



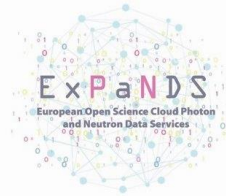
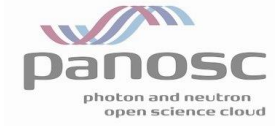
Europe's Photon and Neutron Open Science Cloud for Raw and Processed Data: Aims and Achievements to Date

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. Acknowledgements
2. Managing Photon and Neutron data
3. The Photon and Neutron Open Science Cloud
4. The carbon footprint of raw data
5. How does this benefit Users i.e you?



Acknowledgement of Country

We acknowledge the Traditional Owners of the lands and waters throughout Australia, and pay respect to the Elders past, present and emerging. We recognise the importance of connection to culture, land, kinship and community to the health and wellbeing of Aboriginal & Torres Strait Islander families. We acknowledge the cultural practices and traditions still carried out today and being passed down to future generations.



I'd like to begin by acknowledging the Traditional Owners of the land on which we meet today. I would also like to pay my respects to Elders past and present. I acknowledge the first custodians of this land who gathered an amazing body of knowledge over tens of thousands of years.

I acknowledge the **Committee on Data** of the IUCr. I thank the members of **CommDat** who have played a key role in motivating the work to make **FAIR data reality for the Photon and Neutron** community (and this talk).

A special thanks to **John Helliwell** who led CommDat since the beginning in 2016 up until now.



COMMITTEE ON DATA (COMMDAT)



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<https://www.iucr.org/iucr/governance/advisory-committees/committee-on-data>



WORKSHOP ON RAW DIFFRACTION DATA REUSE: THE GOOD, THE BAD AND THE CHALLENGING



Organized by

Loes Kroon-Batenburg (Netherlands), Selina Storm (Germany), John Helliwell (UK) and Brian McMahon (UK) for the IUCr Committee on Data



<https://www.iucr.org/resources/data/commdat/melbourne-workshop>



CIF Dictionary Workshop Session 1

Room: 216
Chairs: Loes Kroon-Batenburg & James Hester
Session: A118 Raw Diffraction Data Reuse: Warts and All

TODAY - Friday at 1:10 pm – 3:30 pm
Room: 220
Chairs: Nicholas Schwarz & Andrew Gotz
Session: A109 Data-Driven Science: Current Status and Outlook

Room: 207
Chairs: Brinda Vallat & John Helliwell
Session: A014 Databases and Data Management



Next generation of photon sources



Next generation of data sources

1. Current photon sources produce petabytes of data / year
2. Next generation will produce 10-100s of petabytes / year
3. Users + facilities are challenged by the data volumes
4. Reminder: 1 petabyte = 32 year long MP3
Avatar 1 = 1 petabyte,
Avatar 2 = 18 petabytes



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

This talk is about reducing 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

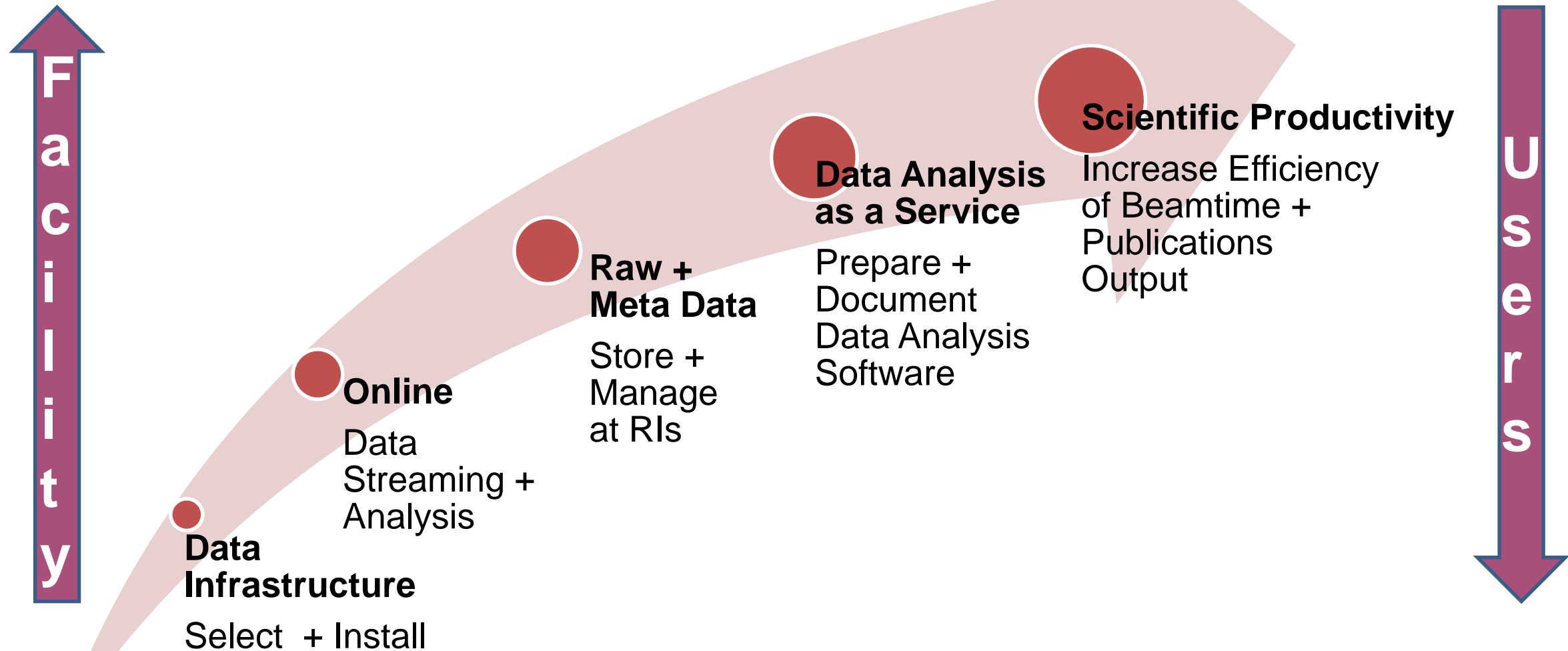
data



Facilities

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

Facilities and Users converging needs for data management



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**

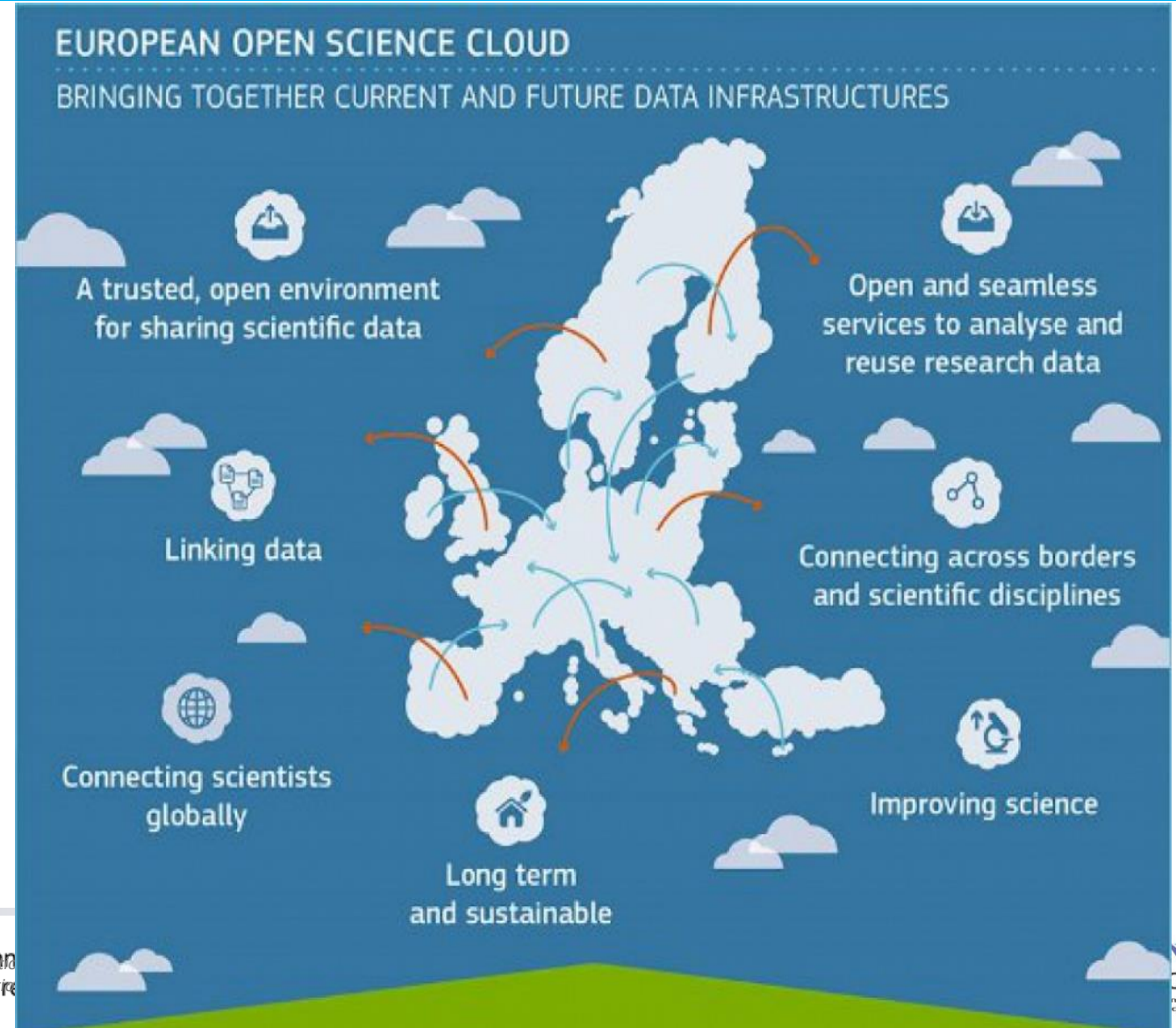


European Open Science Cloud

- 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)



Service dimension of the EOOSC

The EOOSC will provide ~~two million EU~~ researchers with:

- ✓ A catalogue of European research data funded with public money;
- ✓ A catalogue of services to re-use these data;
- ✓ Tools to make their own data open and FAIR;
- ✓ Advanced tools to merge and analyse the data in a secure environment;
- ✓ A simple access gateway to these services (EOOSC Portal).



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.



