PaNOSC & ExPaNDS : résultats des projets EOSC

8th April 2022

Presenters: **Jean-François Perrin** (ESRF)

Contributors: Andy Götz (ESRF) , Patrick Fuhrmann (DESY)

on behalf of PaNOSC + ExPaNDS partners

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.

Quick reminder : The Projects Cheat Sheet

	PaNOSC	ExPaNDS
EU Call	HORIZON 2020 INFRA-EOSC-04	HORIZON 2020 INFRA-EOSC-5B
Description	Cluster of ESFRI PaN Sources	EOSC PaN Data Services
Partners	ESRF, ILL, ESS, EU-XFEL, CERIC-ERIC, ELI-DC, EGI	DESY, ALBA, DLS, ELETTRA, EGI, HZB, HZDDR, Max IV, PSI, Soleil, UKRI
Observers	GEANT EU-DAT National RI's	
Linked 3rd Party	DESY STFC CESNET	
Start – End (Duration)	2018-12-01 – 2022-11-30 [4 Years]	2019-09-01 – 2023-02-28 [3 ½ Years]
Coordinators	A. Götz, G. Bodera	P. Fuhrmann, S. Servan
Budget	12 M Euros	6 M Euros
Home Page	PaNOSC.EU	ExPaNDS.EU
Twitter	@PaNOSC_eu #PaNOSC	@ExPaNDS_eu #ExPaNDS
GitHUB	github.com/panosc-eu	Github.com/expands-eu

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.

PaN facilities covered by PaNOSC/ExPaNDS

PaNOSC

ExPaNDS

Photon (LEAPS)

EGI

eli delivery consortium

CERIC
Central European Research Infrastructure Consortium

Neutron (LENS)

DESY
CESNET
STFC

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panosc photon and neutron open science cloud

ExPaNDS European Open Science Cloud Photon and Neutron Data Services

PaN Open Science Commons - Concept

- **Vision** – create a common space for PaNOSC and ExPaNDS facilities where petabytes of PaN FAIR data, analysis software, notebooks, workflows, and training material can be **F**ound, **A**ccessed (downloaded and/or executed), **R**e-Used + **I**mproved i.e. **FAIR**

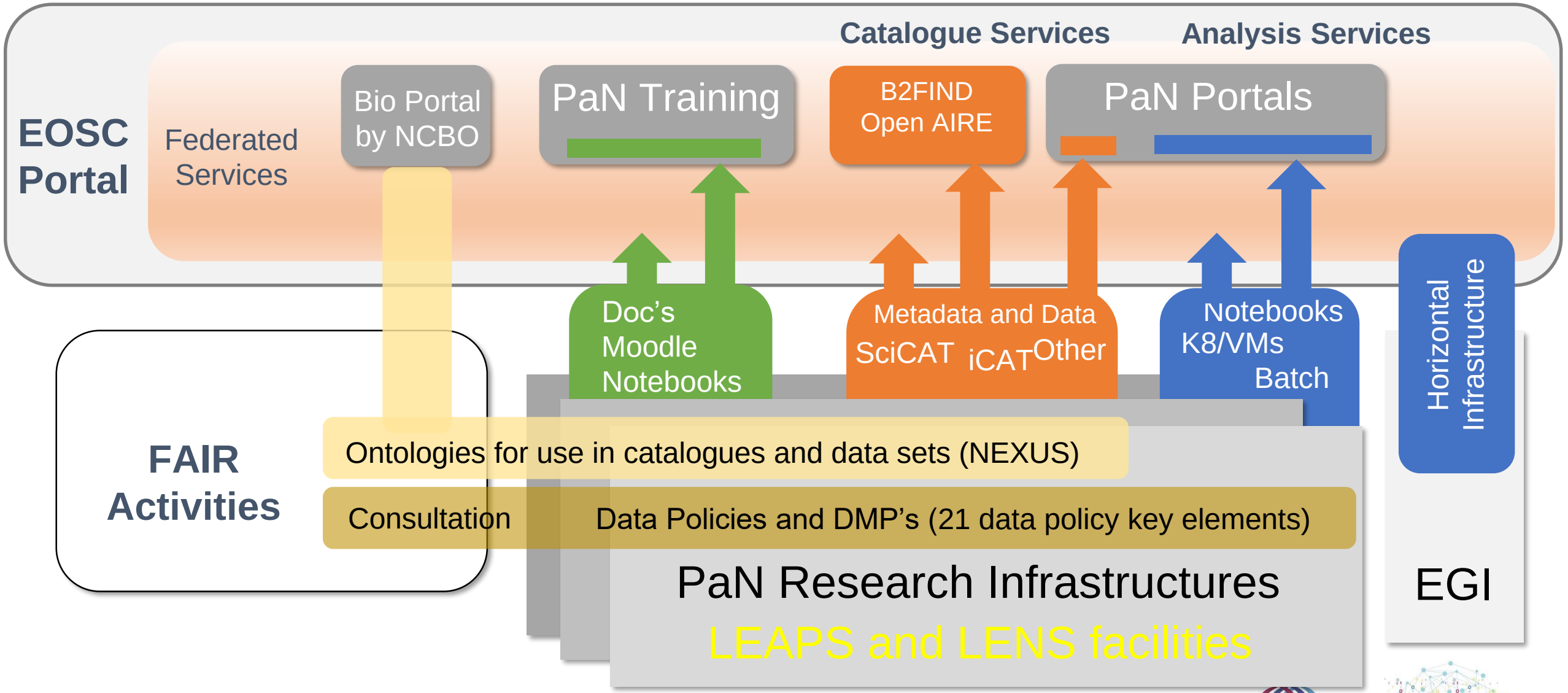
- **Remote access** – the PaN commons will be accessible remotely while being executed locally (close to the data) or via the EOSC (data needs to be moved)

- **Remote users** – the PaN commons will enable and encourage remote users and experiments (urgently required in the post-COVID-19 phase)

10 Primary Outcomes of PaNOSC and ExPaNDS

1. **FAIR data policy** and **DMPs**
2. **FAIR assessment** and common **PID** framework
3. Standardised metadata (**Nexus/HDF5**, PaN ontologies)
4. **Federated search API** for PaN data catalogues
5. **Open Data portal** for searching + downloading data
6. Community **AAI UmbrellaId**
7. **JupyterLab notebooks** and **Nexus/HDF5** files visualisation
8. **Remote data analysis** with VISA + data analysis pipelines
9. **Simulation** software for simulating experimental data (SIMEX)
10. **PaN-learning** platform (pan-learning.org + pan-training.org)

The Big Picture of EOSC in PaNOSC and ExPaNDS



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What did we achieve and what will we have achieved until the end of our projects?

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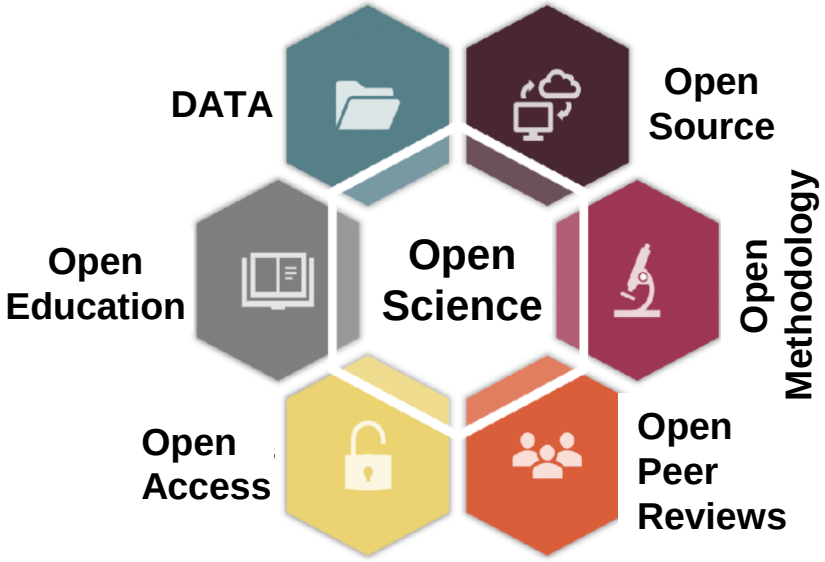

Open Science:
Open Data, FAIR Data Policies, PIDs, catalogues, DMPs .....

