ExPaNDS
European Open Science Cloud Photon and Neutron Data Services

2nd European PaN Symposium

Project results, use cases and the future!

Patrick Fuhrmann (DESY, ExPaNDS), **Andy Götz** (ESRF, PaNOSC)

With contributions by Sophie Servan (DESY) and Jordi Bodera (ESRF)

For the Project teams!

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.

ExPaNDS and PaNOSC in the PaN EU project landscape

DiTARI Proposal

2010 2015 2018 2021

European Open Science Cloud (EOSC)

EOSC Future

2019	2020	2021	2022

ExPaNDS
European Open Science Cloud Photon and Neutron Data Services

panosc
photon and neutron open science cloud

Policies	Common data policy	**FAIR** data policy	Data Management Plans
Analysis	Software Catalogue	Remote analysis	Jupyter
AAI	UmbrellaID	AARC Blueprint	eduTeams
Training	e-neutron		Training platform

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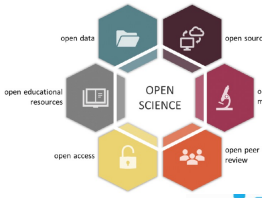
ExPaNDS European Open Science Cloud Photon and Neutron Data Services

Which has a lot of implications .....

BioPortal

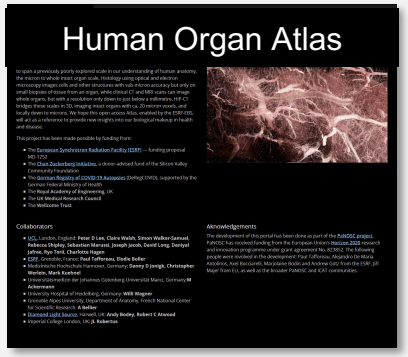
jupyter



EUROPEAN OPEN SCIENCE CLOUD

slurm workload manager

And already some very positive outcomes



Desc… future

Petr Č…

- Describ…
- Public D…
- Publish …
- **R and …**

TELBE Data Analysis wo… and the PaN training pla… Spectra Classification

Jan-Christoph Deinert

- Rendering a workflow i… **PaN training** platform.

DOI, FAIR, an… Case

Frank von D…

- Covid Resea…
- **FAIR**
- **DOIs**

Neutron diffraction from Boro-carbon for efficient structural analysis and defect detection

Mousumi Upadhyay Kahaly (ELI-ALPS)

- Boron-doped diamond (BDD) for high voltage batteries.
- Inelastic neutron scattering
- Simulated with **McStas** code
- **Making use of WP4/5/6 of PaNOSC**

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European Open Science Cloud Photon and Neutron Data Services

How do we achieve our goal ?

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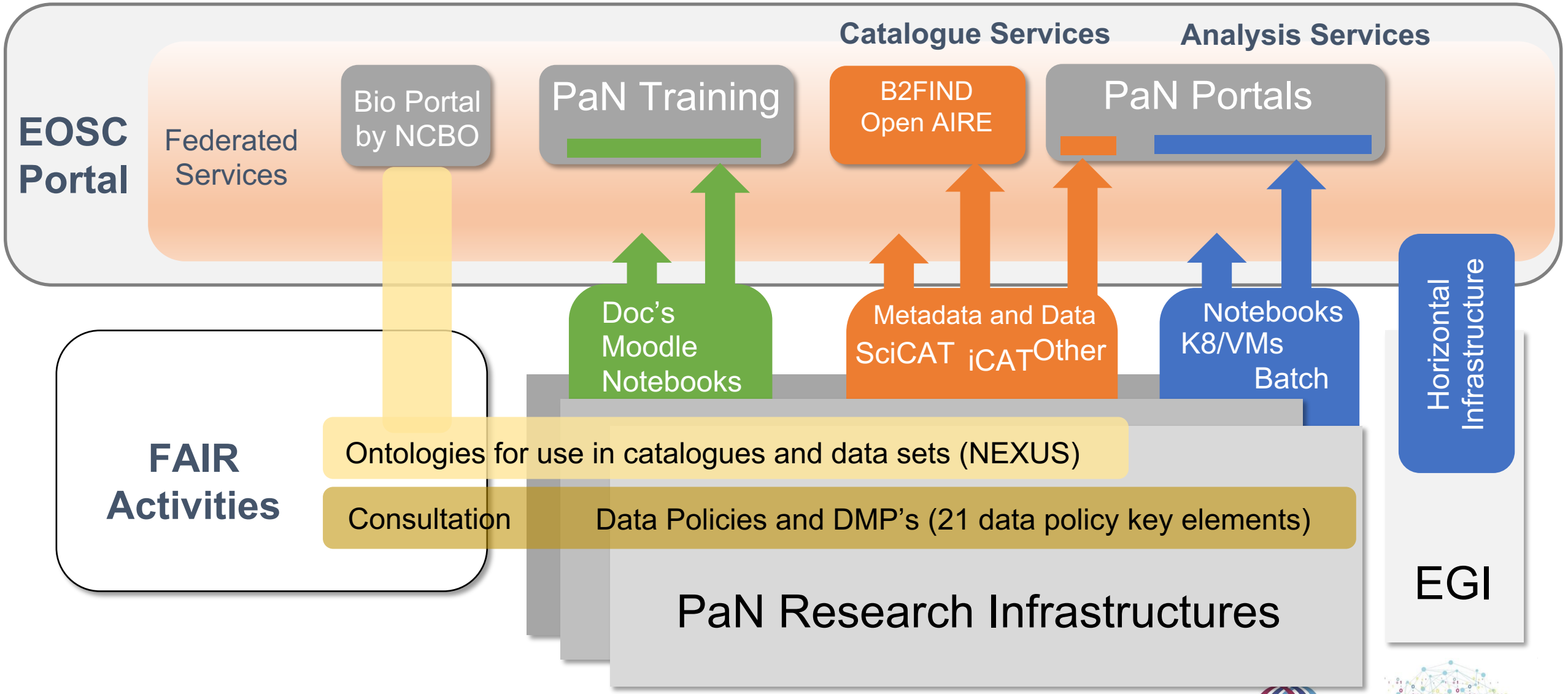
The Big Picture of EOSC in PaNOSC and ExPaNDS



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

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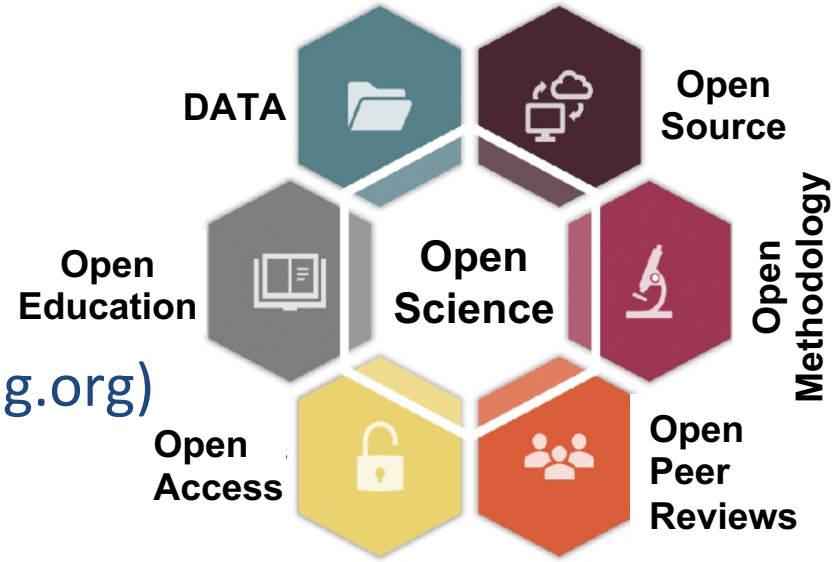
Highlights from PaNOSC and ExPaNDS and table of content.

- From Open Science to FAIR Data
  - FAIR data policy and DMPs FAIR assessment
  - Common PID framework
- Ontologies, Meta Data and standardized searching
  - Standardised metadata (Nexus/HDF5, PaN ontologies)
  - Federated search API for PaN data catalogues
- PaN-learning platform (pan-learning.org + pan-training.org)
- Services
  - Core: Community AAI (GEANT eduTeams)
  - Portable and easy to verified analysis pipelines
  - JupyterLab notebooks and Nexus/HDF5 files visualization
  - Remote data analysis with VISA + portable data analysis pipelines
- Simulation software for simulating experimental data (SIMEX)
  - Only by use case



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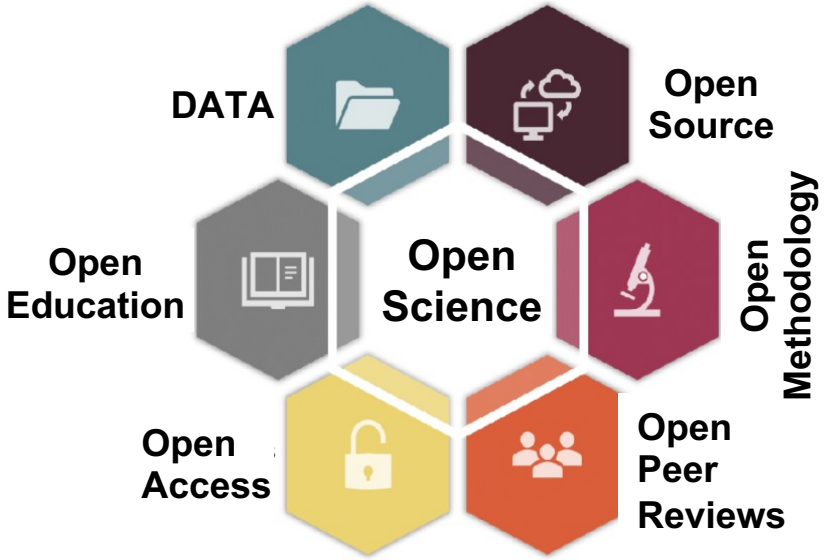

Open Science:
Open Data, FAIR Data Policies, PIDs, DMPs .....

