



ExPaNDS
European Open Science Cloud Photon
and Neutron Data Services

Europe's Photon and Neutron Open Science Cloud for Raw and Processed Data: Aims and Achievements to Date @ ORSO 2024

Andy Götz (ESRF, PaNOSC coordinator)



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.

Talk outline



1. **Achievements of ExPaNDS + PaNOSC**
2. **The Photon and Neutron Open Science Cloud**
3. **Towards the European Open Science Cloud**
4. **How does this benefit Users i.e you?**



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.

Users + Facilities feel the weight of data

Users

- ~~Huge data volumes~~
- ~~Tera → Petabytes~~
- Sample metadata
- Raw data quality
- Data processing
- Data exporting
- FAIR data



Facilities

- Huge data volumes
- Peta → Exabytes
- Data acquisition
- Metadata collection
- Data curation
- Data archiving
- FAIR data



The goal of ExPaNDS and PaNOSC was to reduce the burden on Users to manage and make data FAIR



Users

- **Data scientists**
- Provide metadata
- Keep logbooks
- Data management checklist / plans
- Publish data
- Cite data

data



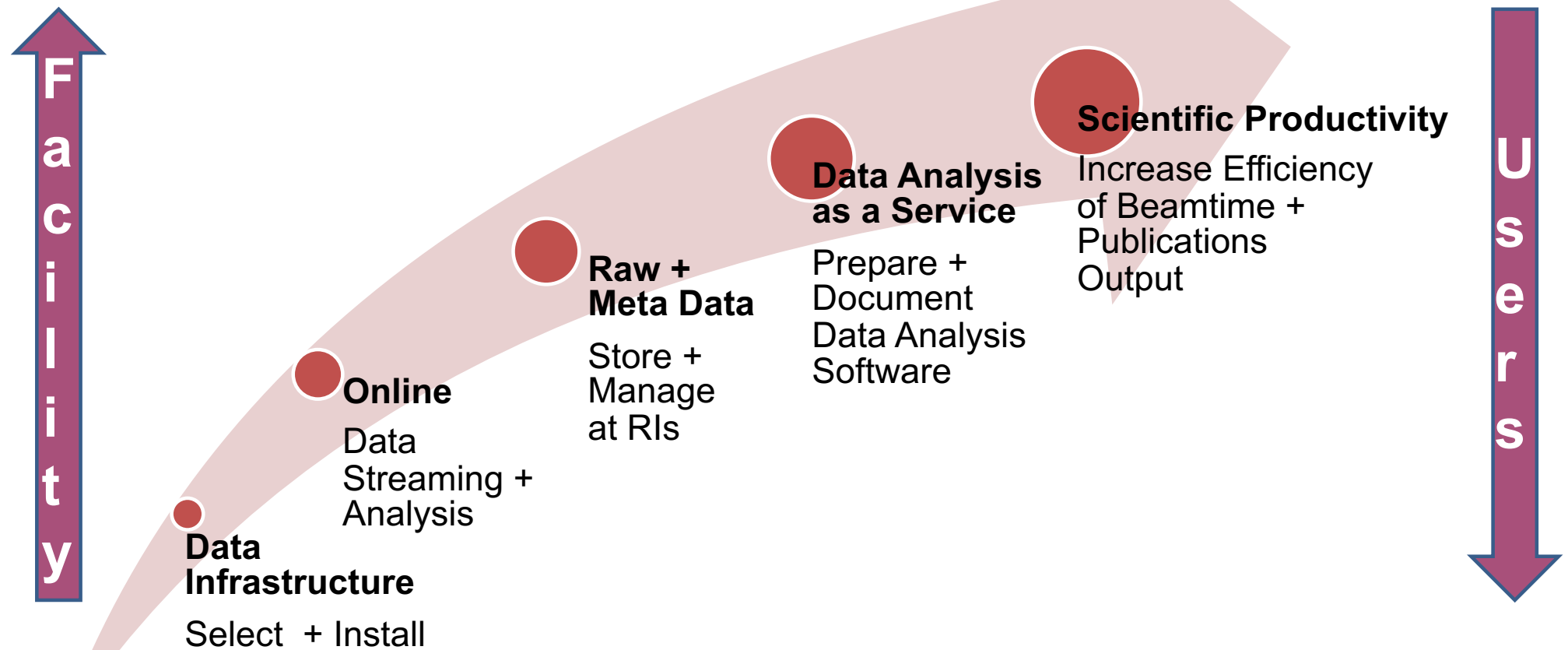
Facilities

- **Data managers**
- Curate raw data
- Online processing
- Metadata catalogues
- Data repositories
- Remote analysis
- Data portals



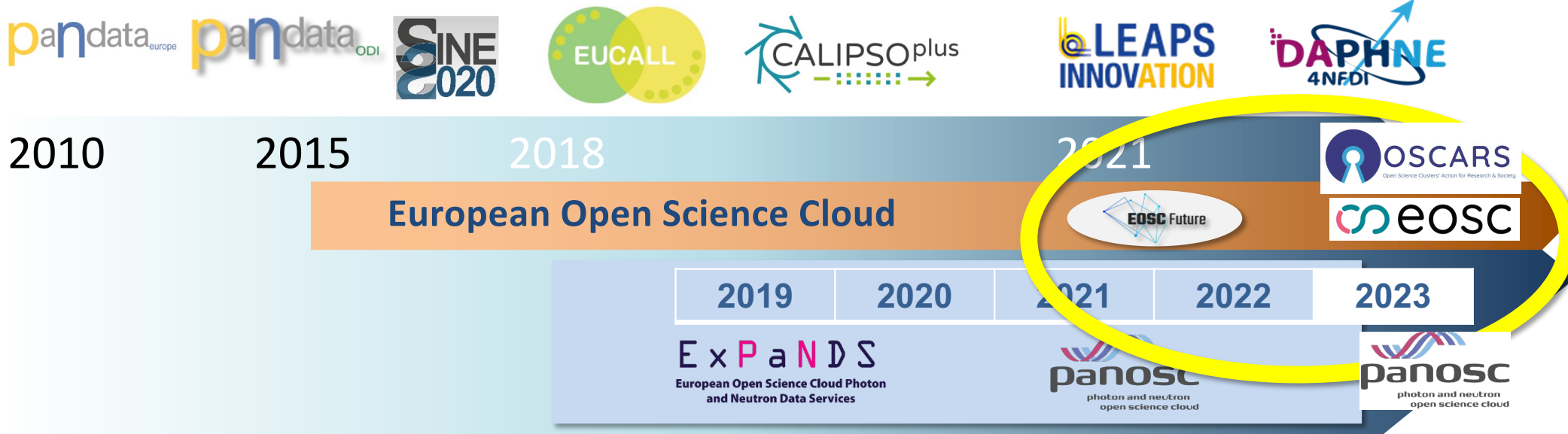
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Facilities and Users converging needs for data management



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.

