



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



2010

2015

2018

2021

European Open Science Cloud (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

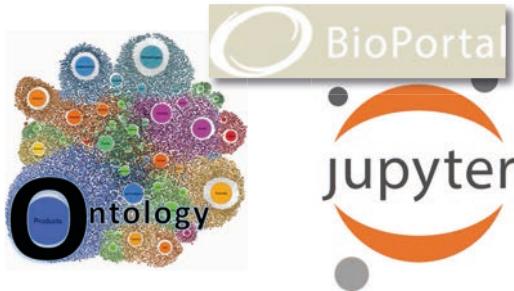


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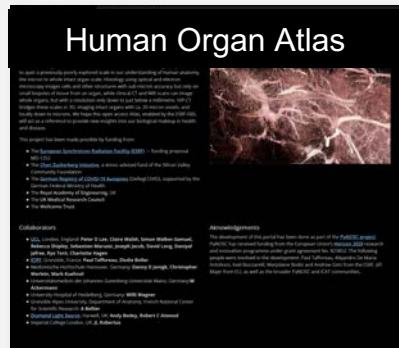


“Making PaN Open Science a reality by supporting our Facilities in enabling FAIR Data.”

Which has a lot of implications



And already some very positive outcomes

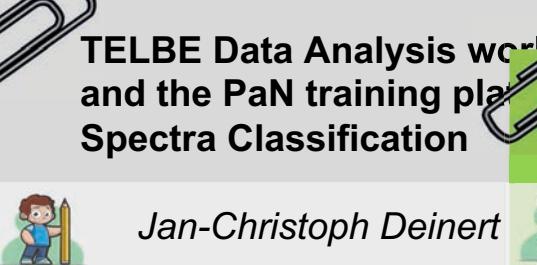


Describing the future

Petr Čech

- Describes
- Public D
- Publish
- R and FAIR

TELBE Data Analysis workflow
and the PaN training platform
Spectra Classification



DOI, FAIR, and
Case



Neutron diffraction from Boron-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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PaNOSC
photon and neutron
open science cloud



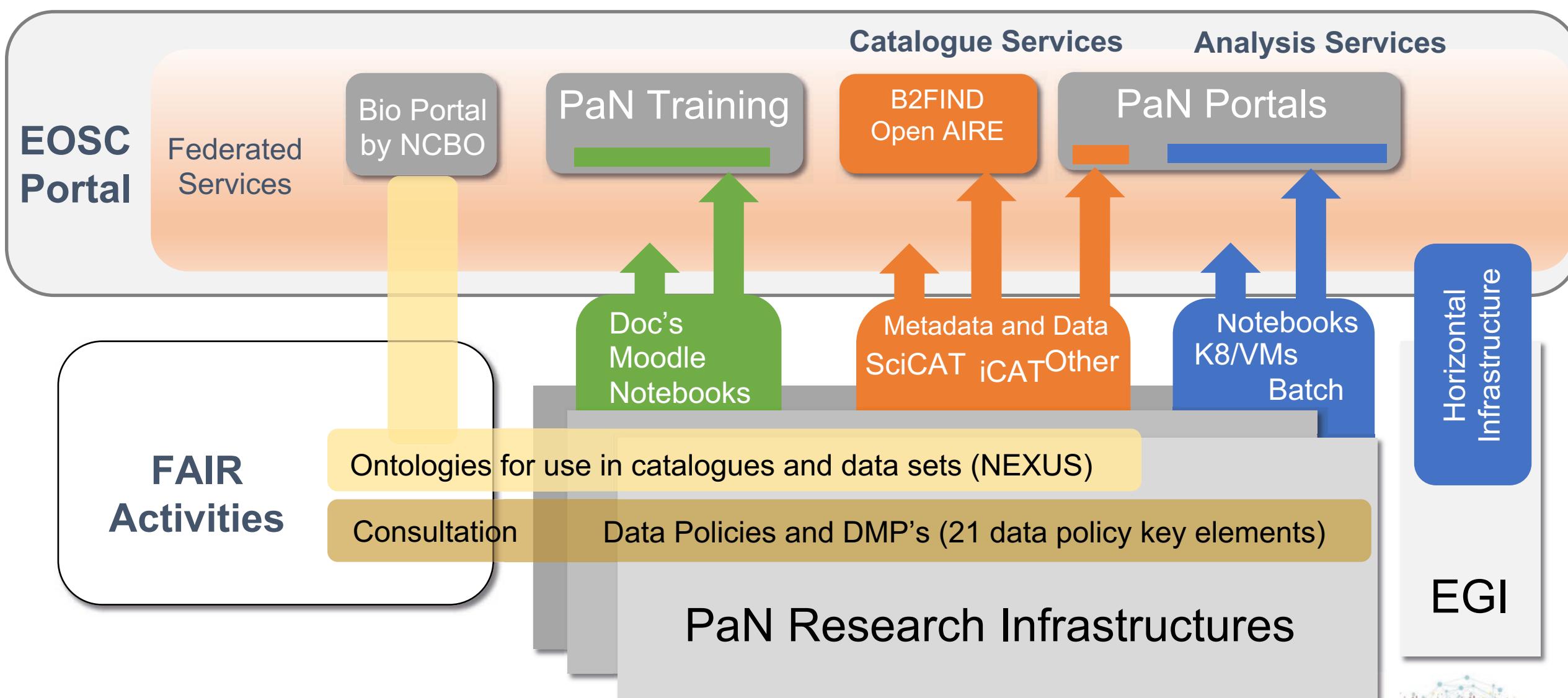
How do we achieve our goal ?



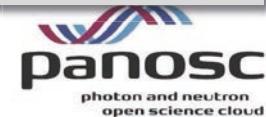
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The Big Picture of EOSC in PaNOSC and ExPaNDS



