



# PaNremains! (an extremely personal view) **For the PaNOSC Finale**

Patrick Fuhrmann (DESY, ExPaNDS coordinator)  
on behalf of the project teams with contributions from Juliane, Lisa from  
DAPHNE4NFDI, Oliver, Thibaud and Kat.



PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

# Continuous support for the PaN community



2010

2015

2018

2021

European Open Science Cloud

EOSC INFRA 23 01 01  
eosc

2019

2020

2021

2022

**E x P a N D S**  
European Open Science Cloud Photon  
and Neutron Data Services

Policies  
Analysis  
AAI  
Training

Common data policy  
Software Catalogue  
UmbrellaID  
e-neutron

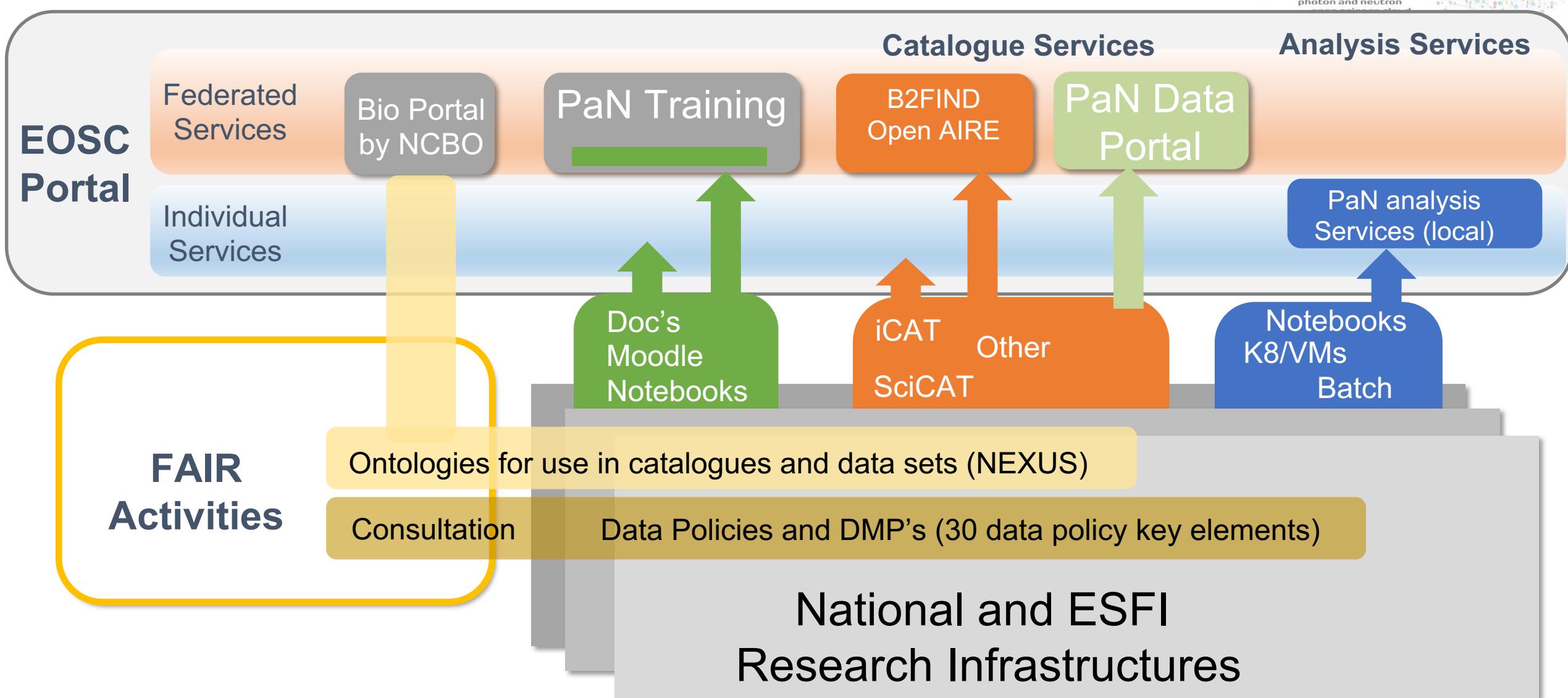
FAIR data policy  
Remote analysis  
AARC Blueprint

Data Management Plans  
Jupyter  
eduTeams  
Training platform



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# The Architecture



PaNOSCExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

# Focused outreach



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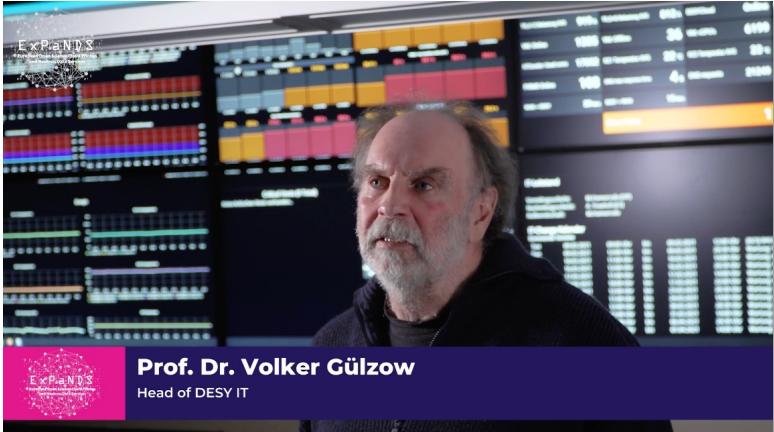
# Target-oriented outreach to different classes of PaN groups (and friendly communities).