European support for the PaN community



Policies
Analysis
AAI
Training

Common data policy
Software Catalogue
UmbrellaID
e-neutron

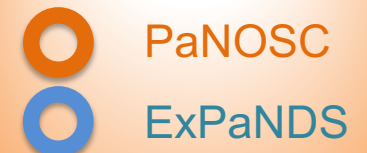
FAIR data policy
Remote analysis
AARC Blueprint

Data Management Plans
Jupyter
eduTeams
Training platform

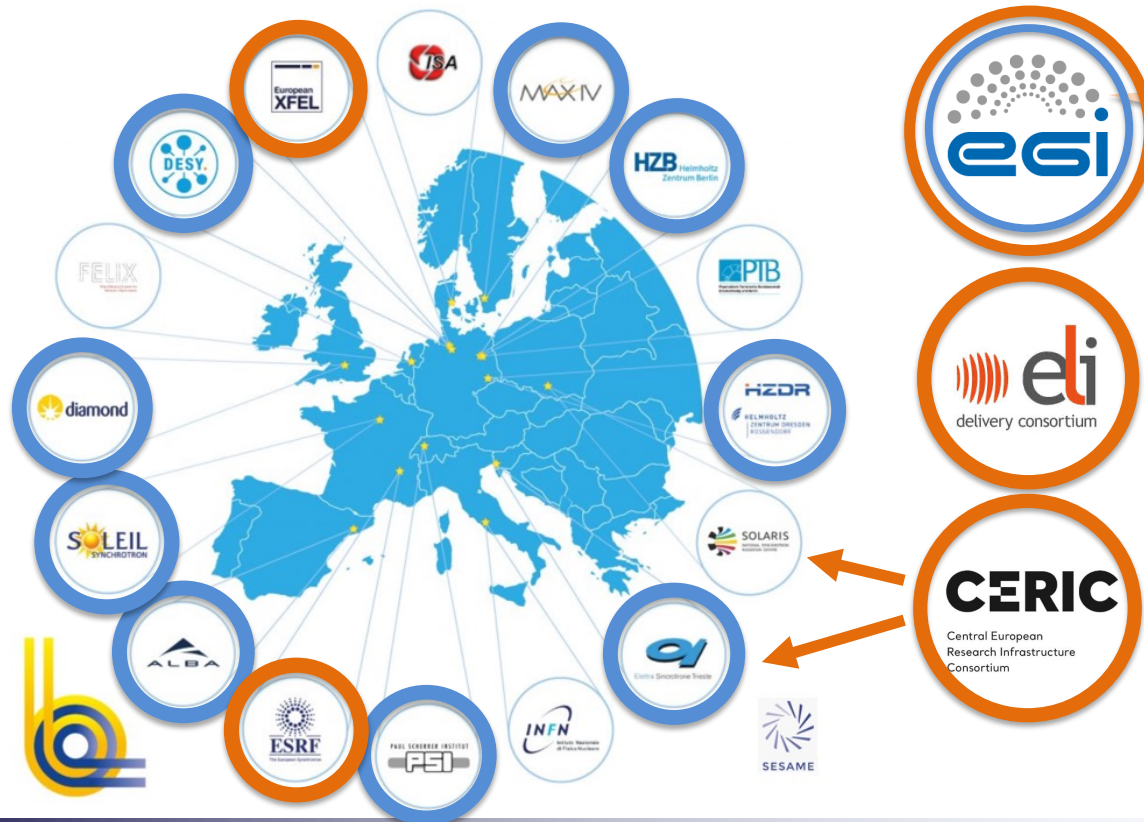


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Two EOSC projects for PaN : PaNOSC and ExPaNDS



Photon (LEAPS)

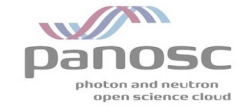


Neutron (LENS),



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PaNOSC + ExPaNDS - Main Achievements

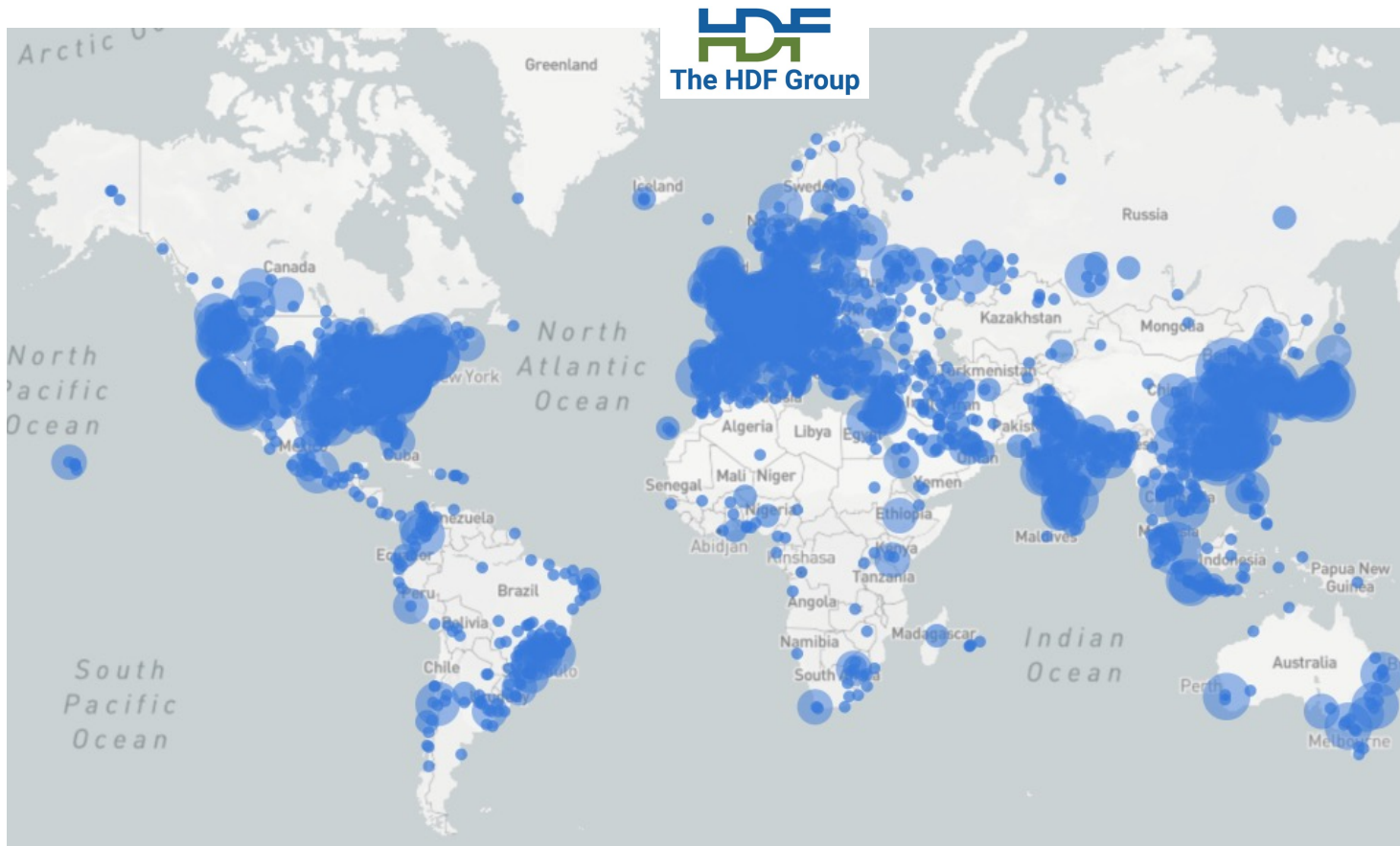


1. **FAIR data policy** and **DMPs**
2. Standardised metadata **Nexus/HDF5 + PaNET** → **Wout's talk**
3. Guidelines for **FAIR data** self-evaluation
4. **Federated search API** for PaN data catalogues
5. **Open Data portal** for searching + downloading data
6. Community **AAI UmbrellaId** → **EduGAIN AAI**
7. **JupyterLab notebooks** and **Nexus/HDF5** files visualisation
8. **Remote data analysis** with VISA + data analysis pipelines
9. **Simulation** software for simulating experimental data (ViNYL)
10. **PaN-training + learning** platform (pan-training.eu)



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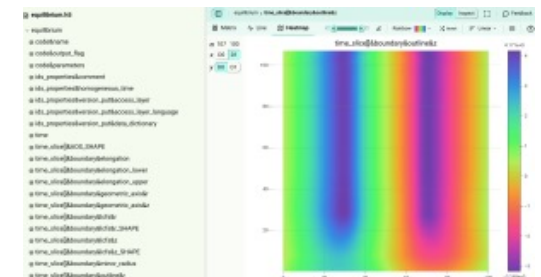
HDF5 is needed to acquire, process and store large datasets and has been adopted as de facto standard across most facilities (with NeXus conventions for metadata)