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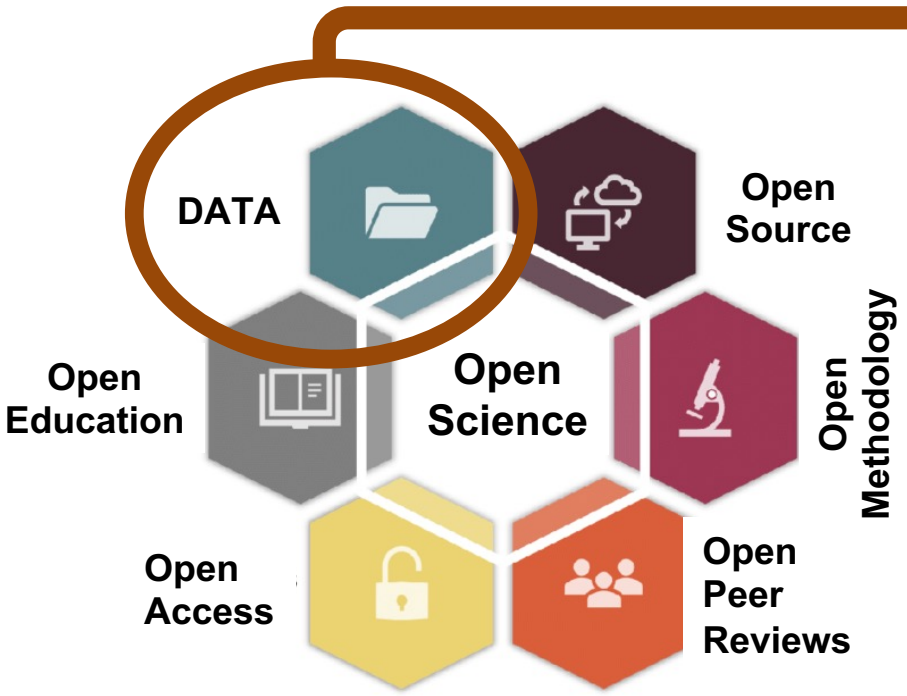
From Open Science to FAIR data.



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

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.

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

We provide

- Data Policy
  - Framework for easy adoption in not so complex cases
  - 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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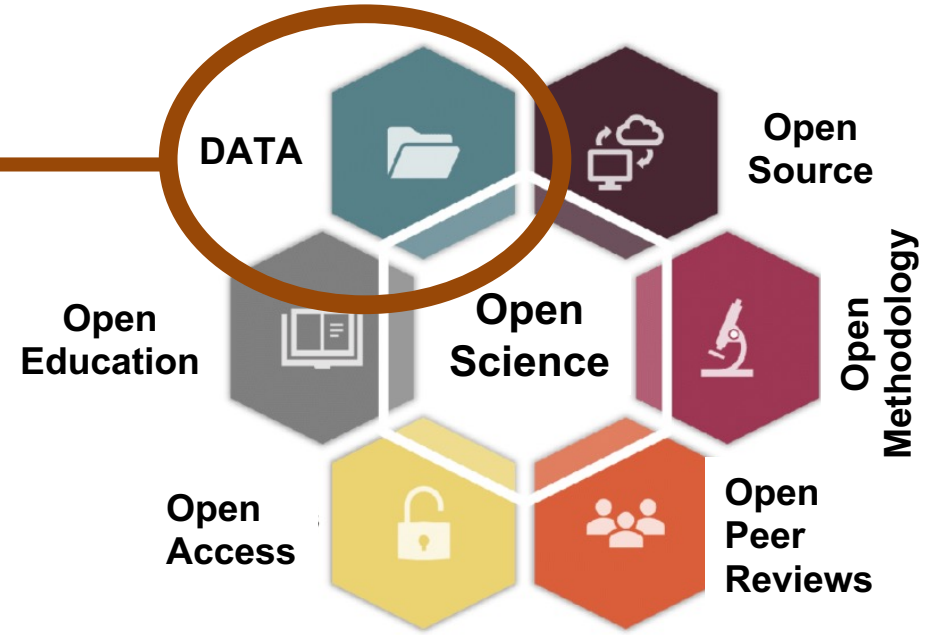
FAIR Data



Meta Data Ontologies, Keywords in Catalogues and NeXus

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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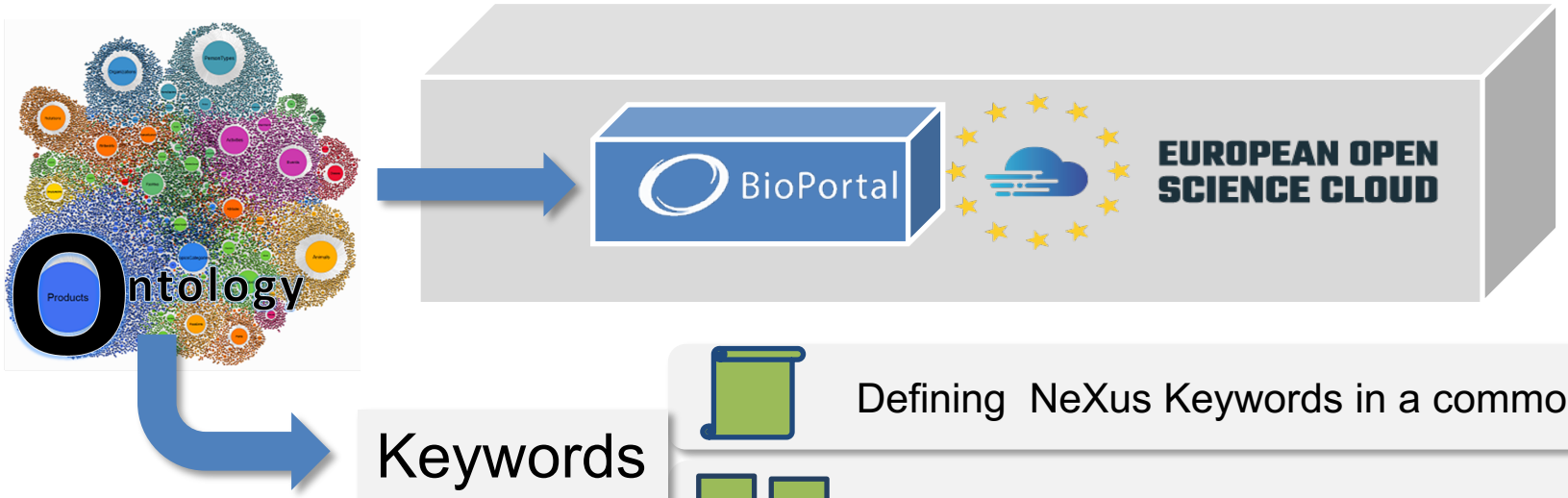
ExPaNDS European Open Science Cloud Photon and Neutron Data Services

Meta Data Ontologies and their consequences



- 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;
- 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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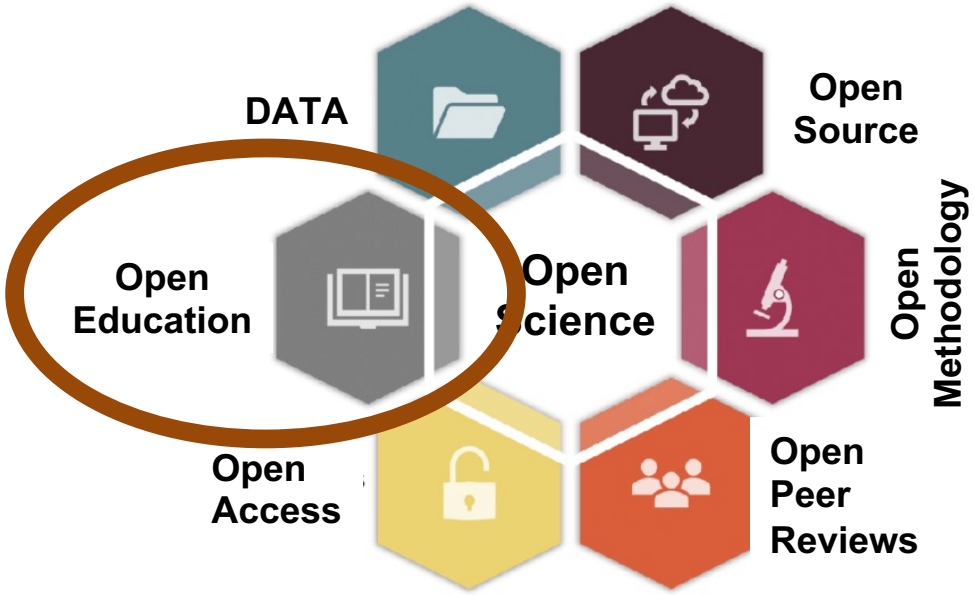
Training and Learning Platform



