



Portfolio material to support training for target groups at all Research Infrastructures (RIs)

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Abstract

We present the deliverable achieved for a *Portfolio material to support training for target groups at all Research Infrastructures (RIs)*. The work represents the achievement of deliverable D3.4 of the Horizon 2020 ExPaNDS project.

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Executive Summary

We report on the status of the portfolio training material in ExPaNDS, created through task 3.6, by providing a description and references of the available material at the time of the report, specifying the target group for each one of them. This work has been facilitated by the use of the pan-training catalogue¹, developed as part of *Work Package 5*, which serves as an entry point for all the ExPaNDS and PaNOSC training material.

We identified four major target groups, from their responsibilities to their role in the data interaction, and we describe the relationship between those target groups and fourteen training materials, among workshops, documents, GitHub repositories and presentation slides. We found that naturally, *software engineers* are benefiting most from the training materials. In addition to *software engineers*, we identified other three target groups, namely *data curators*, *Photon and Neutron (PaN) researchers* and *beamline scientists*.

With this deliverable, we intend to provide to the identified target groups instructions to reproduce the results obtained in the course of the ExPaNDS project and sponsor the adoption of the PaN-training catalogue as the primary source of training material.

It should be noted that some of the material can fit in more than one *Work Package* and it is reported here as long as it relates to *Work Package 3*, in any share. This blending witnesses the joint efforts of all *Work Packages* in the ExPaNDS project and their close interactions.

¹ <https://pan-training.eu/>



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1. Portfolio material to support training for target groups at all RIs

1.1 Background

The work outlined in this document is part of the ExPaNDS project², carried out in close communication with the PaNOSC project³, thus representing the majority of European Photon and Neutron (PaN) sources in coordinated activity to drive forward Findable, Accessible, Interoperable and Reusable (FAIR) facility data and European Open Science Cloud (EOSC) services⁴.

This deliverable:

D3.4: Portfolio material to support training for target groups at all Research Infrastructures (RIs).

aims to collect and explain the training material made available by the project at the time of the report. For each of the materials, the document references the target group(s) it is intended for, which are described at the beginning of the document, and includes a link to the PaN-training catalogue.

1.2 Purpose

The main purposes of this deliverable as alluded to in the original proposal and fleshed out by consultation with PaN community representatives, include:

- To introduce the different target groups for which training material is available.
- To describe each training material, including corresponding links to the PaN-training catalogue.
- To frame each training material to the corresponding target groups.

2. Target groups

We have identified four target groups, which differ based on their interaction with the data, during the collection and production of the training material. The boundaries between groups can be blurred and often a member of one group may have some responsibilities from another group. The training material, although being linked to specific target groups, is thus not limited to them and can serve as documentation to members of other groups. Some examples of mixed responsibilities include the *software engineers* to *data curators* relation and *researchers* to *beamline scientists*.

² <https://expands.eu/>

³ <https://www.panosc.eu/>

⁴ <https://eosc-portal.eu/services-resources>



Funding agencies, even if not directly addressed as target groups, may benefit from knowing that the material is covering a variety of topics and audiences. Additionally, the training portfolio benefits funding agencies by ensuring that all members of the PaN community have easy access to the material necessary to maximise the scientific output from their investment.

2.1 Software engineers

A software engineer is a person who has the responsibility to design, develop, maintain, test, and evaluate software.

Many commonalities among software development and deployment at facilities require extensive documentation. *Work Package 3* is helping collect and produce training material, ranging from data catalogues adoption, EOSC integrations to PaN APIs [1] adoption.

Software engineers are involved throughout the whole deployment and adoption process and this is why most of the training material is addressed to them.

2.2 Data curators

Data curation is the organisation and integration of data collected from various sources. It involves annotation, publication and presentation of the data such that the value of the data is maintained over time, and the data remains available for reuse. Data curation includes "all the processes needed for principled and controlled data creation, maintenance, and management, together with the capacity to add value to data"⁵.