New Features

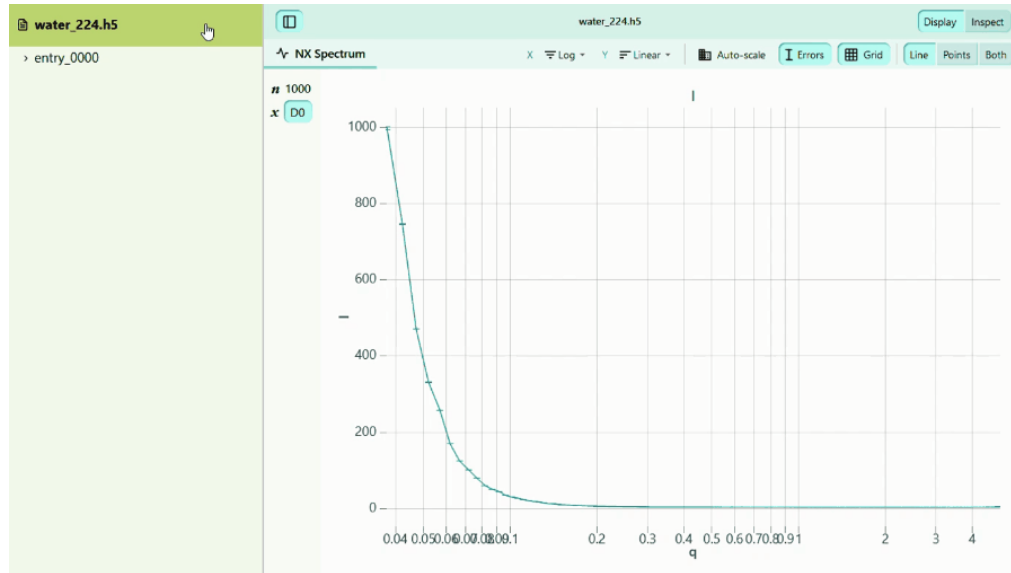
- Multi-dataset I/O
- Selection and vector I/O
- Subfilng VFD
- Multi-Threaded Concurrency (WIP)
- Sparse data storage (WIP)

PaNOSC developed H5Web to make HDF5 even easier



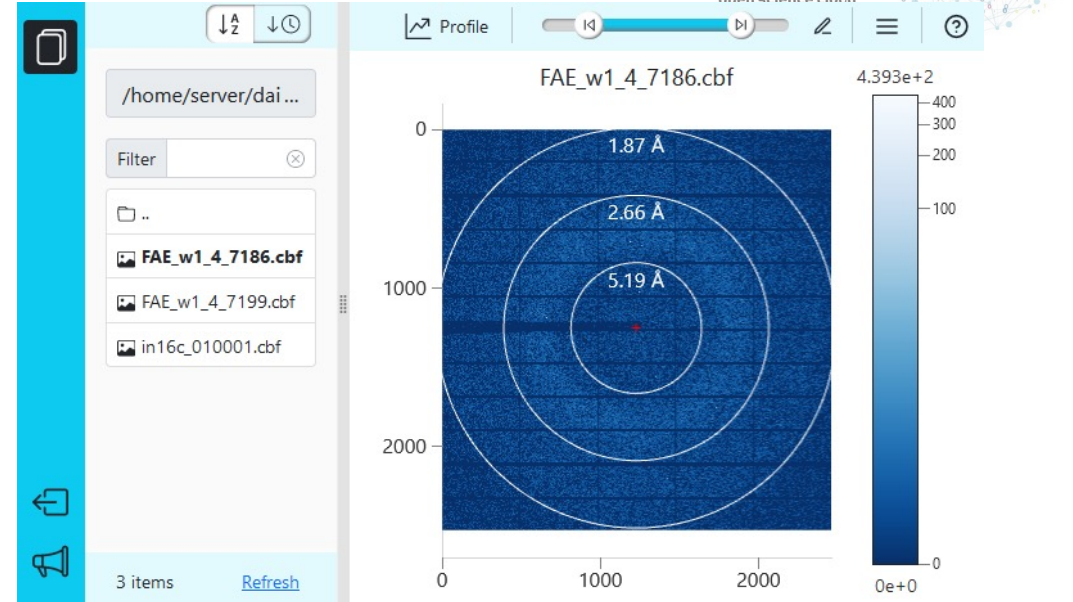
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H5Web Visualization Ecosystem



Generic HDF5 file viewer

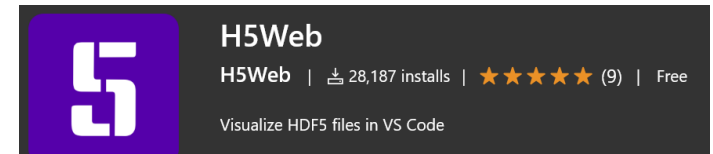
- Integrated into **data portals + web apps (ESRF, EuXFEL, DLS, AS, ...)**, for viewing files generated during experiments
- Available as **JupyterLab** and **VS Code extensions**, and as stand-alone web service, **myHDF5**, for viewing local and remote HDF5 files
<https://github.com/silx-kit/h5web>



A huge thanks to **Brian Maranville** for **h5wasm** !

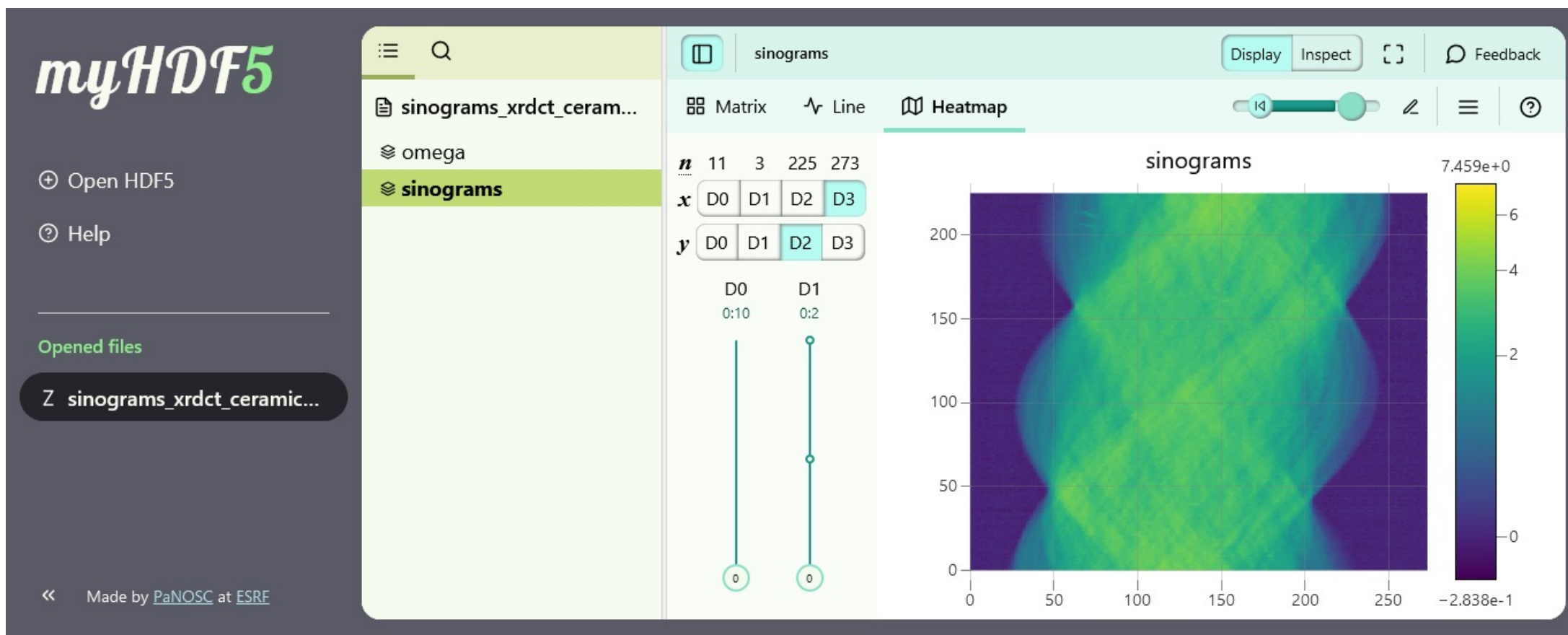


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HDF5 file viewing on the web made easy