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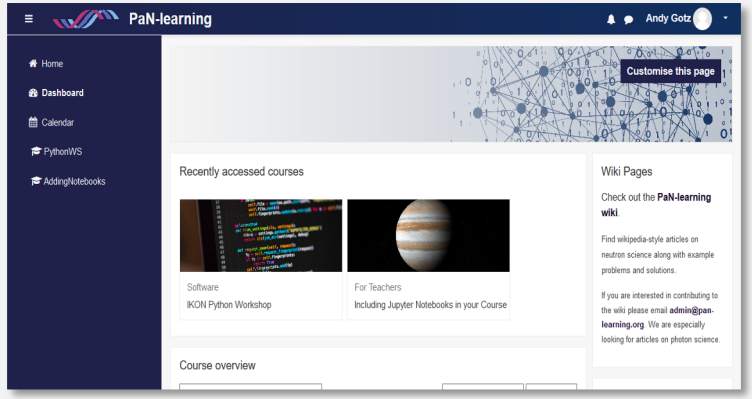
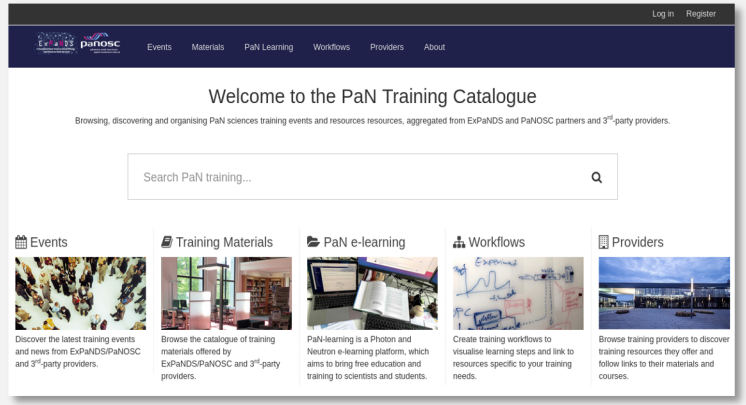
Our contribution to the teaching and learning platform.

- The lack of a central platform for PaN Teaching and Learning has been identified by the facilities.
- 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.

PaN-Training.hzdr.de



PaN-Learning.org



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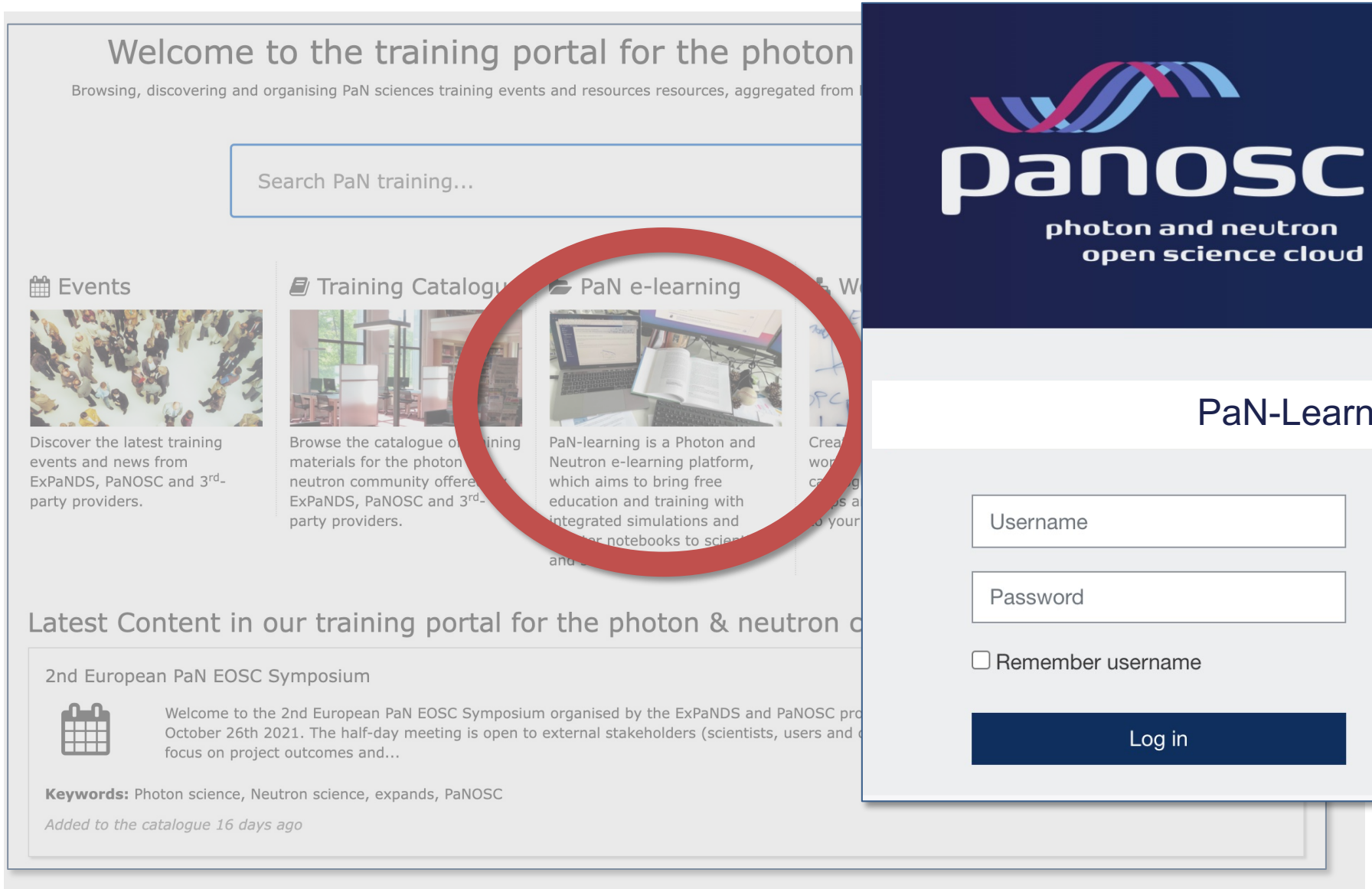
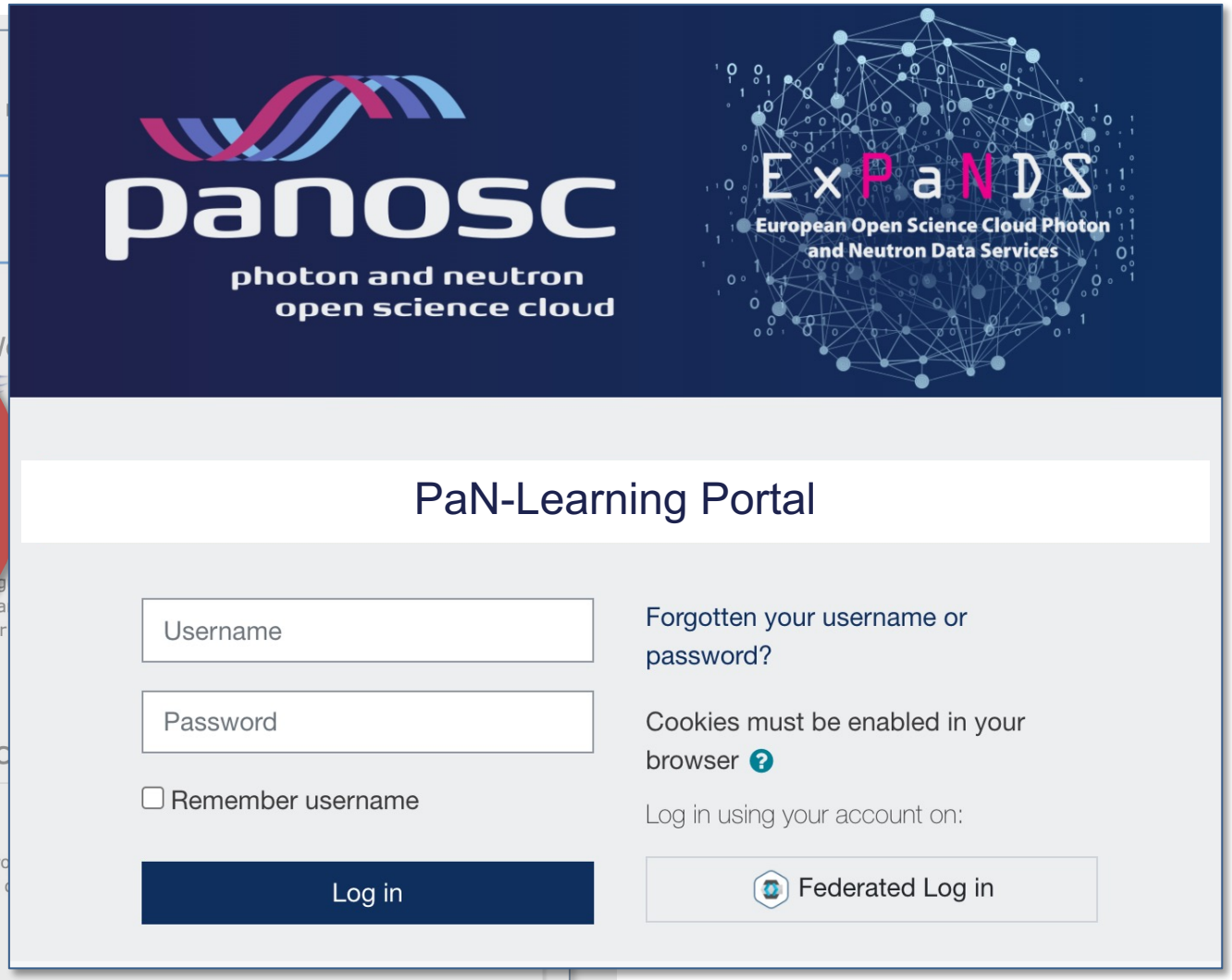
Training and Learning Platforms