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Why are we involving ourselves into those policies?

The ultimate goal is Open Science

Accelerates scientific findings, as it:

- Allows verifiable results;
- Allows to easily find relevant data;
- Reduces the download-data barrier;
- Allows to **re-use data** from other groups or to find data not yet analyzed or published by the original authors, trainings new scientists, development of software, … ;
- We can benefit from similar sciences using synergies;
- Avoid statements like:
  - "The original data can be provided by the author on request!"

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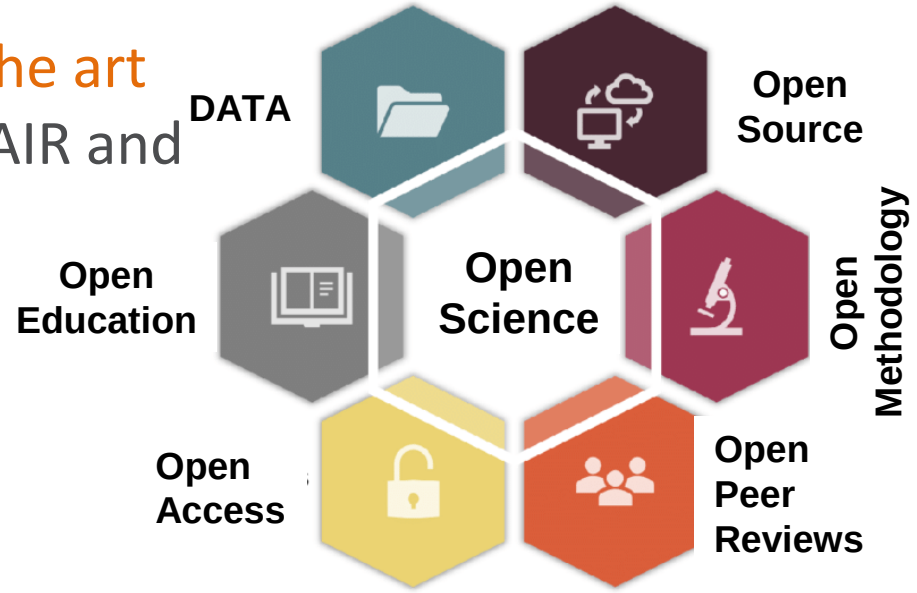
Why are we involving ourselves into those policies,

and why by means of the European Commission?

- The Commission provides us with established, state of the art frameworks to evaluate and implement Data Policies, FAIR and DMP, PID, by funding
  - EOSC with
  - specialized projects like FAIRsFAIR and
  - by supporting international organizations like RDA.
- provides specialized funding for
  - Activities to agree on common standards between the facilities
    'working together makes us stronger'
  - Activities helping us to make our services cross facility portable and EOSC
- However EC is making Open Science a condition.
  - No free lunch!



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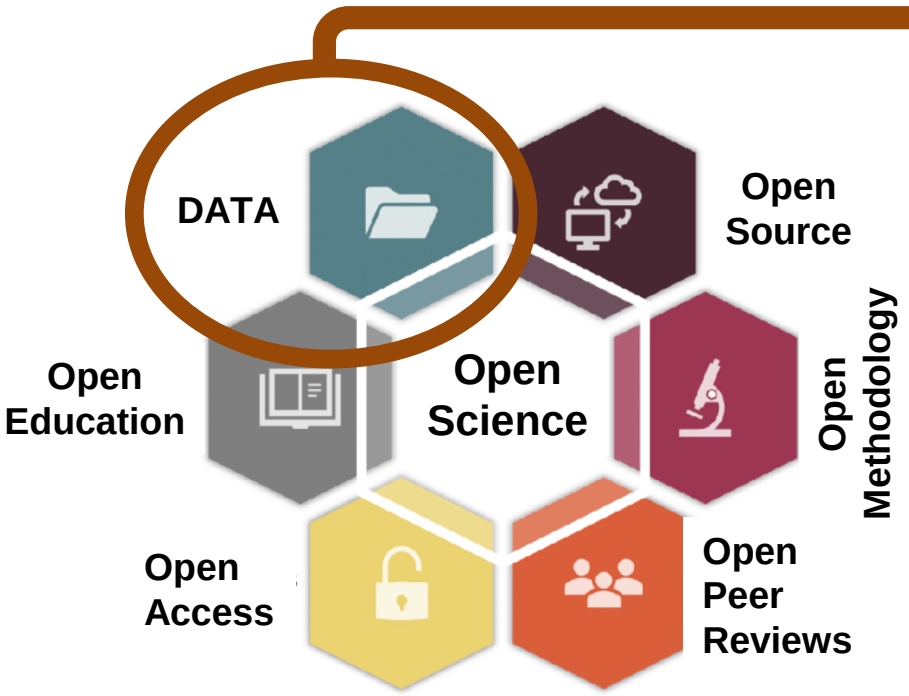
From Open Science to FAIR data.



DOI: 10.5281/zenodo.5205825

Elements of the Data Policy Framework

- FAIR Data
- Rights of Stake holders
- Retention Policy
- Embargo Licenses
- Curation
- Discovery
- FAIR Assess-ment
- DMPs
- ***

- ✓ Global Unique PIDs
- ✓ Contextual Metadata, following community standards (Ontologies)
- ✓ Open Access Protocols (Data, AAI)
- ✓ Human and machine readable access to data and meta data.
- ✓ Standard Fileformats

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Our contribution to Data Polices, DMPs and FAIR data handling.

We provide

- Data Policy Framework for easy adoption in not so complex cases
- Data Policy Guidebook to compose a customized, more complex Data Policy.
- Per Facility consultation
  - We provided the Data Policy Guidebook to the facility responsible person.
  - We provided a facility by facility consultation and discussed the Guide Book.
  - We collected feedback and redesigned accordingly.
  - We help and monitor the implementation or the Policies at the facilities.
- Help on permanent FAIR assessment of the facilities
  - We provide guidelines on how to continuously verify FAIRness of the beamline data taking process, the meta data and the repositories.

