NOBUGS 2022

Building a PaN Data Commons on the PaNOSC and ExPaNDS outcomes

Andy Götz (ESRF + PaNOSC coordinator) + **Patrick Fuhrman** (DESY + ExPaNDS coordinator)

on behalf of and with contributions by

PaNOSC + ExPaNDS WP2, WP3 + WP4, LEAPS WG3

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. What are PaNOSC + ExPaNDS?
2. What are their outcomes?
3. What is a Data Commons?
4. Why build a Data Commons?
5. How to build the Data Commons?
6. Sustaining the Data Commons?
7. What is your role in the Data Commons?
8. Conclusion

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.

The PaNOSC and ExPaNDS H2020 EOSC projects in numbers

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

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

ExPaNDS and PaNOSC in the PaN EU project landscape

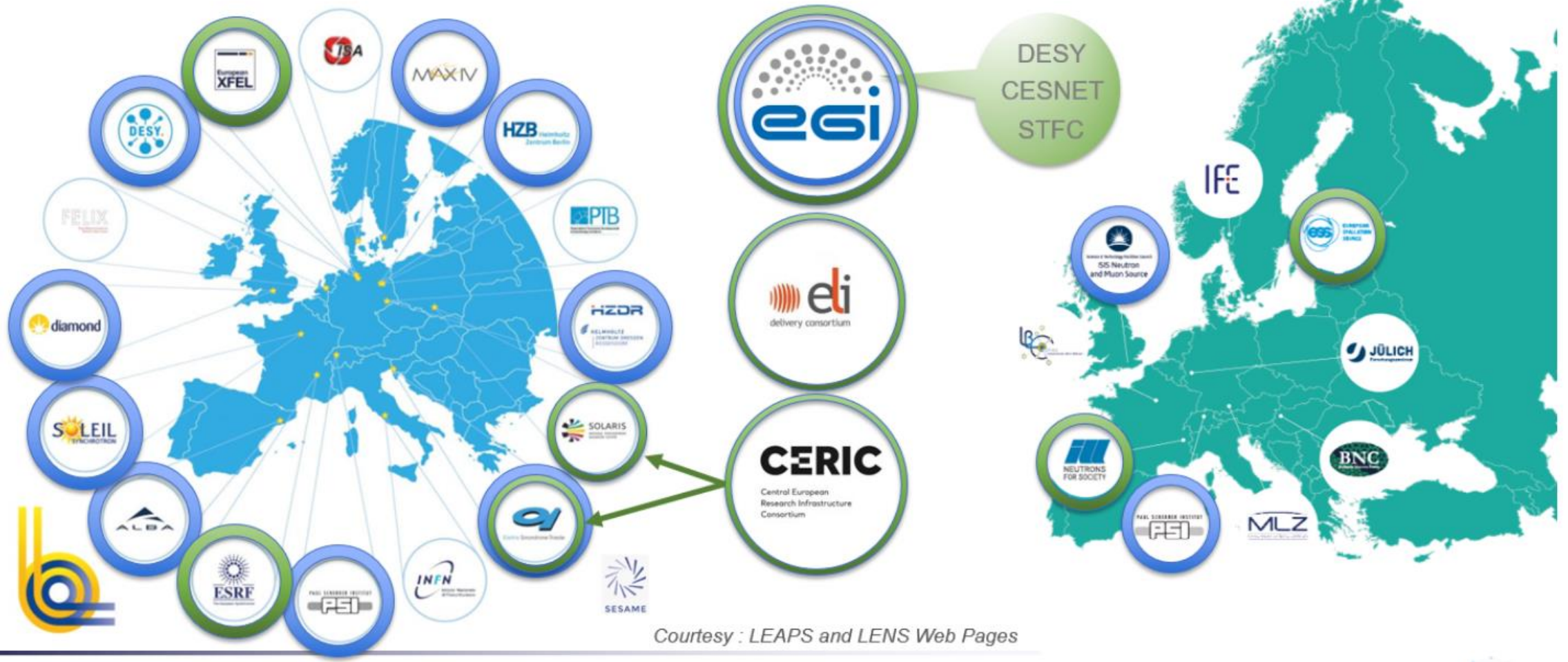
EUROPEAN OPEN SCIENCE CLOUD

PaNOSC

ExPaNDS

Photon (LEAPS)

Neutron (LENS)



Courtesy : LEAPS and LENS Web Pages

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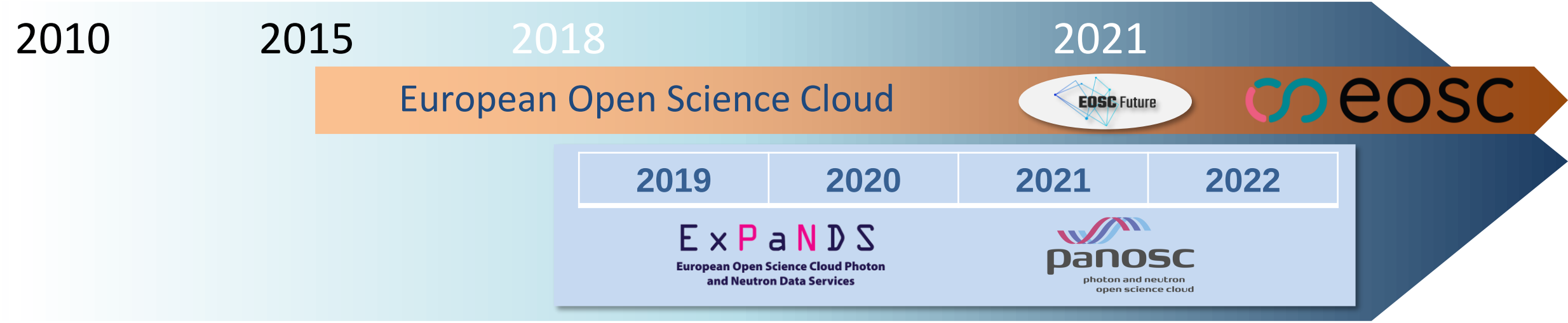
panosc photon and neutron open science cloud

European Open Science Cloud Photon and Neutron Data Services

ExPaNDS and PaNOSC in the PaN EU project landscape



Policies Common data policy **FAIR** data policy Data Management Plans

Analysis Software Catalogue Remote analysis Jupyter

AAI UmbrellaID AARC Blueprint eduTeams

Training e-neutron Training platform

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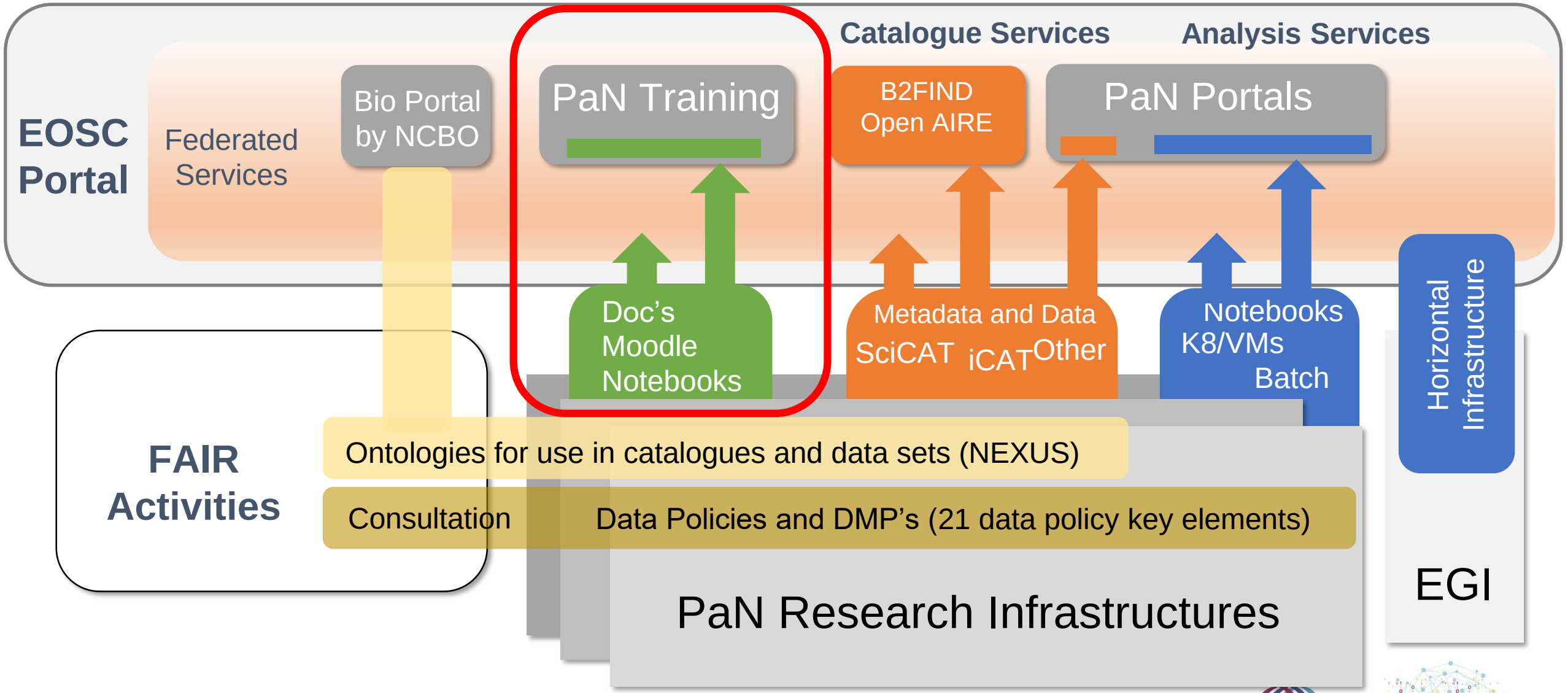
panosc photon and neutron open science cloud

ExPaNDS European Open Science Cloud Photon and Neutron Data Services

The Big Picture of EOSC in PaNOSC and ExPaNDS in EOSC



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10 Primary Outcomes of PaNOSC and ExPaNDS