- Originally planned as replacement for the Zoom-only or cancelled community events and conferences (required by the workplan)
- Presentations and lectures for students
  - Planting the spark of 'Open Science' in young scientists
- Consultations of Facility employees especially Beamline Scientists
  - These are the actual beneficiaries but also our victims.
  - Used as Multiplicators
- Senior Management Interviews
  - Sneaky way to Introduce our projects to our management
  - Important to publicly committing to our FAIR ideas



# Facility Beamline and IT staff



**Prof. Dr. Volker GÜLZOW**  
Head of DESY IT



**Dr. Johanna Hakanpää**  
Beamline scientist in charge at PETRA III (DESY)



**Prof. Dr. Christian G. Schroer**  
Leading scientist at PETRA III and project leader of PETRA IV (DESY)

The Photon and Neutron communities are represented by mechanisms like **LEAPS** for Photon and **LENS** for Neutron. Through those organizations, being connected to the **European Open Science Cloud** we can achieve sustainability.

... and I'm sure that also from the MX user community these wishes are coming that all of the synchrotrons should use the same kind of portals ... and the same kind of **archiving systems** ... And the same kind of **download systems**.

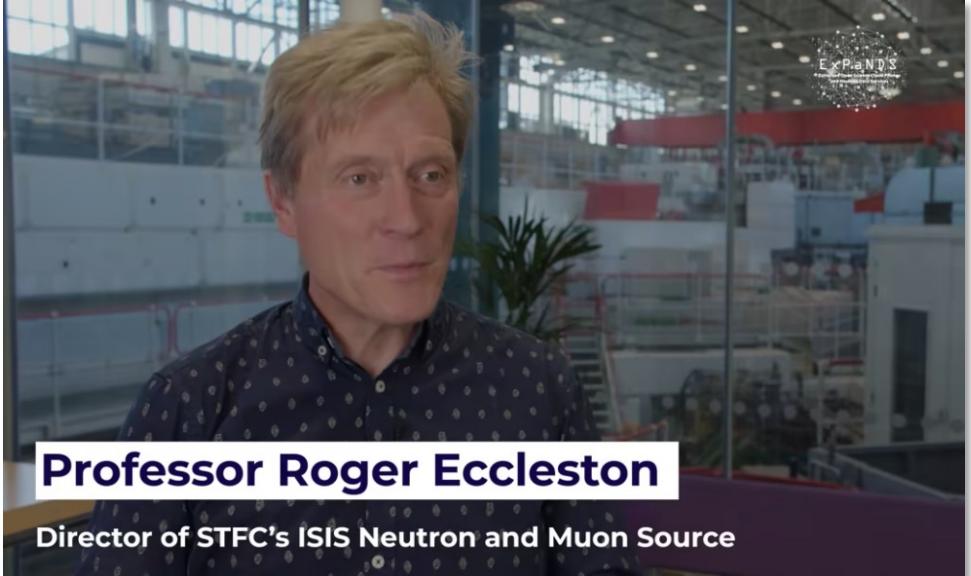
One example [of **interdisciplinarity collaboration**] is showing the extremes .. **were we have scientists from the humanities interpreting old artefacts** that were analyzed by X-Rays.



# Senior Level Engagement



We are increasingly seeing in some communities, the **recognition that by sharing the data** on an appropriate timescale, ideally as soon as possible, there are some **real benefits** to be had. So, I think the challenge, the cultural challenge is to demonstrate to the science community at large that actually the **benefits greatly overwhelm the risks**.



To get optimum value out of having open data ... we need to be inclusive, we need to actually involve as many different facilities and research establishments as possible and that is a **really big coordination job**. What the **ExPaNDS** and **PaNOSC** grants provided is an **excellent basis** for continuing this work on open data and being able to share data.



# Senior Level Engagement



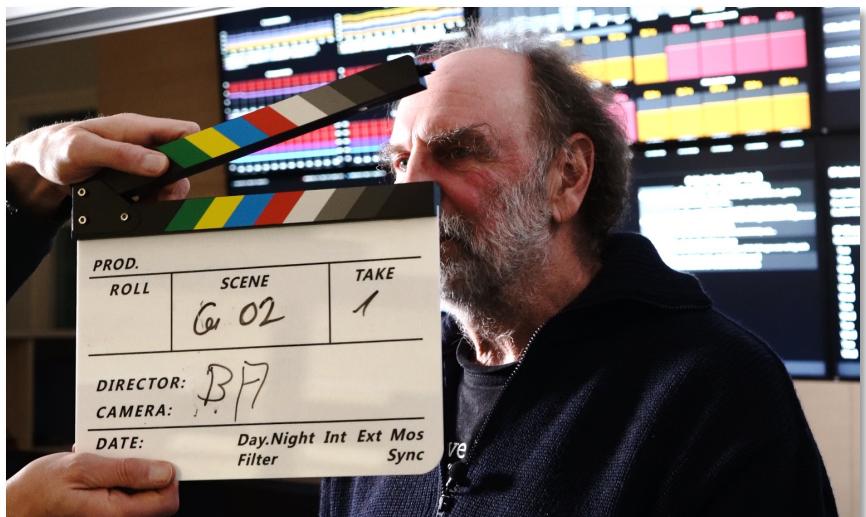
Data collection is not enough,  
advances only come through the  
interpretation of data.