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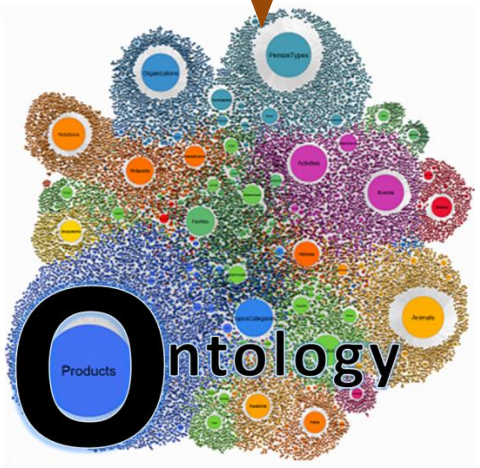
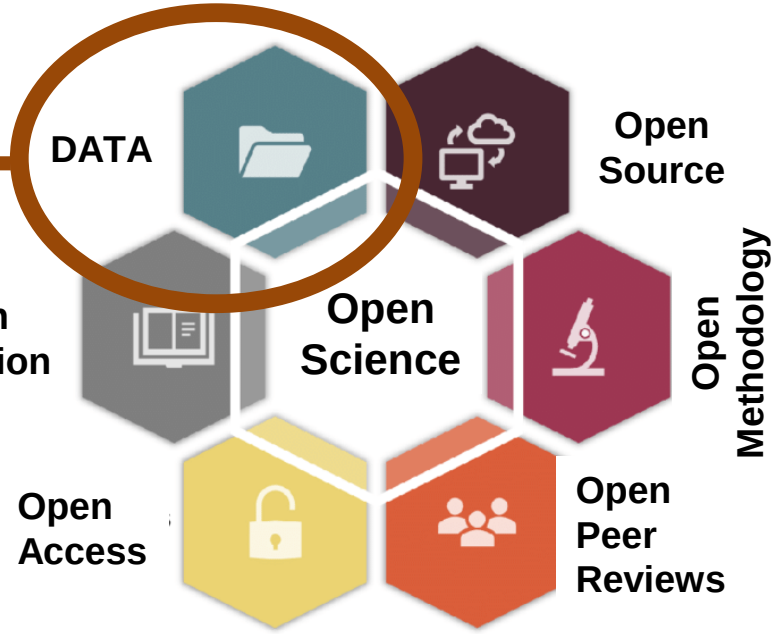
ExPaNDS
European Open Science Cloud Photon and Neutron Data Services





Meta Data Ontologies, Keywords, Catalogues and File Formats

photon

Showing 1 of 1099 Sort: Search Rank

PaN Experimental technique (PANET)

classes 379

The PaNET ontology provides a taxonomy and thesaurus of photon and neutron (PaN) experimental techniques, based mainly on accelerator-based light sources and neutron facilities

Uploaded: 6/19/21

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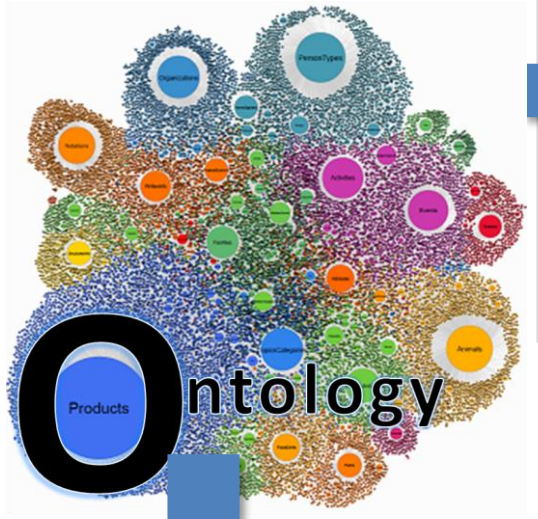
Meta Data Ontologies and their consequences



BioPortal

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Keywords

Defining NeXus Keywords in a common file format like HDF5

Keywords for Meta Data Catalogues and the ‘PaN Search API’

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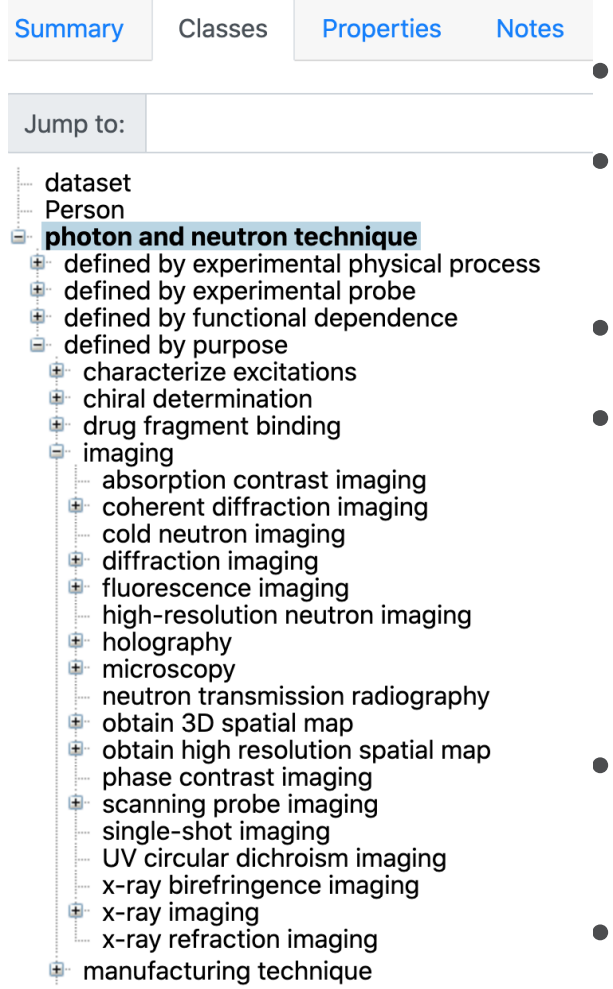
ExPaNDS European Open Science Cloud Photon and Neutron Data Services

Our contribution to Ontologies, NeXus formats and catalogue definitions



- Worked on a common ontology for different techniques in PaN;
- Checked ‘keywords’ for duplication in other sciences and searchability;
- Modelled our Ontology into the BioPortal;
- Working on making the BioPortal (not our service) available through the EOSC Portal;

BioPortal

EUROPEAN OPEN SCIENCE CLOUD

- Publishing hints for catalogues to pick up the right keywords form our ontology;
- Involved in the NeXus definitions following our ontology. (NIAC Involvement).

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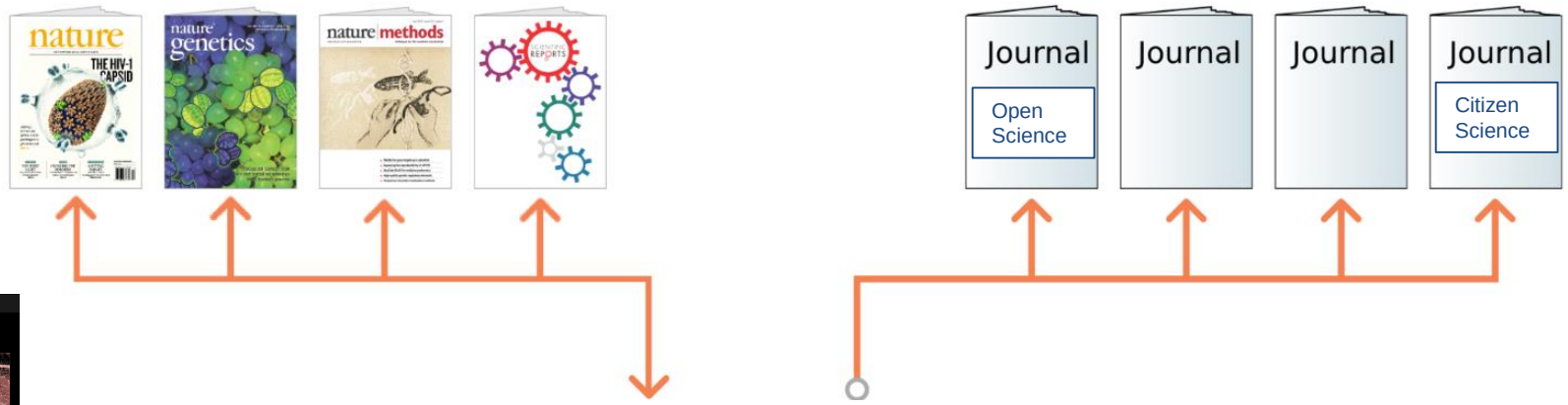
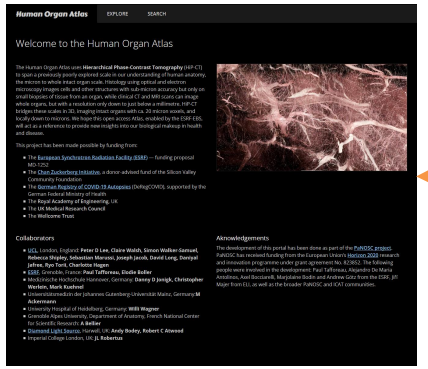
ExPaNDS European Open Science Cloud Photon and Neutron Data Services