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

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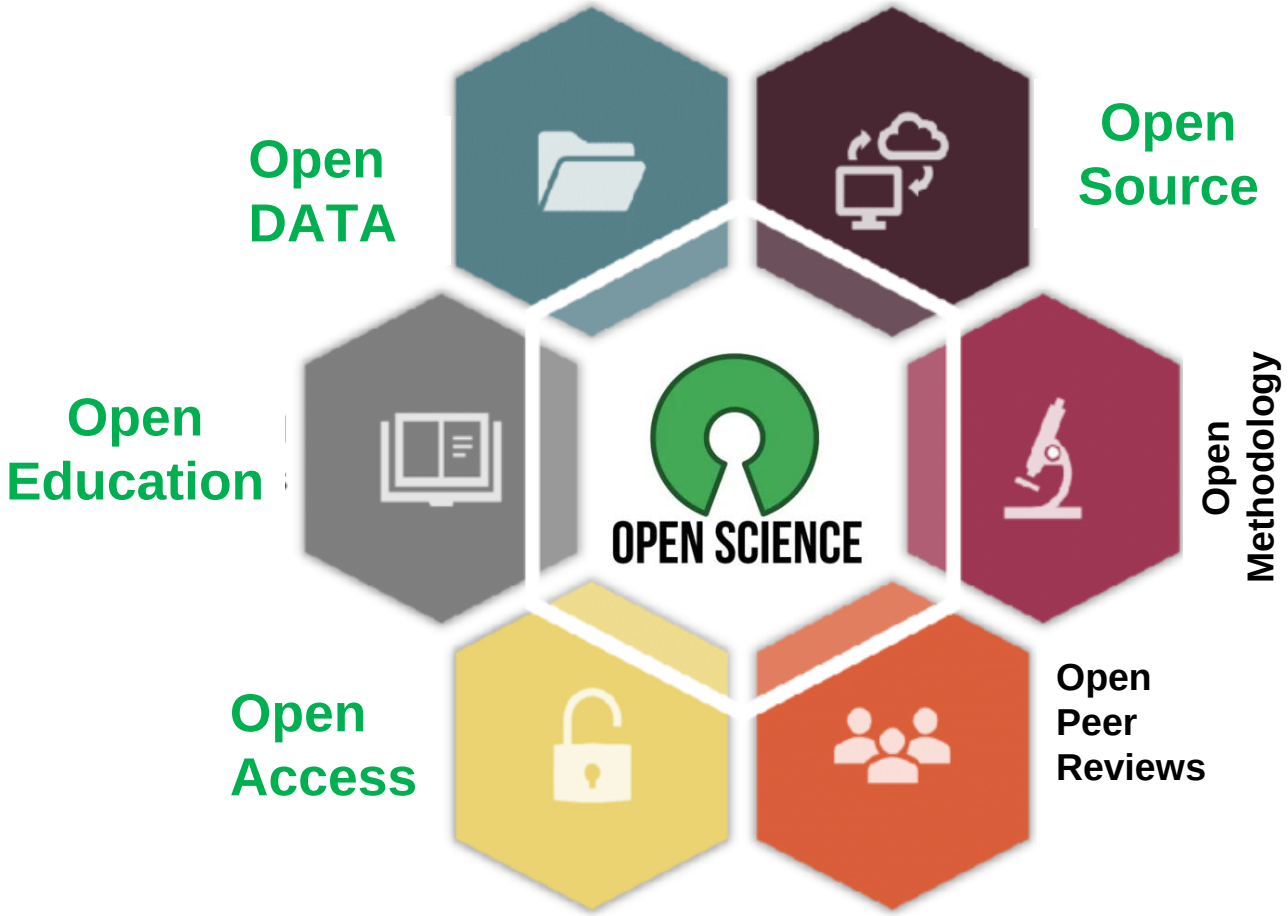
PaNOSC and ExPaNDS and EOSC are contributing to:

OPEN SCIENCE



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We had One Common GOAL

panosc
photon and neutron
open science cloud

ExPaNDS
European Open Science Cloud Photon
and Neutron Data Services

We now have one new Common GOAL

What is a Data Commons

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]

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

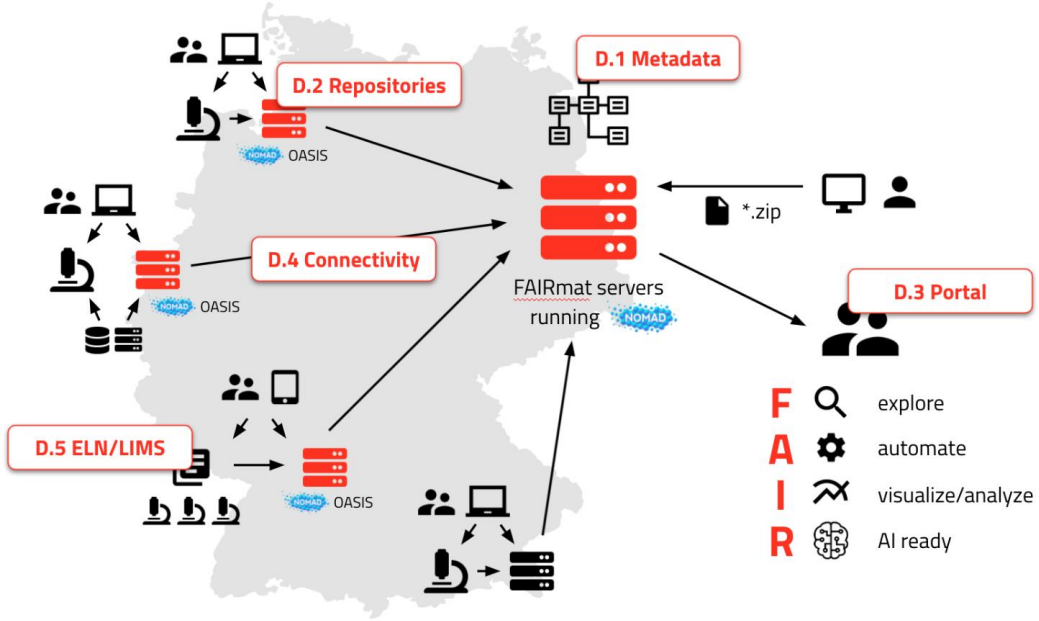
The overarching goal of the NIH Data Commons was to accelerate new biomedical discoveries by developing and testing a cloud-based platform where investigators could store, share, access, and interact with digital objects (data, software, etc.) generated from biomedical and behavioral research.

https://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/

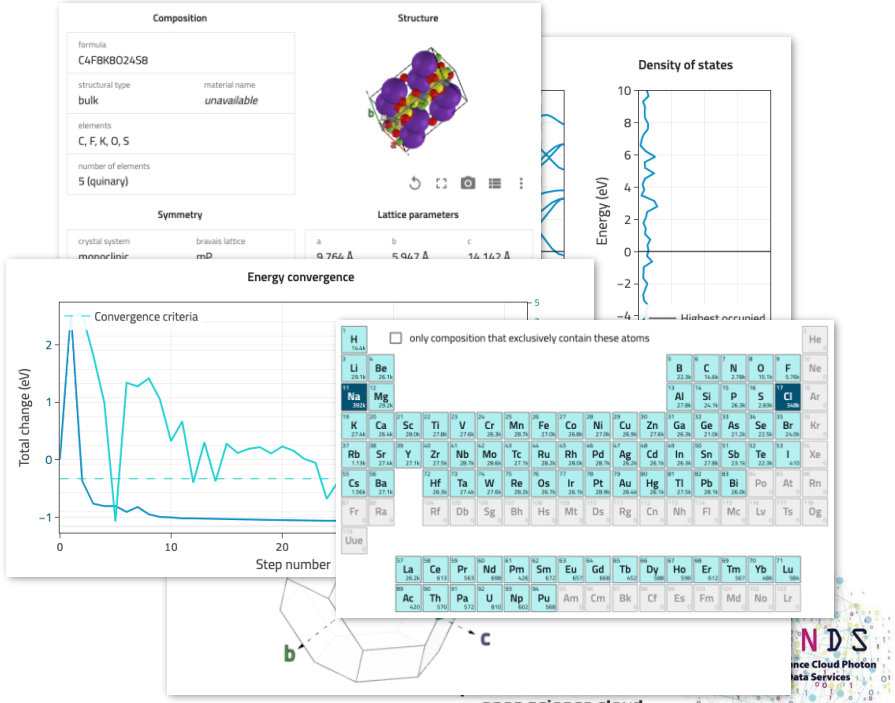
Example of a Data Commons



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** from
- ➔ Use integrated tools to **explore**, **visualize**, and **analyze**