There was always an understandable  
sense of data ownership from the  
scientists who conducted the experiments  
but the interdisciplinary research of today  
requires a new way of thinking.



# And a lots of fun ....



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# Presenting our experience in FAIR Data to other communities.



**iBERGRID** 



**eOSC** SYNERGY



**panosc**  
photon and neutron  
open science cloud

Ibergrid 2022

### PaNOSC and ExPaNDS outcomes

Patrick Fuhrman (DESY, ExPaNDS coordinator) and Andy Götz (ESRF, PaNOSC coordinator) on behalf of the teams

Please see presentation from Oscar Matilla from ALBA Synchrotron (Monday) for more on Synchrotron Science.



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Oscar (ALBA) and myself were invited to present the results of ExPaNDS at the IBERGRID conference.

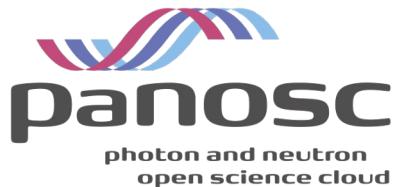


The adaption of Data Lakes for future Large Scale Facilities  
Based on the requirement of Photon Science.



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# VISA portal deployment and the ESCAPE Data Lake



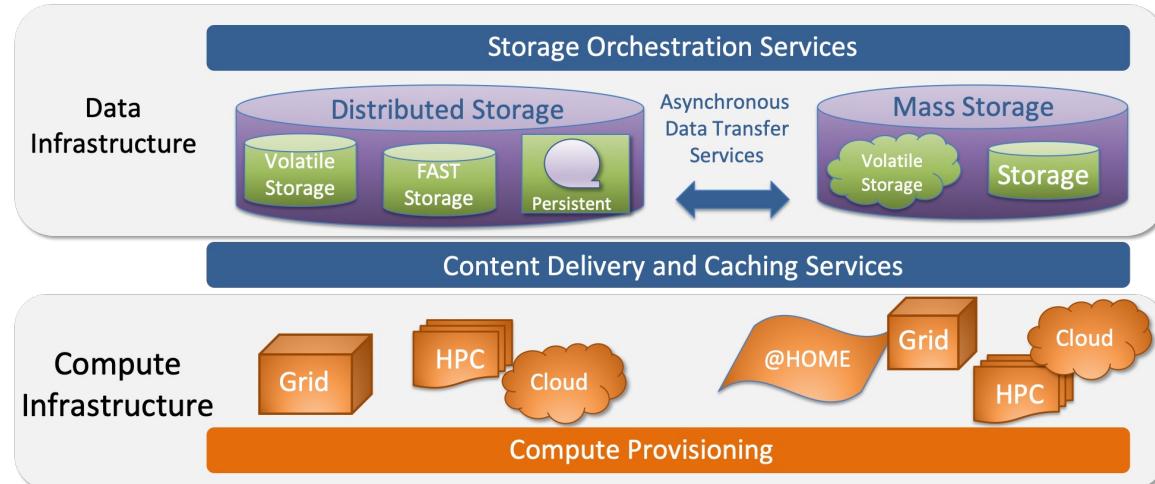
meets



meets

## The Data Lake: World wide data management

Outcome of the ESCAPE (HEP and Astro) Cluster



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# The common analysis portal... Deployment at DESY for PETRA III and European XFEL



## Local Proposal Portal

**DOOR**  
DESY Online Office for Research with Photons



## Local Data and Compute Infrastructure



kubernetes



openstack®

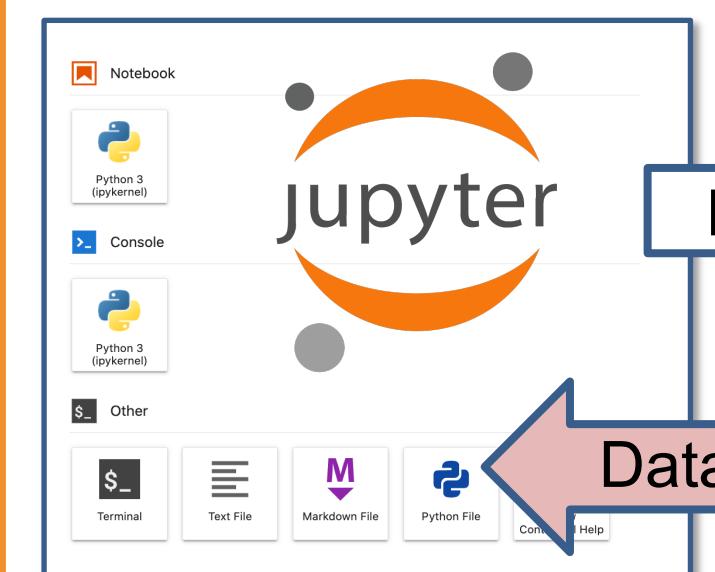


jupyter  
ESCAPE  
European Science Cluster of Astroparticle & Particle Physics INFRA research infrastructures  
Data Lakes