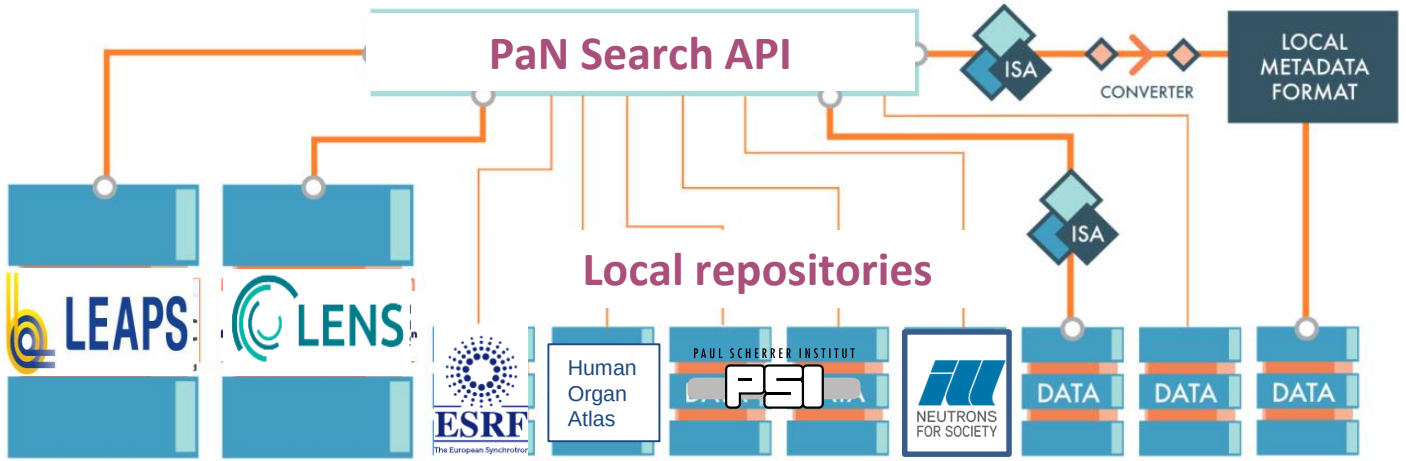
Sustain Published Data ➡ Through PaN Repositories





PaN Open Data Portal

PaN Open Data Repository



ICAT

SciCat

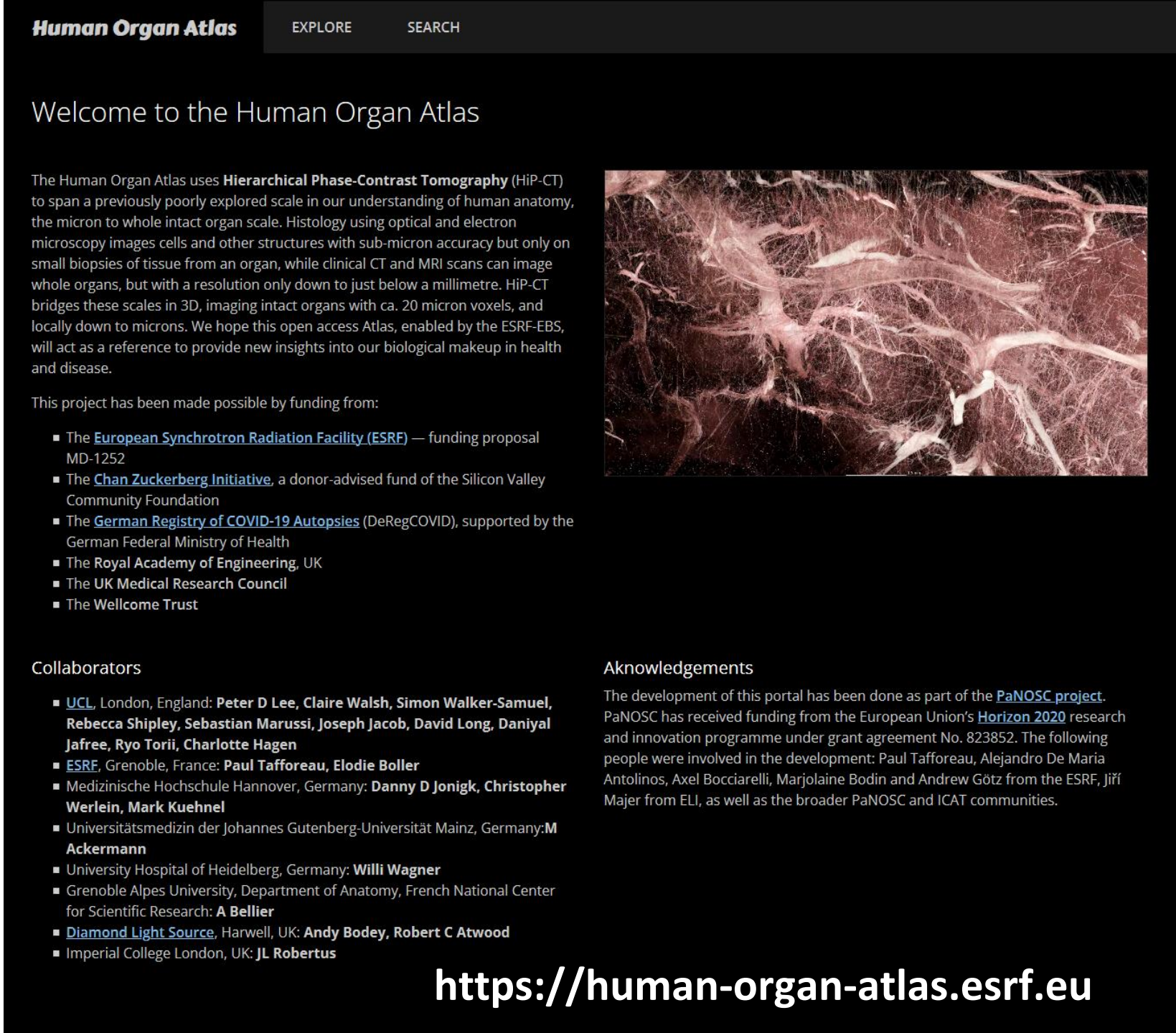
image: http://blogs.nature.com/scientificdata/2013/07/23/scientific-data-to-complement-and-promote-public-data-repositories/

Example of open data publishing:

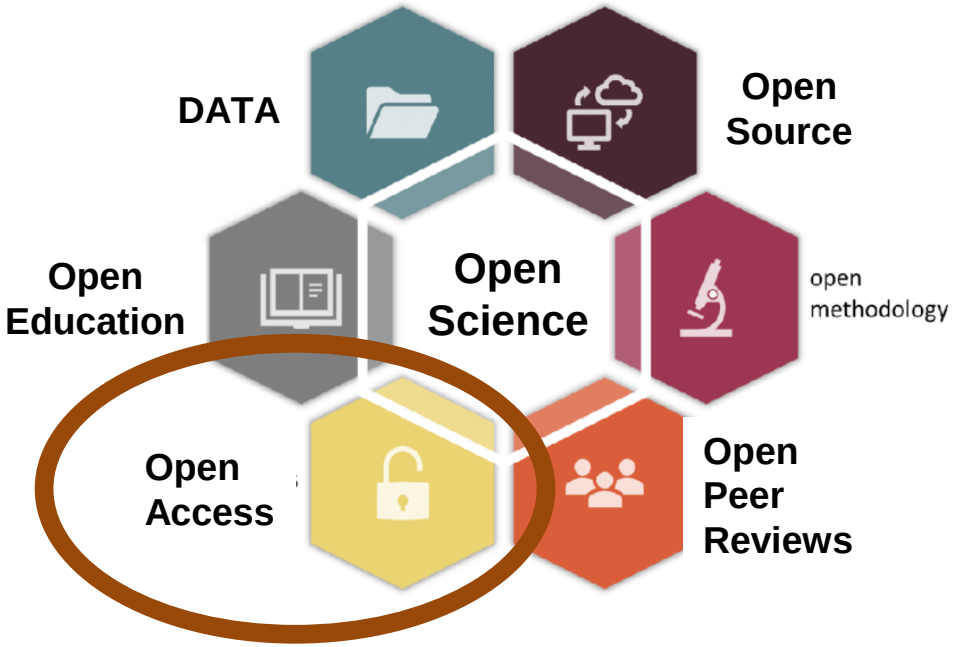
Human Organ Atlas

*Walsh, C.L., * Tafforeau, P., * Wagner, W.L., Jafree, D.J., Bellier, A., Werlein, C., Kühnel ,M.P., Boller, E., Walker-Samuel, S., Robertus, J-L., Long, D.A., Jacob, J., Marussi, S., Brown, E., Holroyd, N., Jonigk#, D.D., Ackermann#, M., Lee#, P.D. **Imaging intact human organs locally resolving cellular structures using hierarchical phase- contrast tomography.** Nat Methods (2021) Accepted

refer to PaNOSC Use Case 23 for more info



Prerequisite for open access : the common AAI



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PaN and EOSC Core service: Authentication and Identity Management (AAI)

- Originally
  - Scientist needed a different identity at each facilities to access their services.
    - Lots of passwords to remember and to loose
    - Difficult with cross facility services.

- UmbrellaID
  - Scientist only needs one identity with UmbrellaID (on top of home identity)
  - 'Catch all' identity providers are no longer state of the art and not trusted.

- Now: eduTeams [GÉANT service] (in progress)
  - Scientist only needs the one identity from his/her home facility!
  - Single Sign On: for cross facility services (data orchestration and automatic analysis)
    - One service can use another services somewhere else on your behalf!
  - Less Prison Time: Legal Issues for IdPs and Services are sorted out (AARC Blueprint)
  - Security: We are part of the European wide CERT system.

- EOSC-Future -> Science agnostic AAI
  - Scientist can use his home Identity for different services cross communities.

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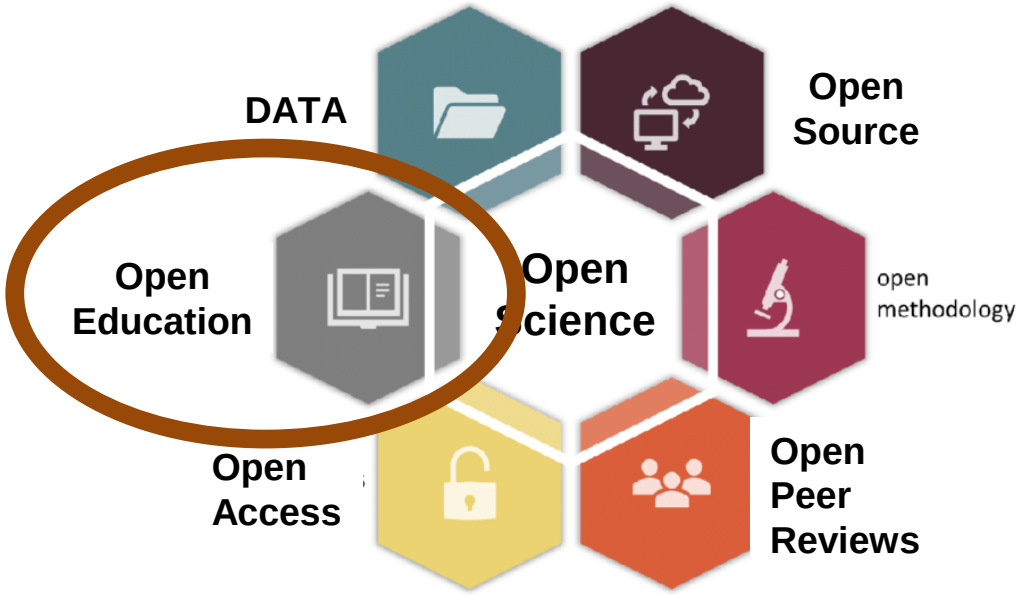
Training and Learning Platform



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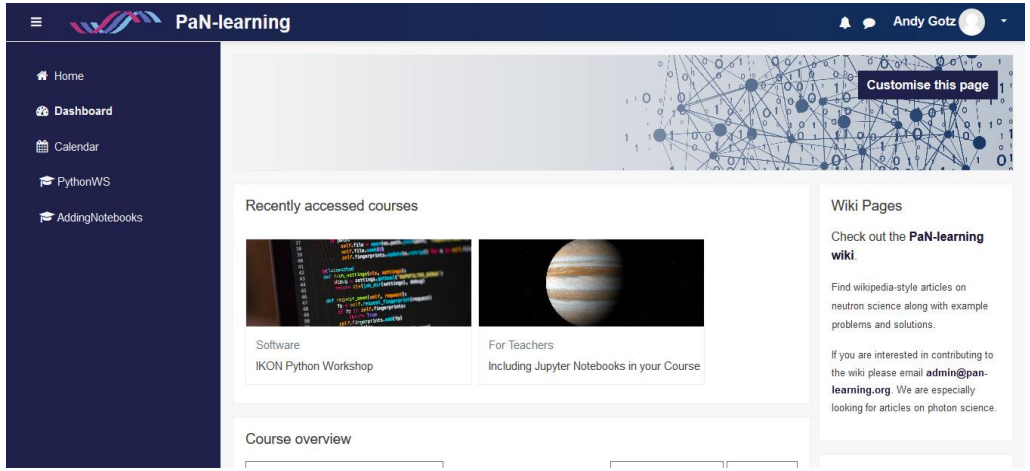
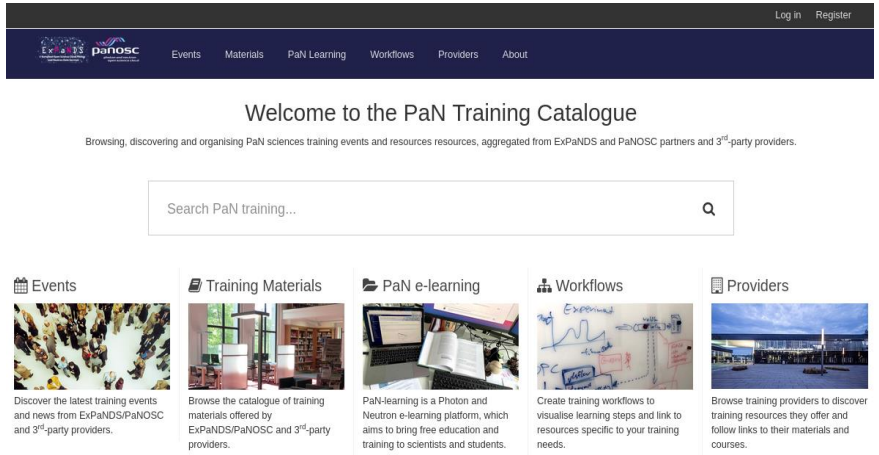
Training and Learning Platforms