<https://myhdf5.hdfgroup.org/>



VISA - Remote Data Processing/analyses



New compute instance

Please fill in the details below to create a new compute instance

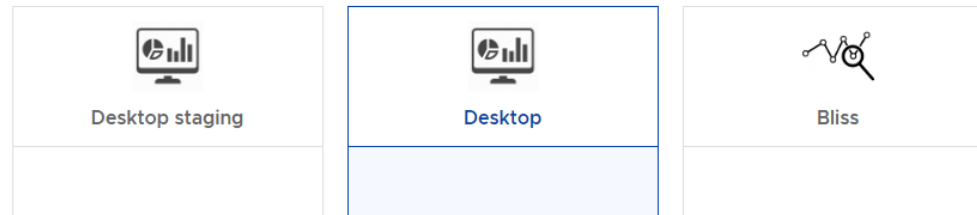
Experiments

Select the experiments you wish to associate with your compute instance

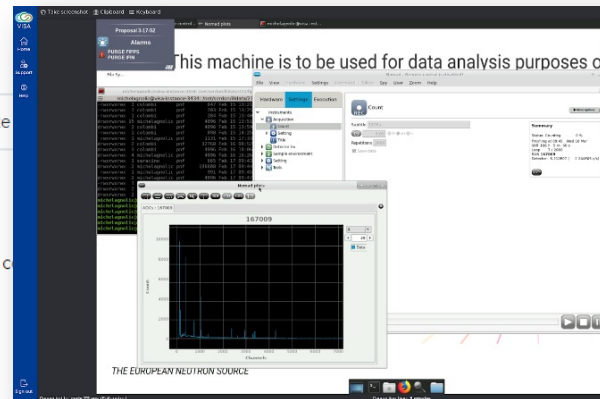
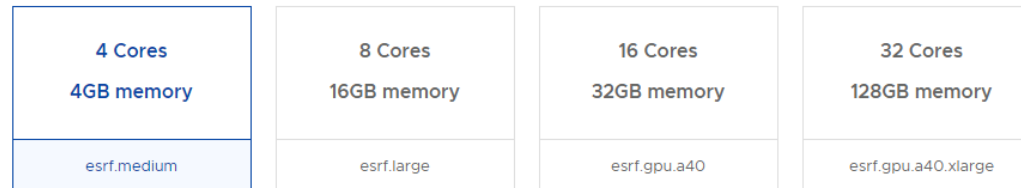
☒ Instance not associated to any specific experiments

Computing Environment

Choose an environment



Choose hardware requirements



Infrastructure for remote data processing / analysis

Users dedicated VM

Access to data

Access to Provisioning of scientific SW using CVMFS and Containers

Access to the GPUs, HPC cluster

Infrastructure based on OpenStack

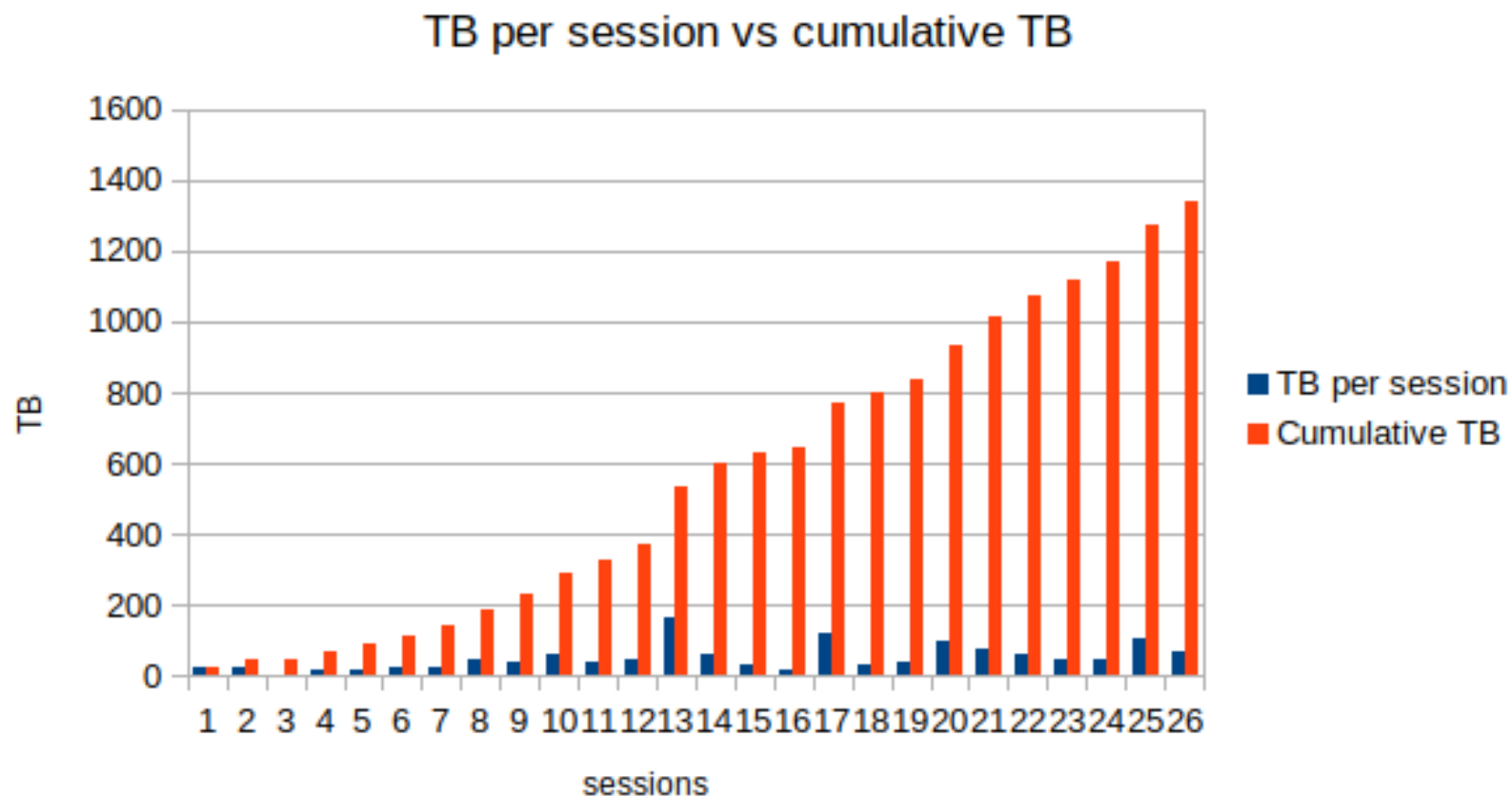
Development led by ILL in the scope of the PaNOSC project



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ESRF-EBS serial crystallography beamline (ID29) produced > 1.2 PB in first 6 months



VISA for ID29 SSX - demo dataset and processing

```
Applications - xfce terminal
Terminal - basus@visa-vm062: /data/projects/open-datasets/visa-demo
File Edit View Terminal Tabs Help
To run a command as administrator (user "root"), use "sudo <command>".
See "man sudo_root" for details.
basus@visa-vm062:~$ cd /data/projects/open-datasets/visa-demo/
basus@visa-vm062:/data/projects/open-datasets/visa-demo$ dh *
-bash: dh: command not found
basus@visa-vm062:/data/projects/open-datasets/visa-demo$ du -hs restored_dataset/
911G  restored_dataset/
basus@visa-vm062:/data/projects/open-datasets/visa-demo$
```