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

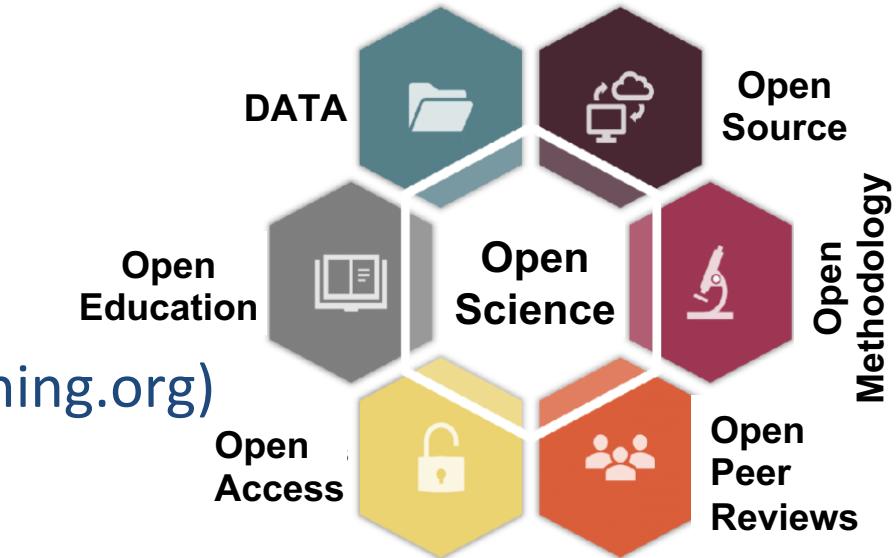


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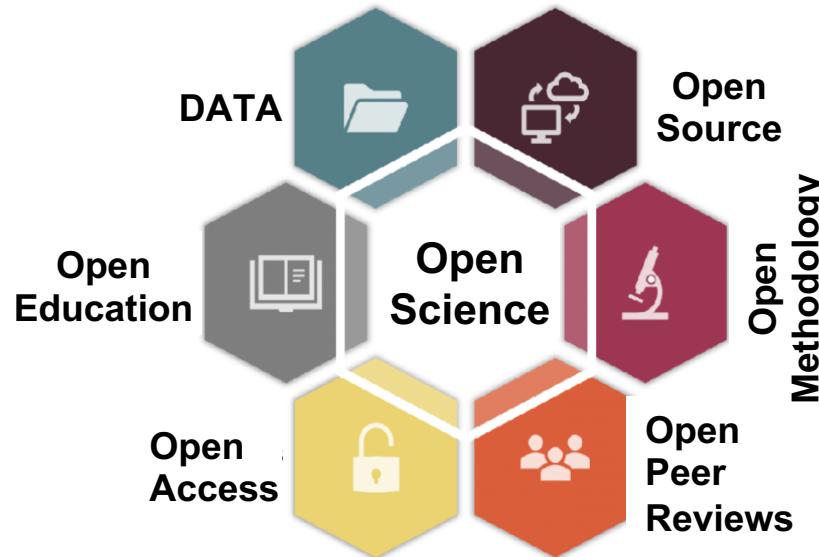
Highlights from PaNOSC and ExPaNDS and table of content.

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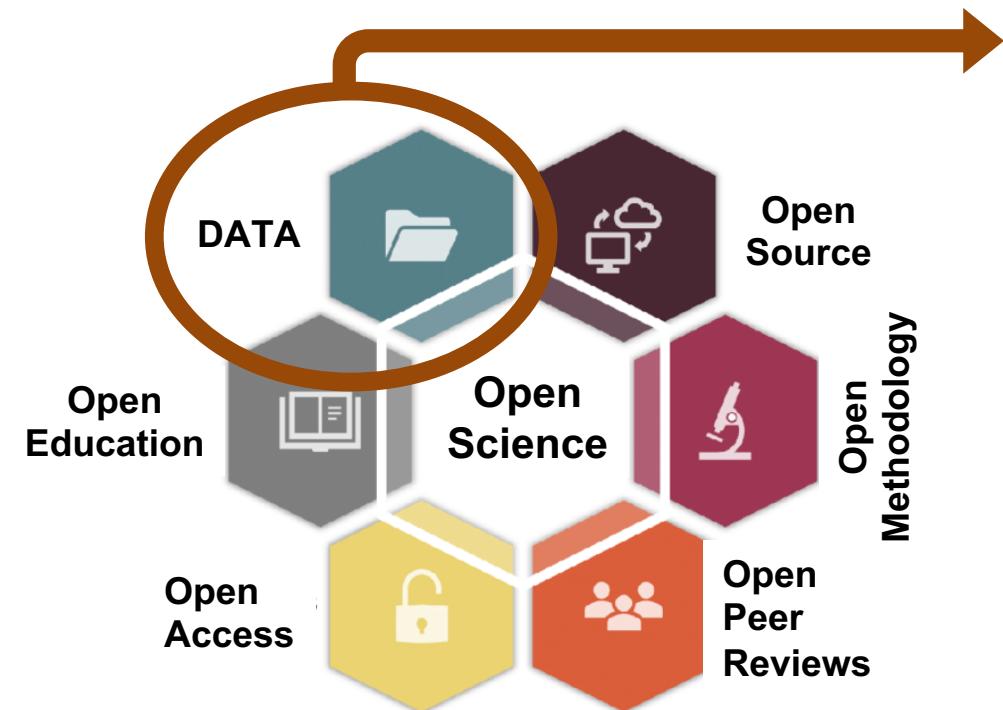
Open Science: Open Data, FAIR Data Policies, PIDs, DMPs



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From Open Science to FAIR data.



DOI: 10.5281/zenodo.5205825

Elements of the Data Policy Framework



- ✓ 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 Policies, DMPs and FAIR data handling.

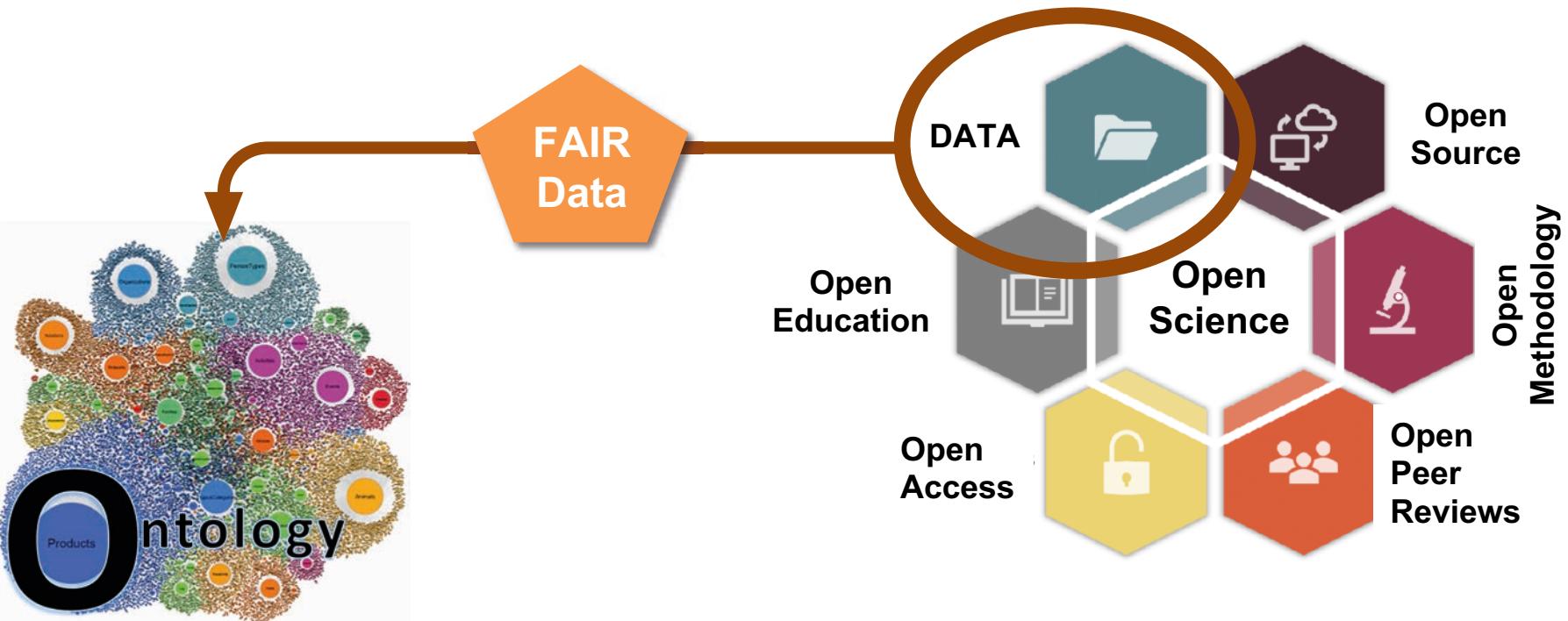
We provide

- **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 of 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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Meta Data Ontologies, Keywords in Catalogues and Nexus

photon

Showing 1 of 1099 Sort: Search Rank ▾

PaN Experimental technique (PANET)