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 Siccó Masholt Room

European Open Science Cloud
New Research & Innovation Opportunities



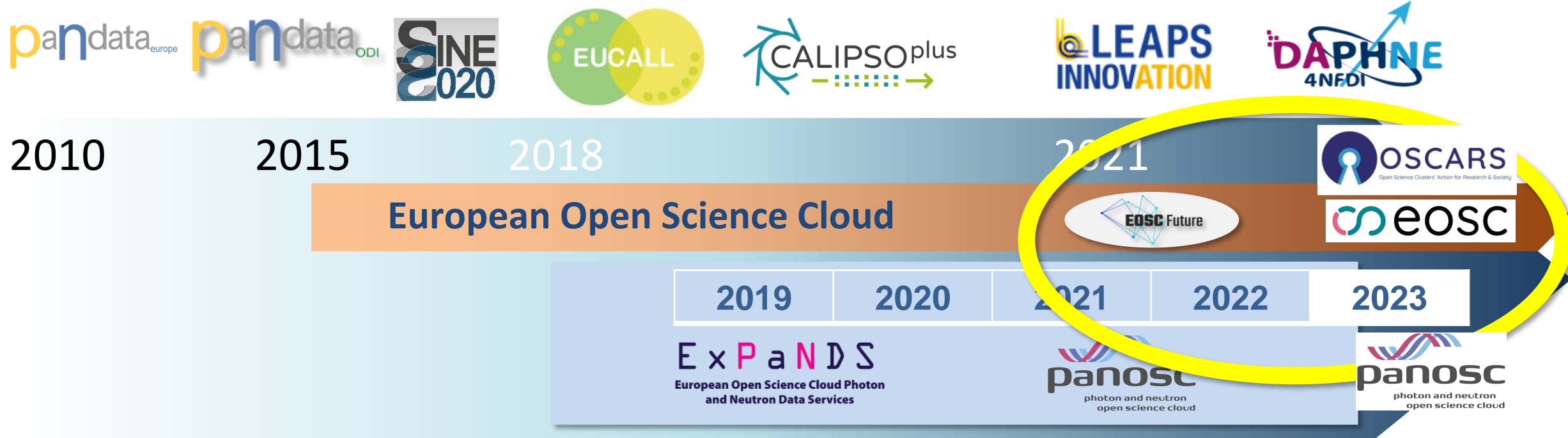
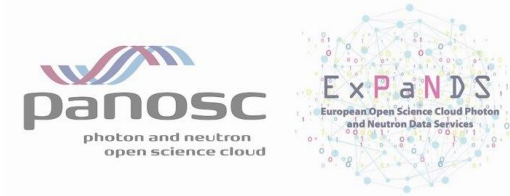
<http://ec.europa.eu/research/openscience/eosc>

#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



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

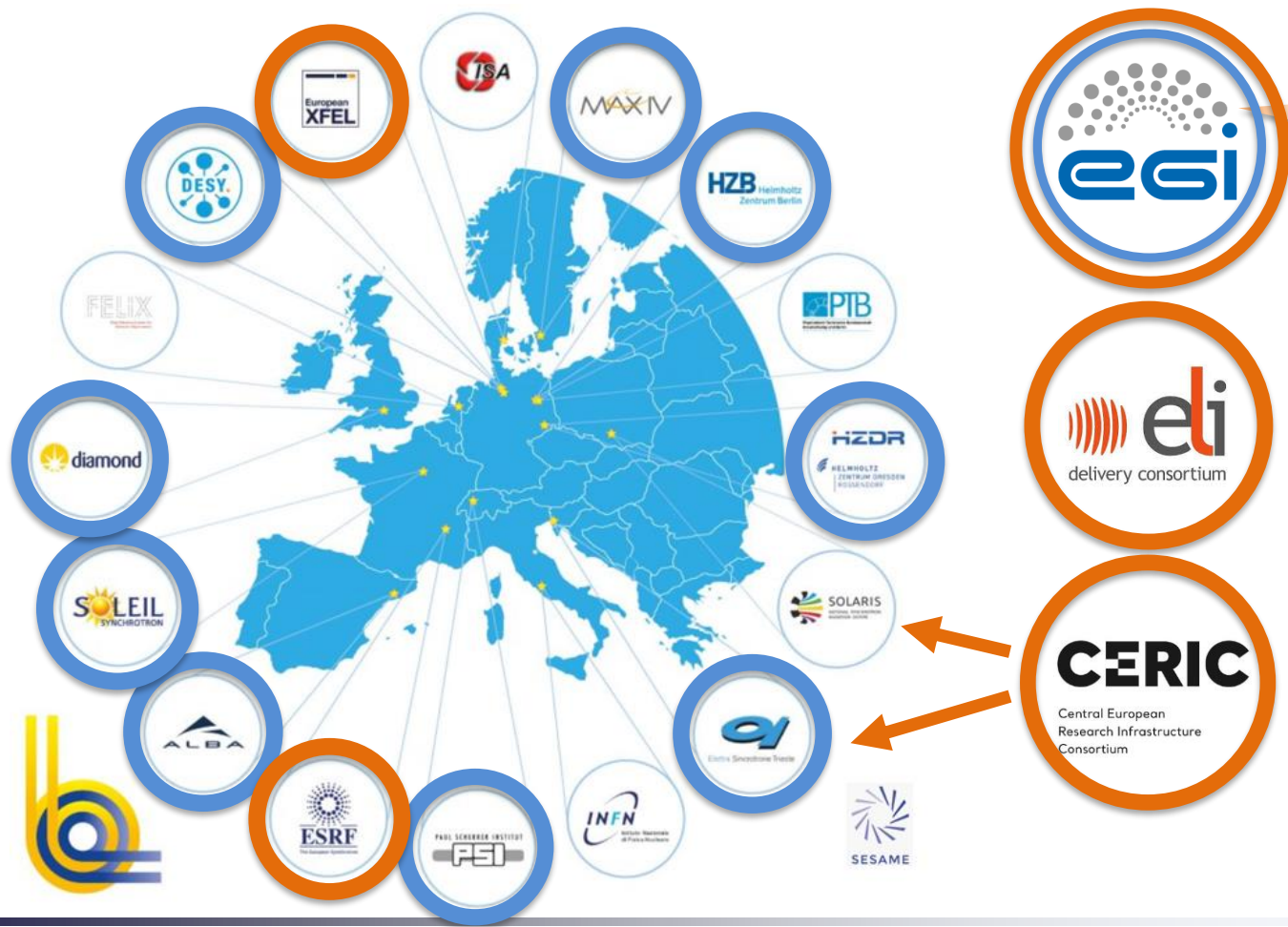


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Two EOSC projects for PaN : PaNOSC and ExPaNDS

○ PaNOSC
○ ExPaNDS

Photon (LEAPS)



Neutron (LENS)



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.

Cross-Domain Research Infrastructure Collaboration for Open Science



SCIENCE-CLUSTERS.eu
Research Infrastructures 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 Commission. Other outcomes of the projects are cornerstones of the clusters' activities: multidisciplinary initiatives with harmonised policies and procedures in their specific scientific domain.



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 opens Q1 2024 (see PaNOSC or OSCARS web site)



ASTRONOMY AND
PARTICLE PHYSICS

Learn more [↗](#)

ENVIRONMENTAL

Learn more [↗](#)

PHOTON AND
NEUTRON SCIENCE

Learn more [↗](#)

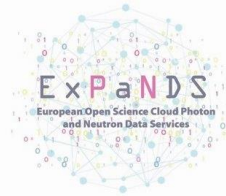
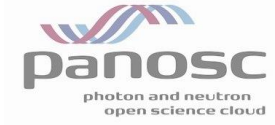


SOCIAL SCIENCES
AND HUMANITIES

Learn more [↗](#)



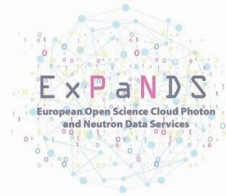
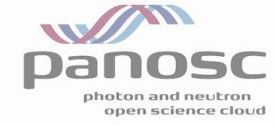
PaNOSC + ExPaNDS - Main Achievements



1. **FAIR data policy** and **DMPs**
2. Standardised metadata (**Nexus/HDF5**)
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 Umbrella**
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-learning** platform (pan-learning.org)




Active Data Management Plans




1. ExPaNDS and PaNOSC have adopted active DMPs
2. Active DMPs are updated at different phases of the project
3. ESS and ESRF have chosen to use DS Wizard developed by Elixir
4. Example of implementation @ ESRF
 1. Automatically generates a DMP automatically for every proposal
 2. 50 out of 82 questions are automatically filled in from DP/User/Data Portals
 3. DMPs offer a structured way to communicate information
 4. Users can use the DMP for satisfy funders requirements
 5. Next step is to use the DMPs to ensure users can manage their **data**



View

Comments TODOs Version history 

Current Phase

Before starting the project/proposal 

- Chapters**
- I. General / Topic
 - II. Content classification / Datas
 - III. Technical classification
 - IV. Metadata 2
 - V. Ethics / General legal issues
 - VII. Storage and long-term preservation / Selection** ✓
 - What are the criteria / rules for the selection of the data...
 - Who selects the data to be archived?

VII. Storage and long-term preservation / Selection


Here the user is asked to define their criteria for archiving data as well as the duration and accessibility of the data.

What are the criteria / rules for the selection of the data (after the end of the project)?  

discussed between the instrument scientist and the user. Normally the instrument scientist can guide the user.

Desirable: *Before starting the project/proposal*

Only raw data with metadata generated by ESRF software will be archived. All raw data necessary to do a complete analysis without redoing the experiment are archived. Processed data can be stored on request.

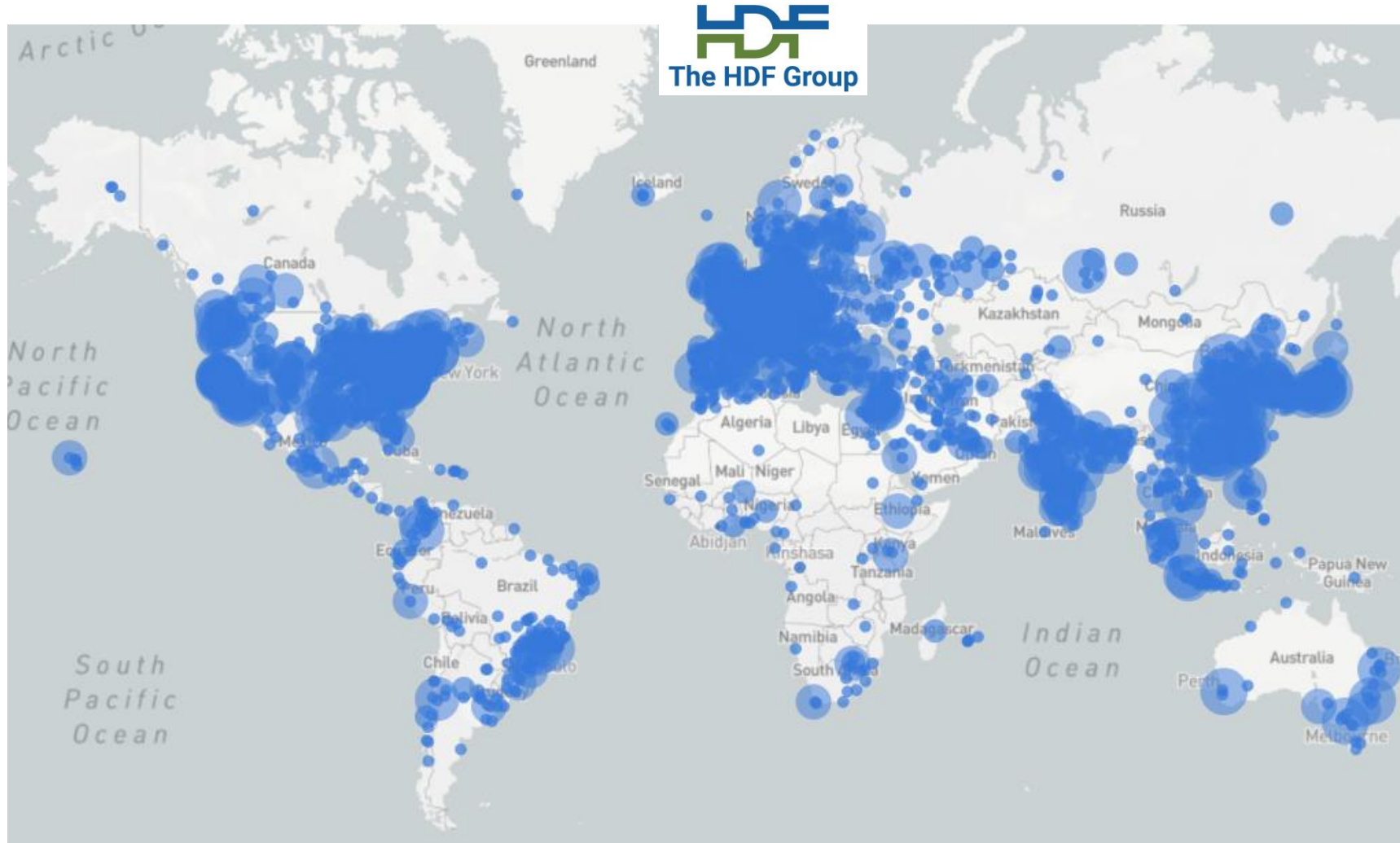
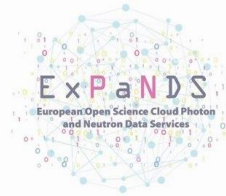
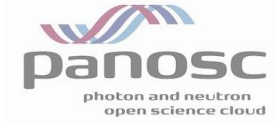
 Clear answer

Answered 21 days ago by admin admin.