Data curators, if compared to software engineers, take an approach more focused on data rather than software and are responsible for ensuring that data is correctly tagged and maintained. This role often overlaps with software engineers and sometimes data consistency is simply another responsibility of software engineers.

2.3 PaN researchers

A Photon and Neutron (PaN) researcher is a scientist working with data obtained from Photon and Neutron facilities.

A key goal of the ExPaNDS project is to improve the FAIRness of data so that users can access existing data and incorporate it into their research. This is why it is important to provide guidelines to PaN researchers, ranging from searching for data to tagging the data, to making data FAIR.

Some of the training material describes resources that require the user to have an account at the PaN facility. Although acquiring access to remote facilities is outside of the ExPaNDS remit, we envision that a federated AAI (Umbrella-ID) will play a role in supporting such access.

Note that FAIR data can benefit researchers from other fields of study; therefore, we make the training material generally available.

⁵ https://en.wikipedia.org/wiki/Data_curation



2.4 Beamline scientists

In accelerator physics, a beamline refers to the trajectory of accelerated particles with the accompanying path segments (guide tubes, diagnostic devices) along a specific path of an accelerator facility. Examples of beamlines include synchrotron light (obtained from a synchrotron source) and neutrons (from a spallation source or a research reactor).

Beamlines usually end in experimental stations. Experimental stations provide the environment in which experiments take place, and typically house the instruments that use particle beams to make measurements. Such experiments can be in many different scientific fields, including particle physics, materials science, chemistry, and molecular biology. Beamlines can also be used for irradiation tests or to produce isotopes.

A *beamline scientist* is someone working at the beamlines and is responsible for the experiment execution and data collection. They may also be responsible for metadata ingestion, which facilitates data curation. It often happens that a beamline scientist is also a PaN researcher.

3. Training material

The subsections which follow report on all the training materials, related to *Work Package 3*, which is available at the time of writing. Each of them follows a predefined structure, consisting of a short description, a list of fitting target groups, the resource type and the link to the PaN-training catalogue. The reader can find more details and the actual resource by following the provided link.

3.1 Develop common rules and best practices between national RI's and harmonise the provision of the EOSC services

Description: By providing the link to the workshop on the 6th and 7th of April 2020, it explains how ExPaNDS is delivering its data services to PaNOSC and EOSC by touching on how to make open datasets available to the EOSC community and how to get the software in the PaN software catalogue, how to get pipelines to run and how to ensure their quality over time.

Target groups:

- **Software engineers:** apart from what is described in section 3.2, software engineers can understand how to publish software in the PaN software catalogue⁶, ensure quality using the *Service Quality as a service by EOSC-Synergy*⁷ [3] and run data analysis as a service in EGI⁸.
- **Data curators:** can extract metadata guidelines as described in section 3.2 and extend them to the fields required by the PaN software catalogue.

⁶ <https://software.pan-data.eu/>

⁷ <https://www.eosc-synergy.eu/>

⁸ <https://www.egi.eu/>



- **PaN researchers:** can understand, aside from what is described in section 3.2, how to browse and search on the PaN software catalogue and how to run data analysis as a service in EGI.

Resource type: Workshop

PaN-training catalogue:

<https://pan-training.eu/materials/develop-common-rules-and-best-practices-between-national-ri-s-and-harmonize-the-provision-of-the-eosc-services>

3.2 Delivering data services to EOSC

Description: Covering the first day of the workshop, which is described in section 3.1, it explains what the OAI-PMH⁹ is and how it can be implemented in SciCat and ICAT. It also covers what B2FIND¹⁰ is and what metadata usage can be done to better expose PaN data. Finally, it provides an overview of what OpenAIRE¹¹ is and offers.