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

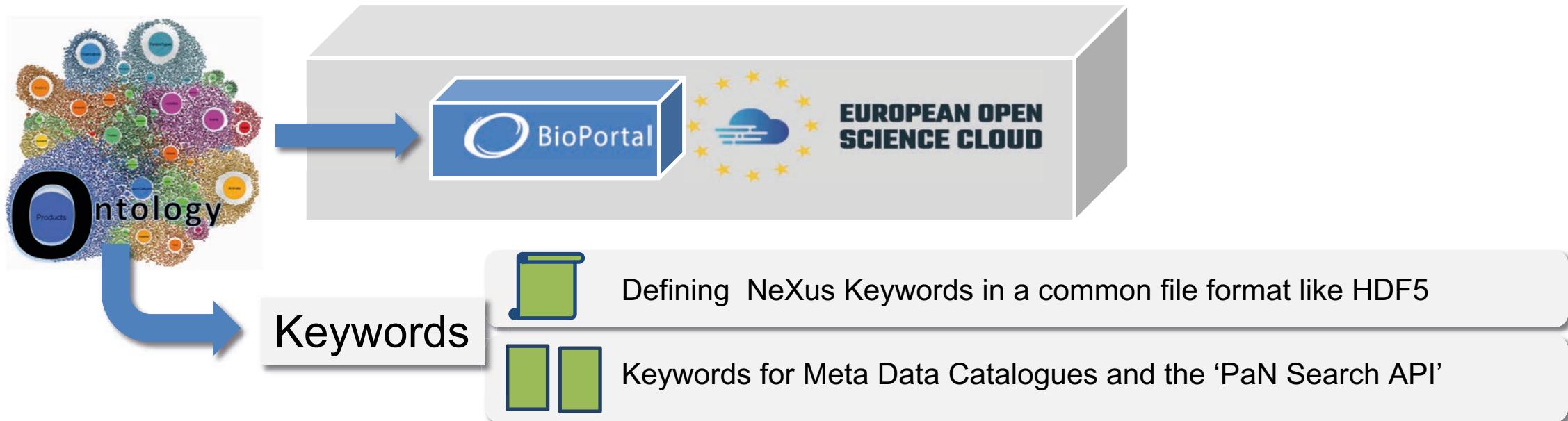
classes
379



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Meta Data Ontologies and their consequences



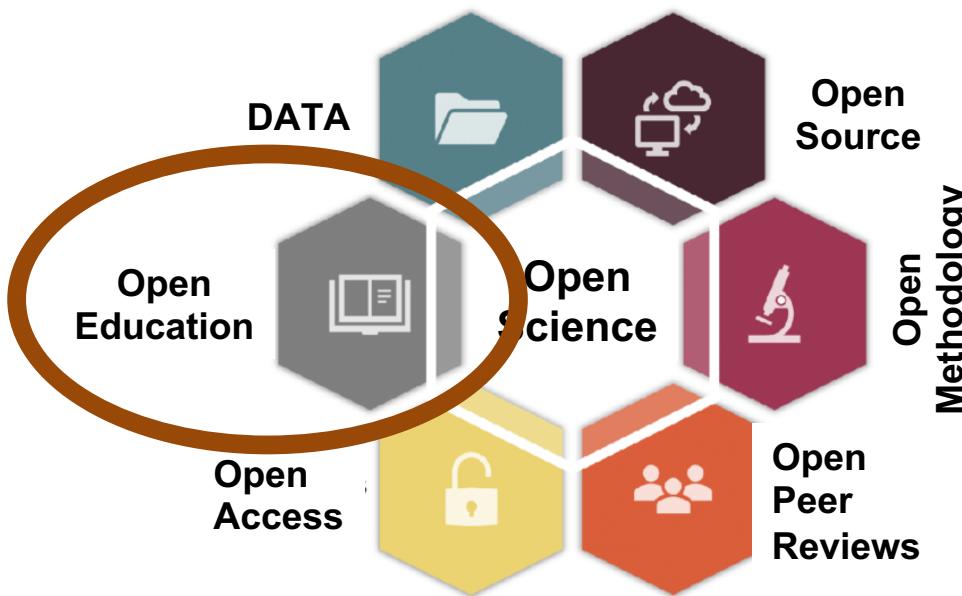
- Worked on a common ontology for different techniques in PaN;
- Checked 'keywords' for duplication in other sciences and searchability;
- Modelled our Ontology into the BioPortal;
- Working on making the BioPortal (not our service) available through the EOSC Portal;
- Publishing hints for catalogues to pick up the right keywords from our ontology;
- Involved in the NeXus definitions following our ontology. (NIAC Involvement).



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Training and Learning Platform



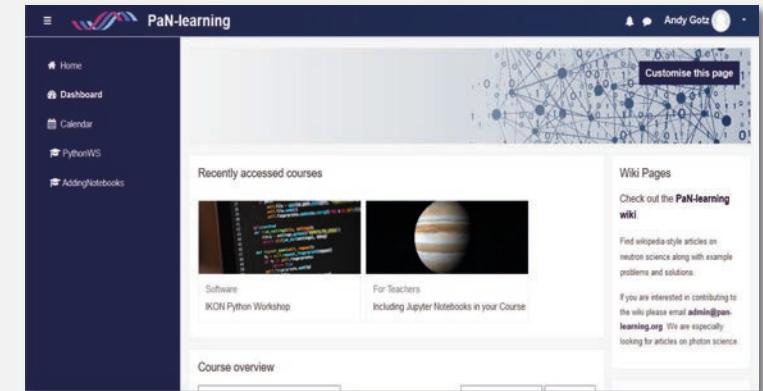
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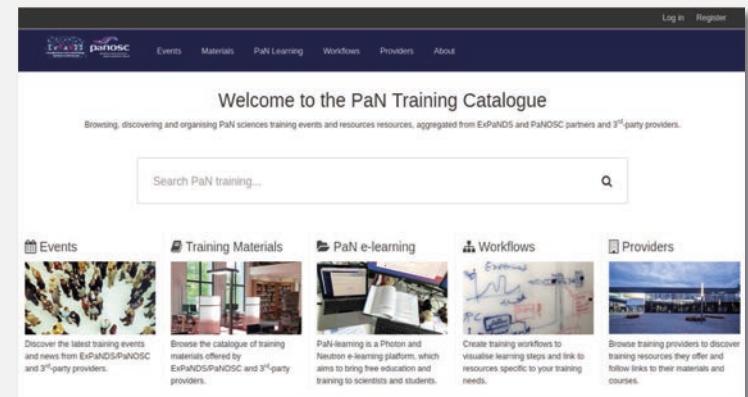
Our contribution to the teaching and learning platform.

- 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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PanOSC
photon and neutron
open science cloud



Training and Learning Platforms

Welcome to the training portal for the photon & neutron community

Browsing, discovering and organising PaN sciences training events and resources resources, aggregated from ExPaNDS and PaNOSC partners and 3rd-party providers.

Search PaN training...



Events



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

Training Catalogue



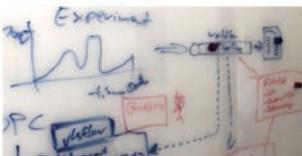
Browse the catalogue of training materials for the photon & neutron community offered by ExPaNDS, PaNOSC and 3rd-party providers.

PaN e-learning



PaN-learning is a Photon and Neutron e-learning platform, which aims to bring free education and training with integrated simulations and Jupyter notebooks to scientists and students.

Workflows



Create simple training workflows directly in our catalogue to visualise learning steps and link resources specific to your training needs.

Providers



Browse training providers to discover training resources they offer and follow links to their materials and courses.

Latest Content in our training portal for the photon & neutron community

2nd European PaN EOSC Symposium



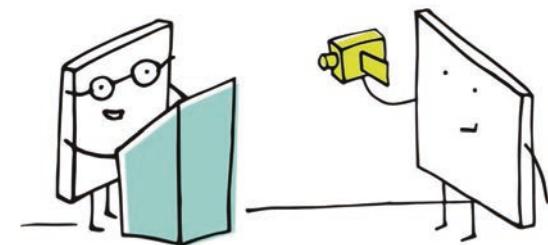
Welcome to the 2nd European PaN EOSC Symposium organised by the ExPaNDS and PaNOSC projects, to be held online, on Tuesday, October 26th 2021. The half-day meeting is open to external stakeholders (scientists, users and decision makers). Our first session will focus on project outcomes and...