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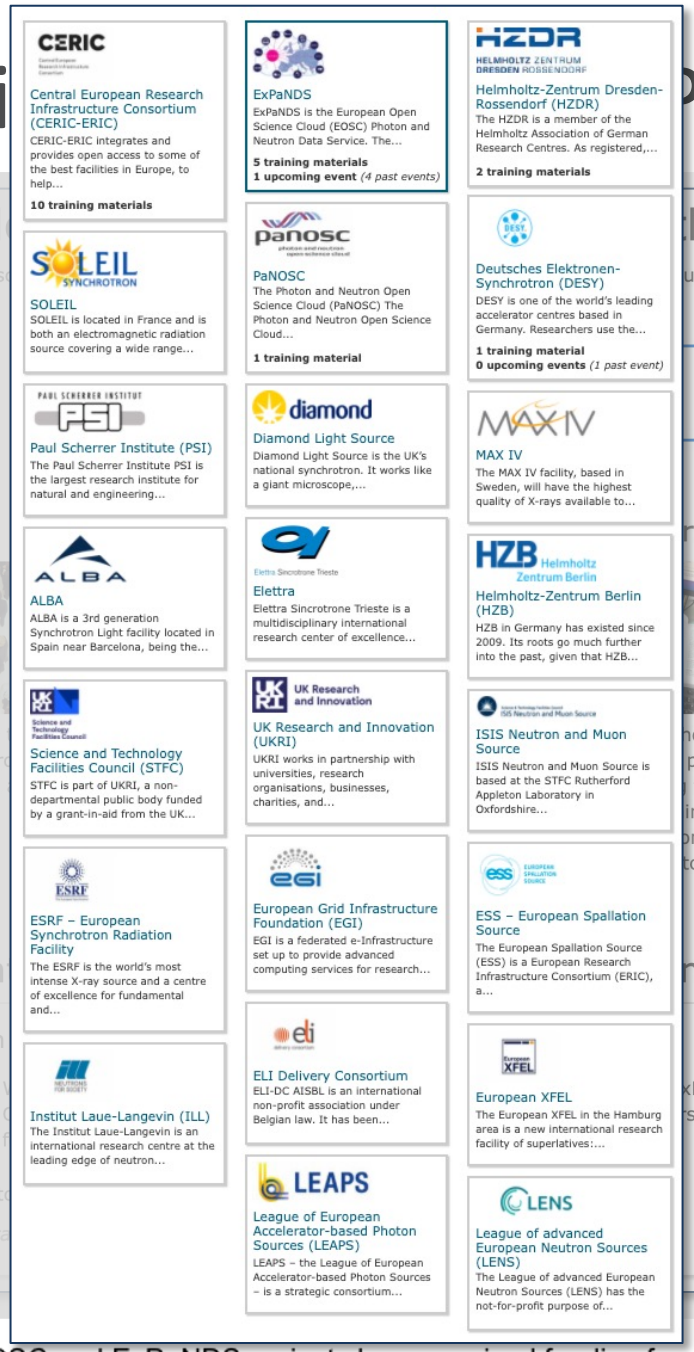
Traini Platforms



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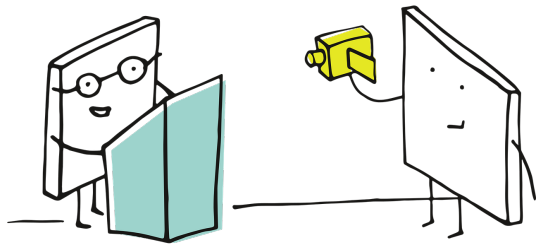

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&

PaN-Learning.org

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Training and Learning Platforms

Welcome to the training portal for

Browsing, discovering and organising PaN sciences training events and resources res

Search PaN training...

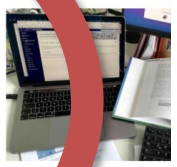
Events

Discover the latest training events and news from ExPaNDS, PaNOSC and 3rd-party providers.

Training Catalogue

Browse the catalogue of training materials for the photon & neutron community offered by ExPaNDS, PaNOSC and 3rd-party providers.

PaN e-lea



PaN-[T]raining is a Ne[w] e-learnin[g] [p]latform that aims to brin[g] [E]ducation and trai[ning] integrated simulat[ion] Jupyter notebooks [for] and students.

Latest Content in our training portal for the photo

2nd European PaN EOSC Symposium

Welcome to the 2nd European PaN EOSC Symposium organised by the October 26th 2021. The half-day meeting is open to external stakehold focus on project outcomes and...

Keywords: Photon science, Neutron science, expands, PaNOSC

Added to the catalogue 16 days ago

ExPaNDS D3.2: Ontologies v1.0

We present ontologies for the domain of photon and neutron (PaN) science. With the primary goal of supporting PaN FAIR dat a catalogue services, we have developed three ontologies: PaN experimental techniques (PaNET), an ontology of NeXus defini tions (NeXusOntology), and a semantic integration...

Keywords: expands, ontology, EOSC, Photon science, experimental techniques, Neutron scie nce, deliverable

Resource type: Document

ExPaNDS D5.4 : PaN Training Catalogue Demo Video

Demo video demonstrating the concept and the features of the PaN Training Catalogue as part of ExPaNDS Deliverable 5.4

Keywords: catalogue, expands, deliverable

Resource type: video

ExPaNDS D2.3: Final data policy framework for Photon and Neutron RIs

ExPaNDS deliverable D2.3: Final data policy framework for photon and neutron RIs, considers how data policies for research i nfrastructures providing photon and neutron facilities should be framed, in particular in the light of supporting open science a nd FAIR data. It builds on and revises the...

Keywords: expands, data policy

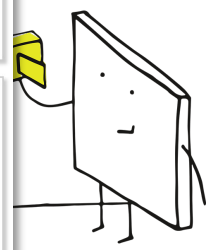
Resource type: Document

Introduction to Soft X-ray Transmission and Emission Microscope, TwinMic at Elettra Sincrotrone Trieste

Introduction to the TwinMic Beamline: Soft X-ray Transmission and Emission Microscope at the CERIC Italian partner facility, Elettra Sincrotrone Trieste ---TwinMic beamline webpage in the CERIC website:...

Keywords: soft X-ray Microscopy, synchrotron, Central European Research Infrastructure Con sortium, CERIC, synchrotron beamline, microscopy, electrochemistry, battery research, Herita ge Science, Elettra synchrotron, Elettra Sincrotrone Trieste, life sciences, microscope