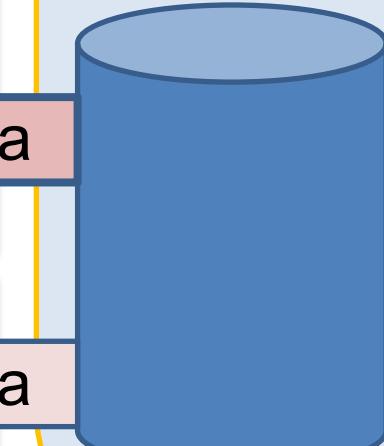
PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

# Connecting facilities



Desktop

Data Location Mgmt



**ESCAPE**  
European Science Cluster of Astronomy & Particle physics ESFRI research Infrastructures

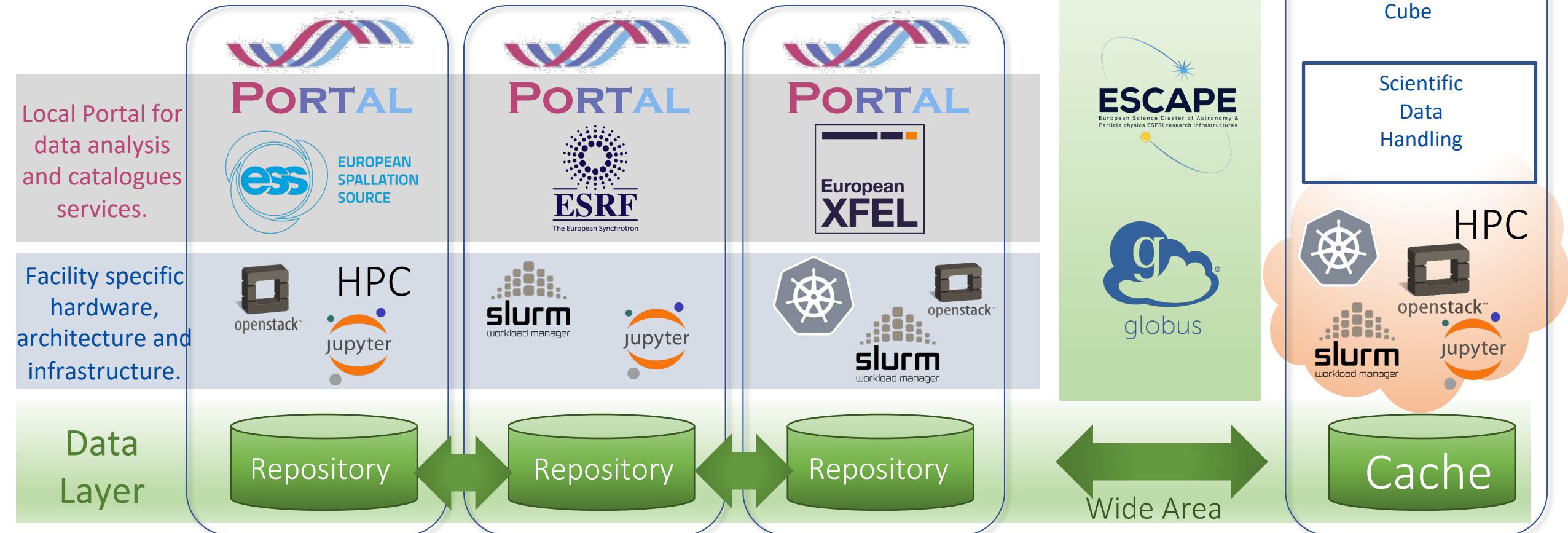
Data Lake



# Use Case : The PaN Data Commons



Outcome of the ExPaNDS and PaNOSC projects (PaN Cluster)



# Further collaborative work with VISA



- For some RI's there is no plan B in terms of Portal
  - So they rely on VISA becoming a success in terms of
    - Development
    - Deployment
  - Puts some pressure on ILL, who don't have the resources to support the entire community.
- So, Majid is trying to compose a small group, initially targeting an MoU (only), supporting ILL with Portal development and deployment.
  - Can become a very challenging process
  - So he really needs your support.
  - E.g. ALBA and VISA Kubernetes integration.



Here you see Majid , taking Arms against a Sea of legal troubles, and by opposing end them.



# The training, catalogue and workflows

*As already completely covered by Andrew M.!*



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# Pan-training.eu/workflows

Scientific topic	
small angle neutron scattering	1
Target audience	
life scientists	2
research data scientist	2
ExPaNDS and PaNOSC project ...	1
PaN Community	1
Keyword	
Jupyter notebooks	2
Pulmonary arterial hypertension...	2
Python	2
imaging	2
synchrotron	2
Higgs	1
Mantid	1
SANS	1
data analysis	1
Show more keywords	▼
Licence	
License Not Specified	6
Creative Commons Attributio...	2
Open Data Commons Attributi...	2

+ Create workflow

## Full-field Tomography at PSI

This workflow has some details on the instrument the data is produced from (TOMCAT beamline) and the infrastructure PSI has concerning their data.