Facilities need to help Users by pre-filling DMPs for them



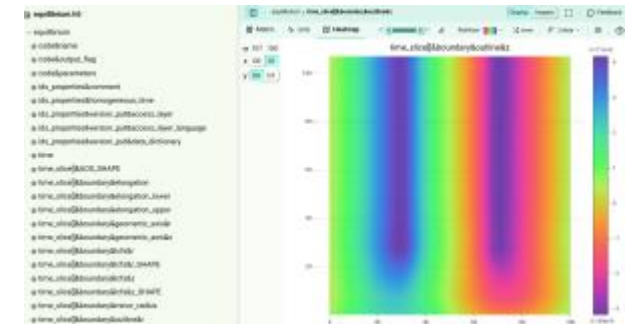
HDF5 is needed to acquire, process and store large datasets and has been adopted as de facto standard across most facilities (with NeXus conventions for metadata)



New Features

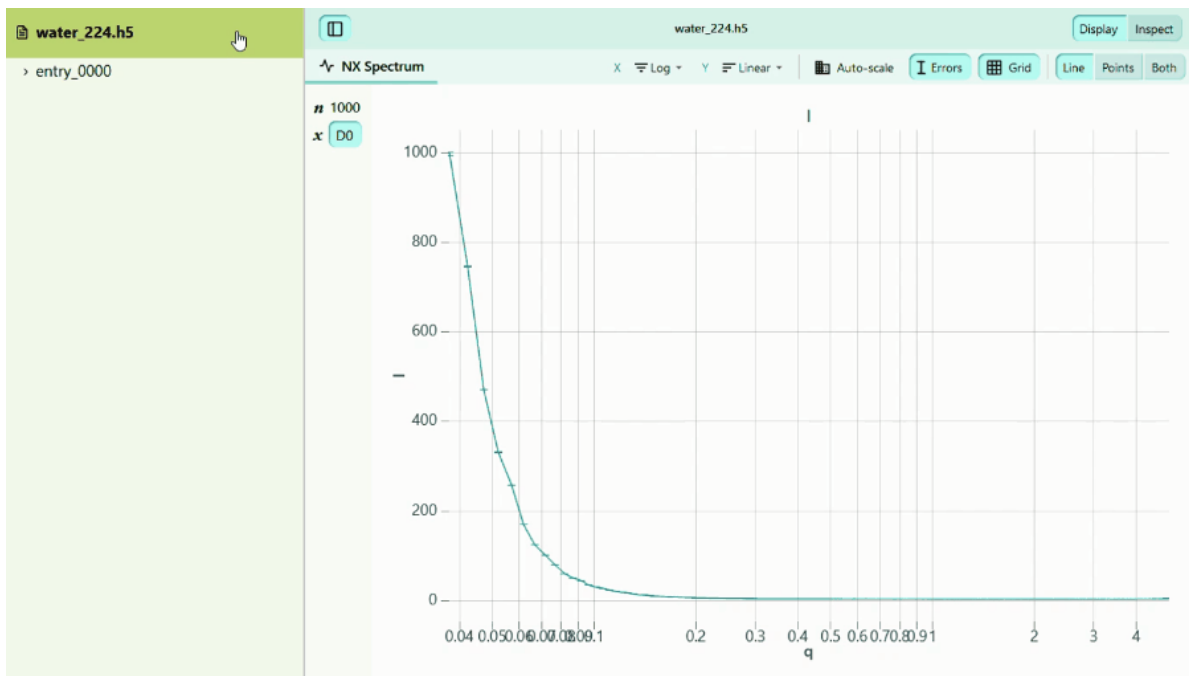
- Multi-dataset I/O
- Selection and vector I/O
- Subfilng VFD
- Multi-Threaded Concurrency (WIP)
- Sparse data storage (WIP)

PaNOSC developed H5Web to make HDF5 even easier

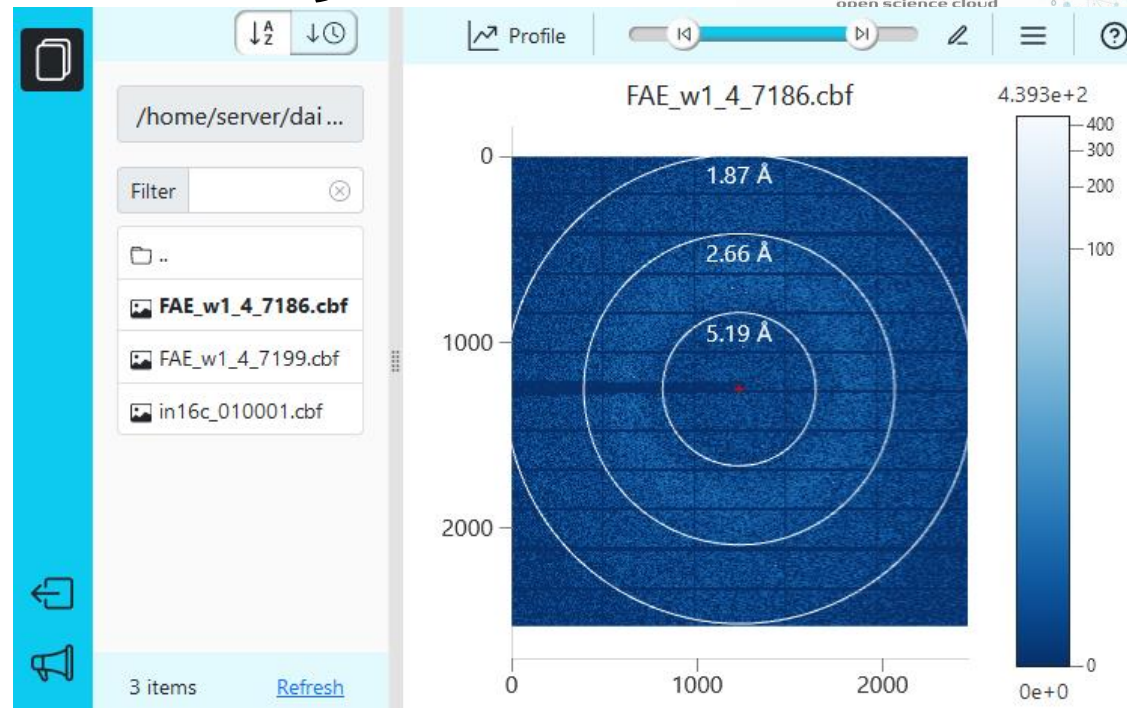


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H5Web Visualization Ecosystem



Generic HDF5 file viewer



Visualization components

- 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>

Used in various web applications at ESRF including:

- **Braggy**, diffraction image viewer (screenshot above)
- **Daiquiri**, beamline control and data acquisition software

H5Web

H5Web | 📄 9,845 installs | ★★★★★ (7) | Free



HDF5 file viewing on the web made easy

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

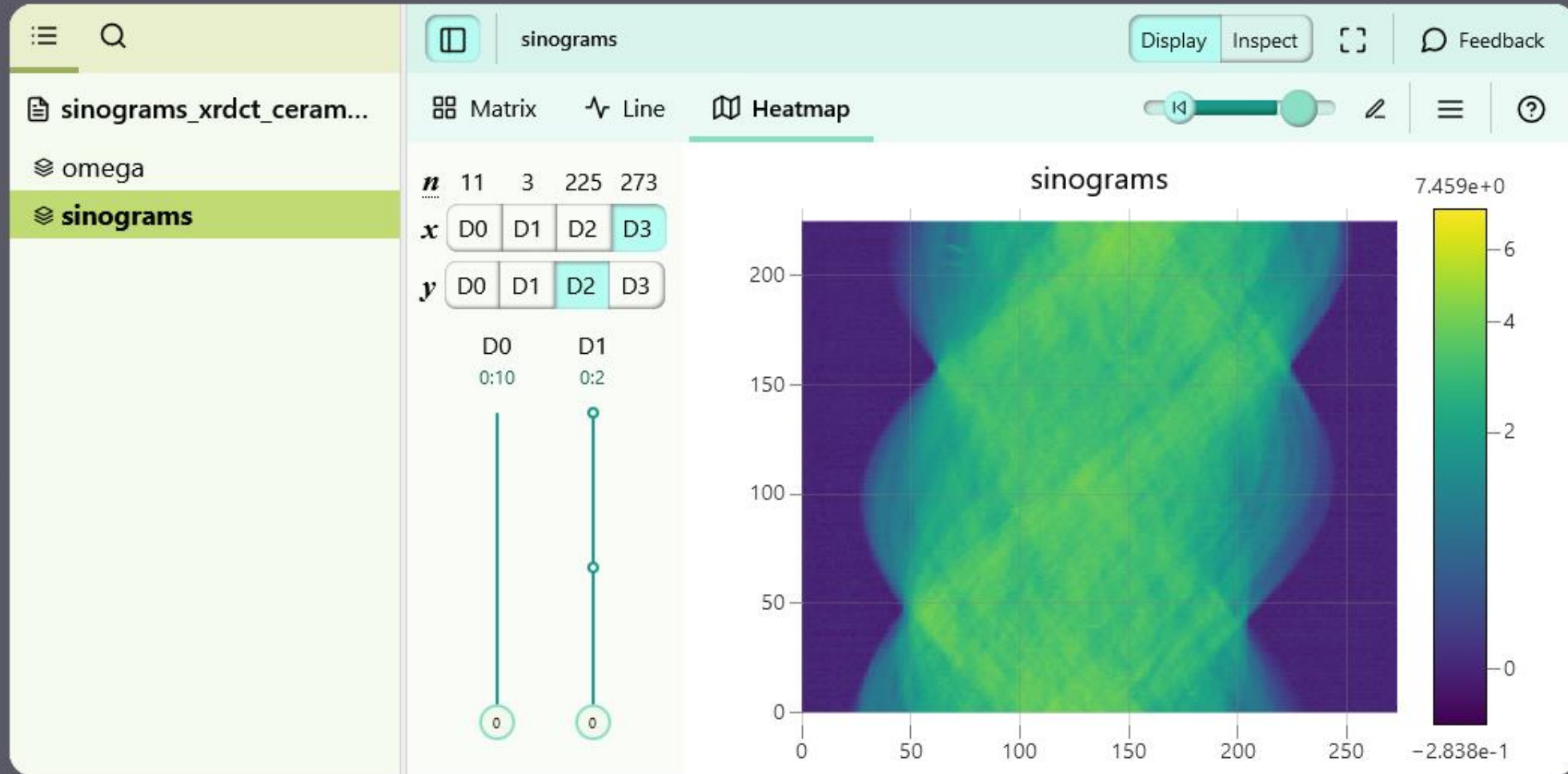
myHDF5

Open HDF5

Help

Opened files

Z sinograms_xrdct_ceramic...



← Made by PaNOSC at ESRF



Data compression is essential to deal with the “too much” data being produced by detectors – register for the workshop here <https://indico.desy.de/event/39343/>

2023 European HDF User Group (HUG) plugins and data compression summit

Sep 19 – 21, 2023
DESY
Europe/Berlin timezone

Overview

Call for Abstracts

Registration

Venue

Accommodation

Organising committee and
sponsorship

Local organiser

✉ david.pennicard@desy.de

On September 19-21, the 2023 European HDF5 Users Group (HUG) summit is going to be held both in-person and virtually at DESY in Hamburg, Germany.

The HDF5 library and toolset have been widely used to simplify management and access to scientific and engineering data with ubiquitous data solutions. This meeting will have a focus on plugins and data compression, which become an increasingly important topic as data volumes grow, and is being hosted in collaboration with the LEAPS-INNOV EU project: <https://www.leaps-innov.eu/>

The HDF Group will give an update on the latest developments within HDF5 and present the roadmap for the future. We will have invited talks and contributed presentations from HDF5 users and developers, discussions on future requirements and developments, and events such as tutorials.

Please use the links in the side panel to register and/or submit your presentation proposal. As well as taking abstracts for presentations on your work, we are keen to get feedback and discussion on next steps with HDF. So, if there are topics or problems you wish to discuss, you are also welcome to let us know via the abstract system, and we could then arrange a discussion slot.