911Gb data collected in 8 min
80K images collected
Users avg collect: 25Tb/12hrs

```
Experimental data
Terminal - basus@visa-vm062: /data/projects/open-datasets/visa-demo/visa_demo/manual_processing
File Edit View Terminal Tabs Help
This is what I understood your unit cell to be:
tetragonal P, unique axis c, right handed.
a      b      c      alpha  beta  gamma
78.80  78.80  38.00 A    90.00  90.00  90.00 deg
List of indexing methods:
0: xgandalf-nolatt-cell      (xgandalf using cell parameters as prior information)
1: asdf-nolatt-cell         (asdf using cell parameters as prior information)
Indexing parameters:
  Check unit cell parameters: on
  Check peak alignment: on
  Refine indexing solutions: on
  Multi-lattice indexing ("delete and retry"): on
  Retry indexing: on
2 images processed, 1 hits (50.0%), 0 indexable (0.0% of hits, 0.0% overall), 0 crystals, 0.4 images/sec.
7 images processed, 6 hits (85.7%), 2 indexable (33.3% of hits, 28.6% overall), 2 crystals, 1.0 images/sec.
19 images processed, 18 hits (94.7%), 7 indexable (38.9% of hits, 36.8% overall), 9 crystals, 2.3 images/sec.
34 images processed, 33 hits (97.1%), 13 indexable (39.4% of hits, 38.2% overall), 15 crystals, 3.0 images/sec.
54 images processed, 49 hits (90.7%), 18 indexable (36.7% of hits, 33.3% overall), 21 crystals, 3.9 images/sec.
63 images processed, 58 hits (92.1%), 19 indexable (32.8% of hits, 30.2% overall), 23 crystals, 1.7 images/sec.
```

manual processing
from command line
2 images/sec

```
Terminal - basus@visa-vm062: /data/projects/open-datasets/visa-demo/visa_demo
File Edit View Terminal Tabs Help
basus@visa-vm062:~$ cd /data/projects/open-datasets/visa-demo/visa_demo/
basus@visa-vm062:/data/projects/open-datasets/visa-demo/visa_demo$ ls
4et8.pdb  ExeCrystFEL_2apj5a6f  ExeCrystFEL_zksoj5_  lyso.cell  lysozyme_PC  run.sh
autoCryst.log  ExeCrystFEL_of012fwg  input.json  lyso.mtz  manual_processing  ssx.process
basus@visa-vm062:/data/projects/open-datasets/visa-demo/visa_demo$ ./ssx.process
./ssx.process: line 6: ssx_proc: command not found
basus@visa-vm062:/data/projects/open-datasets/visa-demo/visa_demo$ module load ssx_proc/20230531
Loading ssx_proc/20230531
Loading requirement: ccp4/8.0 crystfel/0.10.2
basus@visa-vm062:/data/projects/open-datasets/visa-demo/visa_demo$ ./ssx.process
Submitted batch job 521
Submitted batch job 522
Submitted batch job 523
Submitted batch job 524
Submitted batch job 525
Submitted batch job 526
Submitted batch job 527
Submitted batch job 528
Submitted batch job 529
Submitted batch job 530
Submitted batch job 531
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Submitted batch job 550
Submitted batch job 551
Submitted batch job 552
Submitted batch job 553
Submitted batch job 554
Submitted batch job 555
Submitted batch job 556
Submitted batch job 557
Submitted batch job 558
```

CVMFS module to load
softwares
Automated script to access
SLURM cluster

eral, don't store any valuable data on it.

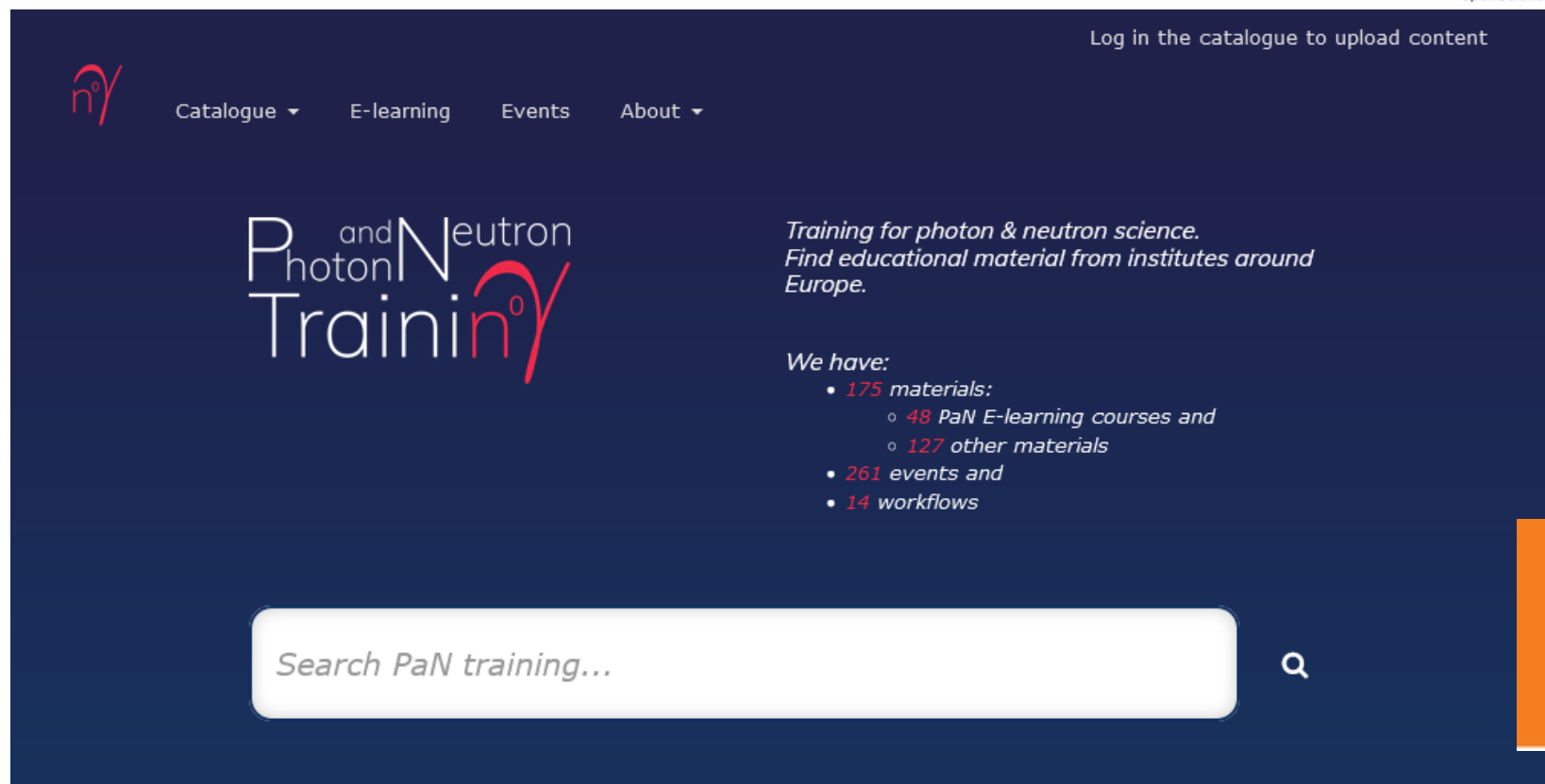
VISA for ID29 SSX – graphical viewers performance acceptable in a VISA virtual machine via browser

The screenshot displays a VISA virtual machine interface. On the left, a sidebar contains the VISA logo, Home, and Help buttons. The main window is divided into several panes:

- Terminal (top left):** Shows command-line output for Coot 0.9.8.8 EL (ccp4). The output includes map statistics (mean: 2.256e-05, sigma: 0.1283, maximum: 0.838, minimum: -0.3266) and a message about swapping atoms in the ASP.
- Terminal (bottom left):** Shows experimental data processing statistics, including the number of images processed, hits, and crystals.
- 3D Viewer (center):** Displays a 3D molecular model of a protein structure, rendered in blue and yellow, with a coordinate system (x, y, z) visible.
- Terminal (top right):** Shows the command-line interface for Coot 0.9.8.8 EL (ccp4).
- Terminal (bottom right):** Shows the command-line interface for the n.sh.x.process script.