- A centralized platform for collecting our highly distributed knowledge, documents and teaching material
  - which was identified at the facilities as important and missing.
- One can see golden thread in the current disparity of content.



https://pan-training.hzdr.de/



https://pan-learning.org

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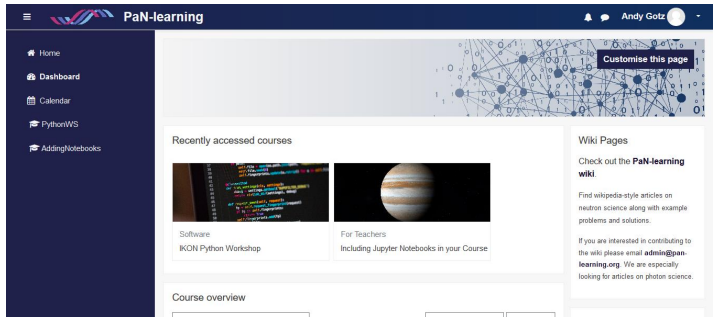
Our contribution to the teaching and learning platform.

- We evaluated available, state of the art technologies for teaching and data collection platforms.
- We introduced a PaN training platform to
  - **create**/store courses and to
  - **collect** existing material.
- We are re-using successful projects developed by
  - **Elixir** (TeSS) and
  - **SINE2020** e-neutrons.



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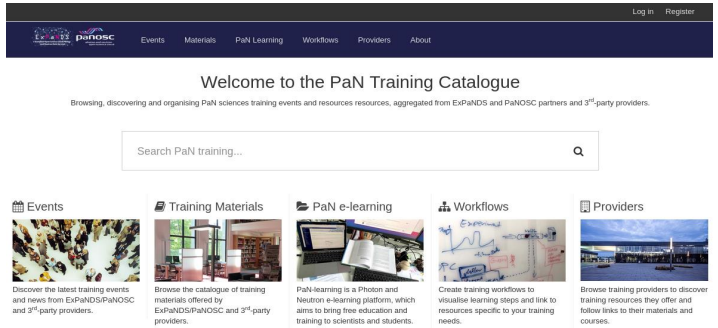

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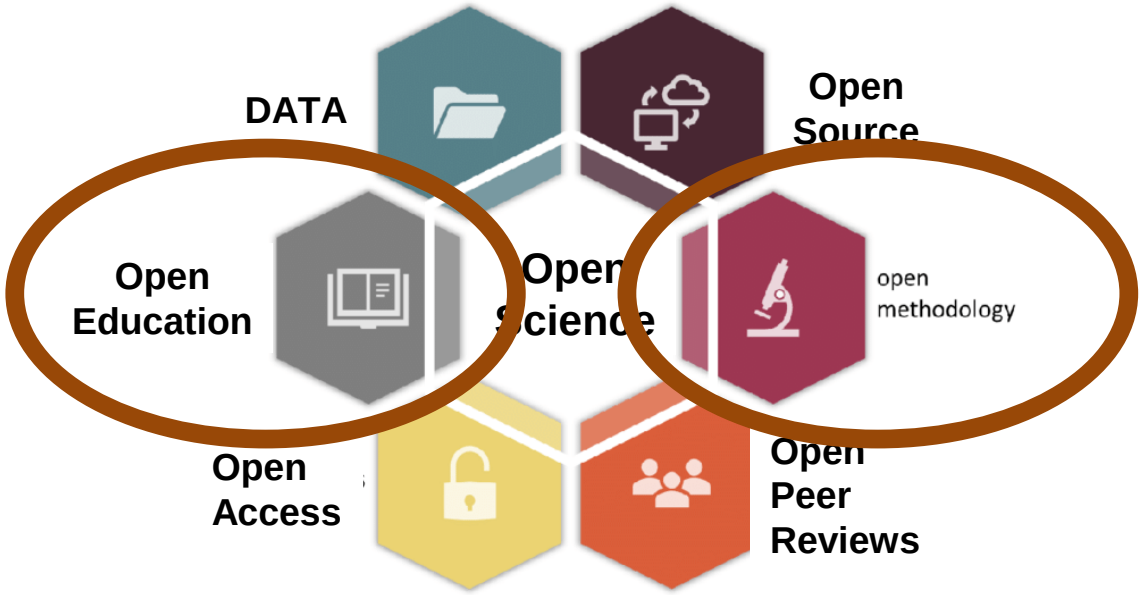
Data analyse services



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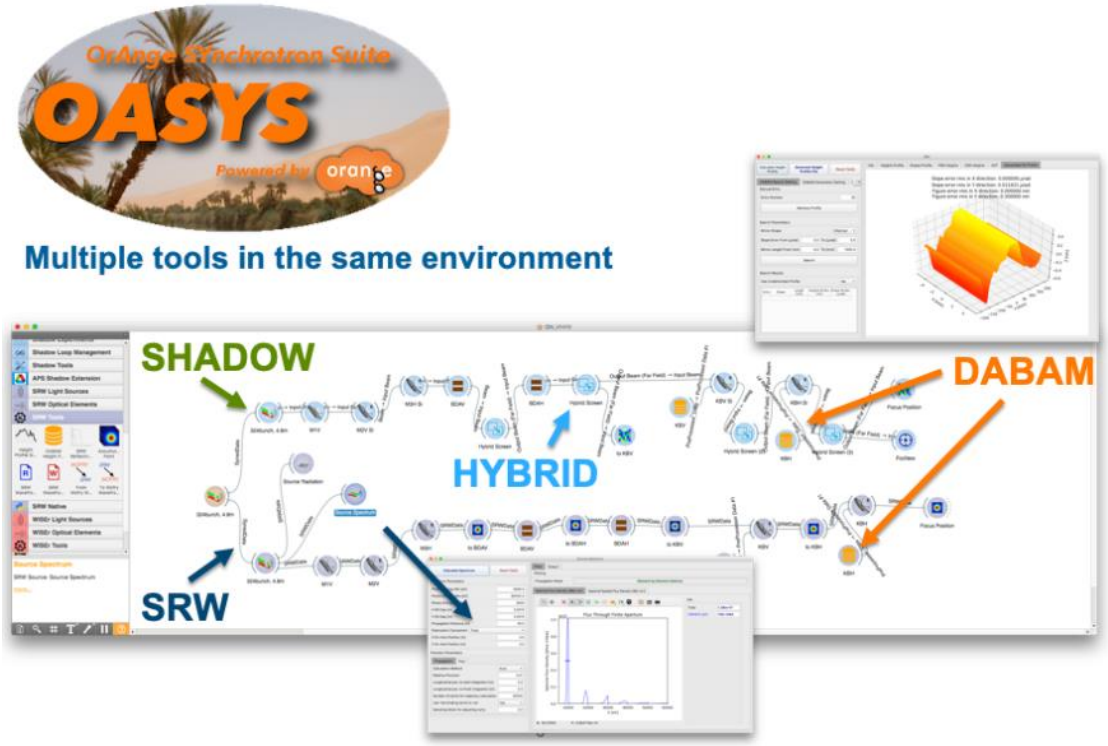
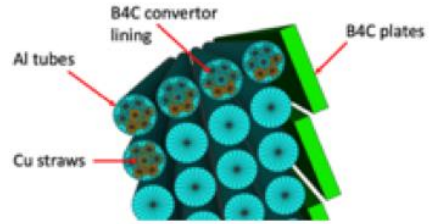
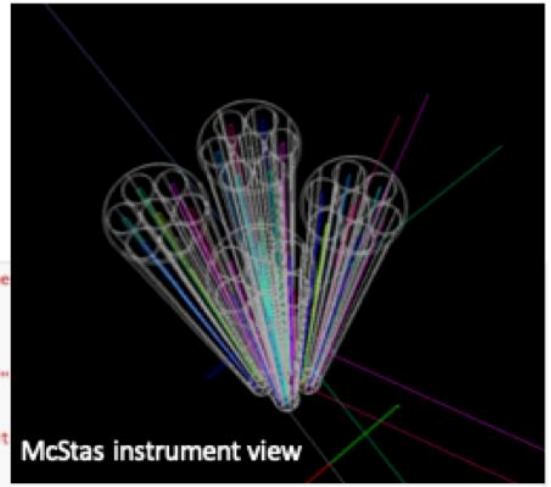
Simulation in PaNOSC provides support to OASYS + McStas








```
In [4]: Al_incoherent = ISIS_SANS2d_Mantid.add_component("Al_incohe
        Al_incoherent.sigma = "4+0.0082"
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        Al_incoherent.unit_cell_volume = 66.4

        Al_powder = ISIS_SANS2d_Mantid.add_component("Al_powder", "
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        Al = ISIS_SANS2d_Mantid.add_component("Al", "Union_make_mat
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        Al.my_absorption = "100*4+0.231/66.4"

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        Cu.my_absorption = "100*4+3.78/47.24"
executed in 9ms, finished 21:52:02 2020-12-15
```