If you are more interested in the science and want to reproduce the data and not bother with the surrounding details/context, please refer to the <a...

## Pulmonary arterial hypertension research

This training workflow shows the combination of the demonstrations from the ExPaNDS mid-term review.

The workflow consist of three steps:

- Basic material to introduce the problem,
- The associated dataset with the related scientific publication and
- Source code and reference to the...

## TELBE Terahertz Spectroscopy

The radiation source ELBE (Electron Linac for beams with high Brilliance and low Emittance) at the Helmholtz Centre Dresden Rossendorf (HZDR) can produce several kinds of secondary radiations. THz radiation is one of them and can be used with a typical pulse frequency of 100 kHz...

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meas  
users

Subsequen

attractive for deployment as a cloud-like use case. Involving EOSC in the analysis and...

number of other facilities. Furthermore, it demonstrates a typical workflow to turn raw data into reduced data, which can then be used by subsequent analysis.

The main...

## Workflow for Adding Training Content

The workflow describes how content can be added to our ExPaNDS/PaNOSC Training Portal Ecosyste



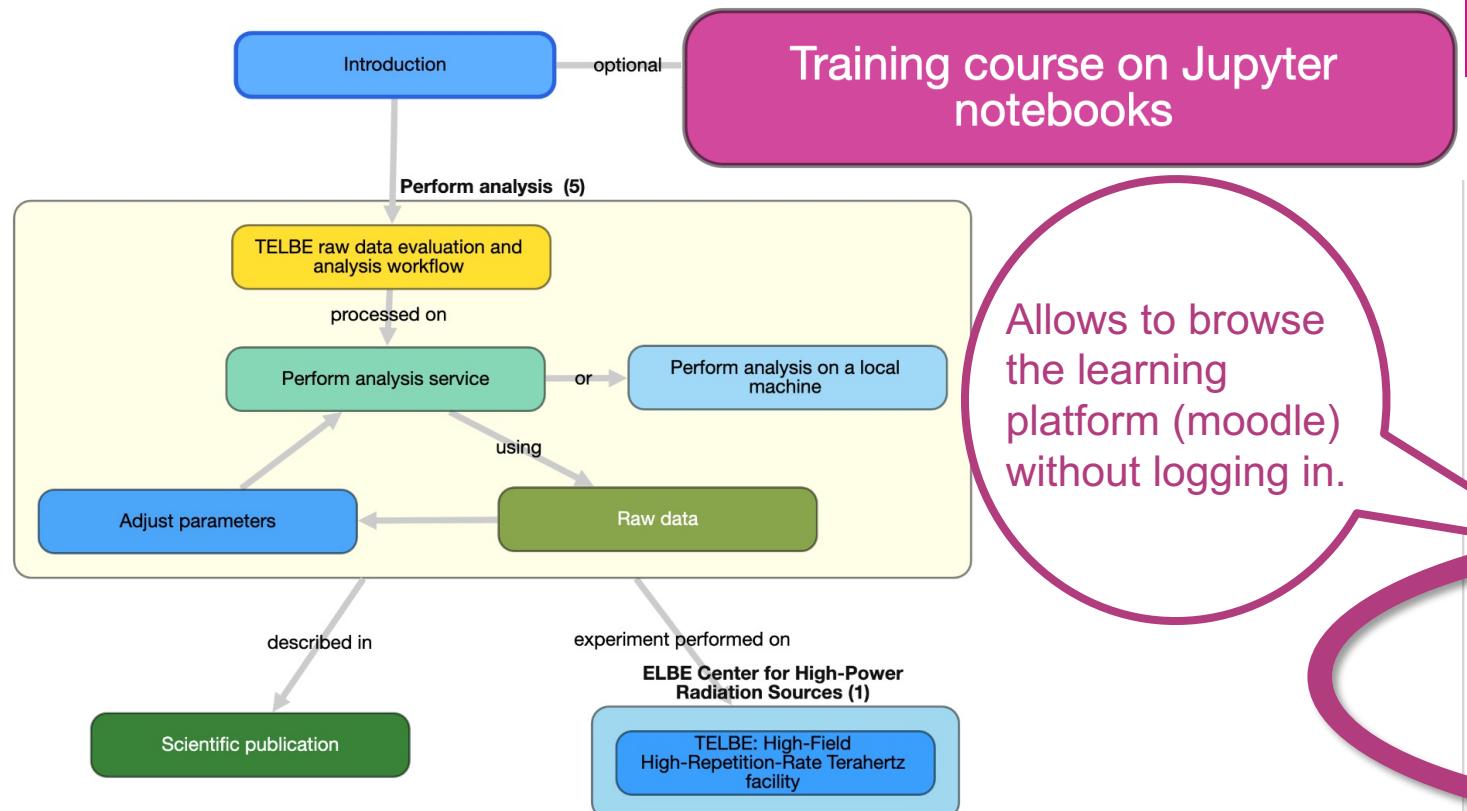
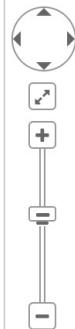
atalogue?