Target groups:

- **Software engineers:** can understand how to expose data and metadata to EOSC services using the OAI-PMH protocol, in particular to B2FIND and openAIRE. The general description of the OAI-PMH enables any data catalogue to develop its OAI-PMH interface. The reader can find explanations and references to ready to use OAI-PMH implementations for ICAT¹² and SciCat¹³ data catalogues. B2FIND and openAIRE documentation is linked in the material for convenience, to enable software engineers to subscribe the implemented OAI-PMH to B2FIND and openAIRE harvesting.
- **Data curators:** following the metadata guidelines required by the OAI-PMH, B2FIND and openAIRE data curators can discover the subset of required metadata fields to enable the integration with these providers.
- **PaN researchers:** can understand how to browse and search on B2FIND and openAIRE.

Resource type: Wiki

PaN-training catalogue: <https://pan-training.eu/materials/delivering-data-services-to-eosc>

3.3 Common search API definition

Description: The document describes the common search API [1] which provides a uniform way via a web portal or computer program to interrogate all data catalogues with specific searches in order to find data of interest. All facilities in the ExPaNDS and PaNOSC community will support this common search API; the mechanism will depend on the data

⁹ <https://www.openarchives.org/pmh/>

¹⁰ <http://b2find.eudat.eu/>

¹¹ <https://www.openaire.eu/>

¹² <https://repo.icatproject.org/site/icat/oaipmh/1.1.1/>

¹³ <https://github.com/SciCatProject/oai-provider-service>



catalogue service in use. By including external links to current implementations for the major metadata catalogues, it provides a progress update of the project and helps research institutes deploy the required software.

Target groups:

- Software engineers: the benefit is twofold: if using ICAT or SciCat, they can understand how to deploy the existing common search API implementation for such catalogue services; if using another type of metadata catalogue service, they can follow the requirements stated by the common search API definition to build an interface to their data catalogue service.
- Data curators: by following the metadata exposed and queried by the common search API, data curators can discover the subset of required metadata fields to enable the integration with these providers.
- PaN researchers: can understand how to use the common search API to search for data relevant to their research topics.

Resource type: Document

PaN-training catalogue: <https://pan-training.eu/materials/common-search-api-definition>

3.4 Report on status, gap analysis and roadmap towards harmonised and federated metadata catalogues for EU national Photon and Neutron RIs

Description: This document contains the results of the gap analysis collected and analysed in November 2020, including a roadmap to achieve harmonised and federated (meta)data catalogues. It also represents deliverable 3.1 of the ExPaNDS project.

Target groups:

- Software engineers: by setting the roadmap, the document helps software engineers to understand the required implementation and deployment steps to achieve the ExPaNDS goals. Furthermore, they can align existing and future work with the effort coming from ExPaNDS, avoiding duplicating work that has already taken place, or will take place through ExPaNDS.
- Data curators: can find an overview of the steps required to achieve FAIR and the needed metadata.

Resource type: Document

PaN-training catalogue:

<https://pan-training.eu/materials/report-on-status-gap-analysis-and-roadmap-towards-harmonised-and-federated-metadata-catalogues-for-eu-national-photon-and-neutron-ris>



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3.5 ExPaNDS D3.2: Ontologies v1.0

Description: This deliverable describes the ontologies created during the course of the ExPaNDS project and mentions the ones which are relevant to it in the context of supporting FAIR data for the PaN communities. In particular, the document describes:

- The PaNET ontology, or PaN experimental techniques ontology, which formalises the definitions and relationships of the multiple experimental techniques used in PaN facilities.
- The NeXus ontology¹⁴, which provides a single controlled vocabulary of the NeXus¹⁵ data format, covering its terms (base class and field names) by flattening and joining the separate namespaces of base classes in a consistent and reversible manner and providing global persistent identifiers for each NeXus term.
- Existing relevant ontologies such as PaNKOS¹⁶, DRAO¹⁷, SRAO¹⁸ and best practices (described in section 7 of the document).

Target groups:

- Software engineers: can implement tools or update existing software for the PaN researchers that include the ontologies definitions and requirements.
- Data curators: following the ontologies description, can understand how to format and ensure data compliance and leverage on a standardised and maintained labelling.
- PaN researchers: growing into the ontologies, can understand what is foreseen to be searchable in the PaN search API.