Topics of interest include, but are not limited to:



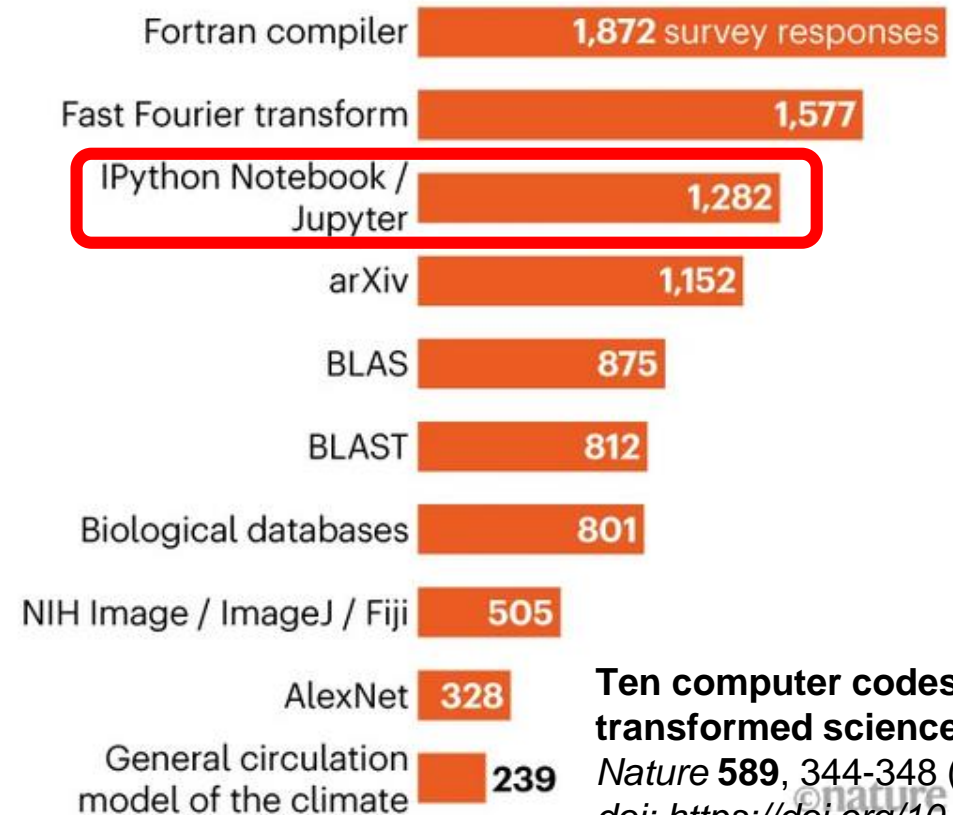
Support for Jupyter notebooks

- **Jupyter service** now available at all PaNOSC and most ExPaNDS sites
- **Jupyter on Slurm** service developed: https://github.com/silx-kit/jupyterhub_moss/
- **H5Web** Jupyterlab plugin developed
- **VISA** provides Jupyter service
- **PaN e-learning** platform provides Jupyter as a service
- **PaNOSC summer school** trained participants to program in Python using Jupyter
- **EGI** provided Jupyter and Binder as a service



TOP CHOICES FOR SCIENCE CODE

Readers voted on which of the ten software codes in this article had the biggest impact on their work. They could choose up to three. Here are the results.



Ten computer codes that transformed science

Nature **589**, 344-348 (2021)
doi: <https://doi.org/10.1038/d41586-021-00075-2>



Open Science with Jupyter notebooks



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



n in one

re-usable

work of others,

PaNOSC provides training on making reproducible publications for FAIR data

https://youtu.be/vStbMUDI_jU



VISA - Remote Data Processing/analyses



VISA

Home

Help

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

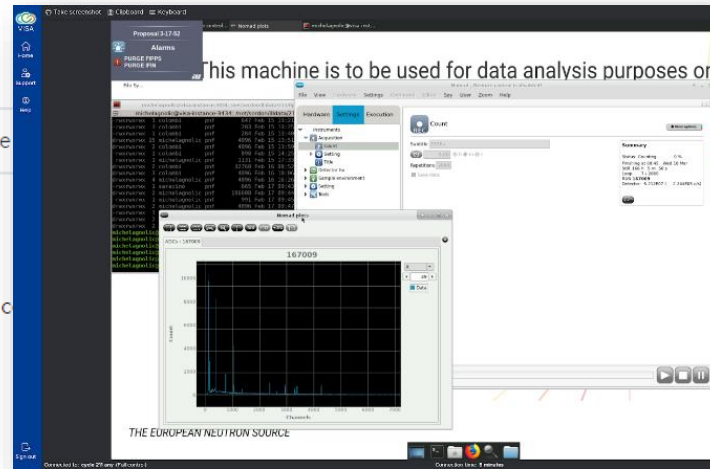
Computing Environment

Choose an environment

 Desktop staging	 Desktop	 Bliss
---------------------	-------------	-----------

Choose hardware requirements

4 Cores 4GB memory esrf.medium	8 Cores 16GB memory esrf.large	16 Cores 32GB memory esrf.gpu.a40	32 Cores 128GB memory esrf.gpu.a40.xlarge
--------------------------------------	--------------------------------------	---	---



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

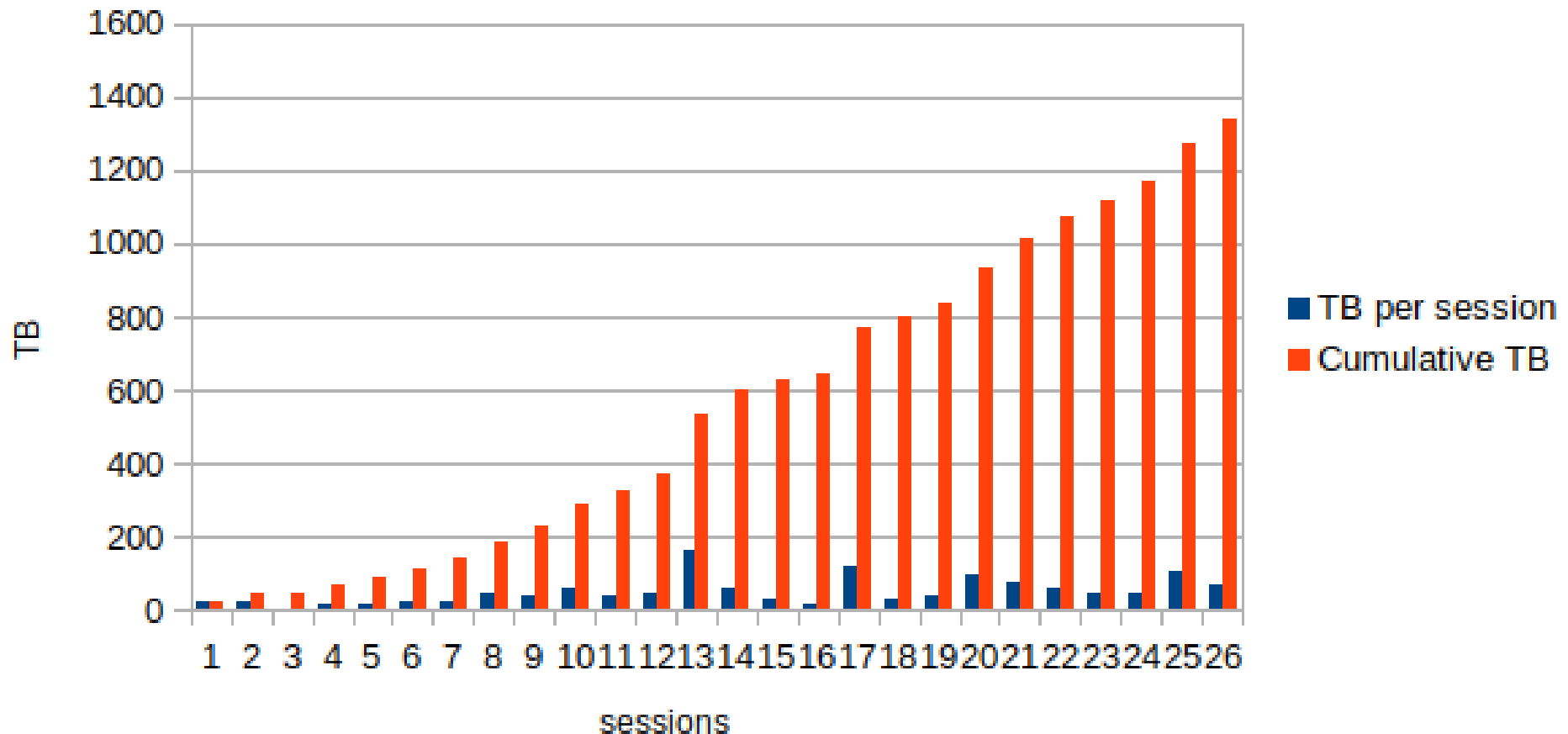
Development led by ILL in the scope of the PaNOSC project

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.



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

TB per session vs cumulative TB



VISA for ID29 SSX - demo dataset and processing

```
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

```
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_zkksoj5_  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

```
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

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 environment. The main window is Coot 0.9.8.8 EL (ccp4), showing a 3D molecular model of a protein structure in blue, with a yellow stick model overlaid. The interface includes a menu bar (File, Edit, Calculate, Draw, Measures, Validate, About, Ligand) and a toolbar with options like 'Reset View' and 'Display Manager'. To the left, a terminal window shows the following output:

```
03955 bounds -0.03961 -0.03949 from bin-number 2464 of 10000
Post-filter Map statistics: mean: 2.
Post-filter Map statistics: min: -0.
Map extents: ..... 180 180 96
Map mean: ..... 2.256e-05
Map sigma: ..... 0.1283
Map maximum: ..... 0.838
Map minimum: ..... -0.3266
(make-and-draw-map-with-reso-with-re
tasetsets/visa-demo/visa_demo/manual_pr
"Fobs:None-specified" "SigF:None-sp
)
(use-graphics-interface-state)
INFO:: backup file name coot-backup/
emo_visa_demo_manual_processing_PROJ
on @.pdb.gz
INFO:: (result) ASP swapped atoms in
INFO:: 1 residues had their atoms sw
(graphics-general-key-press-hook 655
debug:: g.safe_scheme_command() with
)
Key 65515 not found in (python) key
Key 65515 not found in (scheme) key
```

Below this, another terminal window displays processing statistics:

```
Experimental data
Terminal - basus@visa-vm062: /data/projects/ope
File Edit View Terminal Tabs Help
54 images processed, 49 hits (90.7%), 1
crystals, 3.9 images/sec.
63 images processed, 58 hits (92.1%), 1
crystals, 1.7 images/sec.
76 images processed, 70 hits (92.1%), 2
crystals, 2.5 images/sec.
92 images processed, 85 hits (92.4%), 2
crystals, 3.1 images/sec.
98 images processed, 91 hits (92.9%), 3
crystals, 1.2 images/sec.
113 images processed, 104 hits (92.0%),
37 crystals, 2.9 images/sec.
127 images processed, 117 hits (92.1%),
41 crystals, 2.7 images/sec.
c139 images processed, 128 hits (92.1%)
45 crystals, 2.4 images/sec.
^Cbasus@visa-vm062: /data/projects/open-
^C
basus@visa-vm062: /data/projects/open-da
basus@visa-vm062: /data/projects/open-da
basus@visa-vm062: /data/projects/open-da
basus@visa-vm062: /data/projects/open-da
basus@visa-vm062: /data/projects/open-da
basus@visa-vm062: /data/projects/open-da
basus@visa-vm062: /data/projects/open-da
```

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





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 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



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

Log in the catalogue to upload content

Catalogue ▾ E-learning Events About ▾

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...



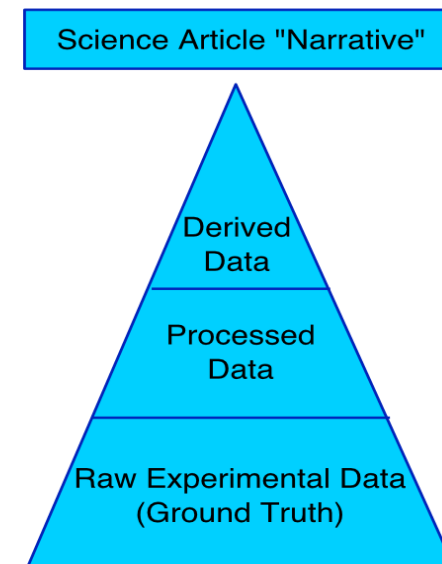
<https://pan-training.eu/>



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**

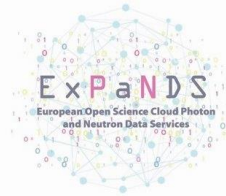
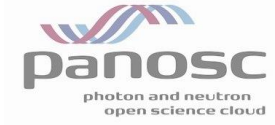


“The vital role of primary experimental data for ensuring trust in (Photon & Neutron) science”

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



What is a Data Commons?



Building a public data commons

The “data sharing for public good” narratives can be traced at least back to 2011, when the United Nations popularized the concept of “data commons”: using privately-owned big data for sustainable development and humanitarian action.^[16] The concept of the data commons is crucial, as it defines both values and institutional setups necessary for valuing access and freedom to operate, over the power to appropriate.^[17]

The overarching goal of the NIH Data Commons was to accelerate new biomedical discoveries by developing and testing a cloud-based platform where investigators could store, share, access, and interact with digital objects (data, software, etc.) generated from biomedical and behavioral research.

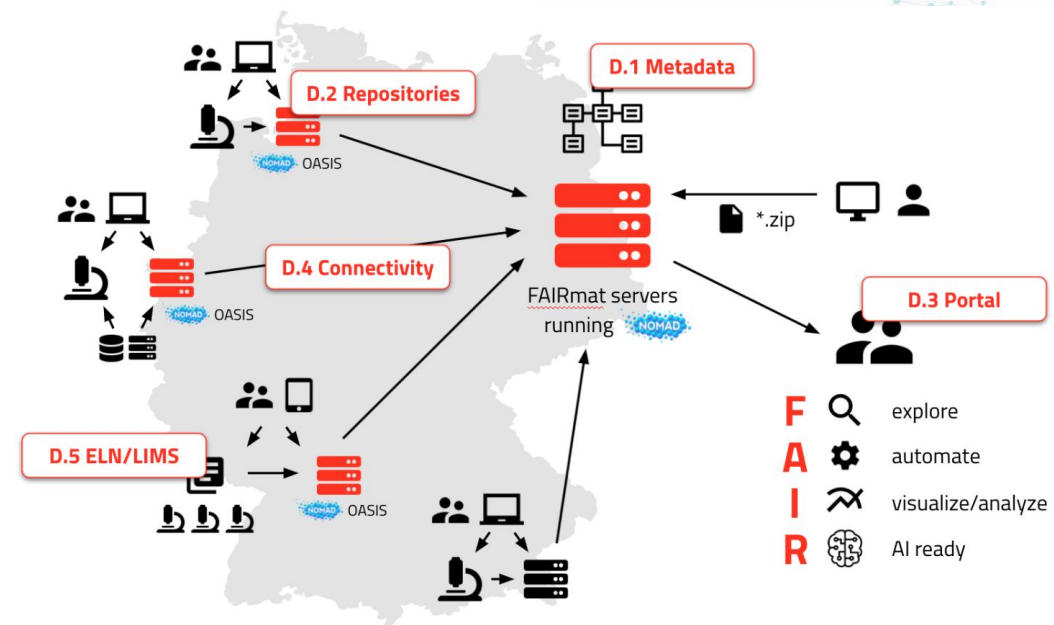
<https://openfuture.eu/publication/public-data-commons/>

<https://commonfund.nih.gov/commons>

Data Commons aggregates data from a **wide range of sources** into a unified database to make it more accessible and useful. More on **why we are building Data Commons**.

<https://datacommons.org/>

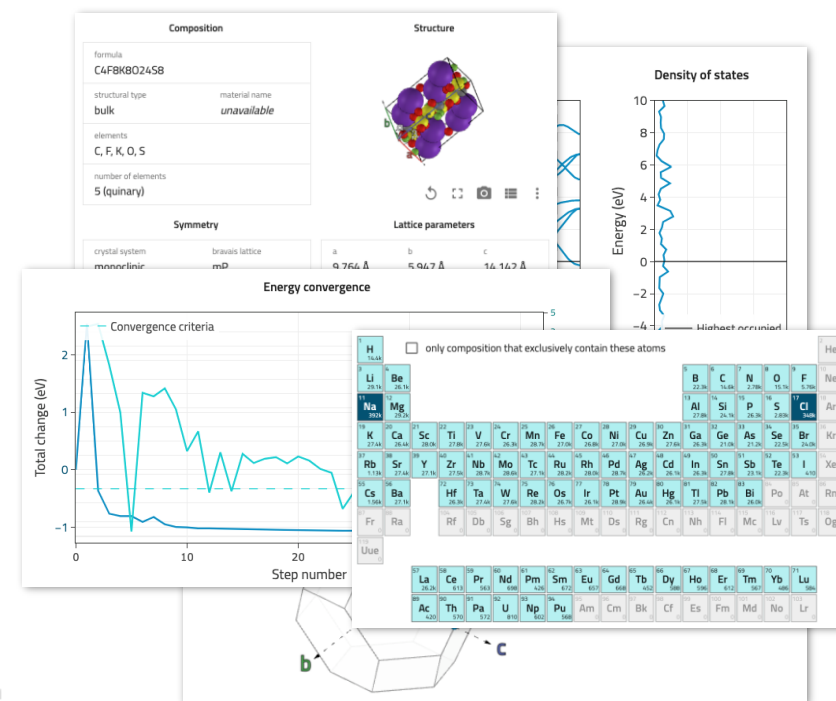
Example of a Data Commons



NOMAD: Publishing research data

More than 12 million of simulations (22 billion quantities) from over 500 authors world-wide

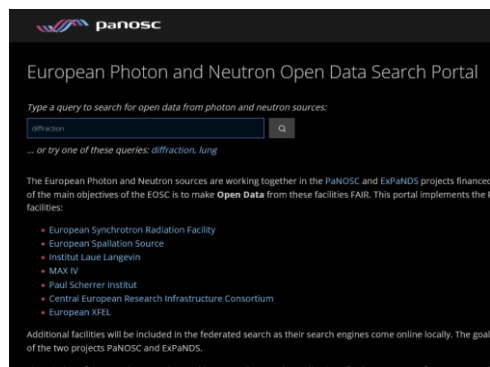
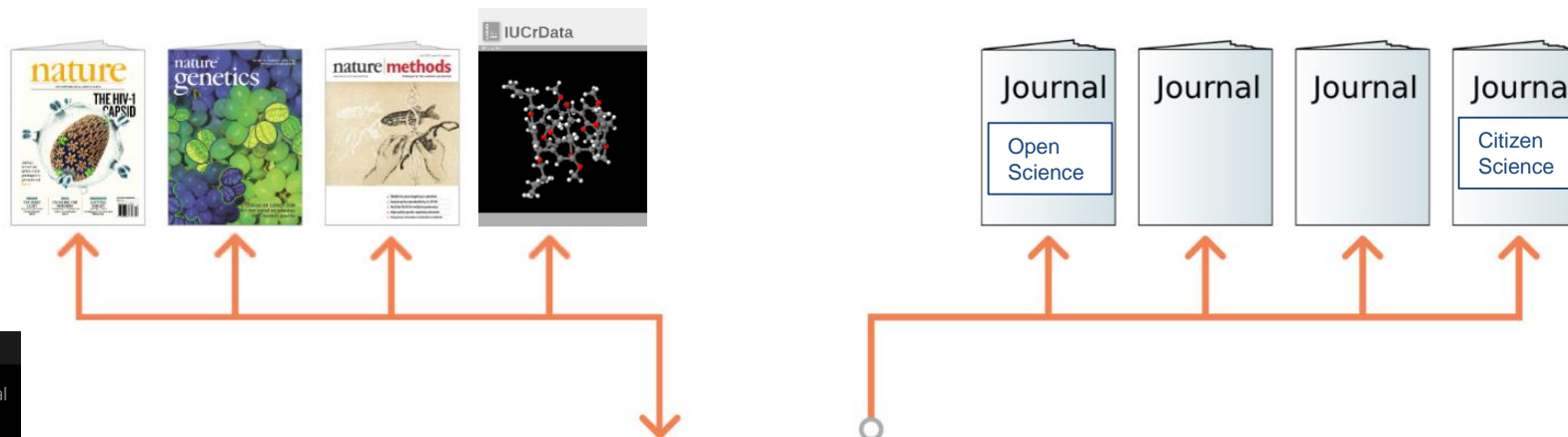
- Free publication and sharing data of data
- Extracts **rich metadata** for more than **50 codes**
- All data in a **raw** and a common **machine readable** form
- Use integrated tools to **explore, visualize, and analyze**



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.

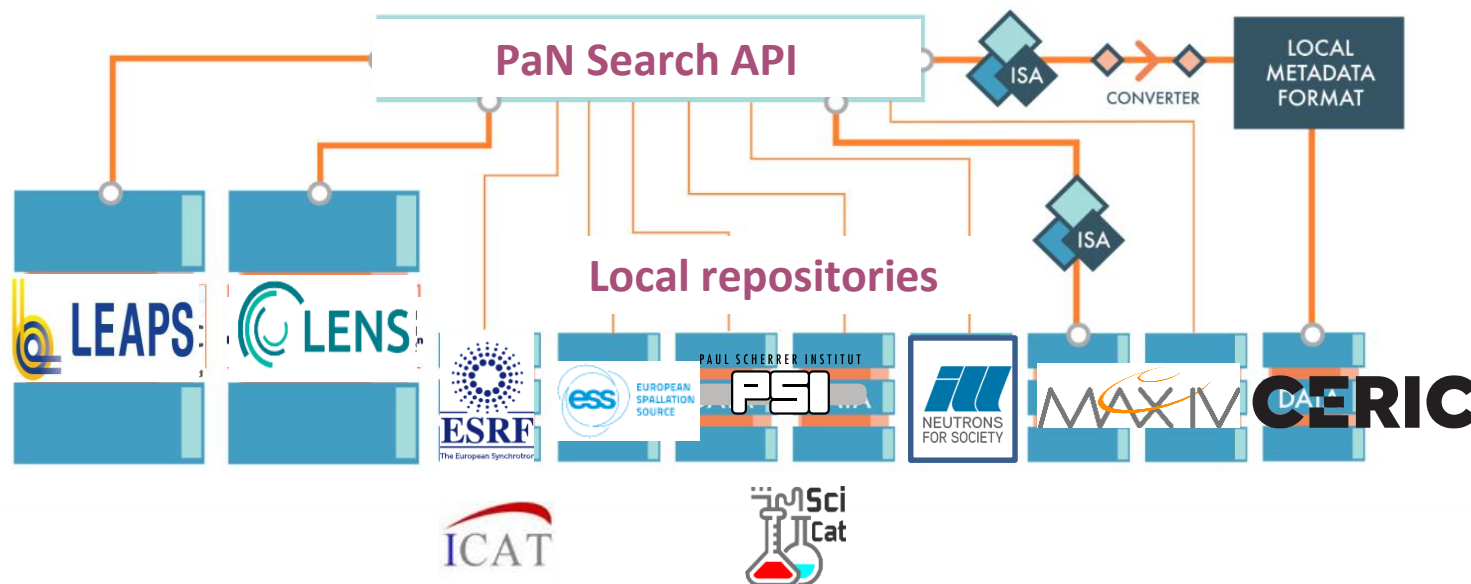
Slide courtesy of Markus Scheidgen

Open Data from federated PaN Repositories



PaN Open Data Portal

PaN Open Data Repository



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



panosc 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 0.900

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 0.900

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 0.900 {?}

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.



Human Organ Atlas - <https://human-organ-atlas.esrf.eu>

Human Organ Atlas

EXPLORE

SEARCH

3D RECONSTRUCTIONS

HELP

Human Organ Atlas

The Human Organ Atlas uses **Hierarchical Phase-Contrast Tomography** 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. To stay up to date, follow [@HiP-CT](https://twitter.com/HiP-CT)



HiP-CT imaging and 3D reconstruction of a [complete brain](#) from the body donor LADAF-2020-31. More videos can be viewed on the [HiP-CT YouTube channel](#).

Funding

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**
- [ESRE](#), 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**



Join us at this workshop on leveraging Open Data
<https://indico.synchrotron-soleil.fr/event/67/>



Leveraging open data from PaN facilities for machine learning

Oct 17 – 18, 2023
Europe/Paris timezone

During the last decade, most European Photon and Neutron (PaN) facilities have adopted **open data policies**, making data available for the benefit of the entire scientific community. At the same time, **machine learning** (ML) is seen as an essential tool to address the exponential growth of data volumes from PaN facilities.