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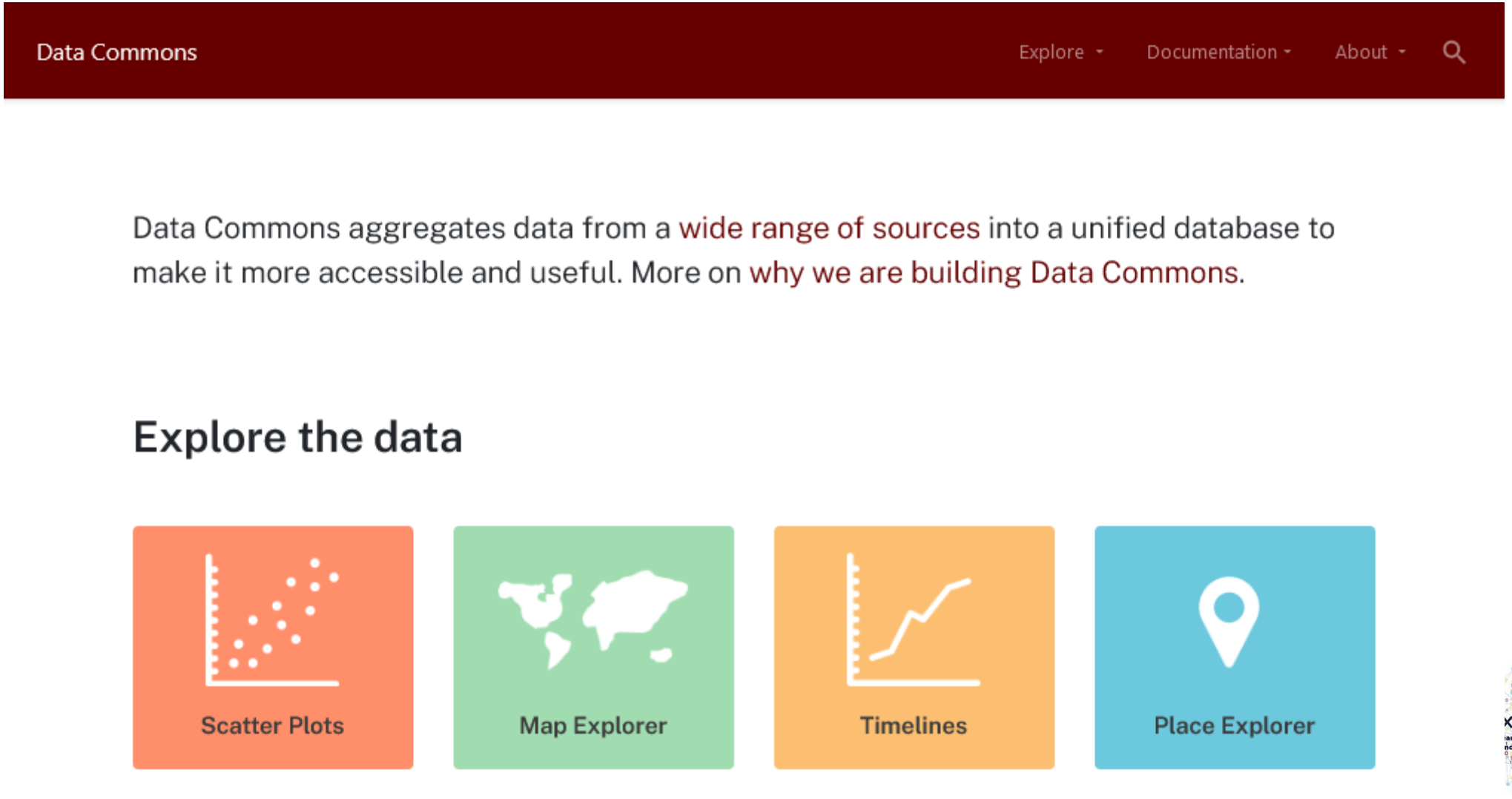
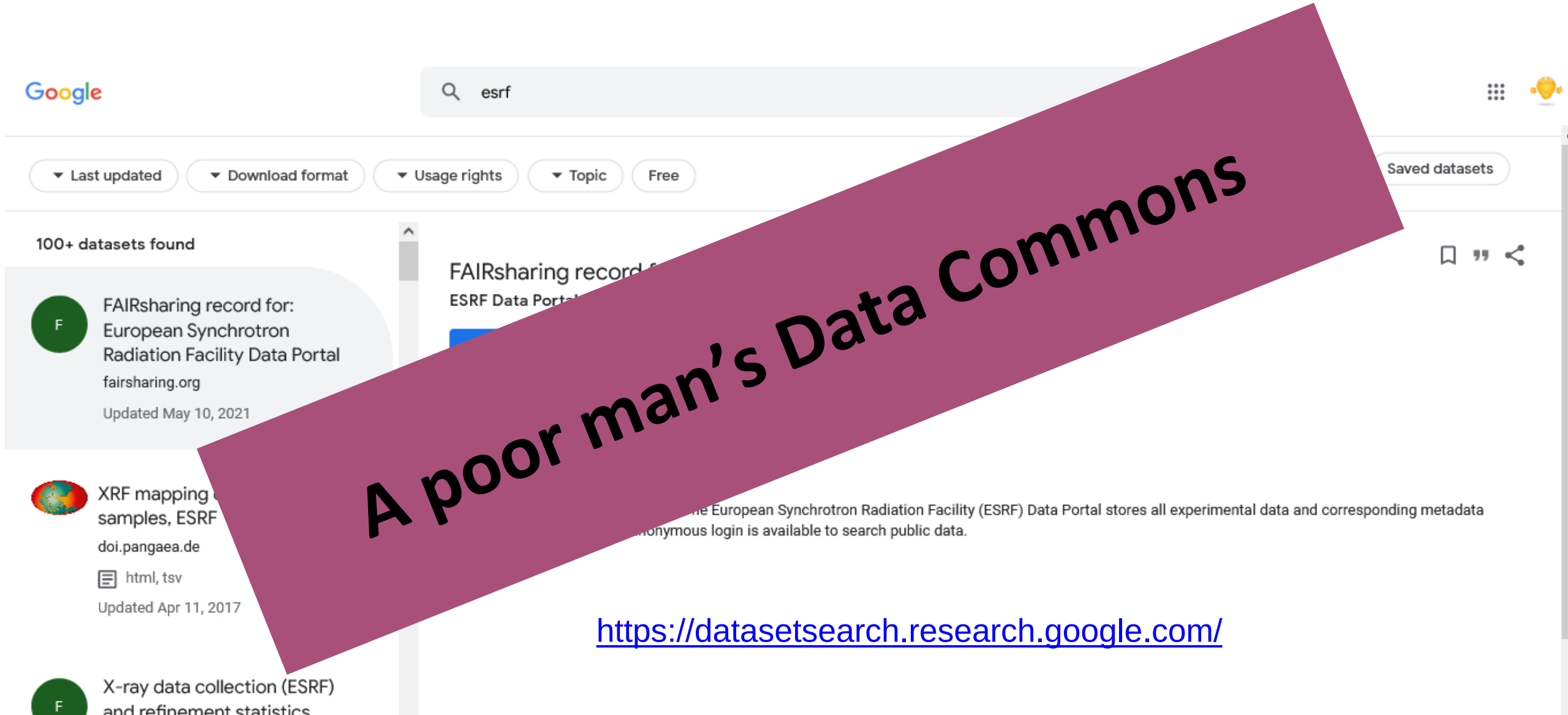
Slide courtesy of Markus Scheidgen

Google Data Commons

https://datacommons.org



Google Dataset Search:



A poor man's Data Commons

https://datasetsearch.research.google.com/

Genomics Data Commons - https://portal.gdc.cancer.gov/

Harmonized Cancer Datasets

Genomic Data Commons Data Portal

Get Started by Exploring:

Projects | Exploration | Analysis | Repository

e.g. BRAF, Breast, TCGA-BLCA, TCGA-A5-A0G2

Data Portal Summary

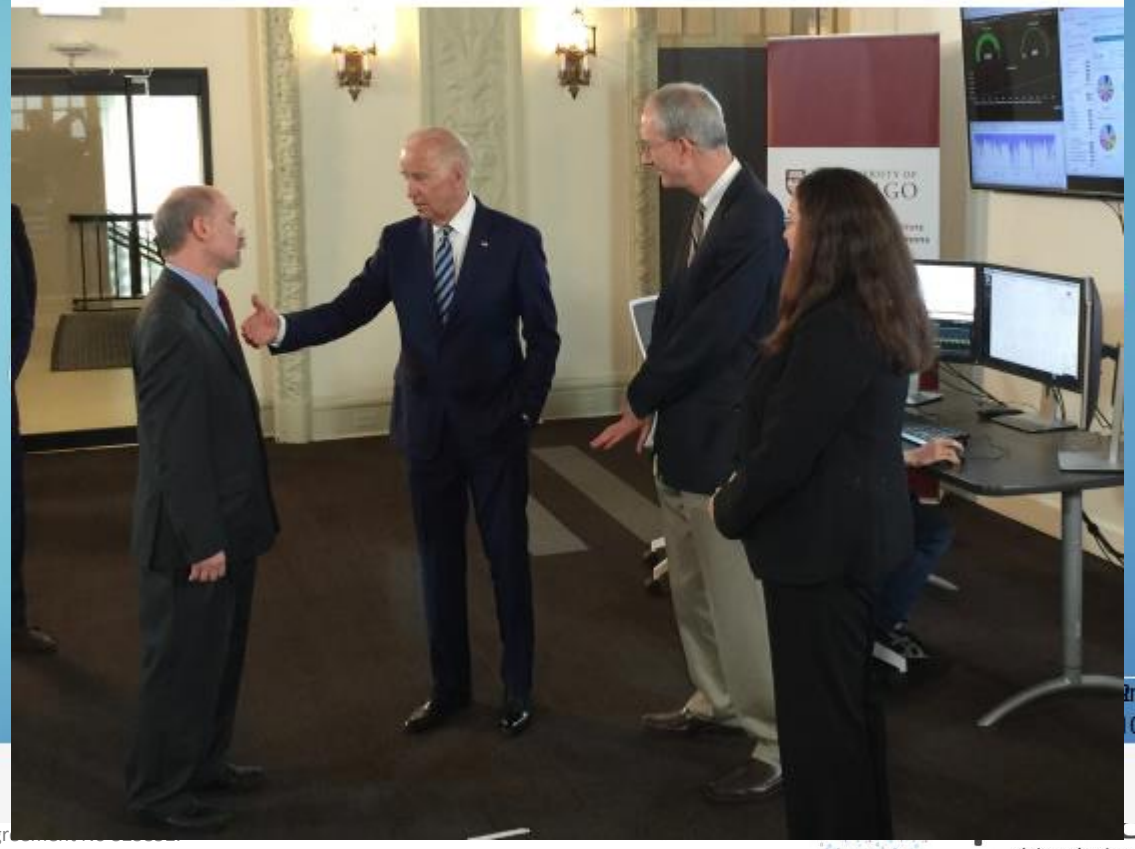
Data Release 34.0 - July 27, 2022

PROJECTS	PRIMARY SITES	CASES
72	67	86,046

FILES	GENES	MUTATIONS
863,977	21,773	2,730,388

I can't tell you how excited I am about this

— Current President of the United States, Joseph R. Biden



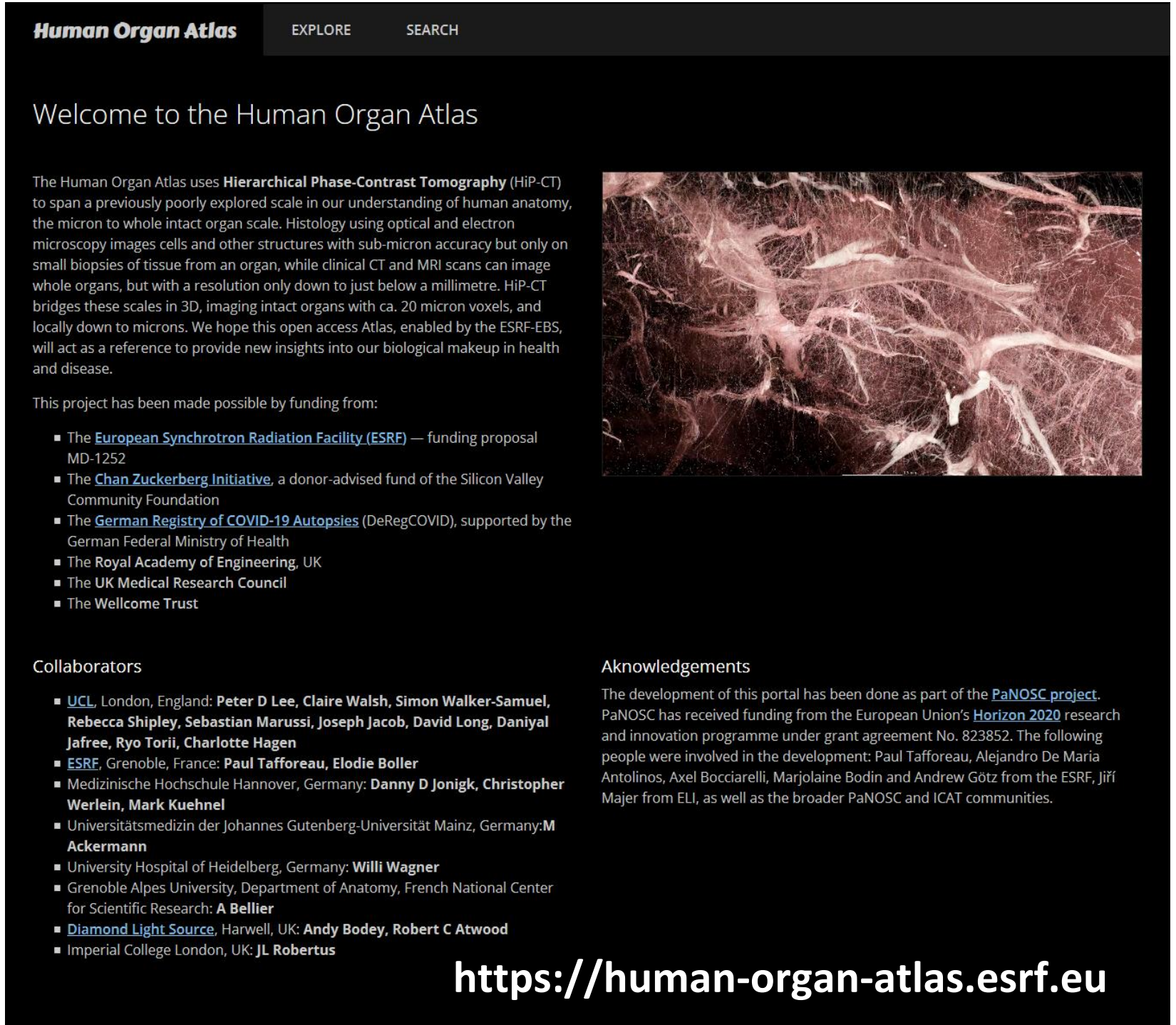
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 857641, respectively.

Example of domain specific open data publishing:

Human Organ Atlas

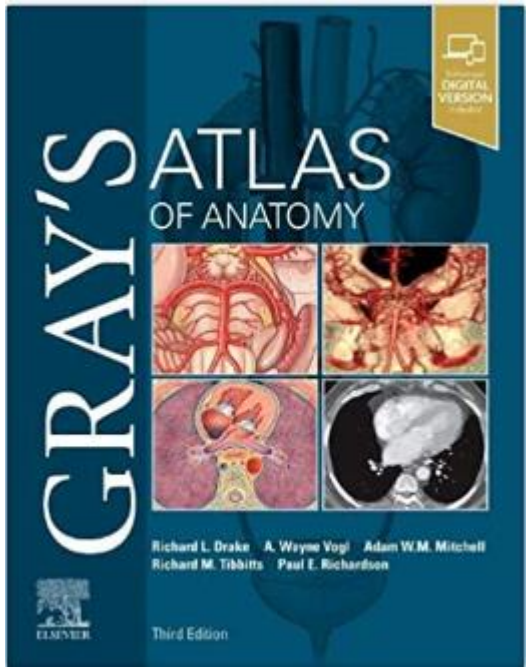
*Walsh, C.L., * Tafforeau, P., * Wagner, W.L., Jafree, D.J., Bellier, A., Werlein, C., Kühnel ,M.P., Boller, E., Walker-Samuel, S., Robertus, J-L., Long, D.A., Jacob, J., Marussi, S., Brown, E., Holroyd, N., Jonigk#, D.D., Ackermann#, M., Lee#, P.D. **Imaging intact human organs locally resolving cellular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

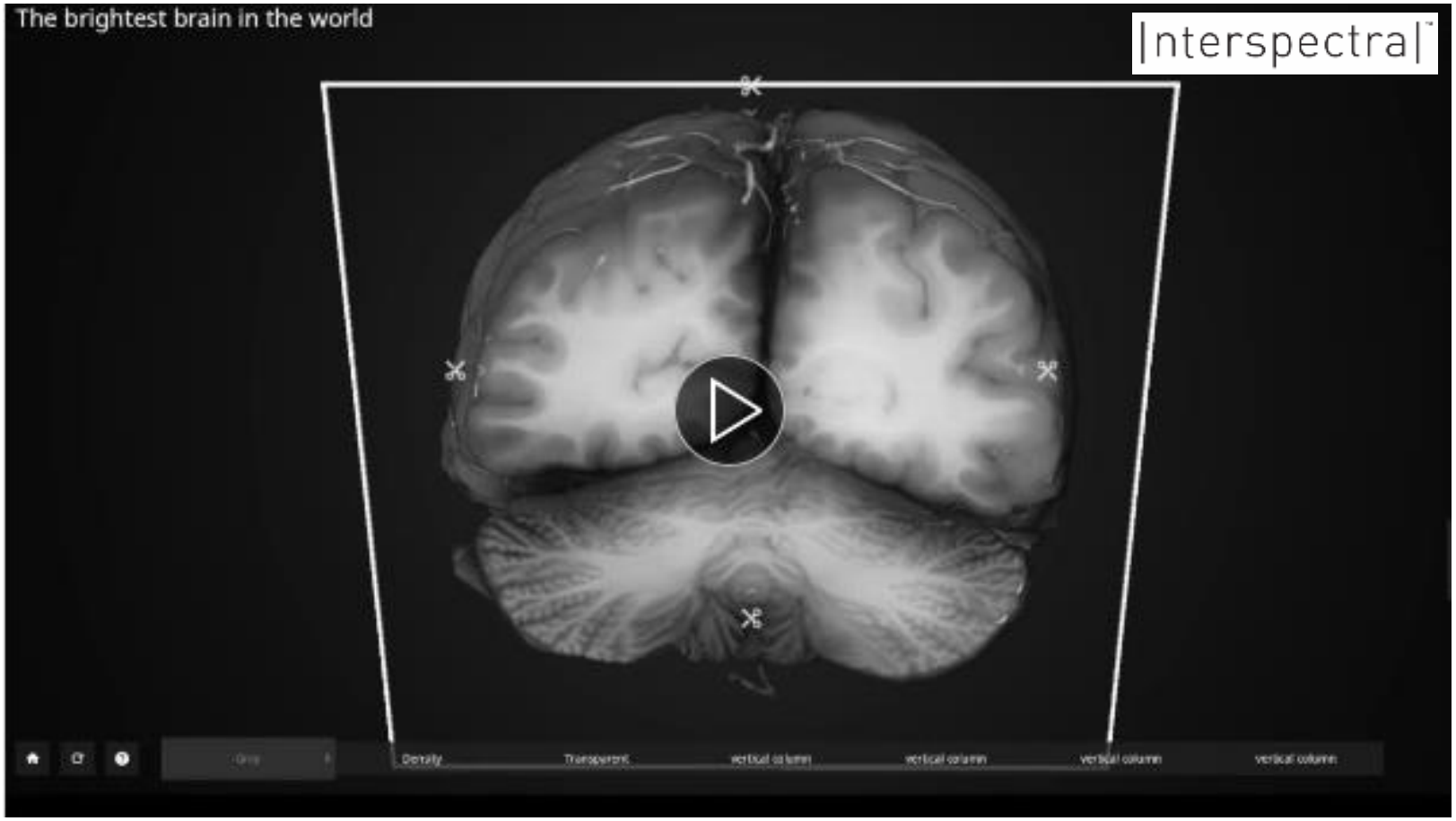
refer to PaNOSC Use Case 23 for more info



Human Organ Atlas FAIR data reuse

Examples of domain specific open data reuse by commercial companies:





https://www.linkedin.com/posts/isabellewegmannhachette_science-3d-visualisation-activity-6975790784402837504-ym8z