Resource type: video



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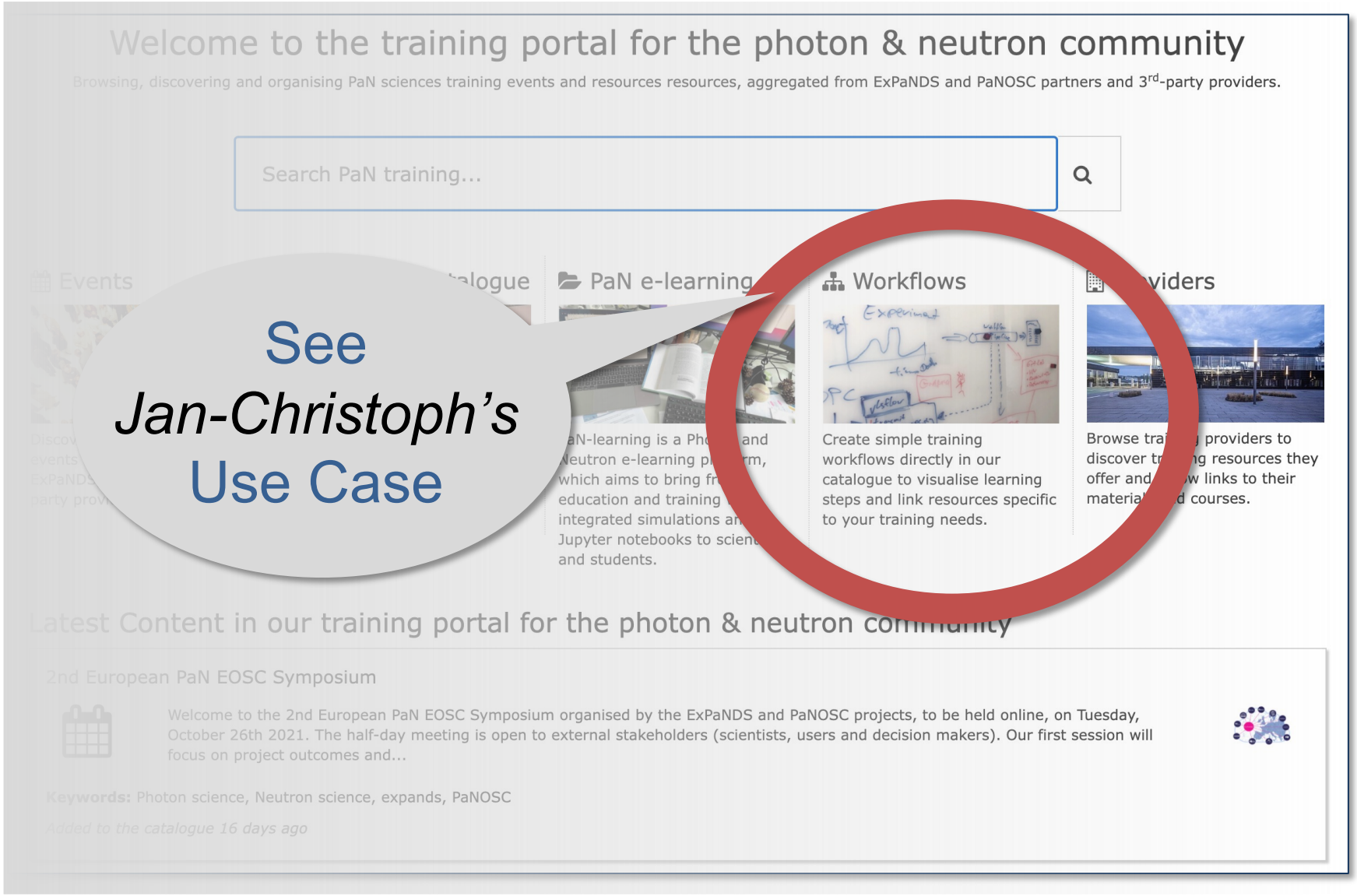
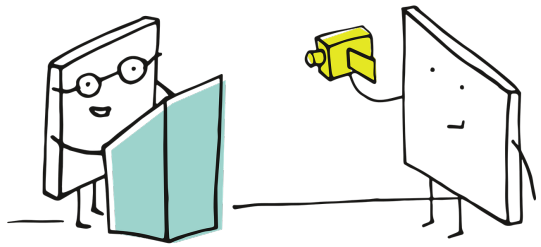
Training and Learning Platforms



See *Jan-Christoph's* Use Case

Now live at



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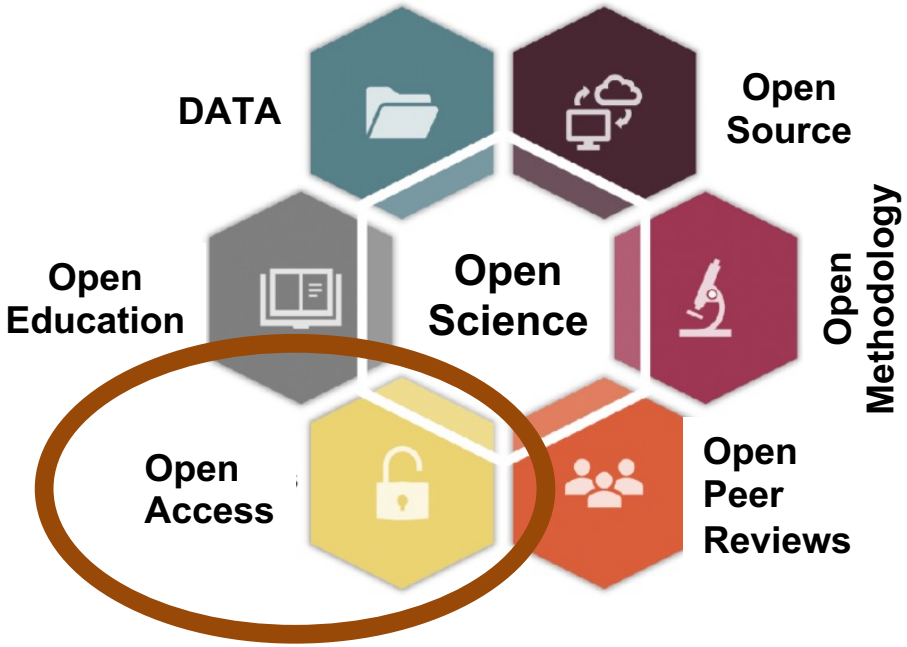
Prerequisite for open access : The common AAI



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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 might not trusted.

- Now: eduTeams [GEANT 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 sciences
  - PaN can co-utilize services from other sciences: e.g. Data Hub and Data Lakes.

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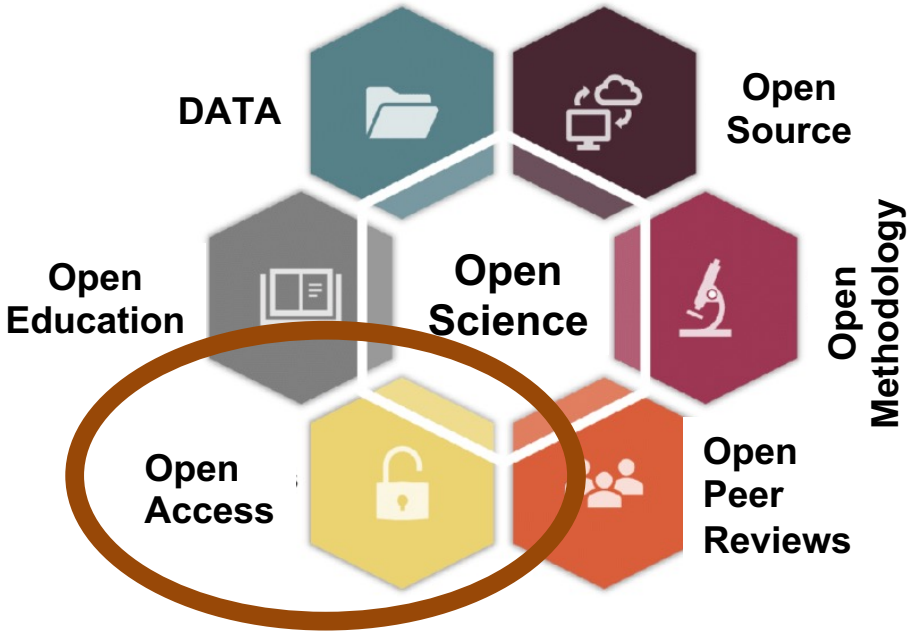
The next generation PaN Facility



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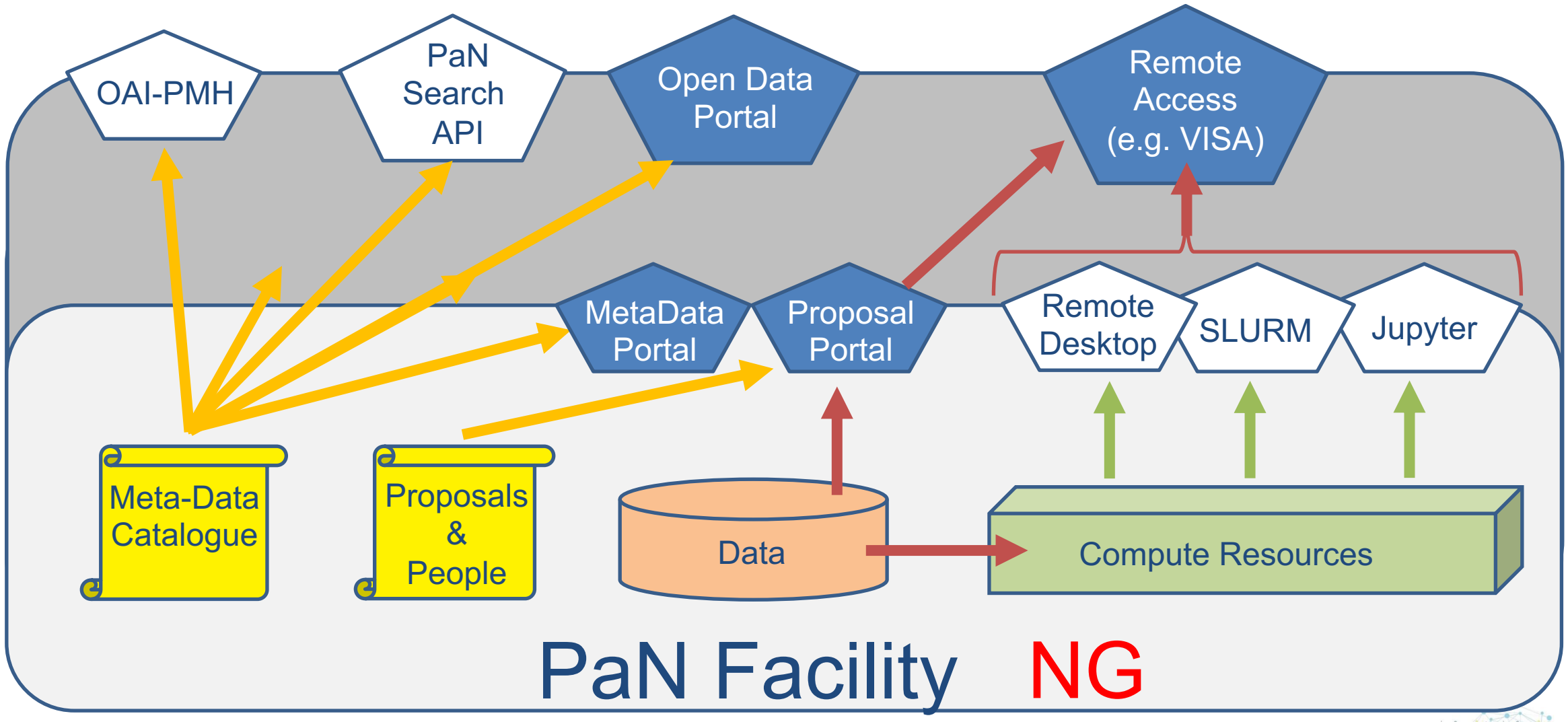
Towards the PaN Facility Next Generation