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

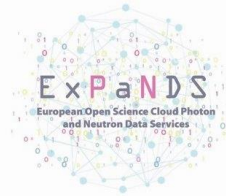
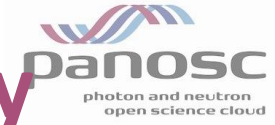


PaNOSC and ExPaNDS projects and innovation programme under the Horizon Europe funding

Not Planning to be adopted (N)
Under evaluation (U)
In progress of being adopted (WIP)



2023 – PaNOSC continues as a community activity



PaNOSC Partners are members of LEAPS + LENS



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.

Vision of Senior Level Engagement



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

To get optimum value out of having open data ... we need to be inclusive, we need to actually involve as many different facilities and research establishments as possible and that is a **really big coordination job**.

What the **ExPaNDS** and **PaNOSC** grants provided is an **excellent basis** for continuing this work on open data and being able to share data.



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

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



LEAPS Data Strategy



Home > The European Physical Journal Plus > Article

LEAPS data strategy

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

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Eur. Phys. J. Plus (2023) 138:617
<https://doi.org/10.1140/epjp/s13360-023-04189-6>

Regular Article

THE EUROPEAN
PHYSICAL JOURNAL PLUS



LEAPS data strategy

Andy Götz^{1,a}, Erwan le Gall^{2,b}, Uwe Konrad³, George Kourousias^{4,c}, Oliver Knodel^{3,d}, Salman Matalgah^{5,e}, Oscar Matilla⁶, Darren Spruce^{7,f}, Ana Valceril Orti⁸, Majid Ounsy⁹, Thomas H. Rod⁹, Frank Schluenzen¹⁰

¹ European Synchrotron Radiation Facility, Grenoble, France

² Institut Laue Langevin, Grenoble, France

³ Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

⁴ Elettra Sincrotrone Trieste, Basovizza, Italy

⁵ SESAME, Allan, Jordan

⁶ ALBA, Cerdanyola del Vallès, Spain

⁷ MAXIV Laboratory, Lund University, Lund, Sweden

⁸ SOLEIL, Saint-Aubin, France

⁹ European Spallation Source ERIC, Copenhagen, Denmark

¹⁰ DESY, Hamburg, Germany

Received: 17 December 2022 / Accepted: 14 June 2023
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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 papers 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.

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



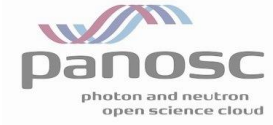
PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

PUMA – Publication and User experiment Metadata Analyser

- The data that **PUMA** can access at ESRF includes information about the instruments and beamlines, techniques, scientific areas, authors, member countries, publications (>40,000), public proposals submitted (>46,000) and accepted (>20,000), and industrial proposals (>1,300).
-
- Additional publication metadata is loaded into PUMA using open data web services (citations, keywords, abstract, authors...)
- PUMA provides a quantifiable view of the data, not only enabling conclusions about the science currently being carried out at the ESRF, but also helping to identify trends.
- It facilitates reporting for the ESRF management and supports strategic planning for the facility.



PUMA – explore corpus



Document Search Institution Search Collections

"van gogh" painting*

From any year to any year

Select year in dropdown lists. For single year selection, you can also click year in below (side column).

Fill expression and press [ENTER] to launch search. Use + for mandatory expressions, - to exclude, | for OR operator, "" for full phrase, * for wildcard and () to group operations. read more

Publications

- Publications filter means JOURNAL_ARTICLE, PROCEEDINGS_ARTICLE, BOOK, E-THESIS
- Proposals available content : ESRF user portal (sms) (1992-2020)
- Publications available content : ESRF library (flora) (2010-2020)
read more

Uncheck search in: title, abstract, keywords, journal title. Check search in: title, abstract, keywords, journal title, fulltext read more

Expand advanced search filters

Active filters - Type: publication Expression: "van gogh" painting*

Search result : 17 documents (0.70s). Showing results 1 to 5

Search result : 17 documents found (with active search filters).

FIRST PREVIOUS 1 2 3 4 NEXT LAST

Export: XLS DOI DOI (WOS)

ADD 17 DOCS to

puma record : 221459 detail , ES record (direct), ES record (proxy)

JOURNAL_ARTICLE : Degradation Process of Lead Chromate in Paintings by Vincent van Gogh Studied by Means of Spectromicroscopic Methods. 3. Synthesis, Characterization, and Detection of Different Crystal Forms of the Chrome Yellow Pigment

doi:10.1021/ac302158b January 2013 (Publication Year : 2013), analytical chemistry (american chemical society (acs))