Keywords: Photon science, Neutron science, expands, PaNOSC

Added to the catalogue 16 days ago

Now live at



PaN-Training.hzdr.de

&

PaN-Learning.org



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Training and Learning Platforms

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Search PaN training...

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PaN-Learning Portal

Username

Password

Remember username

Log in

[Forgotten your username or password?](#)

Cookies must be enabled in your browser [?](#)

Log in using your account on:

 [Federated Log in](#)



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.

Traini

Welcome to the PaN-Training platform! This platform is designed to facilitate learning and training across the photon & neutron community. It provides access to training materials, events, and resources from various providers.

Browsing, displaying, and interacting with the content is easy. You can search for specific topics or providers, filter results by category, and follow links to detailed descriptions and resources.

Discover the latest news and events from our partners: ExPaNDS, PaNOSC, and other providers.

Latest Content

2nd European

Keywords: Photon, Neutron, Data, Training, Learning, Workflows, Providers

CERIC
Central European Research Infrastructure Consortium (CERIC-ERIC)
CERIC-ERIC integrates and provides open access to some of the best facilities in Europe, to help...

ExPaNDS
ExPaNDS is the European Open Science Cloud (EOSC) Photon and Neutron Data Service. The...

5 training materials
1 upcoming event (4 past events)

SOLEIL
SOLEIL is located in France and is both an electromagnetic radiation source covering a wide range...

PaNOSC
The Photon and Neutron Open Science Cloud (PaNOSC) The Photon and Neutron Open Science Cloud...

1 training material
0 upcoming events (1 past event)

POL SCHERER INSTITUT (PSI)
Paul Scherrer Institute (PSI)
The Paul Scherrer Institute PSI is the largest research institute for natural and engineering...

diamond
Diamond Light Source
Diamond Light Source is the UK's national synchrotron. It works like a giant microscope,...

MAX IV
MAX IV
The MAX IV facility, based in Sweden, will have the highest quality of X-rays available to...

ELETTRA
Elettra Synchrotron Trieste
Elettra Synchrotron Trieste is a multidisciplinary international research center of excellence...

HZB
Helmholtz-Zentrum Berlin
Helmholtz-Zentrum Berlin (HZB)
HZB in Germany has existed since 2009. Its roots go much further into the past, given that HZB...

UKRI
UK Research and Innovation
UKRI works in partnership with universities, research organisations, businesses, charities, and...

ISIS
ISIS Neutron and Muon Source
ISIS Neutron and Muon Source is based at the STFC Rutherford Appleton Laboratory in Oxfordshire...

ESRF
European Synchrotron Radiation Facility
The ESRF is the world's most intense X-ray source and a centre of excellence for fundamental and...

EGI
European Grid Infrastructure Foundation (EGI)
EGI is a federated e-Infrastructure set up to provide advanced computing services for research...

ESS
European Spallation Source
The European Spallation Source (ESS) is a European Research Infrastructure Consortium (ERIC), a...

ELI
ELI Delivery Consortium
ELI-DC AISBL is an international non-profit association under Belgian law. It has been...

XFEL
European XFEL
The European XFEL in the Hamburg area is a new international research facility of superlatives:...

LEAPS
League of European Accelerator-based Photon Sources (LEAPS)
LEAPS – the League of European Accelerator-based Photon Sources – is a strategic consortium...

LENS
League of advanced European Neutron Sources (LENS)
The League of advanced European Neutron Sources (LENS) has the not-for-profit purpose of...

Platforms

the photon & neutron community

resources, aggregated from ExPaNDS and PaNOSC partners and 3rd-party providers.

Search

Learning

Workflows

Providers

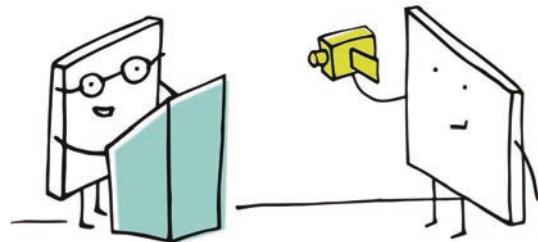
Create simple training workflows directly in our catalogue to visualise learning steps and link resources specific to your training needs.

Join & neutron community

ExPaNDS and PaNOSC projects, to be held online, on Tuesday, 13th October 2020 (scientists, users and decision makers). Our first session will



Now live at



PaN-Training.hzdr.de

&

PaN-Learning.org



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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 data catalogue services, we have developed three ontologies: PaN experimental techniques (PaNET), an ontology of NeXus definitions (NeXusOntology), and a semantic integration...



Keywords: expands, ontology, EOSC, Photon science, experimental techniques, Neutron science, 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 infrastructures providing photon and neutron facilities should be framed, in particular in the light of supporting open science and 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 Consortium, CERIC, synchrotron beamline, microscopy, electrochemistry, battery research, Heritage Science, Elettra synchrotron, Elettra Sincrotrone Trieste, life sciences, microscope

Resource type: video

e at

nzdr.de

g.org



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photon and neutron
open science cloud

Training and Learning Platforms

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Search PaN training...

Events

PaN-learning

Workflows

Providers

See Jan-Christoph's Use Case

Latest Content in our training portal for the photon & neutron community

2nd European PaN EOSC Symposium

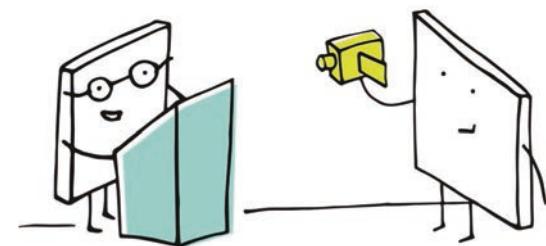
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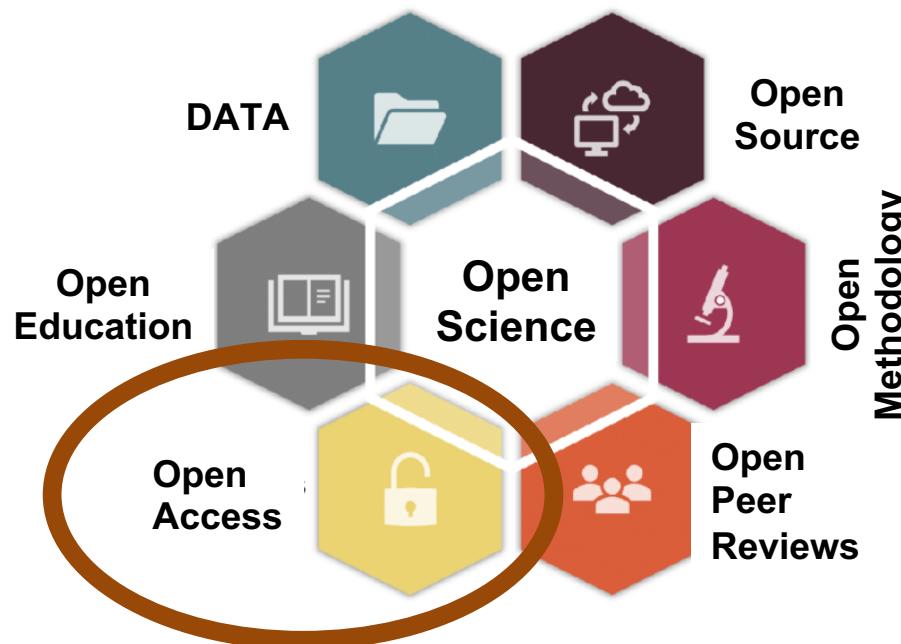
Pan-Training.hzdr.de