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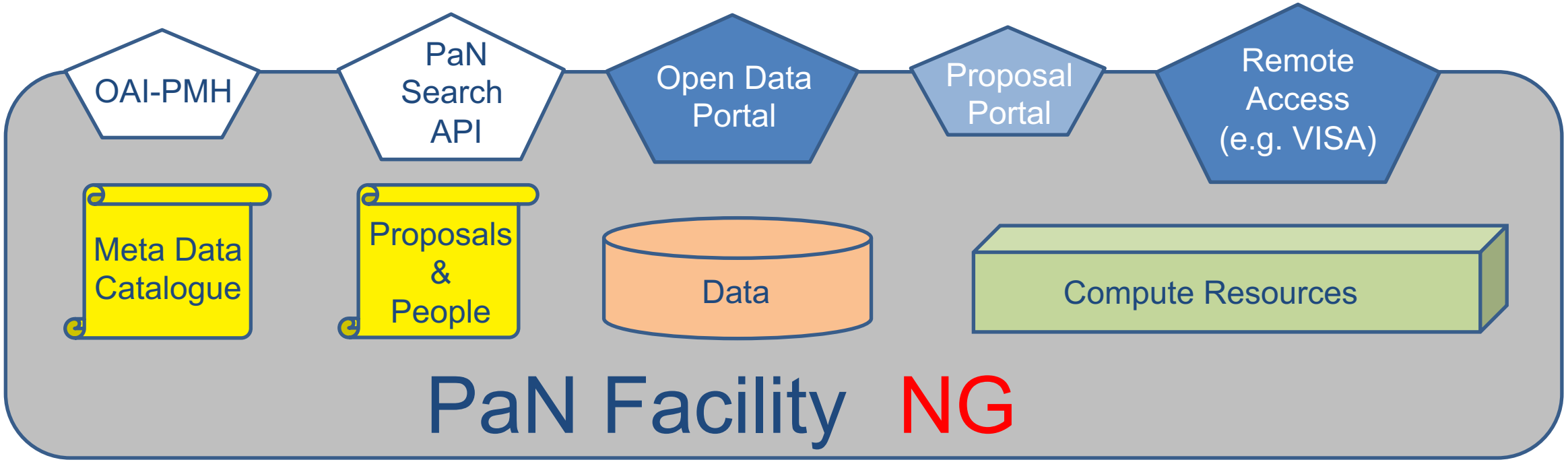
Towards the PaN Facility Next Generation



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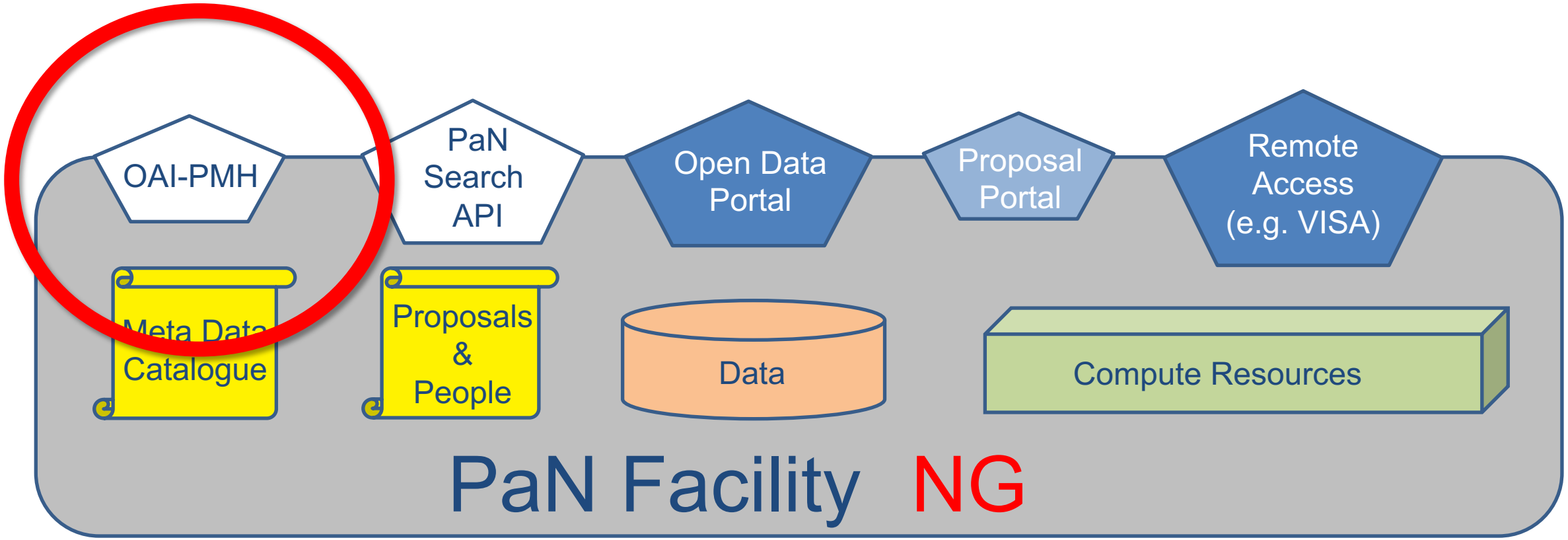
High level harvesting of our PaN treasures.



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Harvesting API

European Open Science Cloud, EOSC

OAI-PMH

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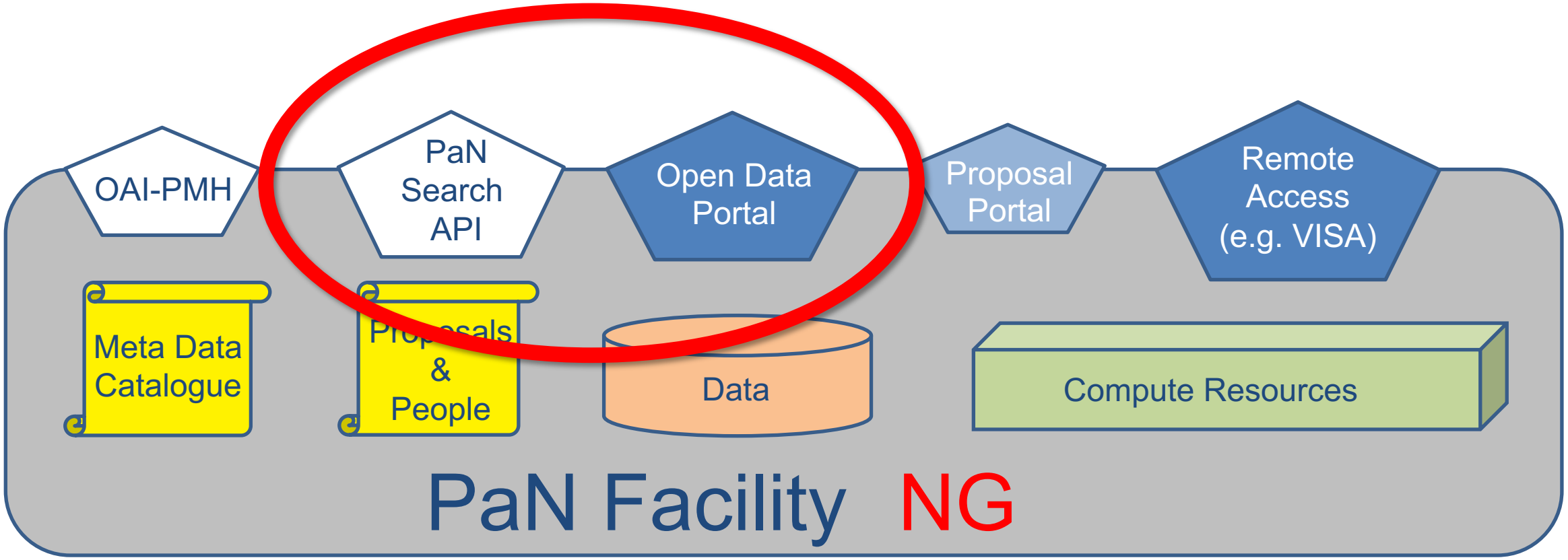
The PaN search API and the Open Data Portal



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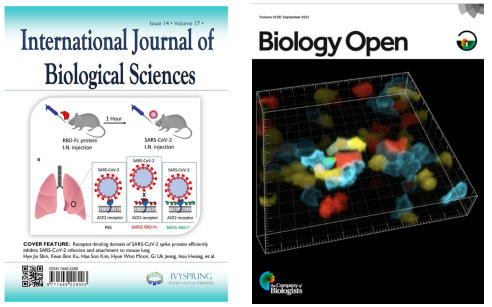
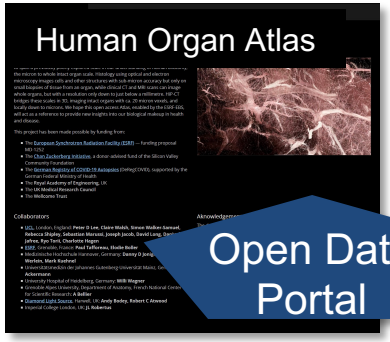
Federated PaN Search and the data portal.