PaNOSC continued simulation activities started in EUCALL with SIMEX, lasers + neutrons

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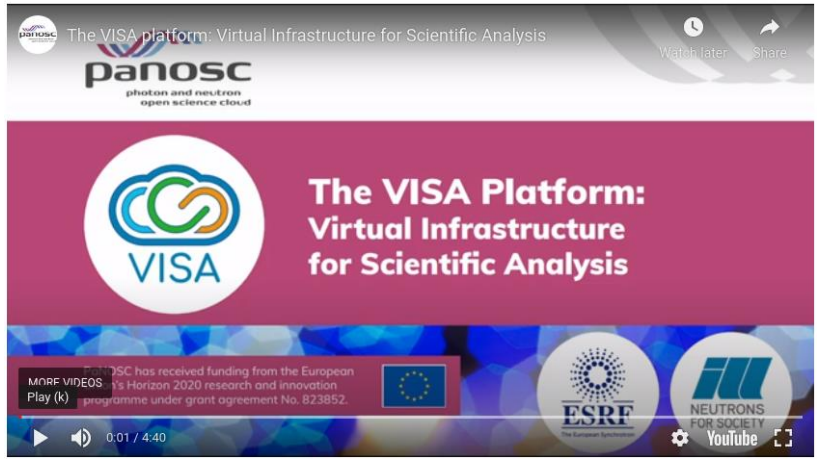
Users need remote data analysis

- Why it’s important
  - next generation of data analysis in globalised research
  - **remote access** to facilities
- What we do
  - develop and deploy **VISA** platform
  - make **Jupyter** notebooks available at all sites
  - make data analysis pipelines **interoperable**
- Provides remote data analysis services in a web browser with access to
  - Experimental data
  - Scientific software
  - Compute ressources
  - Support (IT and Scientific)



https://bit.ly/VISA-video

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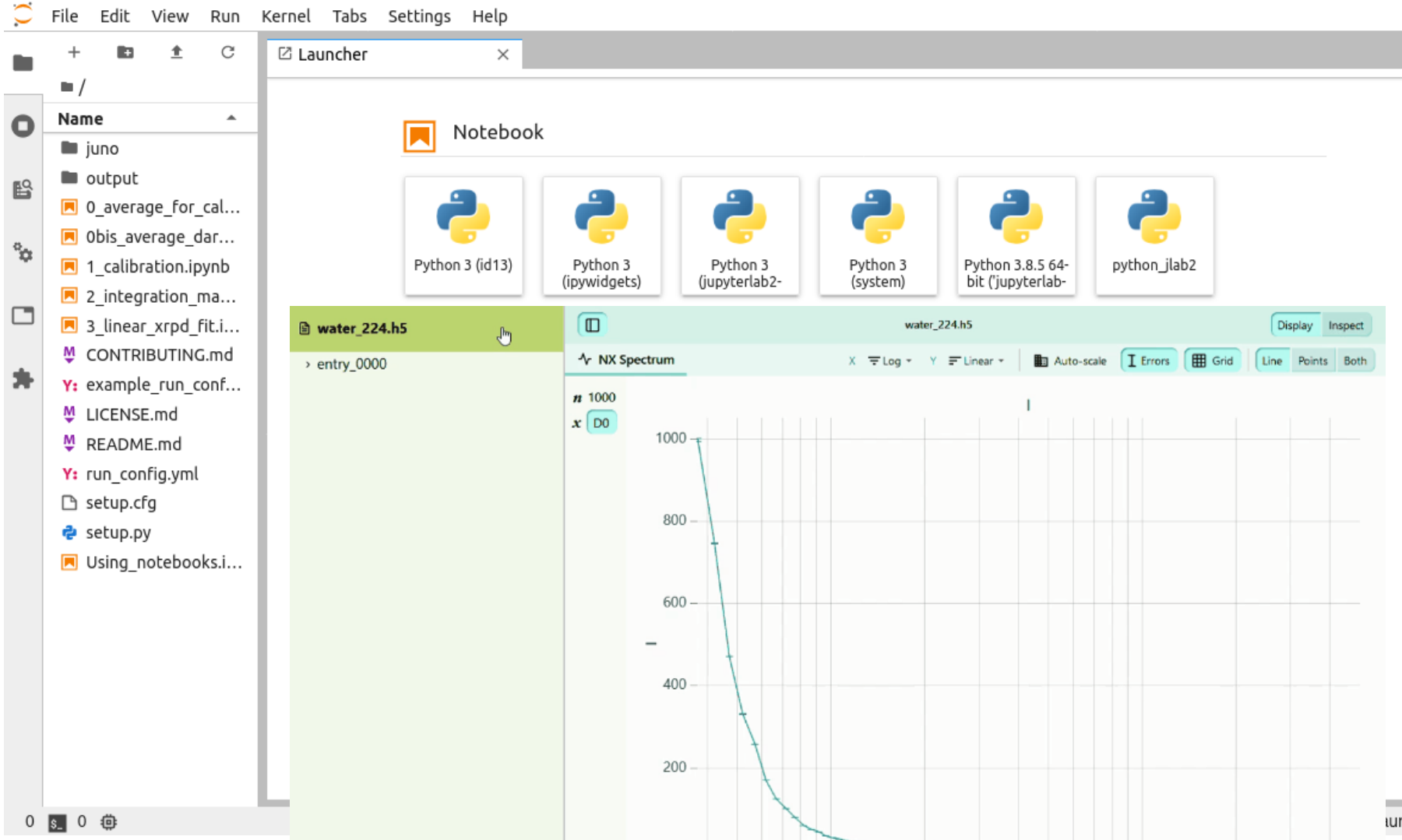
European Open Science Cloud Photon and Neutron Data Services

Remote analysis + visualization with Jupyter notebooks

- **JupyterLab has been widely adopted as remote analysis tool**

- **PaNOSC provides**
  - Jupyter-slurm
  - Nexus/HDF5 visualization
- **PaNOSC + ExPaNDS**
  - Developed for Use Cases