Resource type: Document

PaN-training catalogue: <https://pan-training.eu/materials/expands-d3-2-ontologies>

3.6 ExPaNDS PaN Experimental Techniques (PaNET) ontology

Description: The PaN Experimental Technique (PaNET) ontology provides a taxonomy of experimental techniques relevant for the PaN community. This ontology is being developed as part of *Work Package 3* on EOSC Data Catalogue Services for PaN national RI's of the ExPaNDS project. The development of this work was part of the material described in section 3.5.

The ontology allows adding semantic tags to datasets, and other related research objects, to indicate the experimental techniques that were used to create them. Browsing the GitHub repository, available in the PaN training catalogue link, the user can find meeting minutes, CSV and OWL files with the ontology, releases and the GitHub page¹⁹ with the ontology documentation can be found in the README.

¹⁴ <https://github.com/ExPaNDS-eu/ExPaNDS-nexus-ontology>

¹⁵ <https://www.nexusformat.org/>

¹⁶ <https://github.com/ral-facilities/pankos>

¹⁷ <https://github.com/FAIRsharing/domain-ontology>

¹⁸ <https://fairsharing.org/bsg-s001177>

¹⁹ <https://pages.github.com/>



Target groups:

- Software engineers: can follow the PaNET requirements to implement tools helping the PaN researchers, such as what is described in section 3.9 of this document.
- Data curators: following the PaNET description and visualisation tools, can better understand the taxonomy and its use.
- PaN researchers: can browse the ontology and find available terms which are intended to be used during dataset search.

Resource type: Document

PaN-training catalogue:

<https://pan-training.eu/materials/expands-photon-and-neutron-experimental-techniques-pant-ontology>

3.7 Metadata Catalogue Release

Description: Self-contained, stand-alone data catalogue to support PaN facilities to get started with the adoption of a data catalogue. This material describes the architecture, development and deployment of a reference implementation of a data catalogue consisting of several components, in particular providing a database where to store metadata, some predefined reference metadata, a rest API access layer to the database, a graphical user interface (GUI) for this access layer and the PaN search-API [1], all at their latest version. Crucially, each component is supported by a community maintenance process to allow a managed and agreed approach to modification and extensions in future development.

Target groups:

- Software engineers: can follow the provided documentation to install a “click and play” instance of the data catalogue, including features developed in the PaNOSC ExPaNDS project. It covers aspects from data catalogue evaluation, comparison and proposition to a selected group of internal testers, including researchers and beamline scientists, which benefit especially from the data catalogue UI.
- Data curators: by interacting with the installed metadata catalogue release APIs, can understand how the data is stored, and test ingestion processes and metadata quality checks.

Resource type: Document

PaN-training catalogue: <https://pan-training.eu/materials/metadata-catalogue-release>

3.8 Demonstrate ICAT and SciCat released with APIs compatible with ExPaNDS federated EOSC services

Description: Implementation and deployment of ICAT and SciCat, by providing real examples of their adoption at different facilities. This material has the primary goal of describing the two data catalogues stack and their integration with the EOSC services. It



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thus provides examples that other facilities, currently in the process of adopting a data catalogue and are willing to integrate it with EOSC, can follow.

Target groups:

- **Software engineers:** can find a detailed explanation of the architecture of the ICAT and SciCat data catalogues, with adoption examples from ISIS²⁰, MAXIV²¹ and PSI²². The material can be used to replicate the data catalogue stack during the adoption process and provides a reproducible example of a production environment. By providing high-level diagrams of the PaN search-API, EOSC and Google Dataset search²³ integrations, highlighting the required APIs, software engineers can understand how to disseminate data to these communities.
- **Data curators:** using the available APIs (PaN search-API, EOSC, Google Dataset Search) can discover a subset of required metadata fields and experiment with the returned values.
- **PaN researchers:** can find step by step procedures of interactions with the PaN search-API, EOSC services and Google Dataset Search to search for data. In particular, how they are currently being used at MAXIV and PSI, is described in sections 3.3.2 and 3.4 of the training document.
- **Beamline scientists:** can take ideas for examples of ingestion processes (sections 2.2 and 3.3.1 of the training document).

