptions, services needed to link to the EOSC-core services aren't implemented in ACTRIS yet. The choice of standards and technologies for implementing the EOSC-core services (Appendix I) are sensible and reflect the expertise collected in the EOSC bodies. The simplest solution to the third objective is to use the EOSC-Core technology specification as guideline for the implementation of ACTRIS.

The work on establishing interoperability of services within the atmospheric domain of European environmental Research Infrastructures (fourth objective) has already started during the ENVRI-FAIR project. For data interoperability based on the FAIRness principles, ENVRI-FAIR has created an implementation plan for the atmospheric domain, and implementation has progressed significantly to increase data FAIRness and to converge on FAIRness enabling resources. Some tasks remain concerning data service interoperability, and certainly concerning interoperability of non-data RI services. The best way to continue this work is to continue the work in the ENVRI framework.

For influencing EOSC governance and decisions (fifth objective), at least 2 pathways are thinkable:

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- *Direct influence by ACTRIS ERIC joining the EOSC Association*.
  Joining the EOSC Association will give ACTRIS representatives a direct seat in EOSC bodies. On the other hand, the amount of policy and lobbying work needed to influence these bodies must not be underestimated. ACTRIS would be only one of many members, and building alliances would be essential to succeed.
- *Indirect influence via the ENVRI framework, i.e. by ENVRI having an advisory function for EOSC.*
  While not giving ACTRIS ERIC its own seat in EOSC bodies, this approach would distribute the work of lobbying EOSC on several shoulders in the ENVRI framework, while creating gravity at the same time due to the large number of ENVRI members. However, this option will require consensus within the ENVRI community, and the RIs have very different objectives. This can be complex procedure, particularly after the end of ENVRI-FAIR when the ENVRI community lacks a formal common forum. One promising option can be to work together with the community in the ENVRI hub NEXT project, provided that this proposal (submitted in March 2023) is funded.

The most appropriate approach will depend on the ambition level ACTRIS would like to have towards influencing EOSC governance towards ACTRIS' objectives. This will need to be decided by ACTRIS' governing bodies once ACTRIS ERIC has been established, including a periodic review of the decision. The appropriate approach will also depend on whether the ENVRI community 1) becomes formally established and 2) becomes a formal advisory body for EOSC. If these conditions aren't met, the option of ACTRIS ERIC joining the EOSC Association might still be the most beneficial option for ACTRIS.

6. APPENDIX I: Standards and interfaces used to implement the EOSC-Core part of the EOSC Interoperability Framework[2]

[2] https://eosc-portal.eu/sites/default/files/EOSC%20Future-WP3-EOSC%20Architecture%20and%20Interoperability%20Framework-2021-12-22%5B17%5D%5B6%5D-2.pdf

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EOSC IF Area	Current Standards and Approaches	Goal	Possible Outputs and Impact
Resource Description Framework	EOSC Provider and resource profiles 3.0 and 4.00 developed in EOSC Enhance (recently handed over to EOSC Future), RDF, XML, UML, OpenAIRE guidelines for publication, data and software repositories, OpenAIRE Guidelines for CRIS systems, OpenAIRE-ELIXIR guidelines for bioschema.org (in the making), Scholix.org	Agreed way to describe resources and providers that is shared by the EOSC ecosystem (03, 04, 05, 07) projects	Ensure that EOSC Provider and Resource Profiles 4.0 is adopted by all stakeholders. Records for providers and resources are shared between catalogues Users can search for providers and resources across multiple catalogues to more easily find valuable resources
Identifiers	FAIR Principles, EOSC *PID* Policy and report on the *PID* Architecture, mature Persistent Identifier Frameworks (Datacite, ORCID, DONA, ePIC, EUDAT), initial FREYA *PID* Graph technology, OpenAIRE Research Graph (*PID* graph across all sciences, org registries, author registries, funder registries)	Develop guidelines for providers to select *PID* types, for new *PID* types (e.g. instruments, services, software, organisations), to connect to *PID* Graphs and to implement minimum *PID* Kernel Type Information	EOSC *PID* policy defining how different *PID* approaches can be deployed
AAI	SAML2, OAuth2, OpenID Connect, REFEDS Framework (Sirtfi, R&S, RAF), AARC Blueprint architecture and guidelines, EAWG TF-AAI output on Architecture and Authentication, WISE SCI Trust Framework and AUP which are endorsed by the major Research Infrastructure and e-Infrastructures	Agree on the EOSC AAI Interoperability Guidelines and EOSC Federation Membership requirements	EOSC AAI Federation policy, EOSC AAI Interoperability Guidelines adopted by the Research Infrastructure and *EOSC-Exchange* services
Metadata and Ontologies	Many thematic and community-based metadata schemas and ontologies are	EOSC guidelines for data discovery	Interoperability framework on data discovery and exchange