Traditional Publisher



Open Publisher

Citizen Science



Open Data Portal

Open Data Portal

Open Data Portal

Open Data Portal

PaN Open Data Repository (EOSC)

PaN Search API

ESRF The European Synchrotron

PAUL SCHERRER INSTITUT PSI

DESY.

ALBA

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Elettra Sincrotrone Trieste

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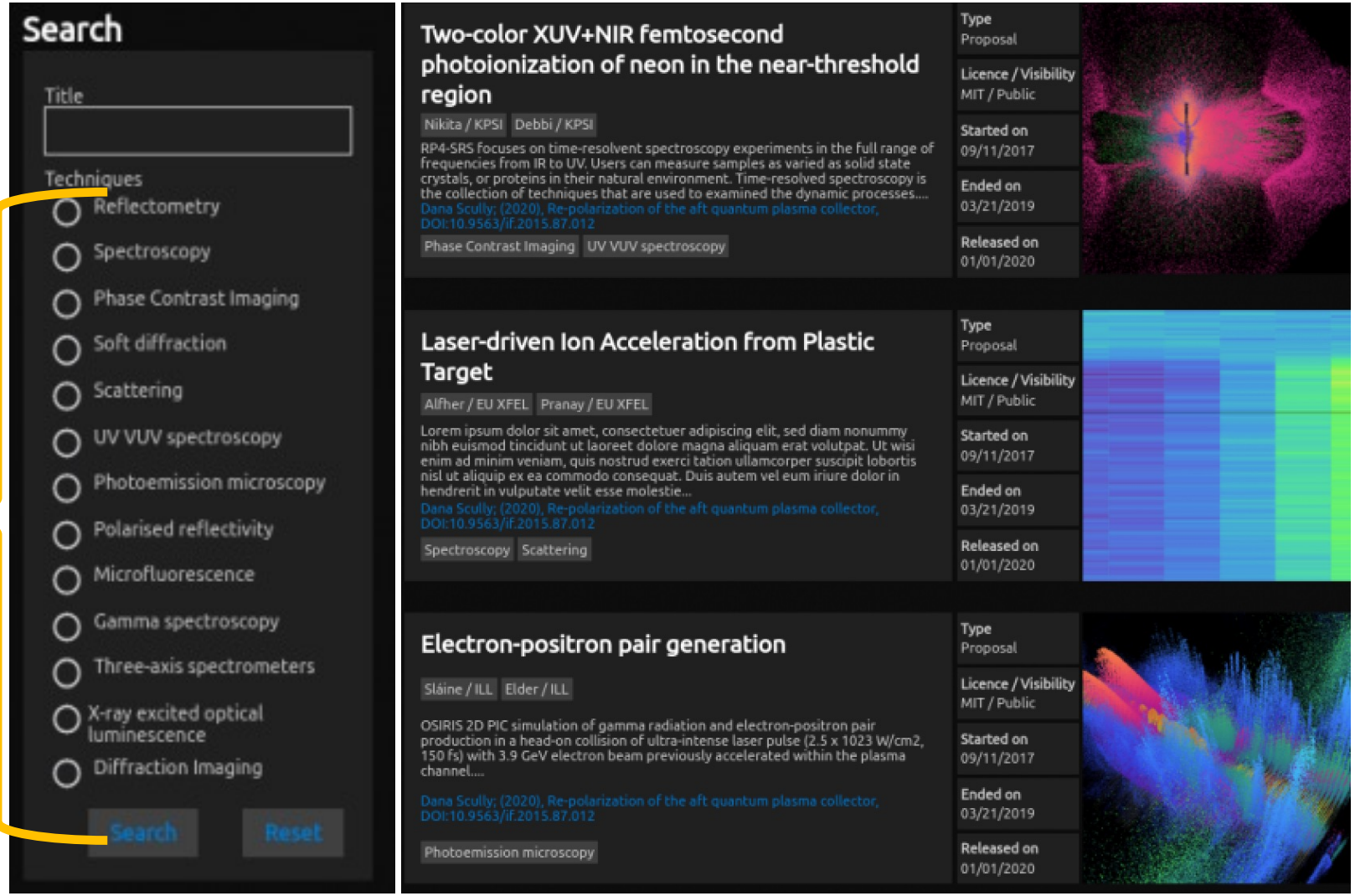
PaN Data Portal

Example for Ontologies

Techniques



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Special Case of the Open Data Portal (Customized)

Human Organ Atlas

The Human Organ Atlas uses **Hierarchical Phase-Contrast Tomography** (HiP-CT) to span a previously poorly explored scale in our understanding of human anatomy, the micron to whole intact organ scale. Histology using optical and electron microscopy images cells and other structures with sub-micron accuracy but only on small biopsies of tissue from an organ, while clinical CT and MRI scans can image whole organs, but with a resolution only down to just below a millimetre. HiP-CT bridges these scales in 3D, imaging intact organs with ca. 20 micron voxels, and locally down to microns. We hope this open access Atlas, enabled by the ESRF-EBS, will act as a reference to provide new insights into our biological makeup in health and disease.

This project has been made possible by funding from:

- The European Synchrotron Radiation Facility (ESRF) — funding proposal MD-1252
- The Chan Zuckerberg Initiative, a donor-advised fund of the Silicon Valley Community Foundation
- The German Registry of COVID-19 Autopsies (DeRegCOVID), supported by the German Federal Ministry of Health
- The **Royal Academy of Engineering**, UK
- The **UK Medical Research Council**
- The **Wellcome Trust**

Collaborators

- UCL, London, England: **Peter D Lee, Claire Walsh, Simon Walker-Samuel, Rebecca Shipley, Sebastian Marussi, Joseph Jacob, David Long, Daniyal Jafree, Ryo Torii, Charlotte Hagen**
- ESRF, Grenoble, France: **Paul Tafforeau, Elodie Boller**
- Medizinische Hochschule Hannover, Germany: **Danny D Jonigk, Christopher Werlein, Mark Kuehnel**
- Universitätsmedizin der Johannes Gutenberg-Universität Mainz, Germany:**M Ackermann**
- University Hospital of Heidelberg, Germany: **Willi Wagner**
- Grenoble Alpes University, Department of Anatomy, French National Center for Scientific Research: **A Bellier**
- Diamond Light Source, Harwell, UK: **Andy Bodey, Robert C Atwood**
- Imperial College London, UK: **JL Robertus**

Aknowledgements

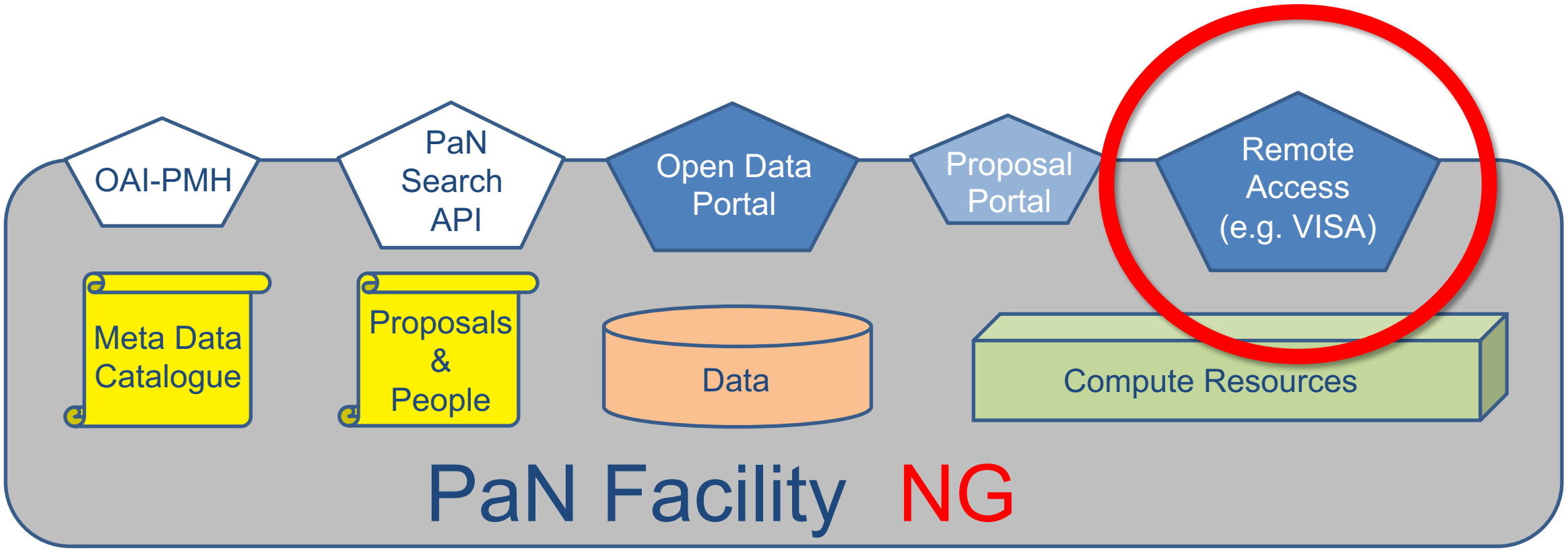
The development of this portal has been done as part of the PaNOSC project. PaNOSC has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852. The following people were involved in the development: Paul Tafforeau, Alejandro De Maria Antolinos, Axel Bocciarelli, Marjolaine Bodin and Andrew Götz from the ESRF, Jiří Majer from ELI, as well as the broader PaNOSC and ICAT communities.