Resource type: Document

PaN-training catalogue:

<https://pan-training.eu/materials/demonstrate-icat-and-scicat-released-with-apis-compatible-with-expands-federated-eosc-services>

3.9 PaNET implementation by the pan-ontologies-API RESTful service

Description: The material describes how to use and implement the pan-ontologies-API²⁴. At a high level, the service works by pulling and caching information from external ontology repositories, and in particular, the *GET /techniques/pan-ontology* endpoint translates the query from the user input (e.g. in the PaN portal) to a new query sent to the search-API, having added the logic from the PaNET ontology. Readers can understand how to use the service and which information it embeds and requires. This work implements the search behaviour when using a PaNET term as described in section 3.5.

Target groups:

- **Software engineers:** interested in using the PaNET ontology [2] in the PaN search-API, as stated by the ExPaNDS project, can find an explanation of its

²⁰ <https://www.isis.stfc.ac.uk/Pages/home.aspx>

²¹ <https://www.maxiv.lu.se/>

²² <https://www.psi.ch/en>

²³ <https://datasetsearch.research.google.com/>

²⁴ <https://github.com/ExPaNDS-eu/pan-ontologies-api>



deployment, behaviour and integration with the PaN search-API. The project is open-source, so it can incorporate any change or suggestions from the community.

- Data curators: following the PaNET links in the training material and understanding how the PaN search-API works, can verify metadata complies with the techniques information from the PaNET ontology.

Resource type: GitHub repository

PaN-training catalogue: <https://pan-training.eu/materials/pan-ontologies-api>

3.10 Scoring workshop

Description: As part of the PaNOSC *Work Package 3* section, this workshop was to illustrate how the Scoring service is designed, how to deploy it and integrate it with the local data catalogue system and the PaN search API. It was followed by a live demonstration of the Scoring service packaged in Jupyter Notebook with a SciCat data catalogue as an example. The score is computed locally at each facility level based on the information or dataset that is accessible only by the facility. All facility scoring results are then merged at the PaNOSC Federated Search before exposing the results to the end-user query. More details on the method used and some definitions of key concepts to compute the score can be found browsing the GitHub link in the PaN-training catalogue.

Target groups:

- Software engineers: can understand how to set up step-by-step the PaNOSC Scoring service on top of the local data catalogue based on the example of SciCat that was used in the demonstration.
- PaN researchers: can understand how the scoring is computed and have a better understanding of the results returned from the PaNOSC Federated Search.

Resource type: GitHub repository

PaN-training catalogue: <https://pan-training.eu/materials/panosc-search-scoring>

3.11 SciCat ingestion approaches

Description: The document describes three approaches to ingest metadata in the data catalogue. Ingesting metadata is one crucial step in the FAIR journey. Being very facility-specific, it is not possible to come up with a standard ingestion process and usually, every facility develops its own mechanism. Here, the document provides two approaches, from facilities using SciCat, to the existing ingestion process, that the reader can take inputs from. A further, more generic approach shows how to interact with the RESTful SciCat APIs to trigger an ingestion process, which serves as a starting point for facilities developing their own ingestion.

Browsing the documentation can also give an overview of SciCat and its components.

Target groups:



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- **Software engineers:** if involved by data curators or beamline scientists, can implement the required software to automatically ingest or ease the manual ingestion process.
- **Data curators:** reading the documentation and with some task overlap with software engineers and beamline scientists, can understand how to populate metadata and enforce their compliance to the facility's requirements.
- **Beamline scientists:** are the principal target of this document, as they are the ones who drive the metadata ingestion at the experiment time. They can understand how to ingest metadata and what are the existing tools that facilitate the process. Finally, they can get in touch with software engineers and data curators to fully, or partially, automate the process.