&

Pan-Learning.org



Prerequisite for open access : The common AAI



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

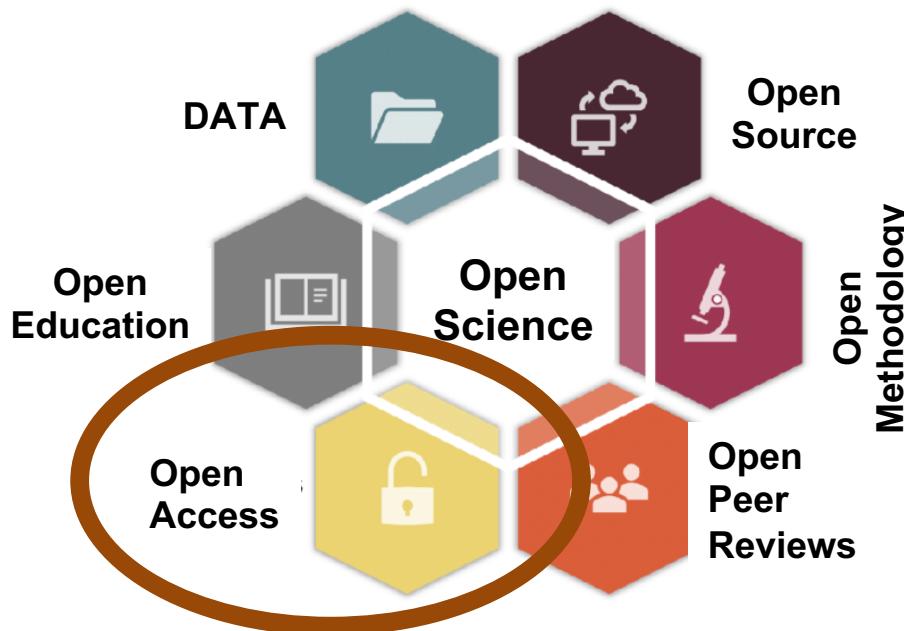
- Originally
 - Scientist needed a different identity at each facilities to access their services.
 - Lots of passwords to remember and to loose
 - Difficult with cross facility services.
- UmbrellaID
 - Scientist only needs one identity with UmbrellaID (on top of home identity)
 - 'Catch all' identity 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.



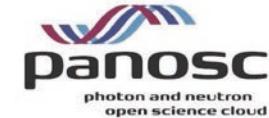
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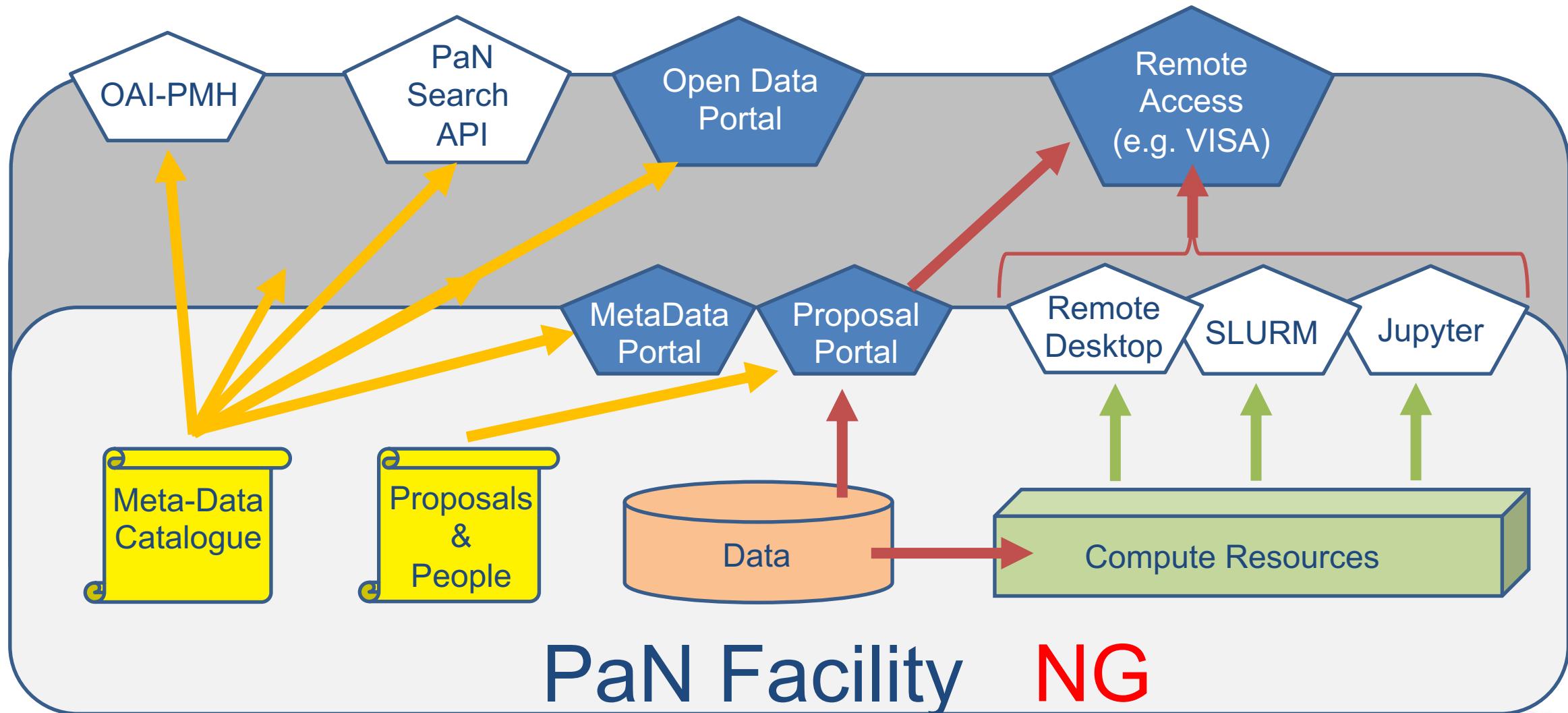
The next generation PaN Facility



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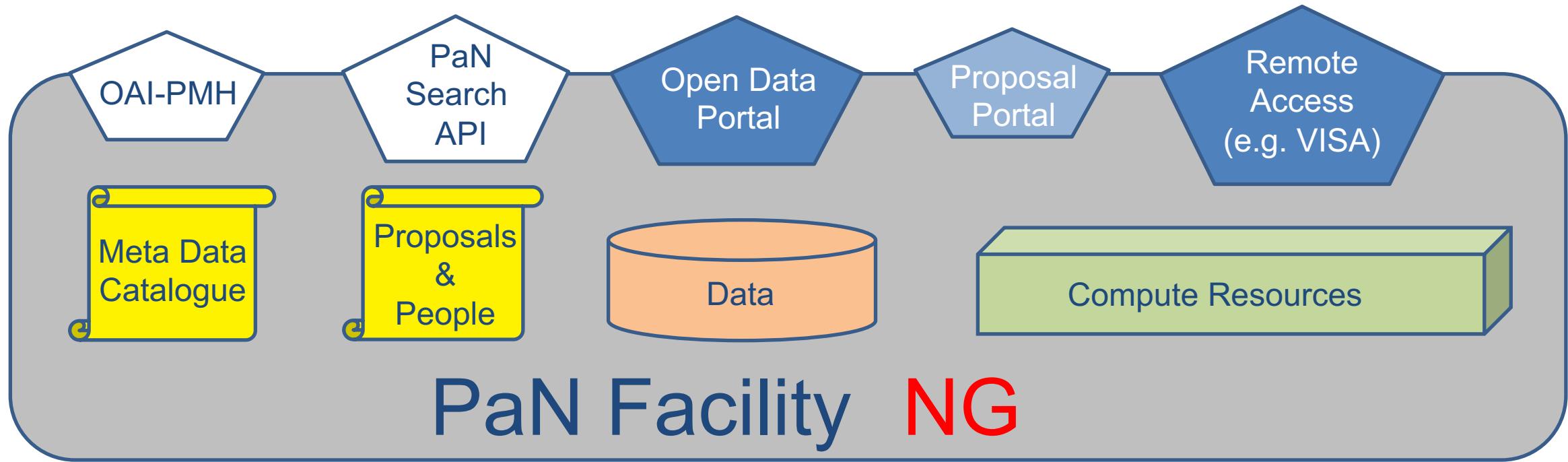
Towards the PaN Facility Next Generation