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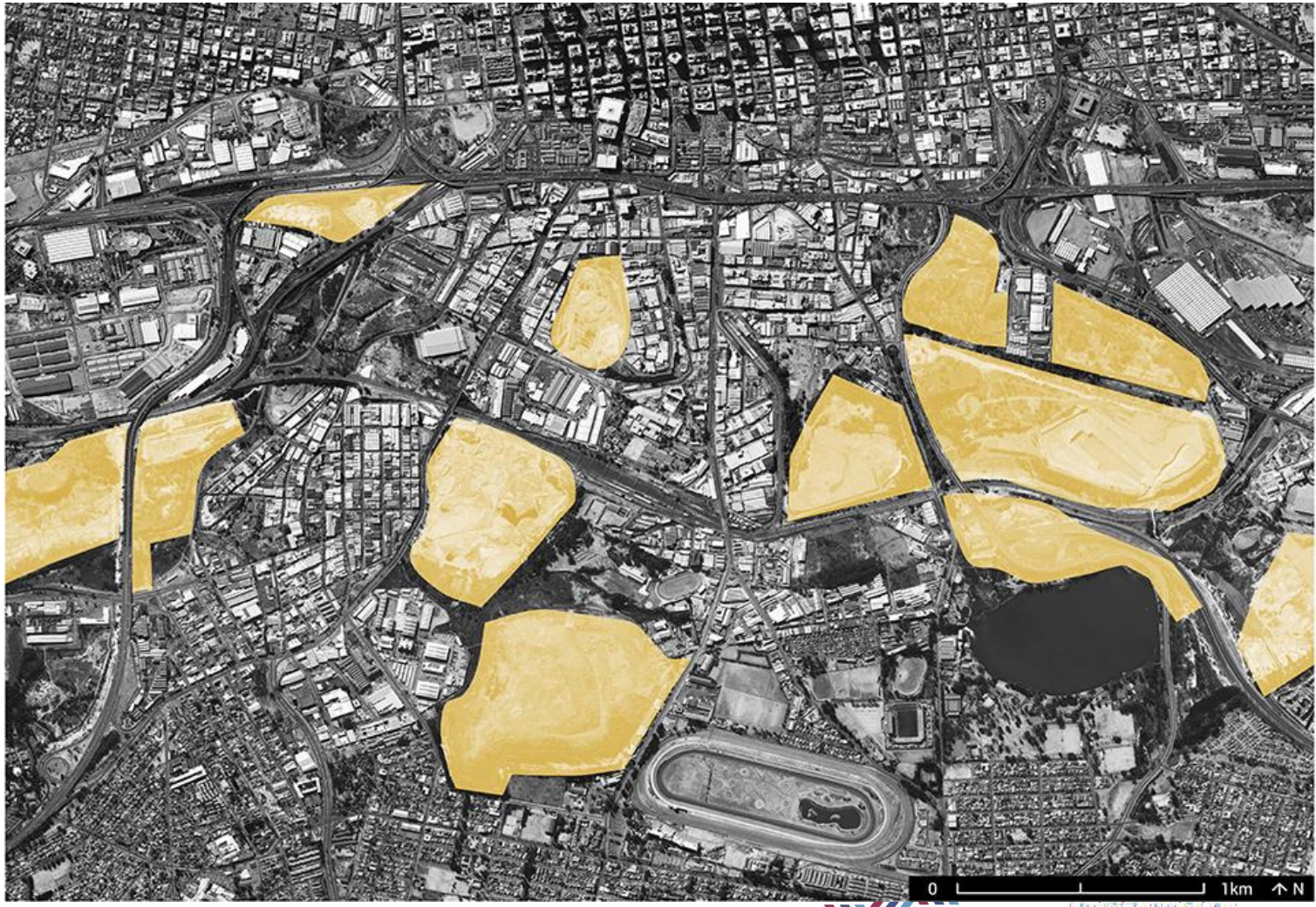
Why make a Data Commons?

Data is sitting around like gold mine dumps …



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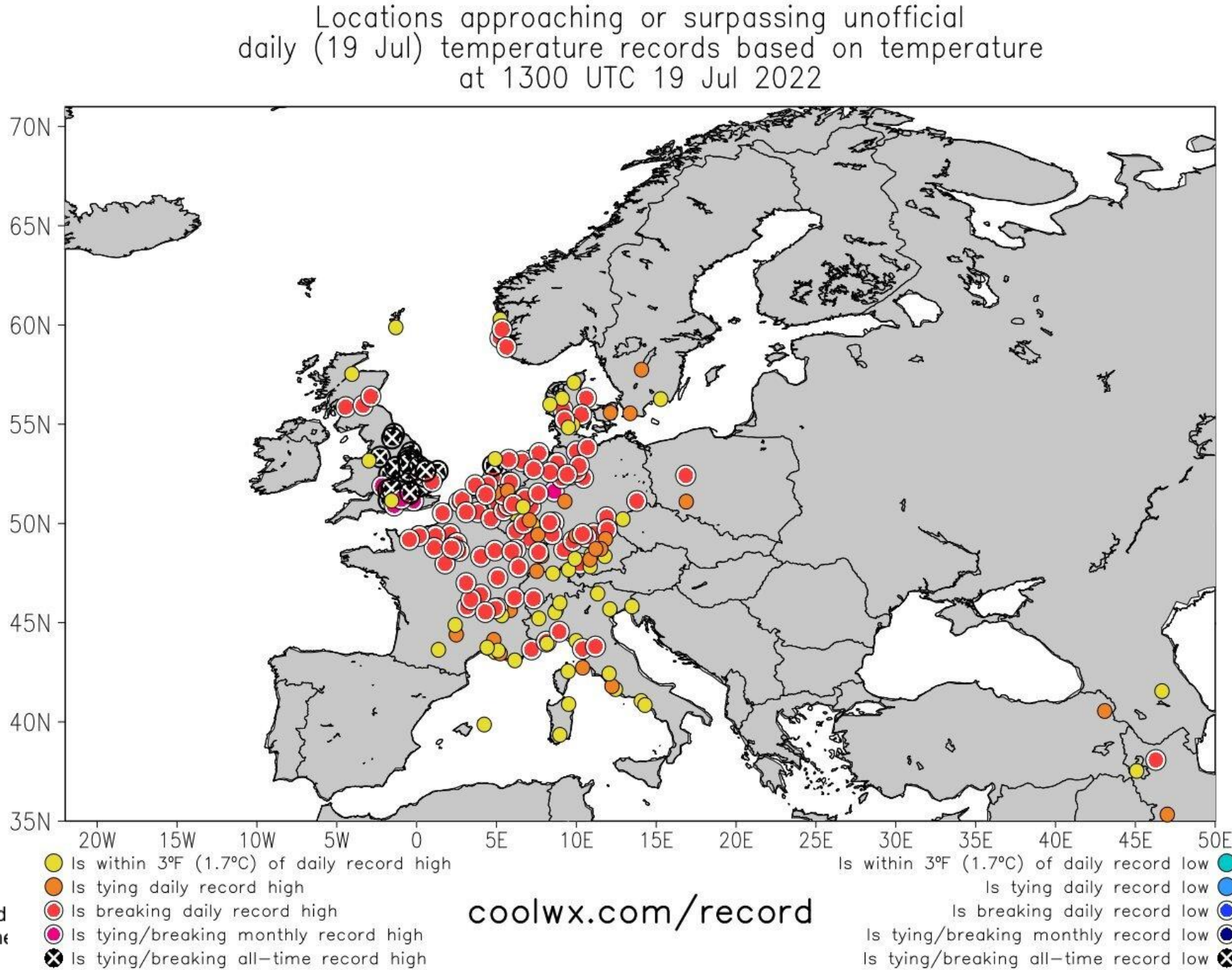
Climate change is more and more visible …



PaNOSC and ExPaNDS projects have received
and innovation programme under grant agreeme

Energy crisis is hitting our labs …

SCIENCE|BUSINESS®

Energy crisis is starting to hit Europe's big science labs

20 Sep 2022 | News

Research infrastructures are worried about the rising cost of running large scientific experiments and are looking for help with paying sky-high electricity bills. One lab has seen a 60% increase in its tariff this year

By Florin Zubaşcu

ALBA synchrotron. Photo: albasynchrotron / Facebook

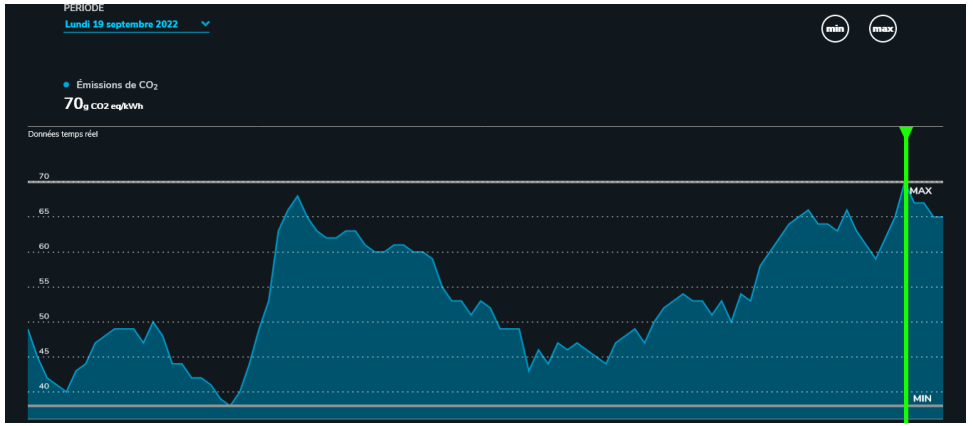
https://sciencebusiness.net/news/energy-crisis-starting-hit-europes-big-science-labs

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

Calculating the carbon footprint of data

- **User Travel -** 3 users fly from Copenhagen to ESRF (380+10 kg CO2e) = 3 x 390 kg
- **Beamtime energy consumption** – 1 week of beamtime (8MW/42) = 190 kWh
- **Data stored on disk** – 100 GB stored on disk (10W x 100 days)
- **Data processing on site** – 1 week of processing on 64 cores (1kW x 1 week)
- **Data transfer** – transfer 100 GB of data back to user (31 kWh)