Resource type: Wiki

PaN-training catalogue: <https://pan-training.eu/materials/scicat-ingestion-approaches>

3.12 DAPHNE4NFDI: Science driven data management solutions for the user community

Description: The folder referenced by the training material contains the slides which were presented during the DAPHNE4NFDI workshop on the 24th of January 2022. In addition to the introductory slides, the reader can find slides covering ICAT and SciCat and explaining how to set the catalogues up and their behaviour. Software engineers, data curators and beamline scientists can understand how to install and interact with the catalogues.

Target groups:

- **Software engineers:** can understand the different components of the data catalogues and realise how to integrate them into the existing infrastructure.
- **Data curators:** can find how to structure data.
- **Beamline scientists:** can find examples of how to ingest data, organise files and add metadata.

Resource type: Workshop

PaN-training catalogue:

<https://pan-training.eu/materials/daphne4nfdi-science-driven-data-management-solutions-for-the-user-community>

3.13 ExPaNDS mid-term review

Description: The training material contains the slides presented during the ExPaNDS mid-term review. The reader can get an overview of the different work packages, including *Work Package 3*, and understand the overall direction and progress of the project. The material presented during the demo gives the reader a step by step example of how to replicate data analysis in multiple facilities.



Target groups:

- PaN researchers: can find a step by step example of how to replicate data analysis in multiple facilities.

Resource type: Workshop

PaN-training catalogue: <https://pan-training.eu/materials/expands-mid-term-review>

3.14 Metadata Catalogue workshop 4th of April

Description: The metadata catalogue is one of the central elements in the research data management of a PaN RI. Different solutions for the implementation are in use, the most common ones are ICAT²⁵ and SciCat²⁶. Some ExPaNDS partners still need to make their choice. This workshop aims to assist this decision making by presenting ICAT and SciCat and highlighting the technical differences.

Target groups:

- Software engineers: can better understand the prerequisites and implied design principles of the respective metadata catalogues. This information is essential to create the tools needed to interact with the catalogues and implement the RI specific workflows around them.
- Data curators: will be informed about the data model that the respective metadata catalogue is based on. This will help them to make the right choices on how to represent the data collected from experiments in the metadata catalogue in the most suitable way. The staff responsible for setting up data management workflows within the RIs, in general, will be assisted in choosing the metadata catalogue implementation that suits the specific needs of their RI best.

Resource type: Workshop

PaN-training catalogue:

<https://pan-training.eu/materials/workshop-on-metadata-catalogues>

4. Future developments

In the remaining time of the project, ExPaNDS and PaNOSC will produce further training material and *Work Package 3* commits to uploading everything to the PaN-training catalogue, to drive even more users to the adoption of FAIR principles.

Two more workshops are planned in the future: an Umbrella-ID²⁷ training shall provide information on mechanisms used for Authentication and Authorization Infrastructure (AAI), such as OpenID Connect²⁸ and assist the participants during a hands-on session to connect

²⁵ <https://icatproject.org/>

²⁶ <https://scicatproject.github.io/>

²⁷ <https://www.umbrellaid.org/>

²⁸ <https://openid.net/connect/>



their facility Single-Sign-On (SSO)²⁹ to Umbrella-ID. Another workshop will discuss options for persistent identifiers for raw data and the metadata to be registered along with those identifiers. Material from both workshops such as the slides will be provided in the PaN-training catalogue.

It is also likely that the existing training materials will evolve.

Conclusions

In this document, we have collected all available training material related to *Work Package 3* activities and outcomes at the time of writing. For each resource, we have emphasised the target groups it covers, distinguishing between four categories: *software engineers*, *data curators*, *PaN researchers* and *beamline scientists*. A dedicated description allows the framing of the training material, easing the browsing of the different sources. A link to the material on the PaN-training catalogue, finally, redirects the reader to the more detailed source.

²⁹ https://en.wikipedia.org/wiki/Single_sign-on



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