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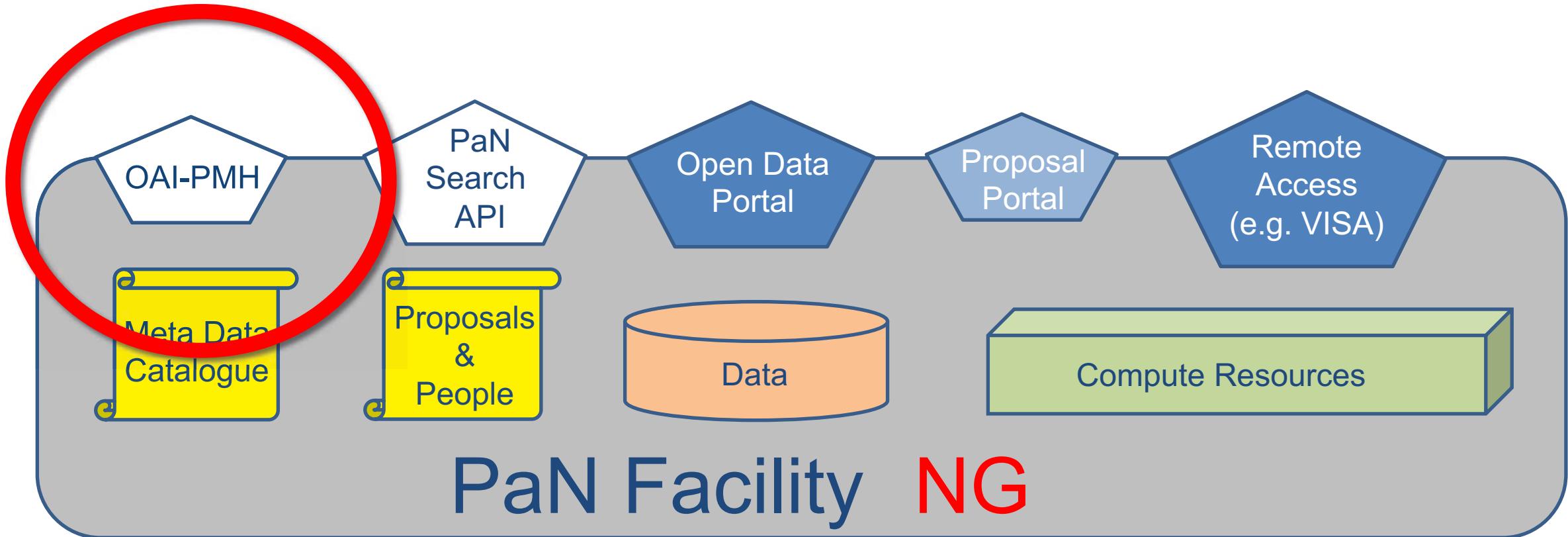
Towards the PaN Facility Next Generation



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High level harvesting of our PaN treasures.