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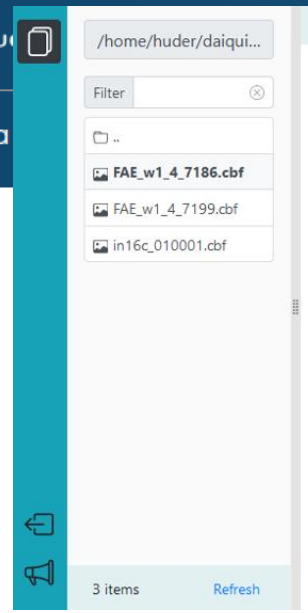
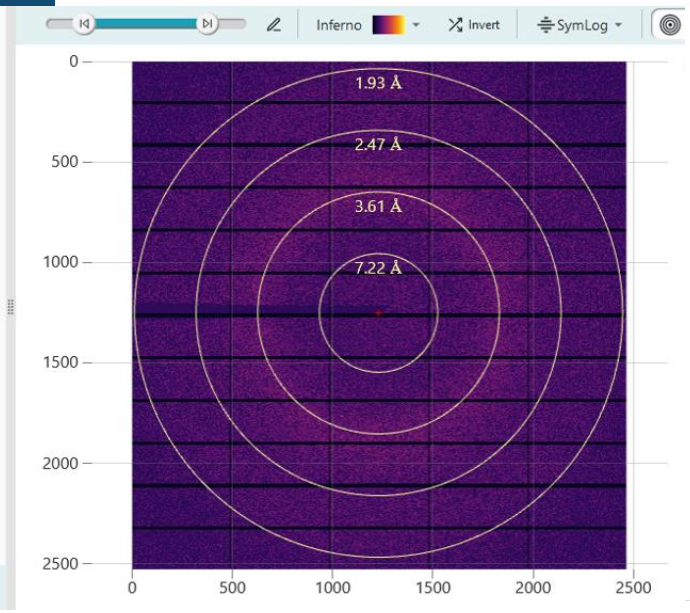
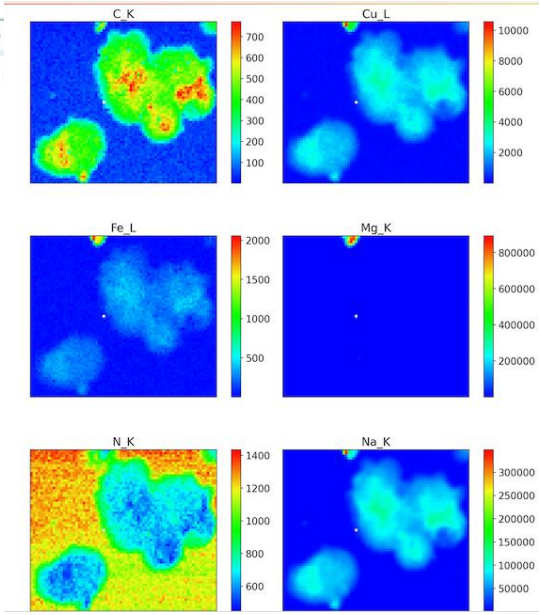
https://www.panosc.eu/all-use-cases/

All Use Cases

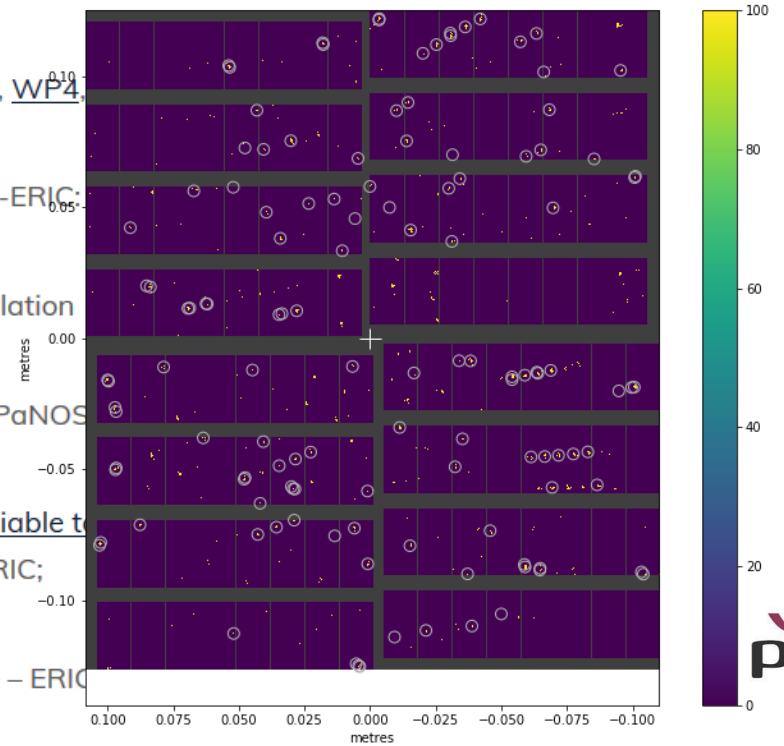
Submit your use case

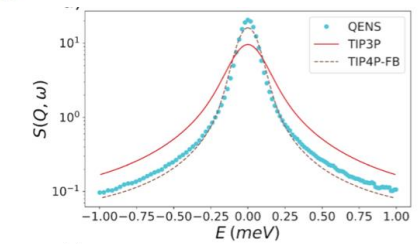


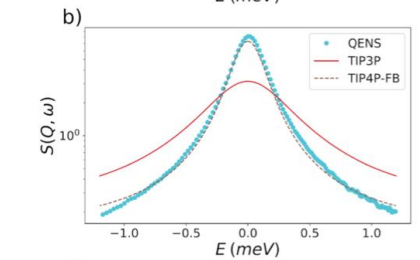


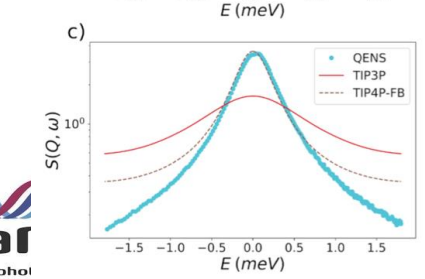


- **Use Case 22** – BRAGGY diffraction image viewer (ESRF; PaNOSC-related WPs: WP3, WP4, WP6)
- **Use Case 21** – Online visualization and analysis of HDF5 PyMCA Output Files (CERIC-ERIC; PaNOSC-related WP: WP4)
- **Use Case 20** – Using an e-learning platform to support presentations (European Spallation Source – ERIC, ESS-ERIC; PaNOSC-related WP: WP8)
- **Use Case 19** – Online visualization and analysis of Bruker NMR output (CERIC-ERIC; PaNOS related WP: WP4)
- **Use Case 18** – In-silico Neutron diffraction from Boro-carbon systems: precise and reliable t for exact structural analysis and defect detection (Extreme Light Infrastructure, ELI-ERIC; PaNOSC-related WP: WP5)
- **Use Case 17** – Reusing data for validation of force fields (European Spallation Source – ERIC ESS-ERIC; PaNOSC-related WPs: WP3, WP4, WP5)









Examples from other clusters in EOSC

- **EOSC-Life**
  - EU COVID-19 portal
- **ESCAPE**
  - High Energy Physics – CERN Open Data
  - Virtual Observatory
- **ENVRI-FAIR**
  - ICOS, DISSCO, …
- **SSHOC**
  - CLARIN, DARIAH, …
- **PaNOSC+ExPaNDS**
  - ISIS, ILL, ESRF, PSI, …

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