CO2e per kwH in France (2022) = 75 g/kWh

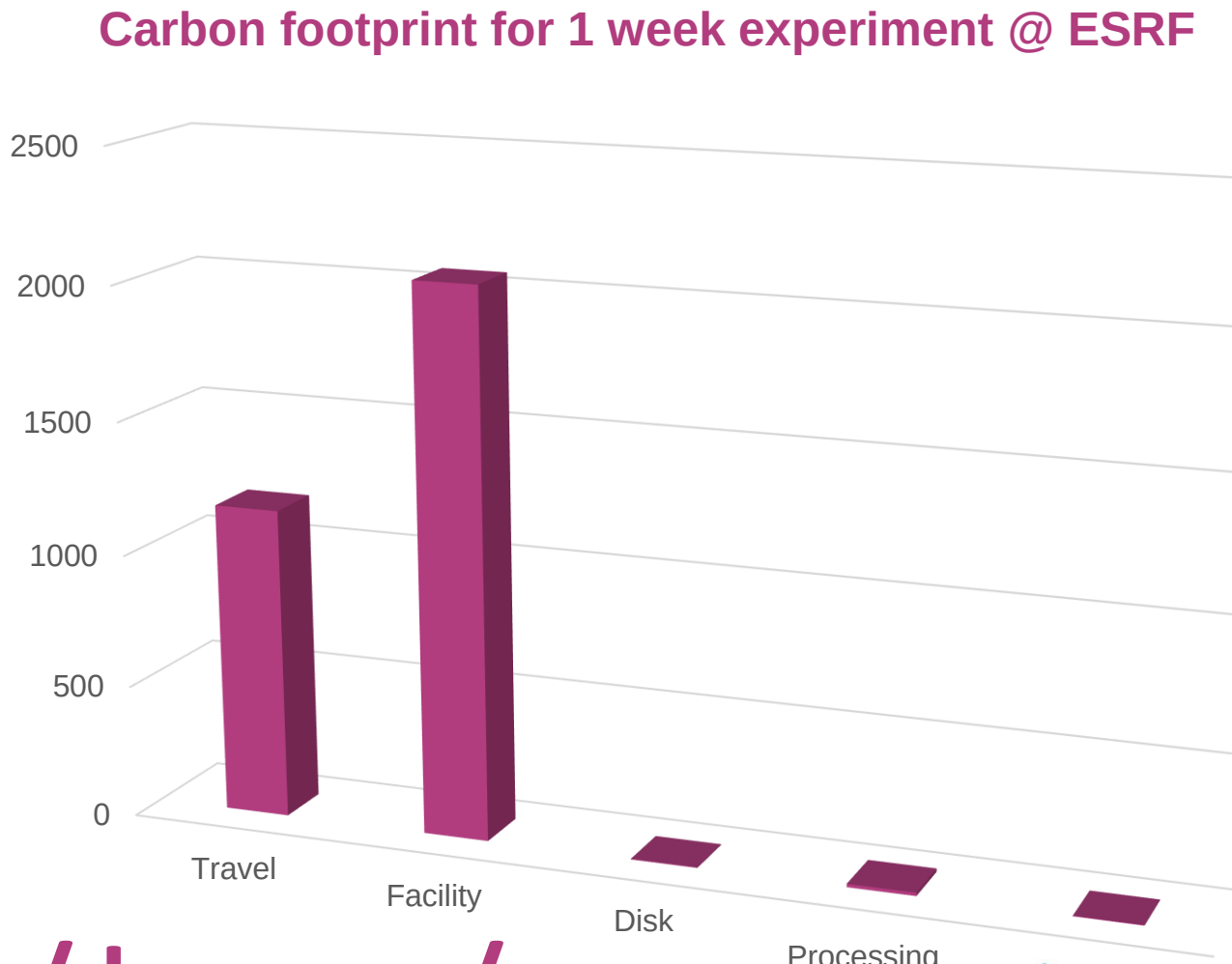


PaNOSC and ExPaNDS pr https://www.rte-france.com/eco2mix/les-emissions-de-co2-par-kwh-produit-en-france#
and innovation programme under grant agreements 823852 and 857641, respectively.

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

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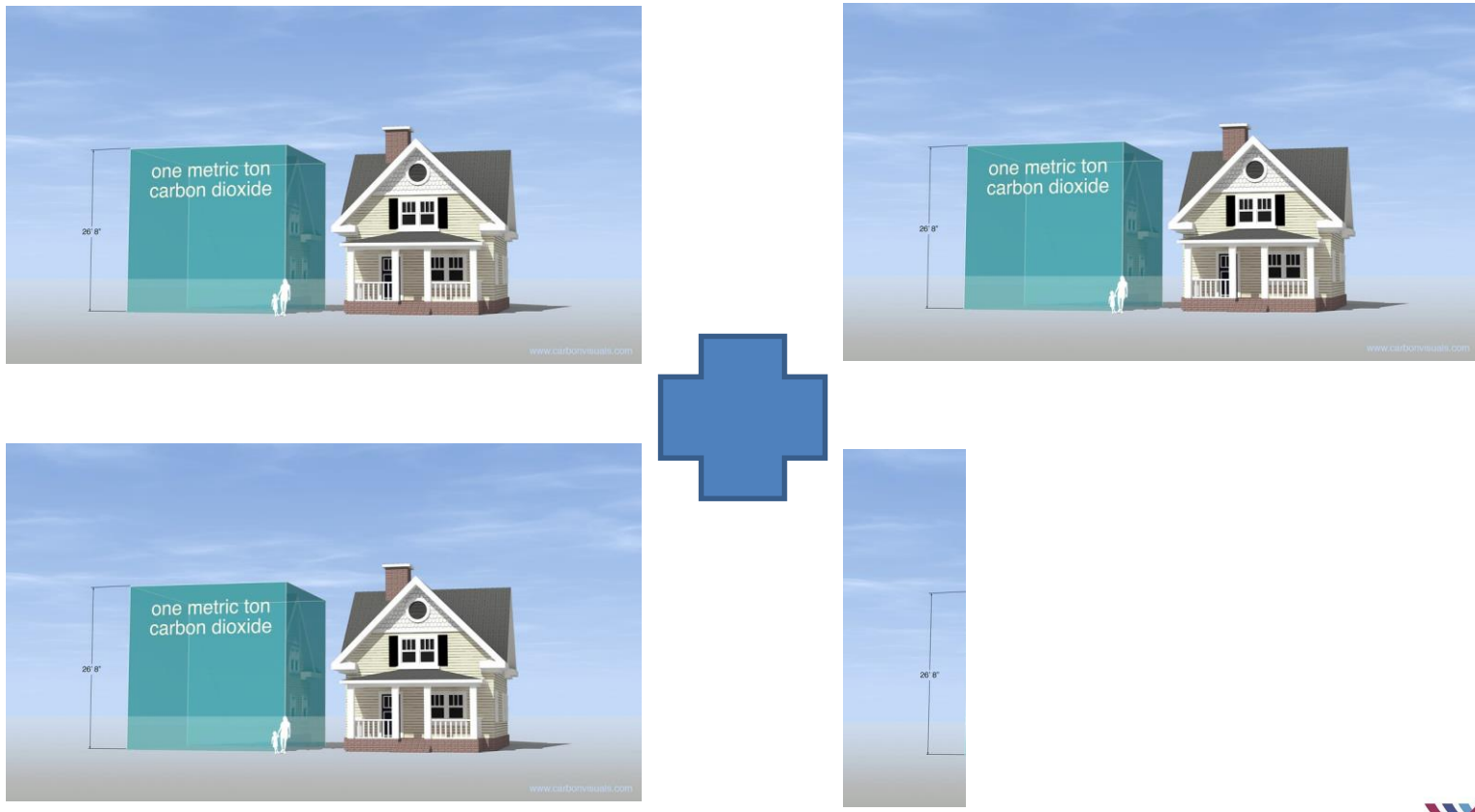
1 week of experiment is equivalent to a cube 30x30x30 metres of CO2



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Carbon footprint of archiving data

- Data stored on tape for 10 years ~ 200 g * 35 = 7 kg

CO2e per kwH in France = **75 g/kWh**

ARCHIVING for 10 years ~ 7 kgs

i.e. 0.2% of the raw data!

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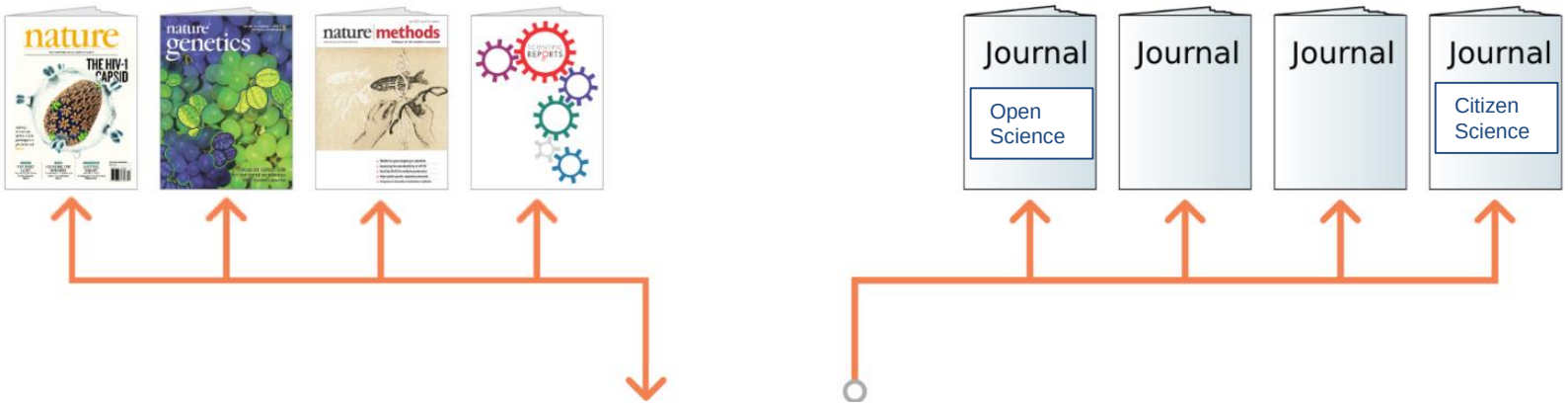
PaN Data Commons - Concept

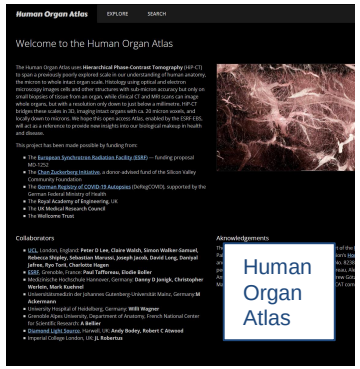
- **Vision** – create a common space for PaNOSC and ExPaNDS facilities where petabytes of PaN FAIR data, analysis software, notebooks, workflows, and training material can be **F**ound, **A**ccessed (downloaded and/or executed), **R**e-Used + **I**mproved i.e. **FAIR**