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Harvesting API

European Open Science Cloud, EOSC

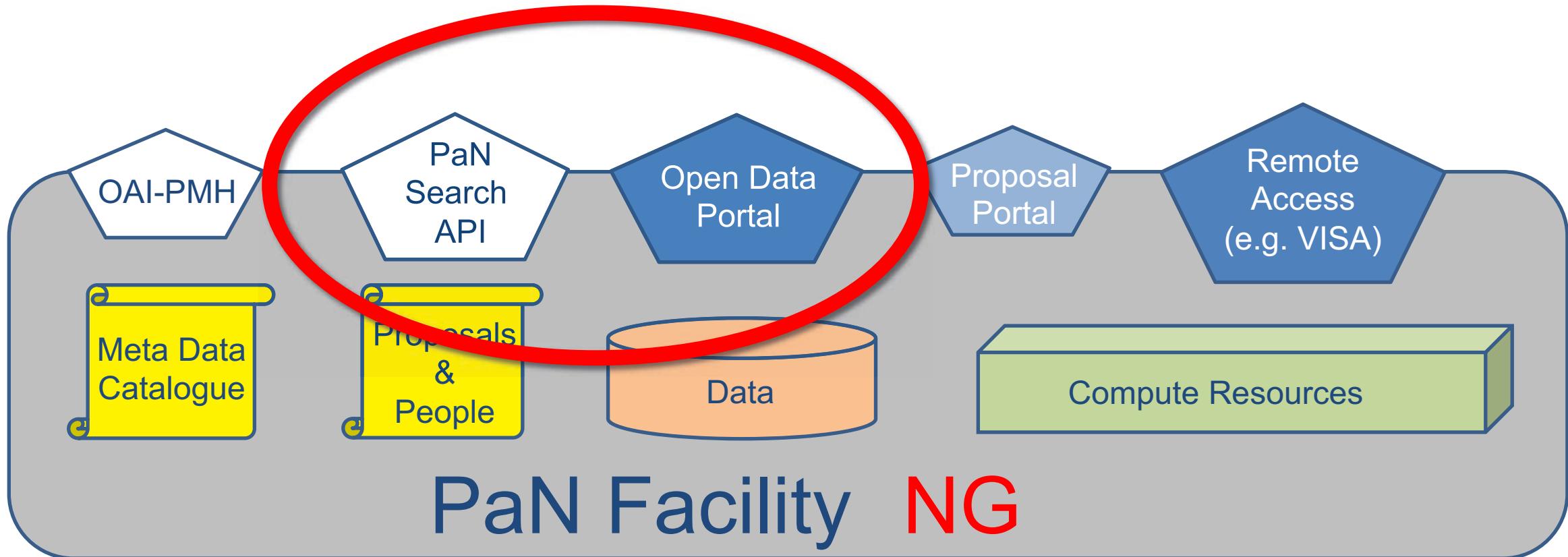


OAI-PMH



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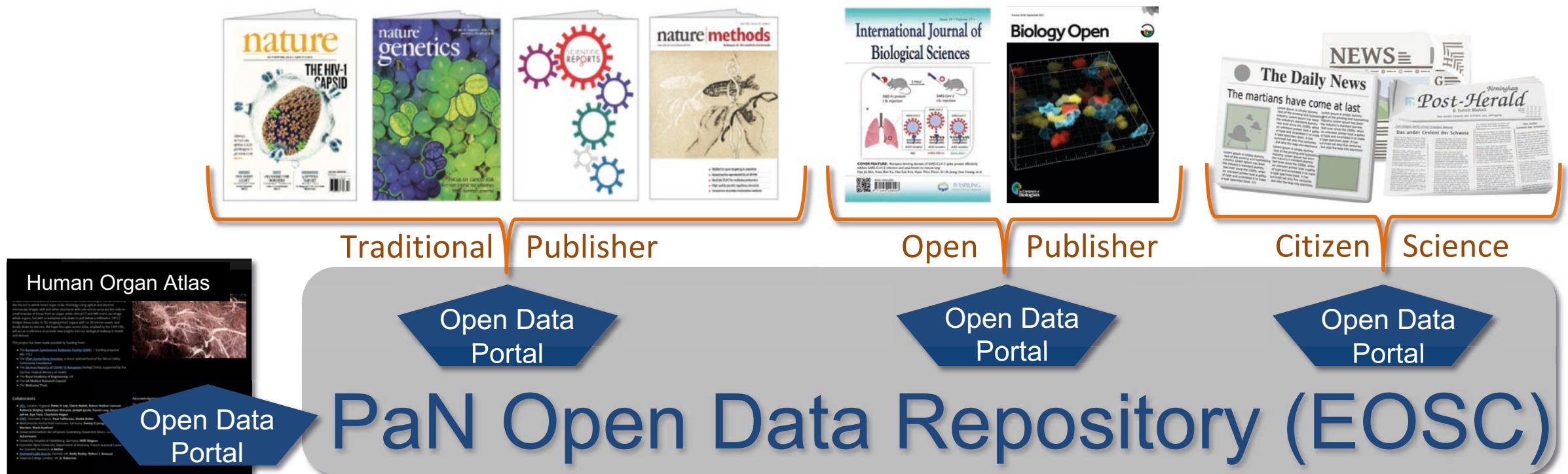
The PaN search API and the Open Data Portal



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Federated PaN Search and the data portal.



PaN Search API



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PaN Data Portal

Example for Ontologies

Techniques

Search

Title

Techniques

- Reflectometry
- Spectroscopy
- Phase Contrast Imaging
- Soft diffraction
- Scattering
- UV VUV spectroscopy
- Photoemission microscopy
- Polarised reflectivity
- Microfluorescence
- Gamma spectroscopy
- Three-axis spectrometers
- X-ray excited optical luminescence
- Diffraction Imaging

Search **Reset**

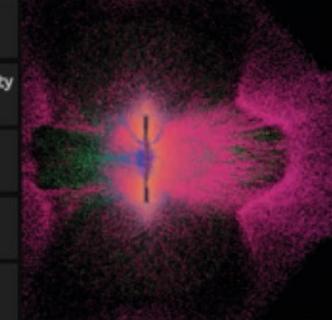
Two-color XUV+NIR femtosecond photoionization of neon in the near-threshold region

Nikita / KPSI Debbi / KPSI

RP4-SRS focuses on time-resolved spectroscopy experiments in the full range of frequencies from IR to UV. Users can measure samples as varied as solid state crystals, or proteins in their natural environment. Time-resolved spectroscopy is the collection of techniques that are used to examine the dynamic processes....
Dana Scully; (2020), Re-polarization of the aft quantum plasma collector, DOI:10.9563/if.2015.87.012

Phase Contrast Imaging UV VUV spectroscopy

Type Proposal
Licence / Visibility MIT / Public
Started on 09/11/2017
Ended on 03/21/2019
Released on 01/01/2020



Laser-driven Ion Acceleration from Plastic Target

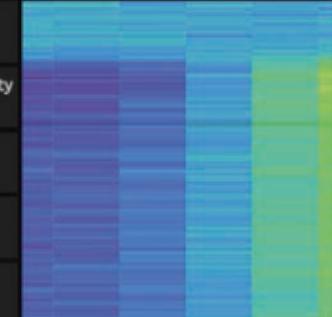
Alipher / EU XFEL Pranay / EU XFEL

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Dana Scully; (2020), Re-polarization of the aft quantum plasma collector, DOI:10.9563/if.2015.87.012

Spectroscopy Scattering

Type Proposal
Licence / Visibility MIT / Public
Started on 09/11/2017
Ended on 03/21/2019
Released on 01/01/2020



Electron-positron pair generation

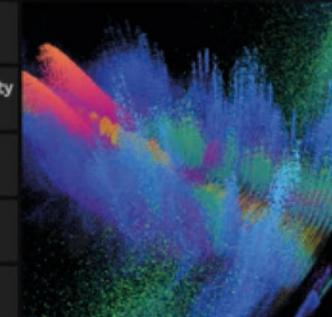
Sláine / ILL Elder / ILL

OSIRIS 2D PIC simulation of gamma radiation and electron-positron pair production in a head-on collision of ultra-intense laser pulse (2.5 x 10²³ W/cm², 150 fs) with 3.9 GeV electron beam previously accelerated within the plasma channel....

Dana Scully; (2020), Re-polarization of the aft quantum plasma collector, DOI:10.9563/if.2015.87.012

Photoemission microscopy

Type Proposal
Licence / Visibility MIT / Public
Started on 09/11/2017
Ended on 03/21/2019
Released on 01/01/2020





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.

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:

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- 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



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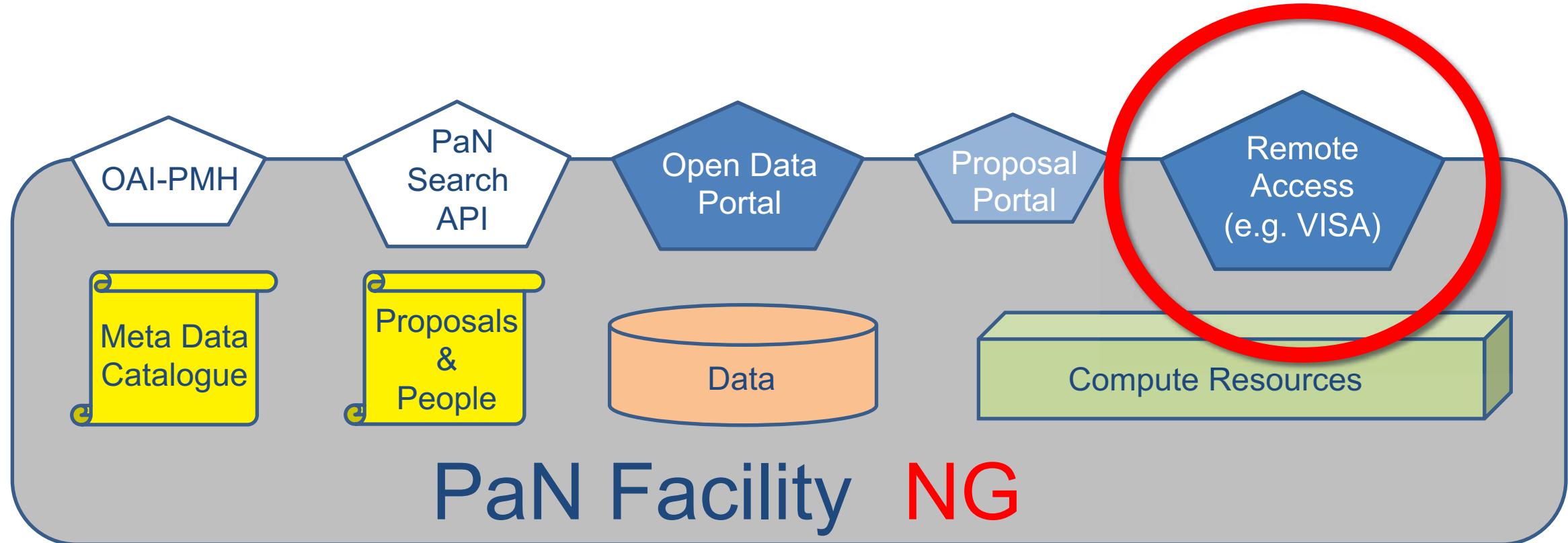
Scientists prepared the Content and displayed by the Customized Open Data Portal.