Refer to PaNOSC Use Case 23 for more info!

Scientists prepared the Content and displayed by the Customized Open Data Portal.

*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

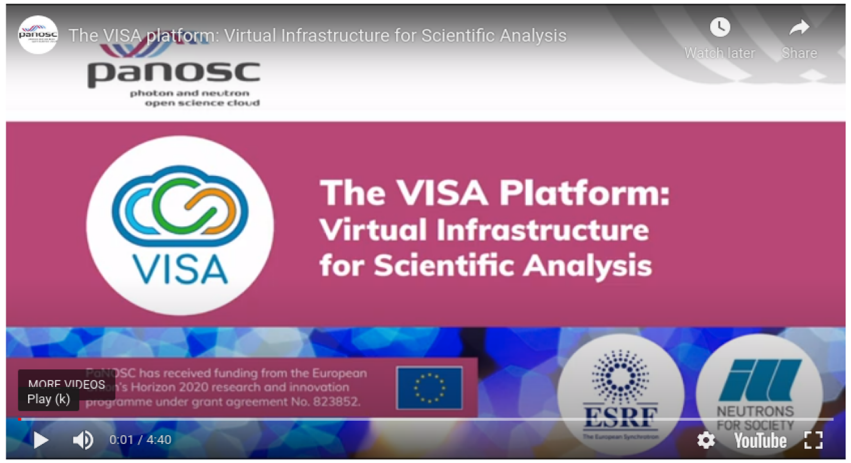
Pan Facility NG VISA Remote Access



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.

Remote data and compute access platform

- Goal: Next generation of data analysis in globalized research;
- **Remote access** to facilities;
- Our solution for a portal: develop and deploy **VISA** platform;
- Make data analysis pipelines **interoperable;**
- Make **Jupyter** notebooks available at all sites;
  - ✓ JupyterLab has been widely adopted as remote analysis-tool
  - ✓ PaNOSC provides:
    - Jupyter-Slurm adaptor.
    - Nexus/HDF5 visualization
  - ✓ PaNOSC + ExPaNDS
    - Developed for Use Cases



https://bit.ly/VISA-video

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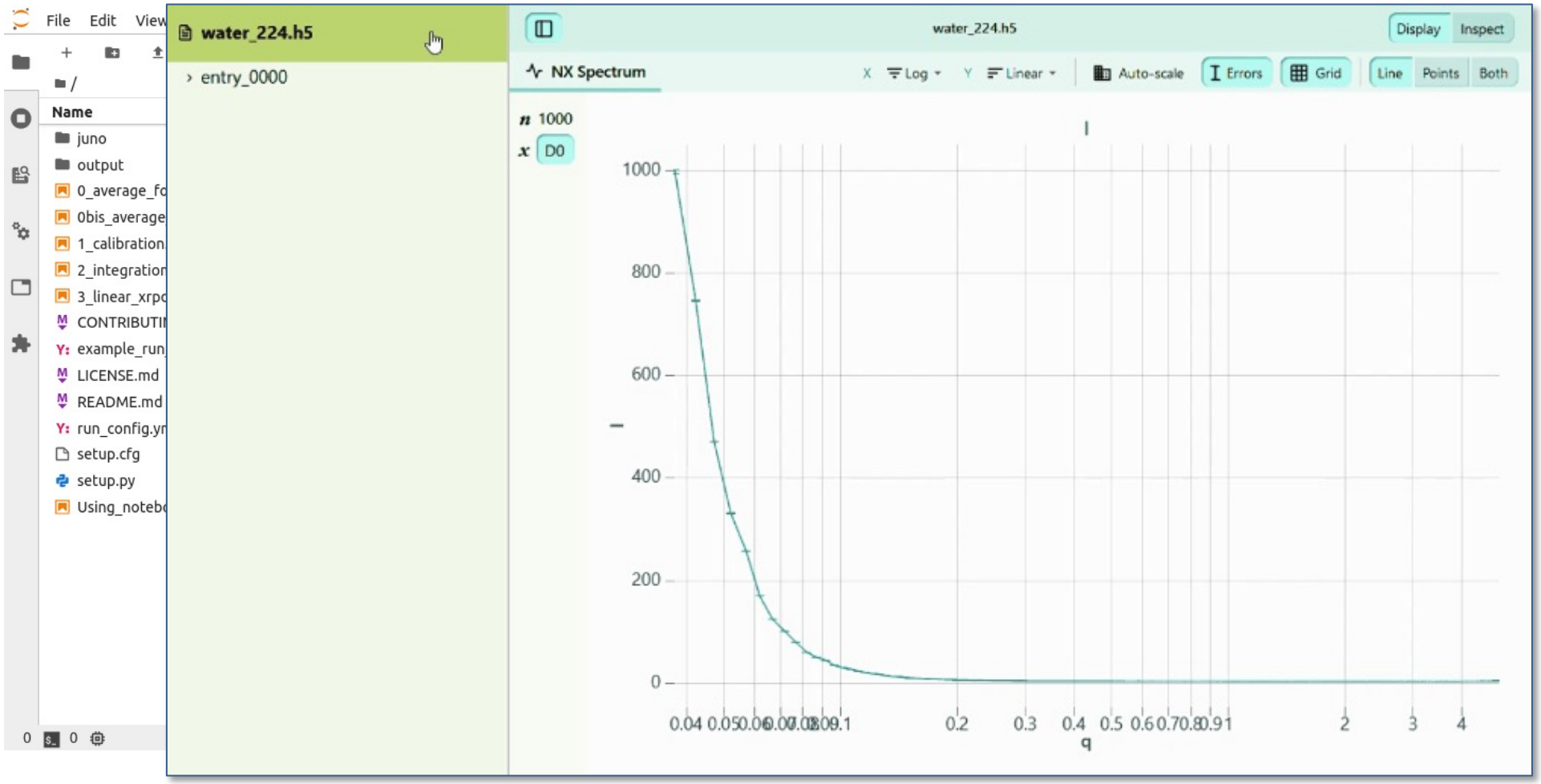
Remote analysis + HDF visualization with Jupyter notebooks



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Quick tour through our use cases of today.

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Our use cases for today.

Describe data by scripts for future reuse

Petr Čermák

- Describing Data as ‘scripts’
- Public Data from ILL
- Publish the scripts on GitHub.
- **R and I in FAIR.**

Neutron diffraction from Boro-carbon for efficient structural analysis and defect detection

Mousumi Upadhyay Kahaly (ELI-ALPS)

- Boron-doped diamond (BDD) for high voltage batteries.
- Inelastic neutron scattering
- Simulated with **McStas** code
- **Making use of WP4/5/6 of PaNOSC**

Machine Learning-based Spectra Classification

Yue Sun

- Example to show how Neural Network-based ML can be used for classifying the system state.
- Shows the importance of **proper file annotation: NeXus**.

Tomography Case Study

Kamel Madi

- Bio-chars from agricultural waste
- Minting DOI’s for precious datasets
- Results are important for a large variety of sciences.
- Water quality, Soil emission of gas
- **So F in FAIR is essential**.
- **Jupyter and WP4 of both projects**

TELBE Data Analysis workflow and the PaN training platform UX Spectra Classification

Jan-Christoph Deinert

- TELBE: Stimulation source for elementary low-energy degrees of freedom in matter.
- Culprate Superconductor
- Rendering this workflow in the **PaN training** platform.

DOI, FAIR, an MX COVID-19 Use Case

Frank von Delft

- Covid Moonshoot consortium is looking for a drug to block SARS-CoV-2
- Screening of the available fragment libraries at Diamond with crystals of the Main Protease of the COVID-19
- **FAIR**
- **DOIs: Linking PDB with Zenodo to maximize dissemination of Information.**

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Open Data Commons and Survey

Next up:

- Facility Survey
- Discussion on consequence of the answer for the Open Data Commons

See Andy's presentation at 11:45

(Stay tuned)

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Thank to all who contributed and will contribute to the success of our two projects
and
enjoy the rest of the day.

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---------- The END ----------

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