The bottom status bar indicates the file path: `...sets/visa-demo/visa_demo/manual_processing/PROJECT_4.1.pdb. Molecule number 0 created.`

Share training material, videos, events, etc. on Pan-training.org



The screenshot shows the Pan-training.org website. At the top right, it says "Log in the catalogue to upload content". The navigation bar includes "Catalogue", "E-learning", "Events", and "About". The main header features the "Photon and Neutron Training" logo. Below this, a text block states: "Training for photon & neutron science. Find educational material from institutes around Europe." A list of resources is provided: "We have: 175 materials: 48 PaN E-learning courses and 127 other materials; 261 events and 14 workflows". A search bar at the bottom left contains the text "Search PaN training...".

Log in the catalogue to upload content

Photon and Neutron Training

Training for photon & neutron science.
Find educational material from institutes around Europe.

We have:

- 175 materials:
 - 48 PaN E-learning courses and
 - 127 other materials
- 261 events and
- 14 workflows

Search PaN training...



<https://pan-training.eu/>



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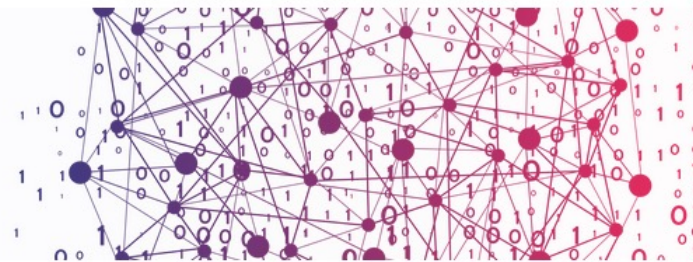
Open Training - courses on Pan-learning.org

Achieving 100% Open Educational Resources:

1. *Publish training material on pan-training.org*
2. *Develop learning material on pan-learning.org*



Photon and Neutron
eLearnin^{n γ}



Welcome to the e-Learning platform

*This e-Learning platform hosts free education and training for scientists and students.
Below you will find courses on both the theory of photon and neutron scattering
and how to use python code or software for data reduction and modelling.*

Login

Username



PaNOSC and E
and innovation p

<https://e-learning.pan-training.eu/moodle/>

FAIR data + Open Science lecture at Hercules School 2024

“The role of the scientist in making data FAIR for reproducible science”

Talk given first time as part of Hercules School in 2024

Rated: 40% Very good, 28% Good, 12% Average

HERCULES
European School

- *“An interesting talk with engaging discussion. Great inclusion in the program”*
- *“Happy this lecture was included.”*
- *“**This teaching is absolutely necessary for our generation.** Although the lecture was severely lacking in nuance and very moralistic (this should definitely be improved for next time), the comments made by the students and the discussions that this sparked were really interesting and made it very enjoyable and reflective about our everyday works. Such deep discussion are much more efficient to change the way of working than “you should do this” type of lecture.”*
- *“This lecture was truly interesting and turn into a debate rapidly even if it was not planned. Maybe change the format to a lecture and debate could be nice for the future.”*
- *“Please push some of the questions/arguments offline earlier to focus on the core topic.”*



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ExPaNDs
European Open Science Cloud Photon
and Neutron Data Services



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

PaN Data Portal - <https://data.panosc.eu>





diffraction

Q

50+ documents found

Facility

all

Technique

Select a technique...

Chemical Formula

Incident Wavelength

min

max

nm

Incident Photon Energy

min

max

eV

Temperature

10.16907/e8effd03-b358-473c-9f66-fa5660b7ffb2

Advances in long-wavelength native phasing at X-ray free-electron lasers

Long-wavelength pulses from the Swiss X-ray free-electron laser (XFEL) have been used for de novo protein structure determination by native single-wavelength anomalous diffraction (native-SAD) phasing of serial femtosecond crystallography (SFX) data. In this work,...

> Details, services ...

Released by **PSI** on January 1st 2020

10.22003/XFEL.EU-DATA-700000-00

Example Data

The European XFEL (EuXFEL) example data proposal contains experimental datasets from various original beam-times, currently covering the techniques of serial femtosecond crystallography (SFX), coherent diffraction imaging (single particle imaging, SPI), X-ray powder...

> Details, services ...




Released by **EuXFEL** on January 1st 2018

10.5291/ILL-DATA.INTER-368

Measurement of 41K's coherent scattering length using powder diffraction

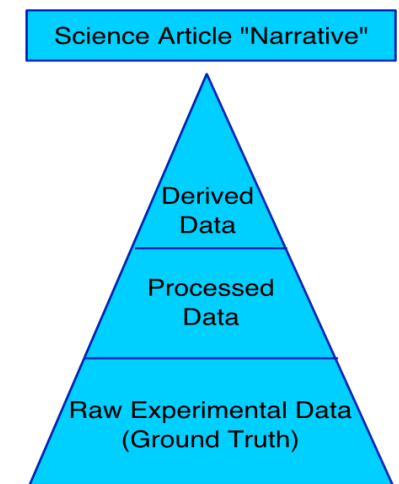
of the two projects PaNOSC and ExPaNDS.

The mission of the PaN data search portal is to contribute to the realization of a data commons for Neutron and Photon science. The search results provide a link to the landing page of the 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 Data Commons - What , Why and How

1. Create new kind of User community –
PaN Open Data User Community
2. Open Data are **findable** via one **portal**
3. Users can analyse the Open Data on their own or request “**Data-Time**” for help
4. Users can **train, analyse, verify, publish**



“The vital role of primary experimental data for ensuring trust in (Photon & Neutron) science”

<https://doi.org/10.5281/zenodo.5155882>



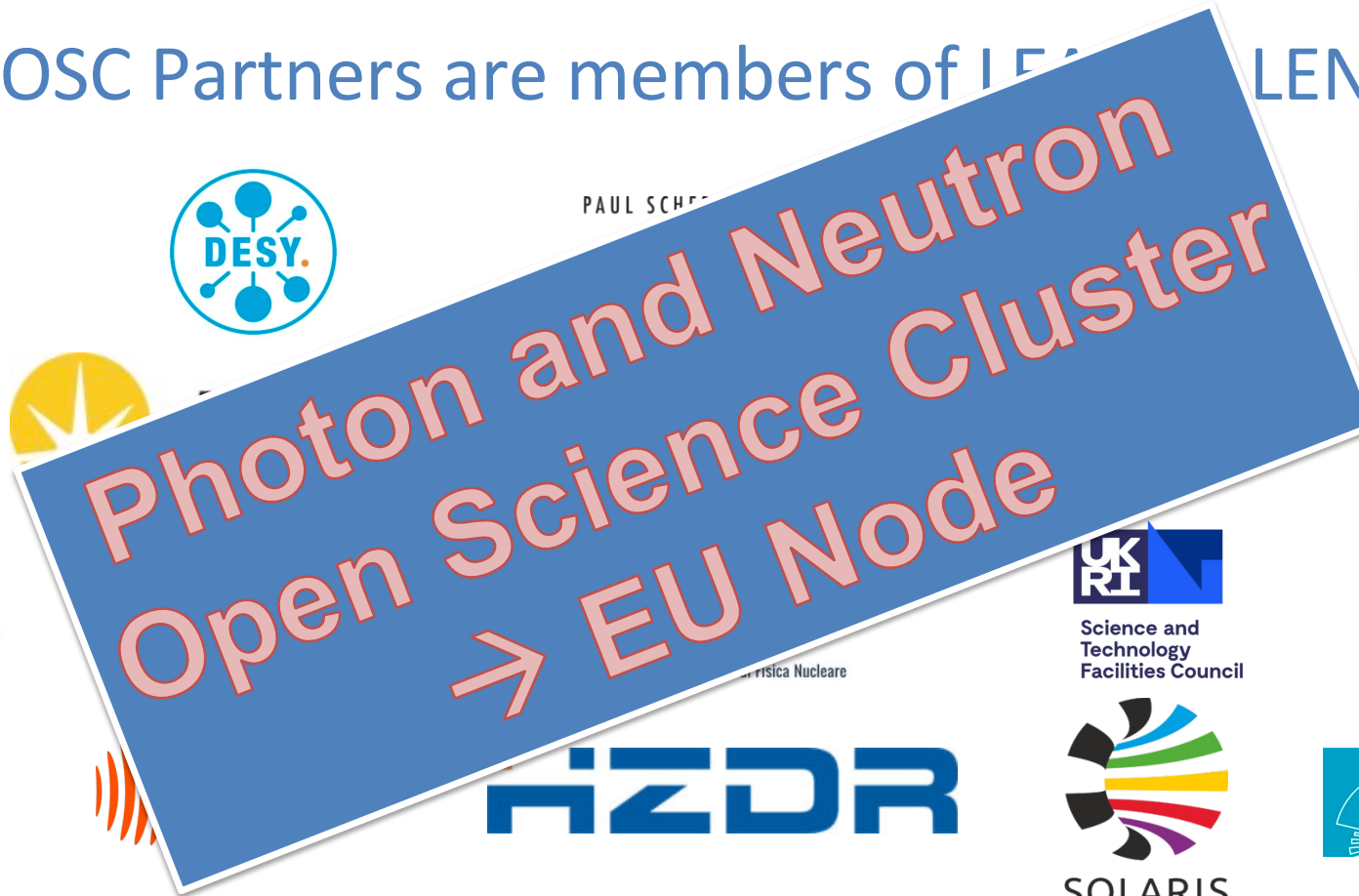
2024 – PaNOSC continues as a community activity