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

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

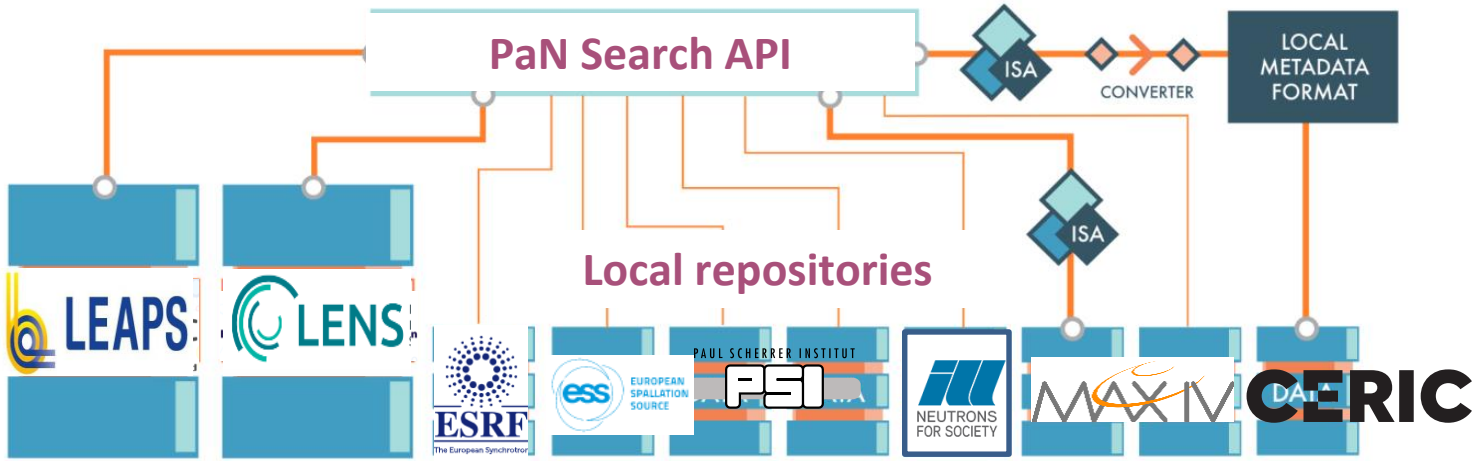
Sustain Published Data ➡ Through PaN Repositories





PaN Open Data Portal

PaN Open Data Repository



ICAT

SciCat

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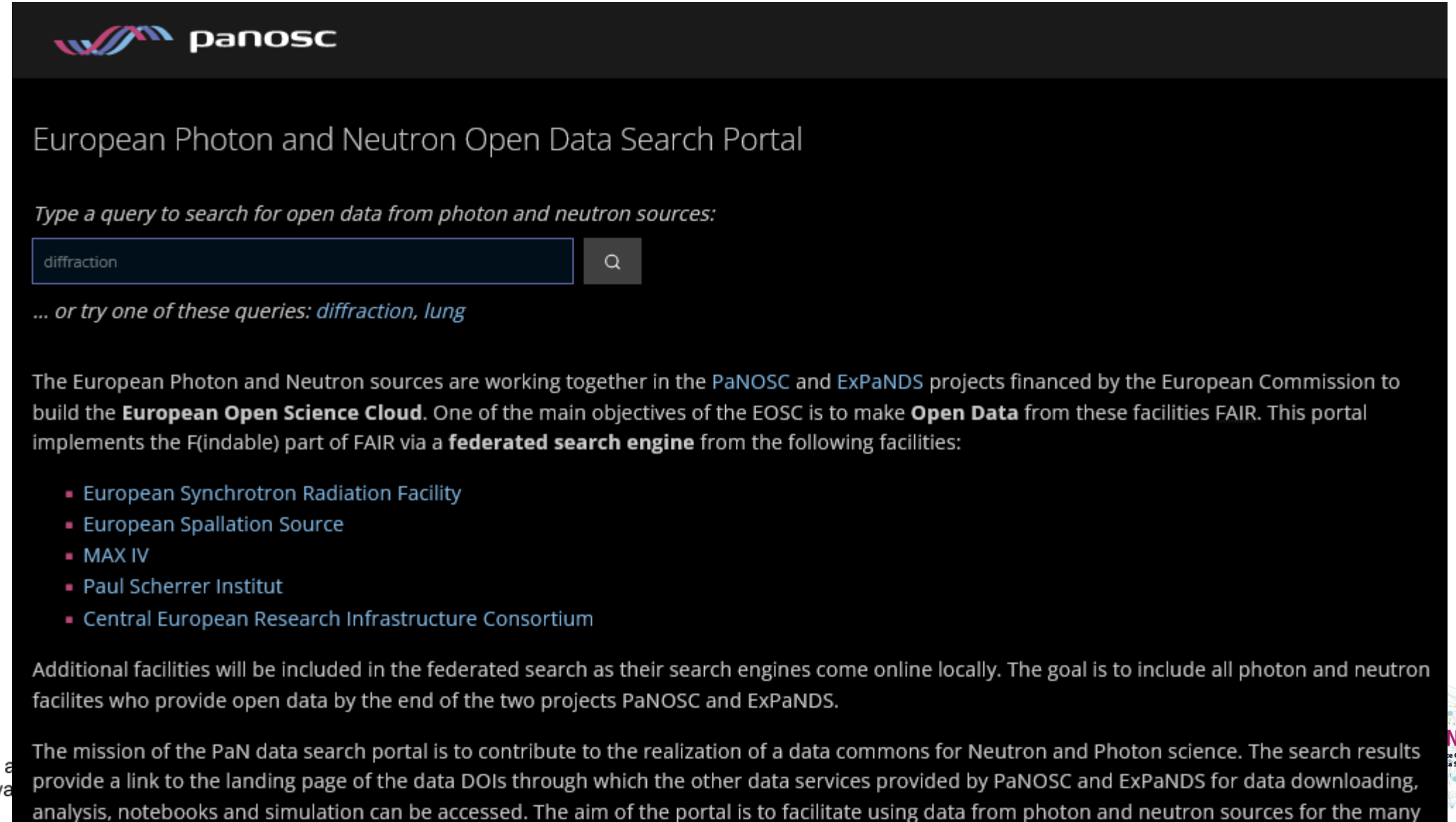
ExPaNDS European Open Science Cloud Photon and Neutron Data Services

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

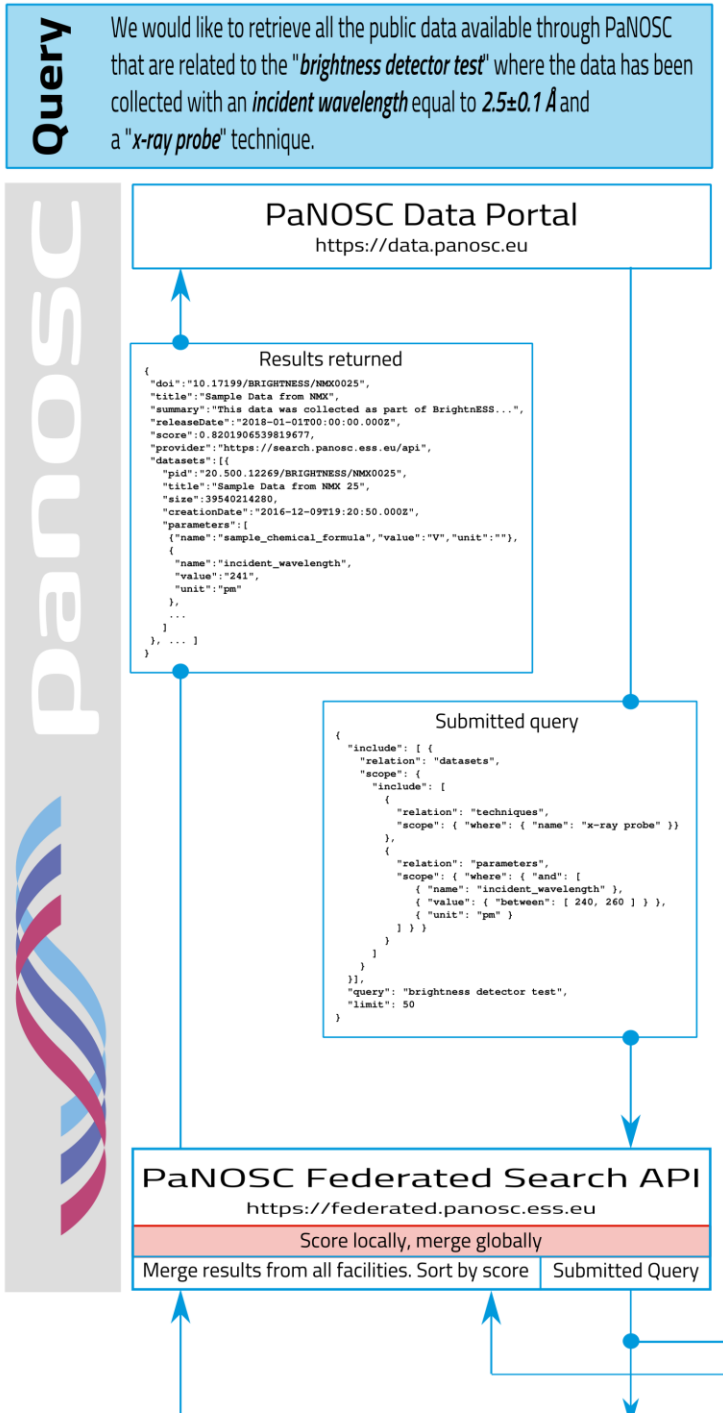
Building the PaN Data Commons on the PaNOSC search portal

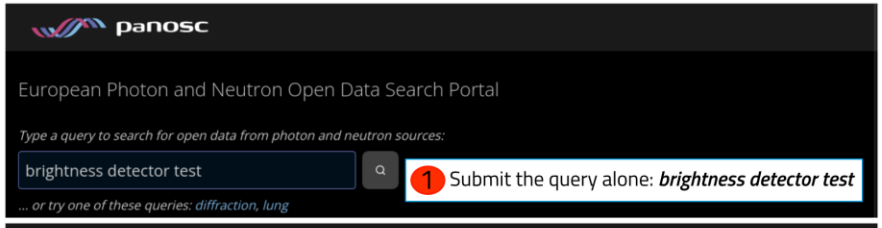


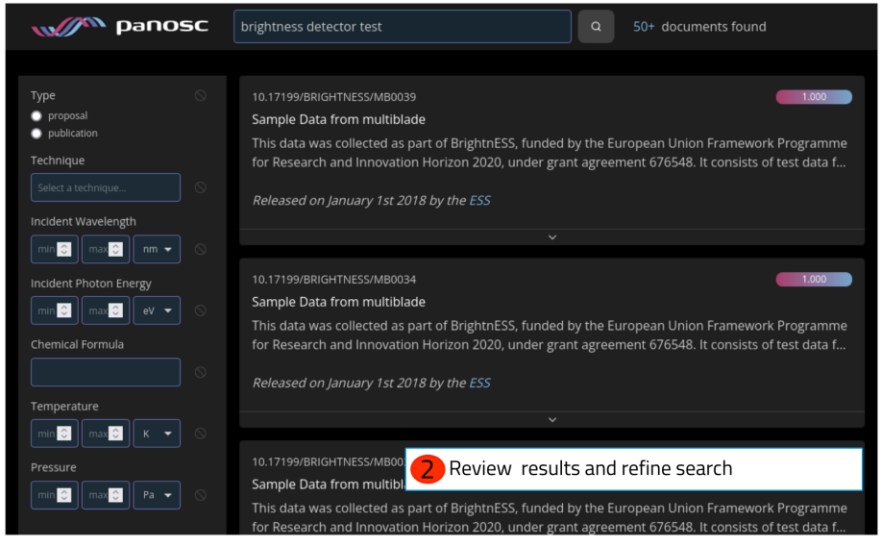
PaNOSC Search API portal @ https://data.panosc.eu