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# HZDR Terahertz Workflow Example

## TELBE Terahertz Spectroscopy



### Training course on Jupyter notebooks

In this workflow we will focus on Jupyter notebooks. Additional Python basics and an introduction to Jupyter notebooks can be found in the blended learning course Illumidesk: Python Course provided by our integrated e-learning platform PAN-learning.

Photon and Neutron eLearning<sup>o</sup>

#### Training materials

e-leraning course on Python basics

Allows to browse the learning platform (moodle) without logging in.



# Link to : e-learning.pan-training.eu -> moodle

Catalogue ▾ e-Learning ▾ Events About ▾

Python Workshop (IKON21)

Participants

Grades

Python Course with McStas and SCIPP

e-Learning

Dashboard

Calendar

## Python Workshop (IKON21)

e-Learning | My courses | Python Workshop (IKON21)

You are enrolled in the course.

### Python Course with McStas and SCIPP

If you have self enrolled onto the course please wait 5 minutes before launching the JupyterHub

Access the course by clicking on the **JupyterHub** link.  
Click **Start My Server > Start** and your container will launch.  
In the folder called **Notebooks** you will find the following:

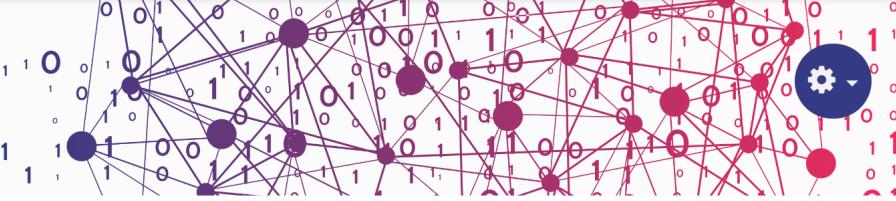
1. **Jupyter basics:** Jupyter notebook introduction.
2. **Python basics:** Basic language principles, Sequence data types, Control structures, Working with functions, Using modules, Input and output, Python 2 vs 3, Python classes.
3. **Using external Libraries:** Scientific libraries numpy, Plotting with matplotlib, Ipywidgets, Fitting scipy, Data analysis library pandas, Testing.
4. **Molecular visualization:** Visualization tutorial, Atomistic simulation environment.
5. **McStas script**
6. **SCIPP**

You can find a copy of the notebooks at <https://github.com/ess-dmsc-dram/python-course-ikon/tree/master/notebooks>

This course was created by the Data Reduction, Analysis and Modelling group of the ESS.  
This version of the course was specifically created for IKON21 in September 2021.

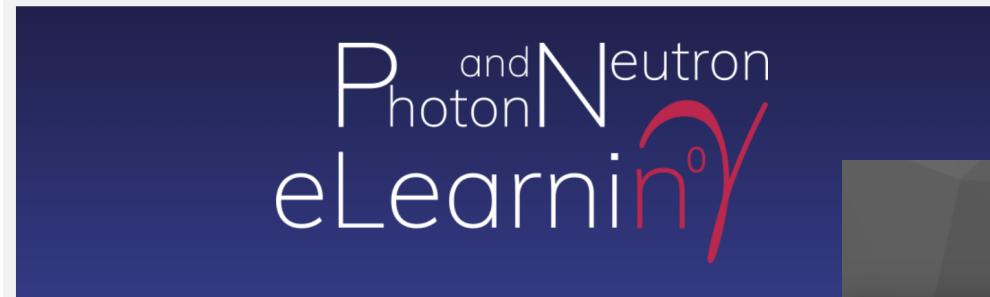
 JupyterHub

 Python Basics Quiz





# Umbrelle (eduTeams) login



Photon and Neutron eLearning

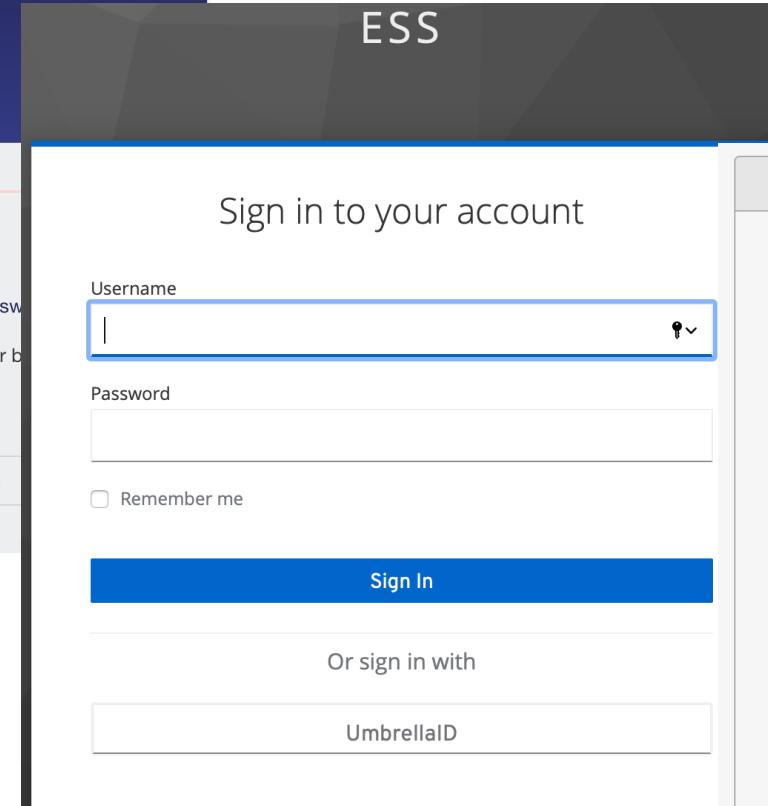
trude.von.richthofen@gmail.com

Forgotten your username or password?