PaNOSC Partners are members of IEF and LENS



PAUL SCHERRER



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Cross-Domain Research Infrastructure Collaboration for Open Science

Research Infrastructures and Communities

The science clusters have grown out of five collaborative projects for linking world-class Research Infrastructures (RIs) to the European Open Science Framework (OSF). Other outcomes of the projects are cornerstones of the clusters' activities. The clusters are multidisciplinary initiatives with harmonised policies and procedures. Each cluster unites multiple RIs in their specific scientific domain.



SCIENCE-CLUSTERS.eu
Research Infrastructures for Open Science



OSCARS
Open Science Clusters' Action for Research & Society

OSCARS will spend 18 million euros on projects on FAIR data and Open Science (150k – 250k euros / project). Call closed, results 26 July 2024 (see OSCARS web site)



ASTRONOMY AND
PARTICLE PHYSICS

Learn more [↗](#)

ENVIRONMENTAL

Learn more [↗](#)

PHOTON AND
NEUTRON SCIENCE

Learn more [↗](#)



SOCIAL SCIENCES
AND HUMANITIES

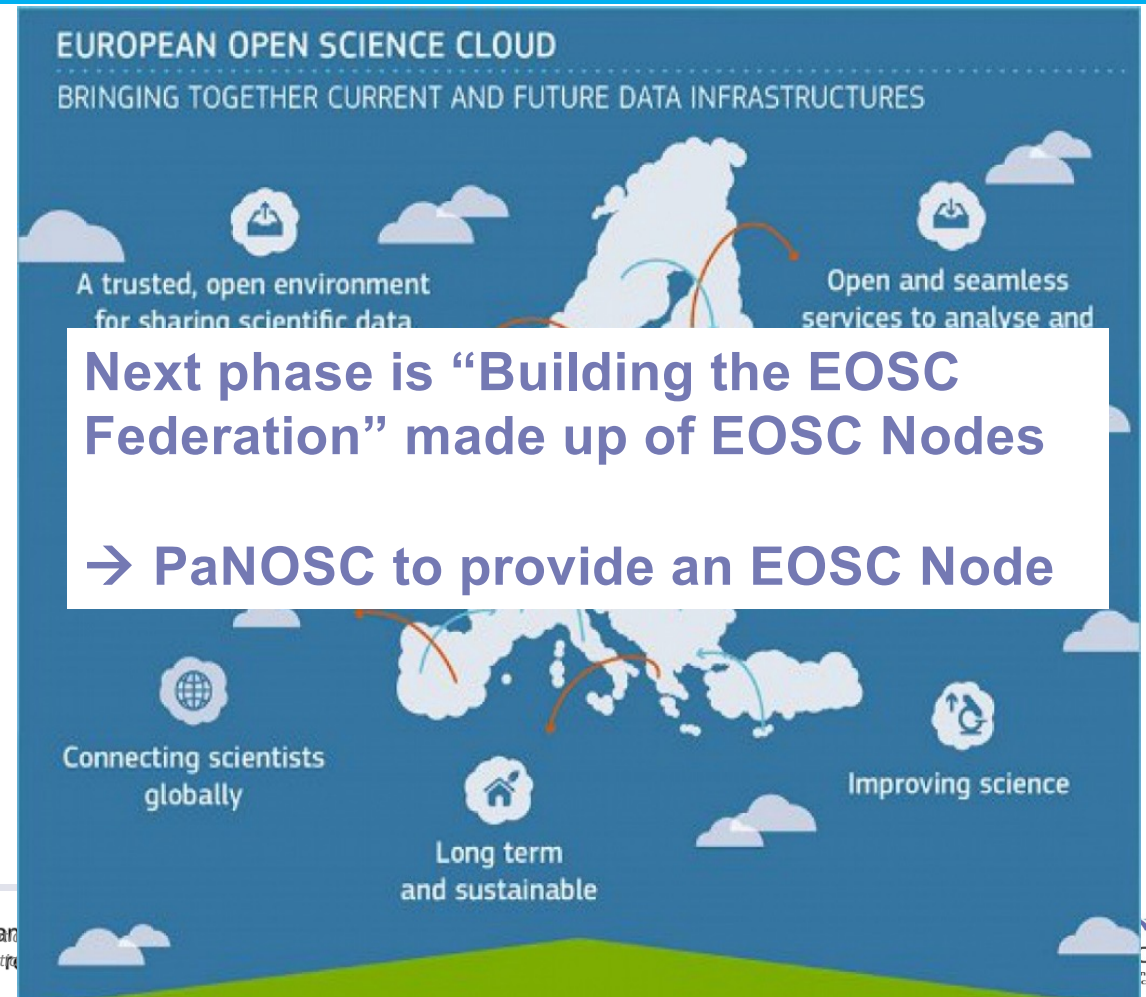
Learn more [↗](#)



European Open Science Cloud - The vision -



- Bridging today's fragmented and ad-hoc solutions; towards a **federation of data infrastructures**
- **FAIR data and services** for data storage, management, analysis and re-use **across borders and disciplines**
- Added value for **data-driven science**, reproducible science, interdisciplinary research, digital innovation (EU DSM)



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IUCr Journals has launched IUCrData's Raw Data Letters

Scientists are encouraged to publish raw data!





IUCrData

ISSN 2414-3146

Crystal structure of the second extracellular domain of human tetraspanin D9: twinning and diffuse scattering

Viviana Neviani, Martin Lutz, Wout Oosterheert, Piet Gros and Loes Kroon-Batenburg*

Department of Chemistry, Structural Biochemistry, Bijvoet Centre for Biomolecular Research, Faculty of Science, Utrecht University, Utrecht, The Netherlands. *Correspondence e-mail: L.m.j.kroon-batenburg@uu.nl

Received 20 April 2021
Accepted 1 May 2021

Keywords: twinning; diffuse scattering; tetraspanin CD9_{EC2}

Remarkable features are reported in the diffraction pattern produced by a crystal of tetraspanin CD9_{EC2}, the structure of which was described previously [Oosterheert *et al.* (2020). *Life Sci. Alliance*, **3**, e202000883]. CD9_{EC2} crystallized in space group *P1* and was twinned. Concurrent with the twinning, diffuse streaks were seen in the direction perpendicular to the twinning interface. Preliminary conclusions are made on packing disorder and potential implications for the observed molecular structure. It is envisaged that the raw diffraction images could be very useful for methods developers in trying to remove the diffuse scattering to extract accurate Bragg intensities or by using it to model the effect of packing disorder on the molecular structure.