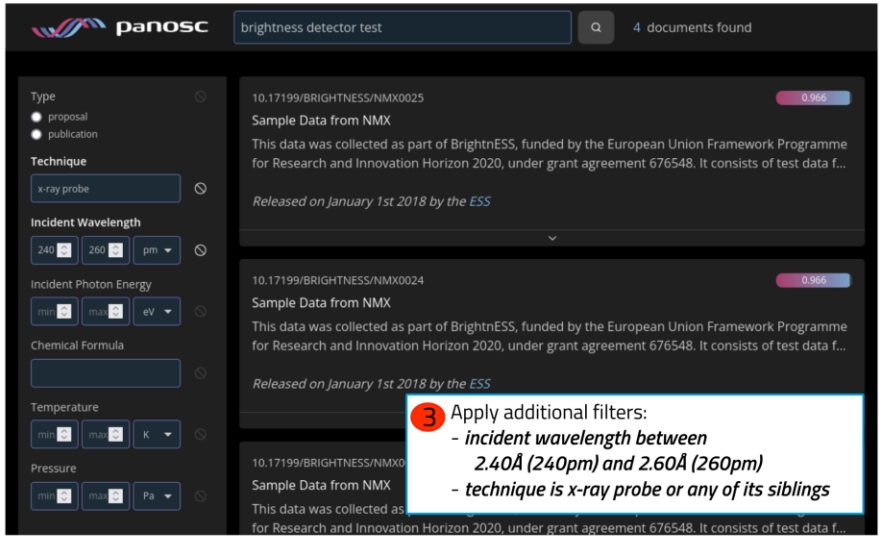
DEMO!

Source: “**SciCat implementation of the PaNOSC Search**” by **Max Novelli** (ESS) et al, https://indico.psi.ch/event/12738/contributions/38937/



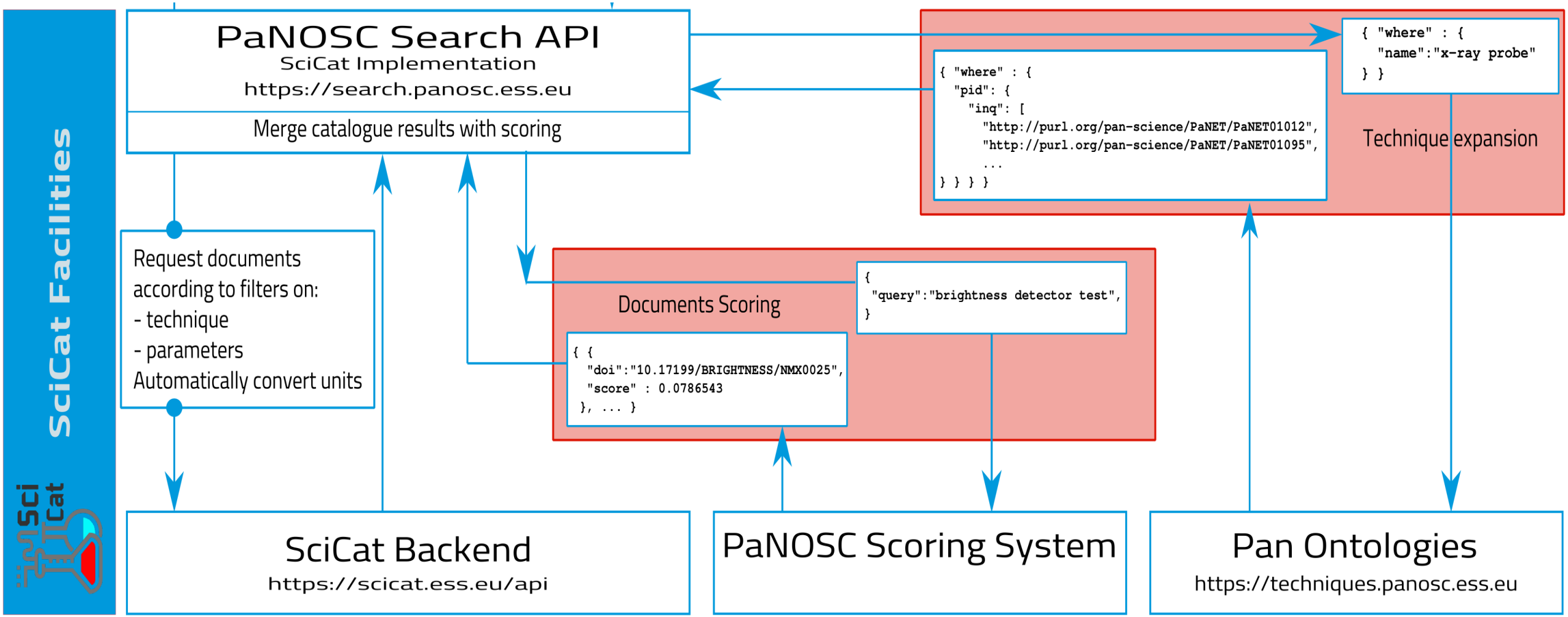






PaNOSC and ExPaNDS projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 823852 and 871072

PaNOSC Search API – implemented on top of SciCat



Source: "**SciCat implementation of the PaNOSC Search"** by **Max Novelli** (ESS) et al, https://indico.psi.ch/event/12738/contributions/38937/

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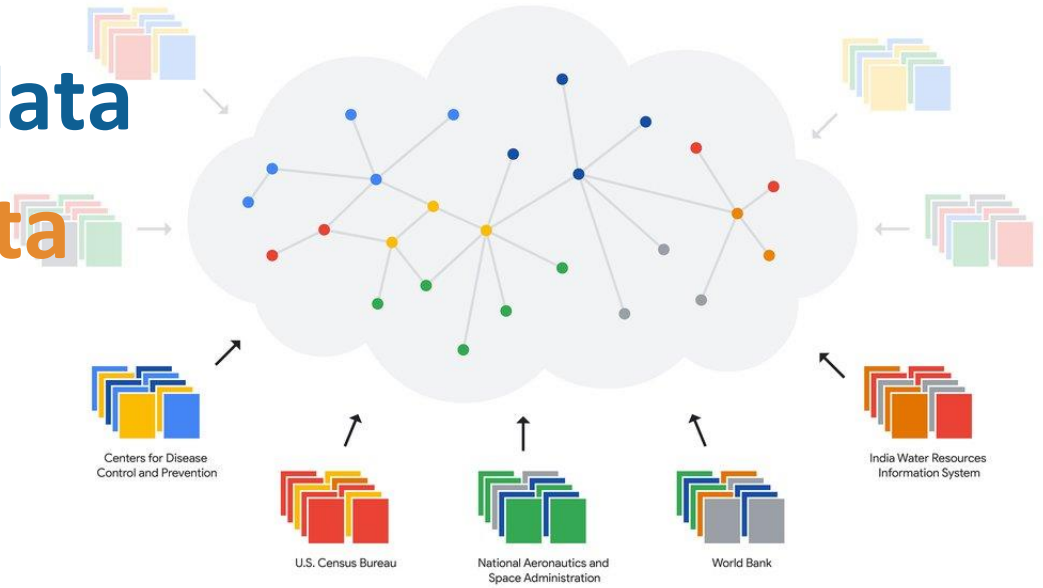
The ExPaNDS project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641.
The PaNOSC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.

What we need from YOU:

1. Implement a open data repository
2. Deploy the PaNOSC Search API + scoring
3. Connect your search endpoint to the PaN Search Portal
4. Data stewards to curate metadata
5. Train your scientists in FAIR data
6. Help build a knowledge graph

Data Commons Knowledge Graph



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Conclusion

1. ExPaNDS and PaNOSC have laid the foundations for a PaN Data Commons
2. The outcomes of the two projects will enable a PaN Data Commons of FAIR data
3. A PaN Data Commons will preserve and increase data reuse
4. Finance to sustain a Data Commons will come from facilities + EOSC
5. The PaN community is on the road to becoming part of the FAIR data landscape
6. Saving our data helps fight climate change and supports open science

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Useful links

- ExPaNDS - https://expands.eu/
- PaNOSC - https://www.panosc.eu/
- EOSC Association - https://eosc.eu/
- PaNOSC data portal – https://data.panosc.eu

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Sources used for carbon footprint estimates

- **User Travel -** https://calculator.carbonfootprint.com/calculator.aspx?tab=3
- **Beamtime energy consumption** – ESRF electrical monitor + control system
- **Data stored on disk** – https://www.buildcomputers.net/power-consumption-of-pc-components.html
- **Data processing on site** – https://www.buildcomputers.net/power-consumption-of-pc-components.html
- **Data transfer+storage in cloud** – https://medium.com/stanford-magazine/carbon-and-the-cloud-d6f481b79dfe
- **Tape storage -** https://datastorage-na.fujifilm.com/reducing-carbon-emissions-through-the-data-tape-ecosystem/
- **CO2 by kWh in France** - https://www.rte-france.com/eco2mix/les-emissions-de-co2-par-kwh-produit-en-france#

PaNOSC and ExF https://sciencebusiness.net/news/energy-crisis-starting-hit-europes-big-science-labs
and innovation programme under grant agreements 823852 and 857641, respectively.