Authors : monico letizia; janssens koen; miliani costanza; brunetti brunetto giovanni; vagnini manuela; vanmeert frederik; falckenberg gerald; abakumov artem m.; lu yinggang; tian he; verbeeck j.; radepont marie; cotte marine; hendriks ella; geldof muriel; van der loeff luuk; salvant johanna; menu michel

Keywords : CORPUS_INFO : flora_esrf_pub_with_esrf_instrument flora_esrf_pub_with_esrf_staff flora_esrf_pub

PUMA : new PUMA keyword

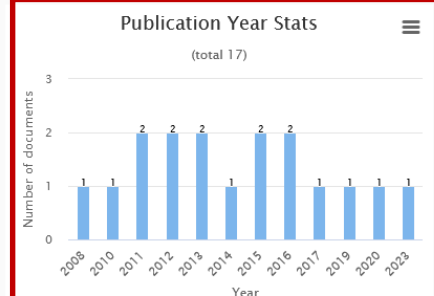
Abstract : the painter, vincent van gogh, and some of his contemporaries frequently made use of the pigment chrome yellow that is known to show a tendency toward darkening. this pigment may correspond to various chemical compounds such as pbcro4 and pbcr1-xso4, that may each be present in various crystallographic forms with different tendencies toward degradation. investigations by x-ray diffraction (xrd), mid-fourier transform infrared (ftir), and raman instruments

Institutions : (show affiliations)

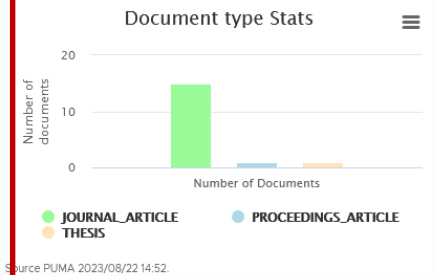
University of Perugia, Perugia, IT	University of Antwerp, Antwerpen, BE	National Research Council, Rome, IT	Institute of Molecular Science and Technologies, Milano, IT	Perugia, IT	Deutsches Elektronen-Synchrotron DESY, Hamburg, DE
French National Centre for Scientific Research, Paris, FR	Laboratoire d'Archéologie Moléculaire et Structurale, UMR5175, Paris, FR	European Synchrotron Radiation Facility, Grenoble, FR	Van Gogh Museum, Amsterdam, NL	Cultural Heritage Agency of Netherlands, Amersfoort, NL	Kroeller-Müller Museum, Ede, NL
Center for Research and Restoration of Museums of France, (UMR171)					

abstract text
- "orange/pale yellow areas of 12 van gogh paintings" by Vincent van gogh Studied by Means of "the painter, vincent van gogh, and some of his "Degradation Process of Lead Chromate in Paintings" - demonstrating that van gogh effectively made use of "on van gogh's portrait of gauguin (van gogh)

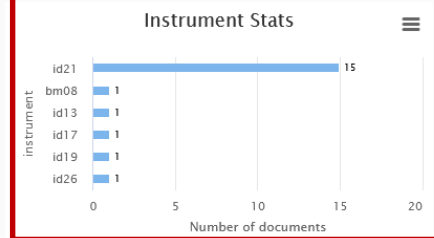
Instruments : id21 (ESRF) Unspecified (PETRA III)



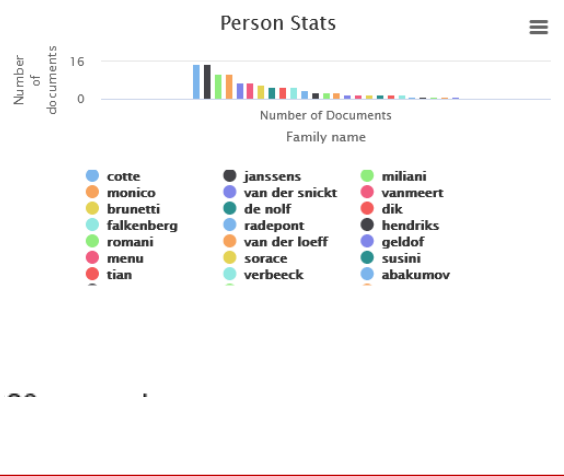
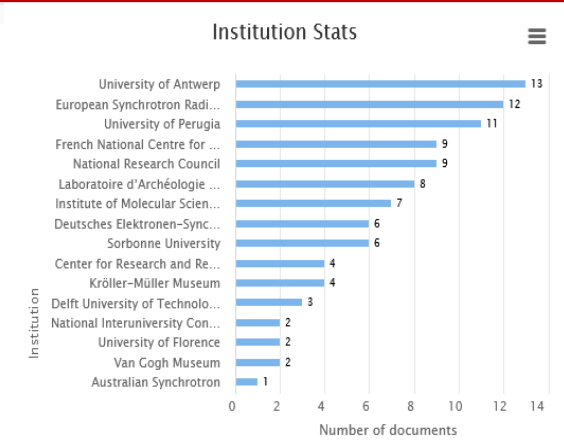
Click year column to filter by year Source PUMA 2023/08/22 14:52.



Source PUMA 2023/08/22 14:52.



- Explore corpus using advanced search
- Proposal & publications
- Full text search (title/abstract/pdf text)
- Instruments, institutions, authors, journals.



PUMA – custom searches

- Topic collections (proposal/publications) can be created within PUMA for custom reporting.
- **Example : “sustainable energy research”, “neurodegenerative diseases research” “human organ atlas”**
- Dashboard based on your custom collection is then available to report on various metrics (Country, institutions, instrument used, open access, journals, citations...)
- In production at **ESRF** + **ILL**, soon at **SOLEIL** (as part of an EU project)
- Contact Renaud Duyme @ ESRF if you are interested

Clarivates : Web Of Science & Incites.

Positive

- Extended publication corpus (contains all scientific publications)
- Advanced publication categorisation (“citation topics”)
- Advanced KPI indicators (Incites)

Negative

- Generic tool not built for Instrument Facilities
- No direct integration with Facility publication corpus
- No Proposal/Experiment/Instruments stats
- Searches only on title/abstract (full publication content not available)
- No Open Data stats



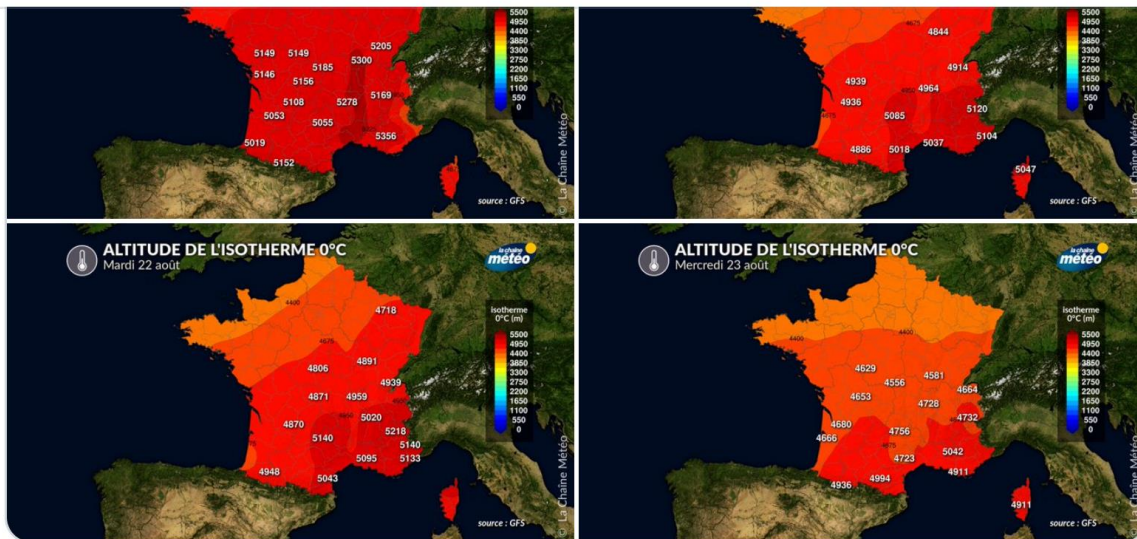
La Chaîne Météo

@lachainemeteo · Suivre



Jusqu'à mercredi, l'isotherme 0°C se situera aux alentours de 5000 mètres d'altitude dans le sud de la France (il dégèlera au #Mont_Blanc !). Prudence si vous avez prévu de randonner en haute montagne près des glaciers alpins qui seront fragilisés par ces températures... Voir plus

Le Parisien



11:50 PM · 20 août 2023



74 Répondre Copier le lien

Lire 4 réponses



Horizon 2020 research y.

ESRF IT devices electrical consumption

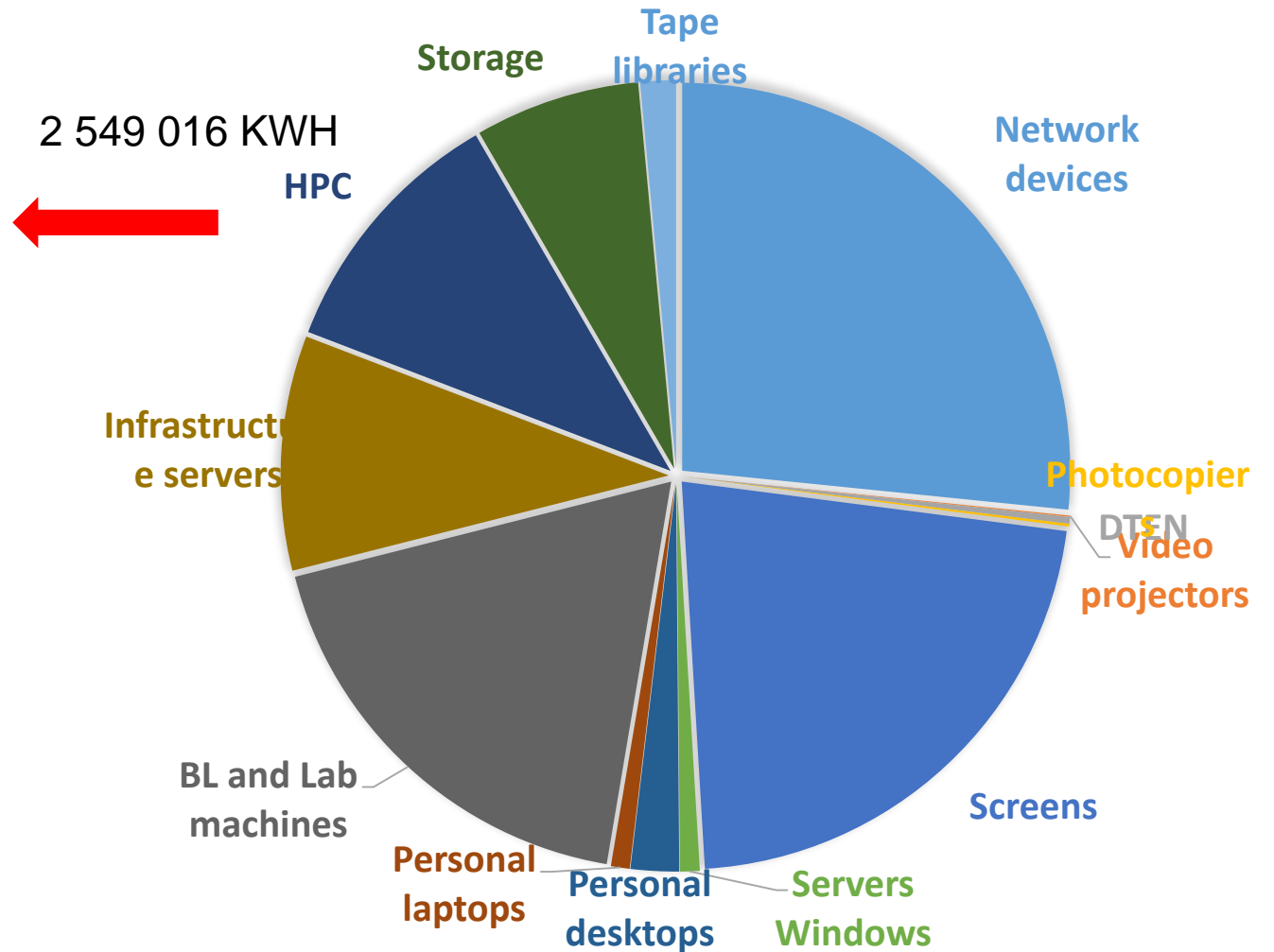
ESRF Electrical consumption e.g. 2018

Poste	Consommation
MACHINE	35 200 000 kWh
HQPS	3 056 000 kWh
CTA (hors central et common)	4 610 000 kWh*
SRE	3 745 000 kWh
Lignes et Laboratoires	3 439 500 kWh
Eclairage	2 080 000 kWh*
Eclairage lignes labos	1 529 000 kWh*
SEG	2 675 000 kWh
Data center central	1 146 500 kWh*
Common building	953 000 kWh
Pertes transformateurs	814 000 kWh*
Extracteurs (hors central, common et GH)	836 500 kWh*
SEB	854 500 kWh
Data center CTRM	600 200 kWh*
Central building	239 500 kWh
SEC	322 000 kWh
SEI	437 000 kWh
SAP	405 000 kWh
SRX	322 000 kWh
Guest houses	284 000 kWh
LOB	221 500 kWh
Station pompage	39 000 kWh
Autres	1 575 000 kWh*
Total	65 385 MWh

* Estimations d'après puissances installées et profils de fonctionnement

Source TID BIG 2018

ESRF Electrical consumption – IT Only



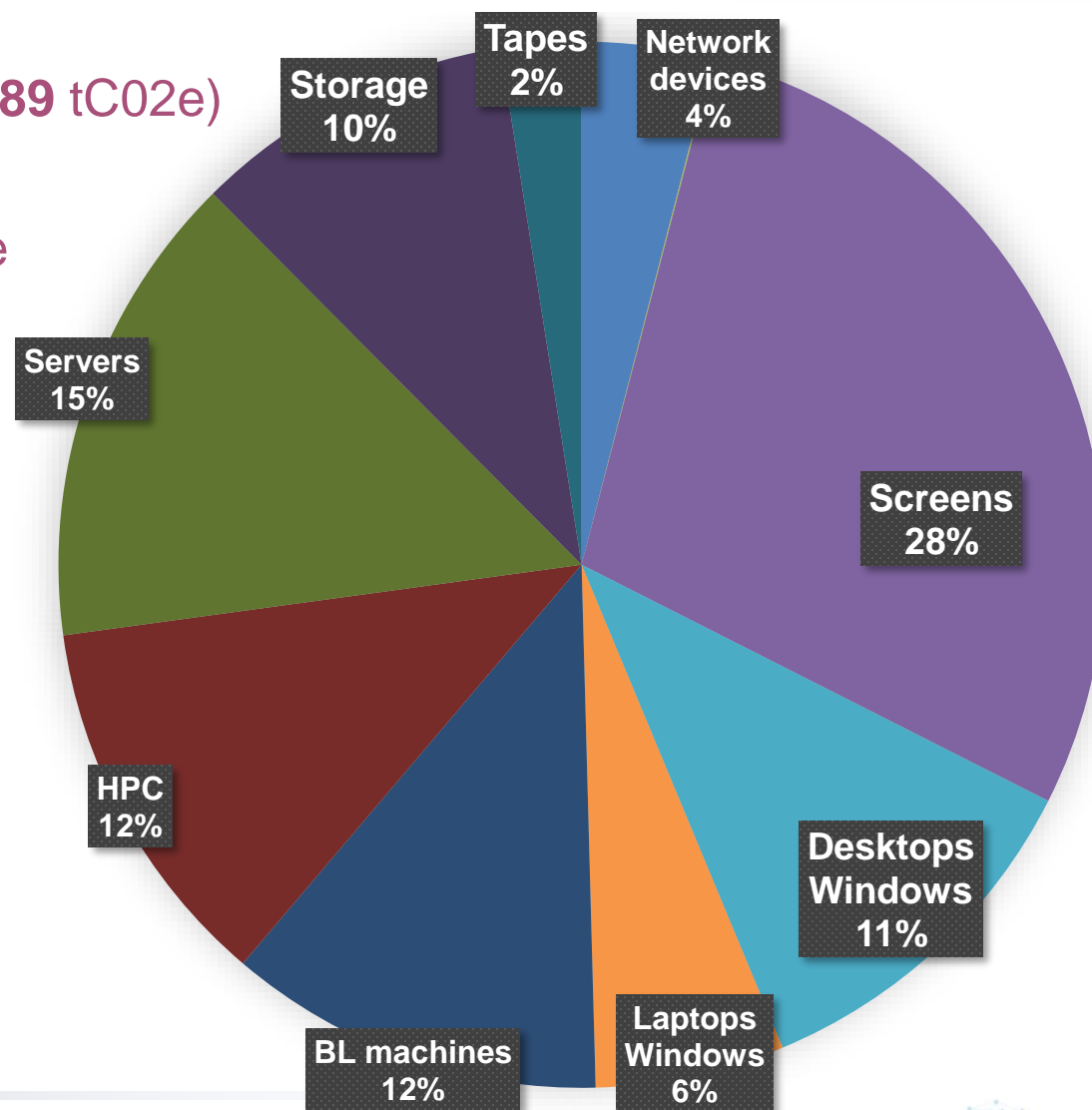
IT – impact on climate in 2021