Raw data



Structure



Raw diffraction data

HDF5 data file, DOI: <https://doi.org/10.5281/zenodo.1234567>

Metadata ImgCIF file, DOI: <https://doi.org/10.1107/S2414314622000384/me6134.cif>

[CheckCif for Raw Data]

checkImgCIF report

ImgCIF checker version 2022-07-16

Checking block 5886687 in he4557img.cif

Running checks (no image download)

=====

Testing: Required items: PASS

Testing: Data source: PASS

Testing: Axes defined: PASS

Testing: Our limitations: PASS

Testing: Detector translation: PASS

Testing: Scan range: PASS

Testing: All frames present: PASS
All frames present and correct for SCAN1

Testing: Detector surface axes used properly: PASS

Testing: Pixel size and origin described correctly: PASS

Testing: Check calculated beam centre: PASS

Testing: Check principal axis is aligned with X: PASS
Testing presence of archive:

Testing: All archives are accessible: PASS

Running checks with downloaded images

=====

Testing image 4: Image type and dimensions: PASS

Raw data table generated from the CIF

Raw data	
DOI	https://doi.org/10.5281/zenodo.5886687
Data archive	Zenodo
Data format	HDF5
Data collection	
Beamline	Diamond I04
Detector	
Temperature (K)	
Radiation type	Synchrotron X-ray source
Wavelength (Å)	0.979491
Beam centre (mm)	-166.874, 172.497
Detector axis	-Z
Detector distance (mm)	-287.22
Swing angle (°)	
Pixel size (mm)	0.075 × 0.075
No. of pixels	4148 × 4362
No. of scans	1
Exposure time per frame (s)	

Scan axis	ω, X
Start angle, increment per frame (°)	0.0, 0.1
Scan range (°)	360.0
No. of frames	3600

Where PaNOSC can help ORSO activities



6th ORSO Workshop: *The output is expected to be a joint paper on Metadata and the setting up of a reflectometry data base for shared data.*

1. **FAIR data policy** – ORSO database policy issues
2. **Standardised metadata** – adoption of **Nexus/HDF5 + PaNET**
3. **JupyterLab notebooks** – provide examples + training
4. **ORSO Database** – to be included in PaNOSC EOSC Node
5. **Remote data analysis** – provide VISA service linked to processing pipelines in PaNOSC EOSC Node
6. **Reflectometry training** – register training material pan-training.eu
7. ORSO to identify a **PaNOSC contact person**



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Conclusion



1. **The Photon and Neutron Open Science Cloud (PaNOSC) is implementing a Data Commons of FAIR data in EOSC**
2. **Facilities have the role of managing data for Users**
3. **Users role is to enrich metadata, publish and cite data**
4. **ORSO must continue its good work on metadata, databases + training material!**



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Thank you

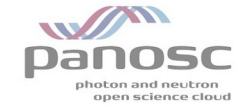


1. **PaNOSC + ExPaNDS** collaborators
2. **ESUO, ENSA, LEAPS** and **LENS** facilities
3. **IUCr Committee on Data**
4. **Users** for use cases, data and feedback
5. **European Commission** for funding PaNOSC + ExPaNDS
6. **ESRF** colleagues **Jean-Francois Perrin, Daniele de Sanctis, Gerd Heber** (HDF Group) and the **EC** for slides



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.

How can the EC help solve the data issues?



1. **European Commission funds common activities**
2. One of the activities of **European Data Strategy** is the **European Open Science Cloud (EOSC)**
3. **Photon and Neutron sources in Europe** are seen as part of the **EOSC as data providers**



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Not a cloud from Brussels, but a research Data Commons driven by the stakeholders

Your opinion on implementing the EOSC

The survey is closed;
you can view here the results as they stand

Vienna
Declaration
2018

EOSC
declaration
2017

EOSC
Association
2020

EOSC SUMMIT

12 June 2017 - Brussels
Charlemagne building - Sicco Masholt Room

European Open Science Cloud
New Research & Innovation Opportunities



<http://ec.europa.eu/research/openscience/eosc>

#EOSC

Together, we can create a European Research Data Commons that will not only benefit Europe but help tackle the societal challenges worldwide. EOSC-A



Open Science with Jupyter notebooks



- Notebooks document
- If used app
- For example
- Notebooks
- Currently, I before they



n in one

e-usable

work of others,

PaNOSC provides training on making reproducible publications for FAIR data
https://youtu.be/vStbMUDI_jU



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Adoption (in October 2022) of PaNOSC+ExPaNDS outcomes

FACILITY	FAIR data policy	DMPs	DOIs	Nexus HDF5	Search API	Open Data Portal	AAI	Jupyter Lab	VISA	VINYL/OASYS/McStas	Pan-learning/training
ALBA	P	P	WIP	WIP	WIP	WIP	P	Y	WIP	N	U
DESY	WIP	WIP	WIP	Y	WIP	P	WIP	Y	U	Y	WIP
CERIC-ERIC	Y	WIP	Y	WIP	Y	Y	Y	Y	Y	Y	Y
DIAMOND											
ELETTRA	Y	WIP	Y	Y	Y	Y	Y	Y	Y	Y	Y
ESRF	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
ELI-ERIC	Y	Y	P	Y	Y	Y	WIP	Y	Y	Y	Y
ESS	Y	Y	Y	Y	Y	Y	Y	WIP	WIP	Y	Y
EuXFEL	Y	WIP	Y	WIP	Y	Y	WIP	Y	WIP	Y	Y
FELIX	Y	P	WIP	U	U	WIP	U	U	N	N	U
HZB	Y	P	WIP	Y	P	Y	P	U	U	U	U
HZDR	Y	WIP	Y	N	U	Y	Y	Y	P	WIP	Y
ILL	Y	WIP	Y	Y	WIP	Y	Y	Y	Y	Y	WIP
MAX-IV	WIP	U	Y	Y	Y	Y	Y	Y	U	U	U
PSI	Y	WIP	Y	WIP	Y	Y	WIP	WIP	N	N	N
PTB	Y	WIP	Y	WIP	N	Y	N	N	N	N	N
SOLARIS											
SOLEIL	Y	WIP	WIP	Y	WIP	WIP	Y	WIP	WIP	U	Y
SESAME	Y	U	P	Y	P	WIP	P	P	N	Y	N



PaNOSC and ExPaNDS projects and innovation programme under

Not Planning to be adopted (N)

Under evaluation (U)

In progress of being adopted (WIP)



panosc
photon and neutron
open science cloud

LEAPS Data Strategy



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LEAPS data strategy

Regular Article | [Open Access](#) | Published: 17 July 2023 | 138, Article number: 61

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Regular Article

THE EUROPEAN
PHYSICAL JOURNAL PLUS



LEAPS data strategy

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- ⁵ SESAME, Allan, Jordan
- ⁶ ALBA, Cerdanyola del Vallès, Spain
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Abstract The continuous evolution of photon sources and their instrumentation enables more and new scientific endeavors at ever increasing pace. This technological evolution is accompanied by an exponential growth of data volumes of increasing complexity, which must be addressed by maximizing efficiency of scientific experiments and automation of workflows covering the entire data lifecycle, aiming to reduce data volumes while producing FAIR and open data of highest reliability. This paper briefly outlines the strategy of the league of European accelerator-based photon sources user facilities to achieve these goals collaboratively in an efficient and sustainable way which will ultimately lead to an increase in the number of publications.



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<https://doi.org/10.1140/epjp/s13360-023-04189-6>