Cookies must be enabled in your browser.

Remember username

**Log in**



ESS

### Sign in to your account

Username

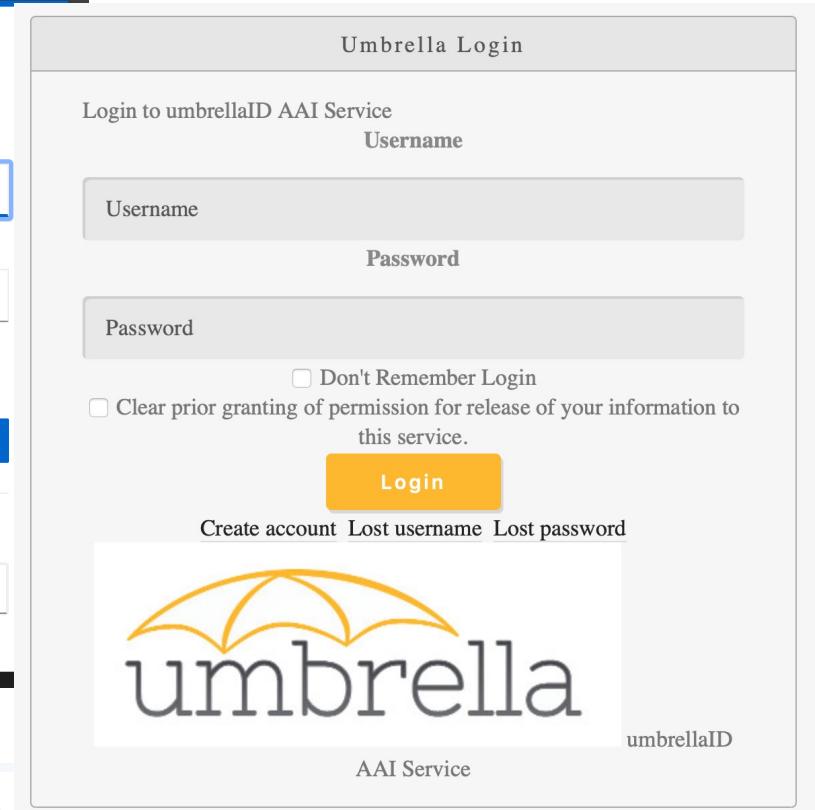
Password

Remember me

**Sign In**

Or sign in with

**UmbrellaID**



### Umbrella Login

Login to umbrellaID AAI Service

Username

Password

Don't Remember Login

Clear prior granting of permission for release of your information to this service.

**Login**

Create account Lost username Lost password



umbrellaID

AAI Service

# Link to the source 'github' and Jupyterhub



jupyterhub Home Token 1395 ➔ Logout

Start My Server

master		python-course-ikon / notebooks /	Go to file
	wpotrzebowski	Added exercise description	9f8d594 19 days ago
..			🕒 History
	1_jupyter_basics	Merge pull request #79 from moving-northwards/patch-4	14 months ago
	2_python_basics	Corrections after review from Wojtek, thanks for the review!	3 years ago
	3_using_external_libraries	matplotlib notebook -> widget, add scippneutron and ess to env file	7 months ago
	4_molecular_visualization	Removed unneeded ASE notebook	14 months ago
	5_McStas	Cleared notebooks.	14 months ago
	6_scipp	Added exercise description	19 days ago



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## FAIR policies and self assessment.



## Elements of the Data Policy Framework



DOI: 10.5281/zenodo.5205825

- Global Unique PIDs for data and instruments!
- Ontologies for PaN techniques (for catalogues and NeXuS)
- Open Access Protocols (Data, AAI)
- Human and machine readable access to data and meta data.
- Community standards for Contextual Metadata
- Standard File-Formats



# Self Assessment for sustained FAIRness

Deliverable D2.6 (on the way)



- Enabling the facilities to assess their FAIRness themselves;
- Finding a responsible person at each facility;
- Educate those individuals through workshops and individual; counseling in FAIR procedures;
- Providing a mechanism for measuring FAIRness;
- Executing a first supervised assessment.