*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

Refer to PaNOSC Use Case 23 for more info!



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

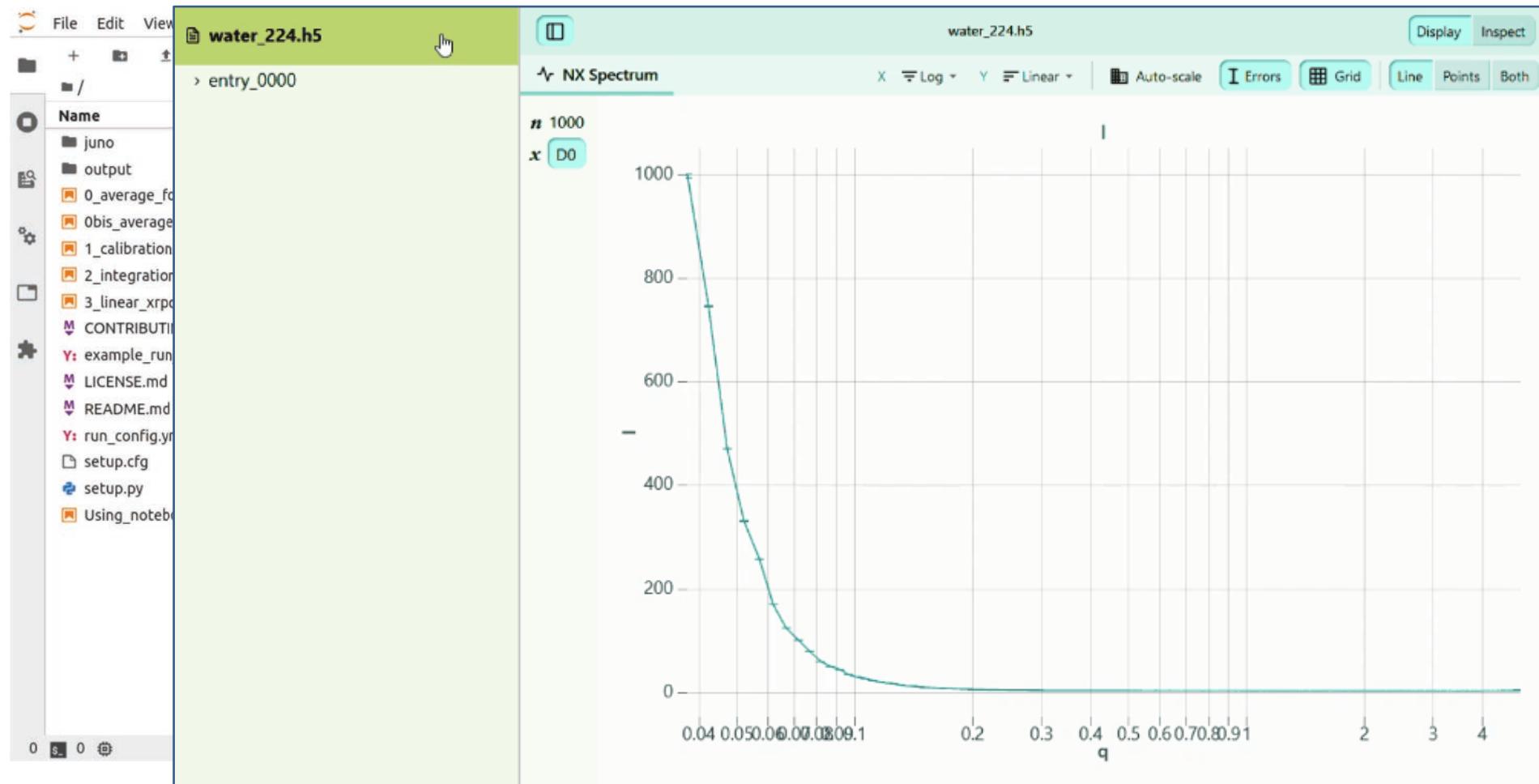


<https://bit.ly/VISA-video>



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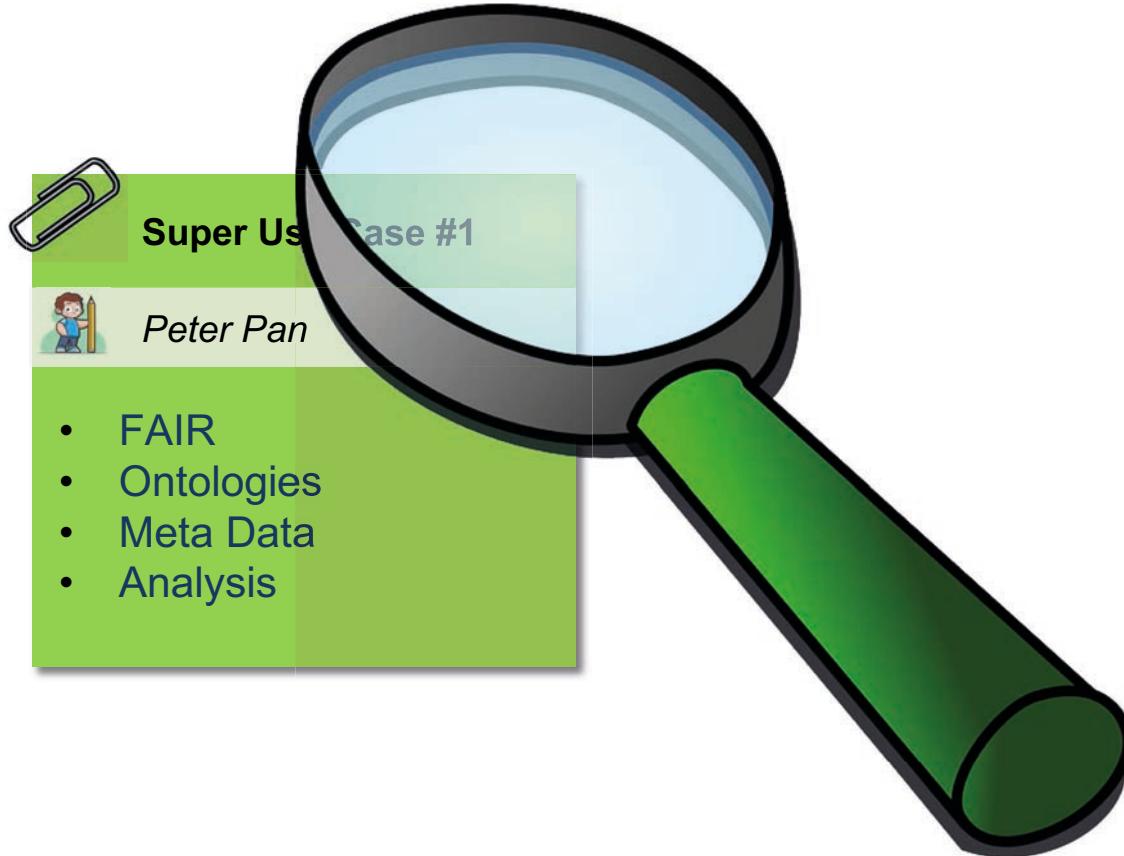
Remote analysis + HDF visualization with Jupyter notebooks



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 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.**



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

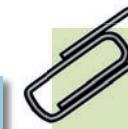


Neutron diffraction from Borocarbon for efficient structural analysis and defect detection



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**.



DOI, FAIR, an MX COVID-19 Use Case



Frank von Delft

- Covid Moonshot 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.**



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.

panosc
photon and neutron
open science cloud



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)

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



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.