Elec consumption 2021 (2 549 016 kWh x 35 gC02 = 89 tC02e)

+
(Manufacturing + Transport) / Equipment life time

=

**3.08 kt
C02equ**



Source

- IT Elec. consumption 2021 : TID ITS.
- Manufacturing & transport : Suppliers (Dell, Lenovo...)

Equivalent – CO₂e

Entrez une quantité de CO₂e ci-dessous

3 000 000

kg CO₂e

3kt CO₂e IT carbon footprint at ESRF for 1 year

c'est autant d'émissions que pour fabriquer, consommer ou parcourir :

13 045 180
km en avion

↑ Comparer

1 271 186 441
km en tgv

↑ Comparer

13 786 765
km en voiture

↑ Comparer

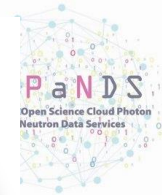


**395 return flights
Geneva/Melbourne
(16512 km)**

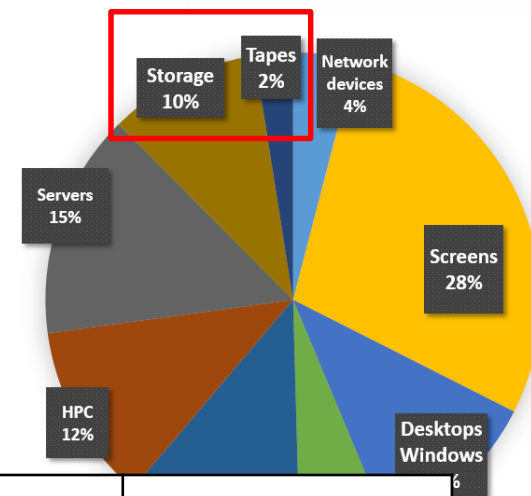
ADEME Tool to calculate CO₂e equivalent for different objects :
<https://impactco2.fr/convertisseur>

ADEME : In France average emission is 10t CO₂ per year per person, should be reduced to 2t.

Disk vs Tape storage for a year



Disk storage vs Tape over a year (source IBM, FUJI, LENOVO)



Tape library with 1000PB (LTO8)

	KgC02	#	time life (years)	Total KgCO2 (manufacturing + transport)	Electrical consumption	Total KgCO2	Volume PB
Elements		8000	10	15	5333.333333		
Robots		836	2	15	111.4666667		
drives		45	33	6	247.5		
tapes		7	51200	6	59731.78		9
Total					65424	1123	66 KgCO2/PB

Tape library with 220 PB (LTO8)

	KgC02	#	time life (years)	Total manufacturing KgCO2	Electrical consumption	Total KgCO2	Volume PB
Elements		8000	10	15	5333.333333		
Robots		836	2	15	111.4666667		
drives		45	33	6	247.5		
tapes		7	11000	6	12833.33333		220
Total					18526	1123	89 KgCO2/PB

Disk storage (Spinning disks – GSS Lenovo)

	KgC02	#	time life (years)	Total manufacturing KgCO2	Electrical consumption	Total KgCO2	Volume PB
Storage Servers (GSS Lenovo)		54000	4	5	43200	10 443	53 643
							20
Total					43200	10443	2682 KgCO2/PB

and innovation programme under grant agreements 823852 and 857641, respectively.



Estimated carbon footprint of experiment



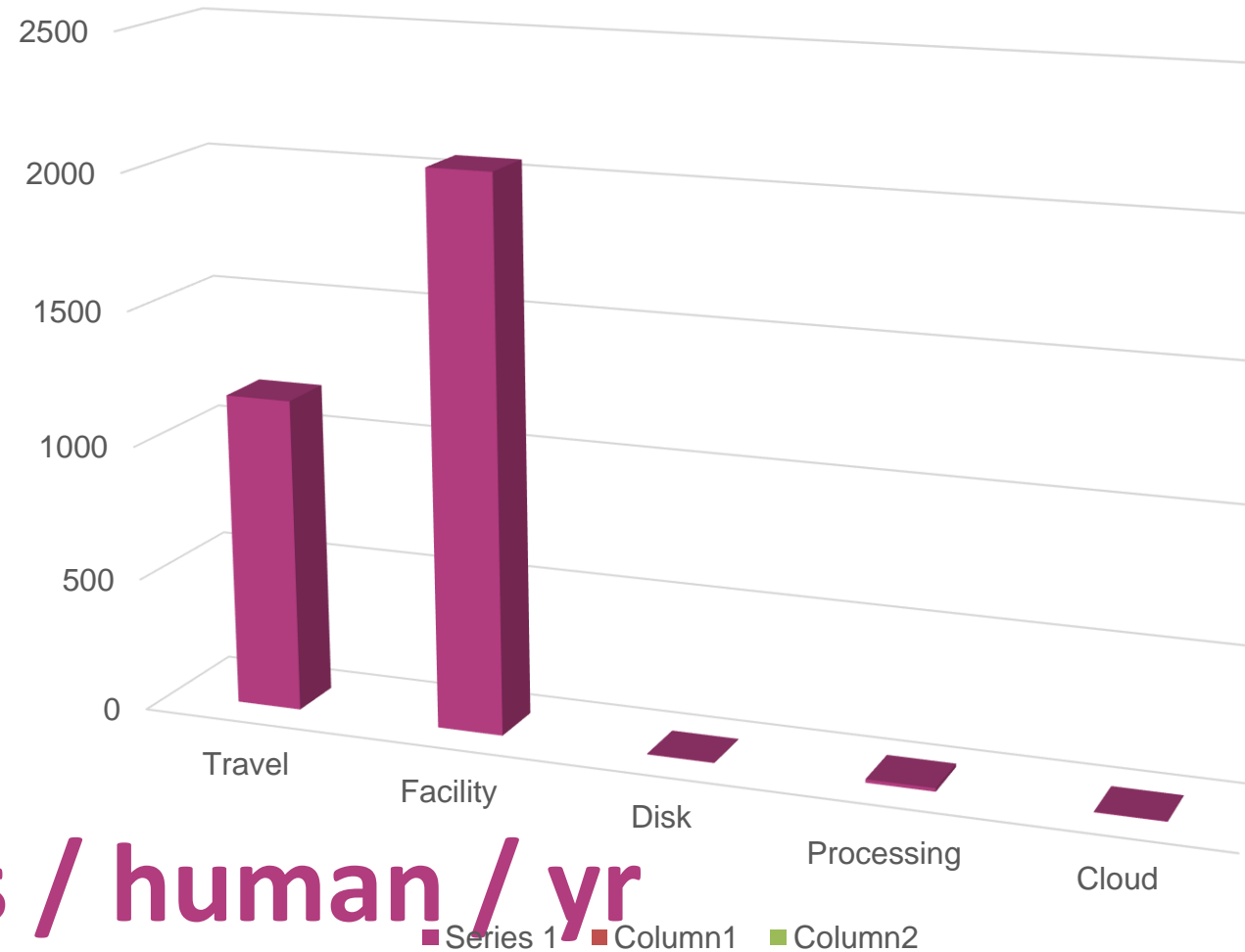
- User Travel = **1170 kg**
- Beamtime energy consumption = **2056 kg**
- Data stored on disk = **1.8 kg**
- Data processing on site = **12.6 kg**
- Cloud transfer = **2.3 kg**

CO₂e per kWh in France = **75 g/kWh**

TOTAL = 3.253 tons !

Sustainable Goal = 5 tons / human / yr

Carbon footprint for 1 week experiment @ ESRF



Carbon footprint of archiving data

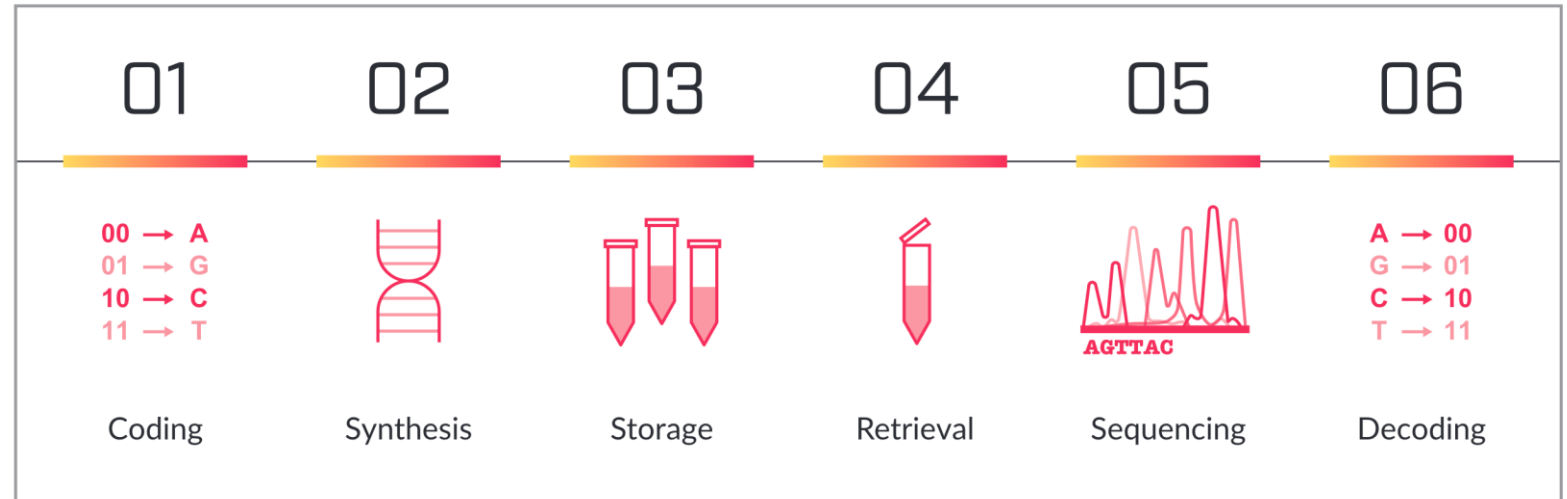
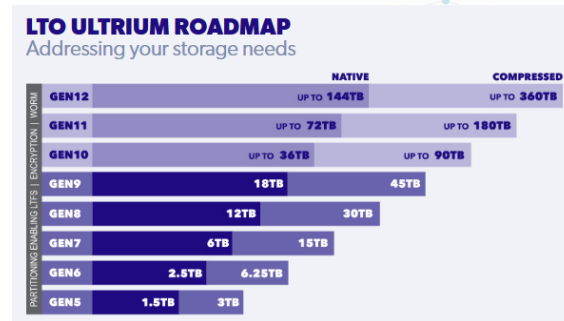
- 200 GB Data archived on tape for 10 years (full tape library)
~ 13 g * 10 yrs = 130 grams

- ARCHIVING raw data for 10 years
4e-6 % of CO₂eq of beam time
to acquire the raw data!



DNA – the ultimate storage medium for raw data?

“Experiments have confirmed the high theoretical information density of nearly **455 billion GB** of data per gram i.e. **455 petabytes / gram**, ~6 orders of magnitude greater than even the most advanced magnetic tape storage systems”



How DNA storage works



Matange, K., Tuck, J.M. & Keung, A.J. DNA stability: a central design consideration for DNA data storage systems. *Nat Commun* **12**, 1358 (2021). <https://doi.org/10.1038/s41467-021-21587-5>



IUCr Journals has launched IUCrData's Raw Data Letters

Scientists are encouraged to publish raw data!

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 x 0.075
No. of pixels	4148 x 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

[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: PASS

Testing: All archives are accessible: PASS

Running checks with downloaded images

Testing image 4: Image type and dimensions: PASS



ISSN 2414-3146

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

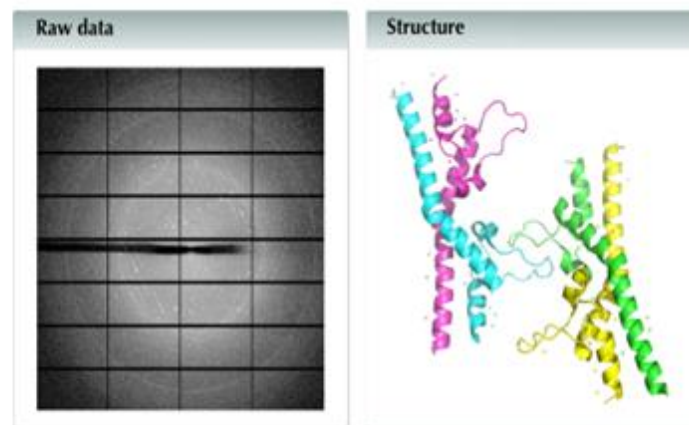
Viviana Neviani, Martin Lutz, Wout Oosterheert, Piet Gros and Loes Kroon-Batenburg*

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

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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 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>

Uni
espe





PaNOSC
@Panosc_eu

*“If you don't
want to share
data why
become a
scientist?”*

← **Thread** Interview w @Claire_L_Walsh, Senior
Research Fellow at @uci & @esrfsyncrotron, and part
of the team who developed (w PaNOSC contribution)
the #HumanOrganAtlas, an online data portal of
human organs scanned w @hip_ct technology at 20µm
per voxel

 bit.ly/3Mk3yc5



Interview with
Claire Walsh (UCL - ESRF)
on the Human Organ Atlas



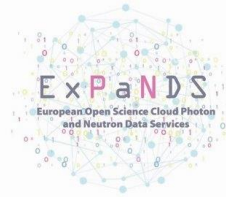
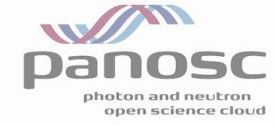
Conclusion



- 1. The Photon and Neutron Open Science Cloud is implementing a Data Commons of FAIR data and will provide data to the scientific community**
- 2. Facilities have the role of managing data for Users**
- 3. Users role is to enrich metadata, publish and cite data**
- 4. IUCr CommDat must continue its good work!**



Thank you



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