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# Continuous self assessment

Deliverable D2.6



## Basic Principles

- Linking back to the FAIR Principles;
- Identifying and taking advantage of what existing FAIR evaluation frameworks have to offer ;
- taking account of the relationships between existing FAIR evaluation approaches ;
- Relating clearly to the processes and practices of PaN RI's

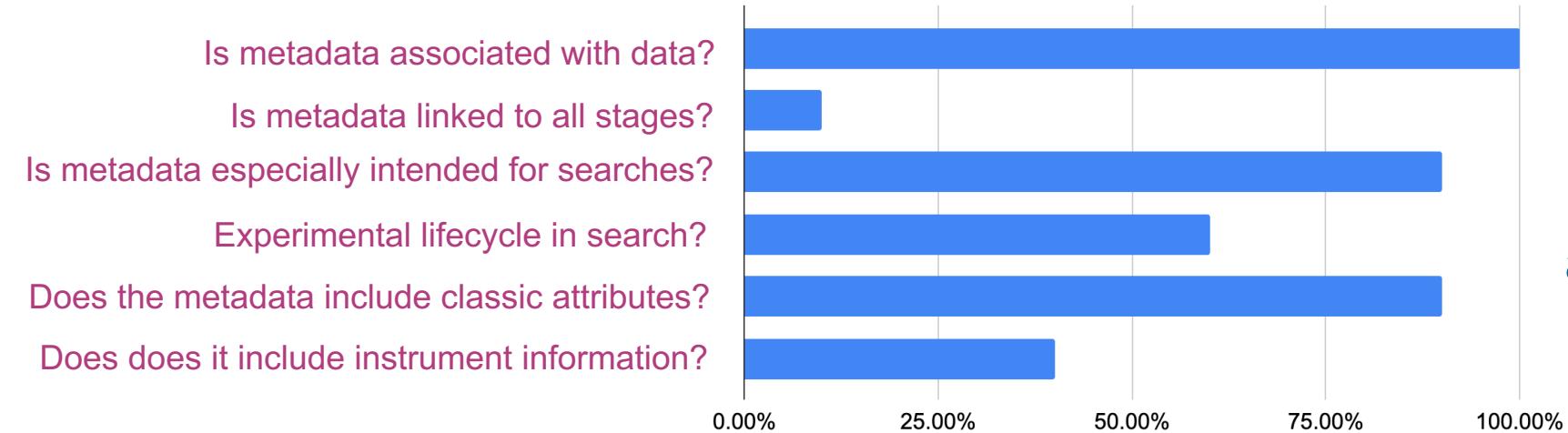
## Topics covered (27 questions based on existing FAIRness tools)

- Existence, completeness and richness of metadata
- Search (Flexibility and Capability) ;
- Standardization;
- Indexing and harvesting of metadata my machines;
- PID's;
- Access to data by users and possibly my machines;
- Curation of data;
- Reflection of the assessment process.



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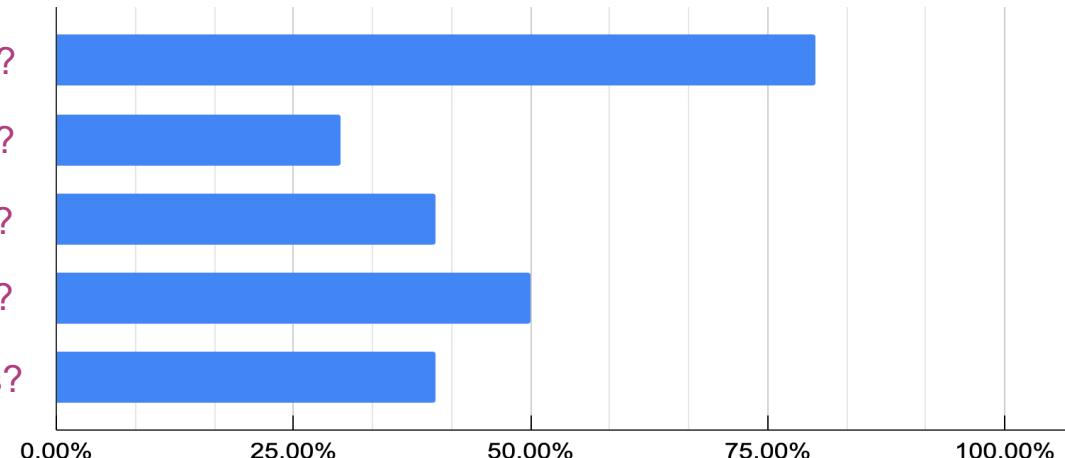
# Diverse results of the first questionnaire and headroom for improvements!



Metadata, catalogues and searches

## Indexing and PIDs

- Can your metadata being retrieved by an API?
- Do you provide an OAI-PMH Interface?
- Do you at least map to OAI-PMH?
- Do you provide Hyperlinked PID's?
- Are you using unpublished private PID's?





And last but not least :



National Research Data Infrastructure  
The aim of the national research data infrastructure (NFDI) is **to systematically manage scientific and research data, provide long-term data storage, backup and accessibility, and network the data both nationally and internationally.**



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# Cooperation with DAPHNE4NFDI



- The main goal of DAPHNE is to make data from photon and neutron experiments "FAIR", thereby making scientific work more efficient and gaining more knowledge from the data
- DAPHNE4NFDI will help to secure the sustainability of ExPaNDS even beyond the project term
- Example:

*"The DAPHNE4NFDI Executive board recommends that the DAPHNE participants test and evaluate SciCat at their home labs in universities and at facilities - if possible.*

*They should provide feedback and indicate where further collective development is required - including deployment and integration[...]"*





Finally, on behalf of ExPaNDS, let me thank you guys for this challenging but friendly collaboration with amazing results.

And particularly, from WP1 and my perspective, thanking Andy for allowing our WP1 and myself to participate in your management meetings and Nicoletta for our exciting common work in preparation of events and conference and the Symposia.