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	available, guidelines for data discovery and metadata harvesting from OpenAIRE and EUDAT, DataCite guidelines for registering DOIs. EOSC-hub interoperability guidelines on Metadata Management and Data Discovery: https://wiki.eosc-hub.eu/display/EOSCDOC/Metadata+Management+and+Data+Discovery	Exchange and cross-walks on basis of existing guidelines	
Accounting for services	Cloud VM Usage Record, OGF StAR record, Grid job usage record, Grid summary job record, ARGO Messaging Service EOSC-hub Interoperability guidelines: https://wiki.eosc-hub.eu/display/EOSCDOC/Accounting .	Agreed usage records to track consumption of EOSC resources Agreed interfaces to collect accounting records from EOSC providers	Interoperability framework for service providers for automated reporting of accounting and usage metrics
Monitoring	Nagios Plugin API, ARGO API, Apache Avro, REST and JSON API, ARGO Messaging Service EOSC-hub Interoperability guidelines: https://wiki.eosc-hub.eu/display/EOSCDOC/Monitoring	Agreed definition of service availability and reliability in EOSC Agreed interfaces to collect monitoring information from EOSC providers	Interoperability framework for monitoring service availability and reliability of services in the EOSC Catalogue
Order Management	API for providers to define service offers and related parameters v1 from EOSC-hub API for EOSC order handling v1 from EOSC-hub	Agreed interfaces to manage service offers and orders	Interoperability framework for order management and for automatic exchange of the orders with service providers
Accounting for research products	COUNTER Code of Practice, OpenAIRE Guidelines and APIs, MakeDataCount Guidelines and APIs	Agreed protocol and exchange format for pull/push exchange of usage data	Interoperability Framework enabling the collection of research data usage statistics across EOSC data repositories
Helpdesk	X-GUS protocol implemented over SOAP	Agreed paths to integrate a helpdesk in the Federated EOSC Helpdesk	Federated EOSC Helpdesk framework for EOSC providers

	EOSC-hub interoperability guidelines: https://wiki.eosc-hub.eu/display/EOSCDOC/Helpdesk	Agreed interfaces between helpdesks	
Data platforms for processing	POSIX, WebDAV, CDMI, S3, OneData	Agreed interfaces for transparent data ingesting, movement, and processing in distributed and hybrid cloud environments, including containers and notebooks	Interoperability framework for transparent data ingesting, movement, and processing in distributed computing resources
Data Publishing and Open Data	SWORD, DOIP, FedoraCommons, DSpace, B2SHARE, Zenodo, DataCite, OpenAIRE guidelines for Data Archives, OpenAIRE PROVIDE, B2FIND guidelines, EDMI, Schema,org, OAI-PMH, RO-Crate	Agreed macro-features and interfaces for a digital repository, an infrastructure component that is able to store, manage, and curate Digital Objects and return their bitstreams when a request is being issued	Interoperability framework for digital repositories in EOSC
Cloud Compute Containerisation and Orchestration	OpenStack API, Open Virtualisation Format (OVF), Paas orchestrators, Kubernetes, Docker Swarm, Mesos, TOSCA EOSC-hub interoperability guidelines: https://wiki.eosc-hub.eu/pages/viewpage.action?pageId=68224522 https://wiki.eosc-hub.eu/display/EOSCDOC/PaaS+Solutions	Agreed interfaces and orchestrators to create VMs and containers into cloud resources	Interoperability framework to federate cloud resources in EOSC
HTC-HPC Compute	TOSCA, OpenStack API, Kubernetes, Distributed Resource Management Application API, QCG (DRMAA) EOSC-hub interoperability guidelines: https://wiki.eosc-hub.eu/pages/viewpage.action?pageId=63438908	Agreed interfaces and orchestrators to deploy and manage clusters on HPC and HTC resources	Interoperability framework to deploy and orchestrate clusters on demand on HPC and HTC resources and manage batch job processing

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