



**ExPaNDS**

European Open Science Cloud Photon  
and Neutron Data Services



# PaNOSC and ExPaNDS Overview

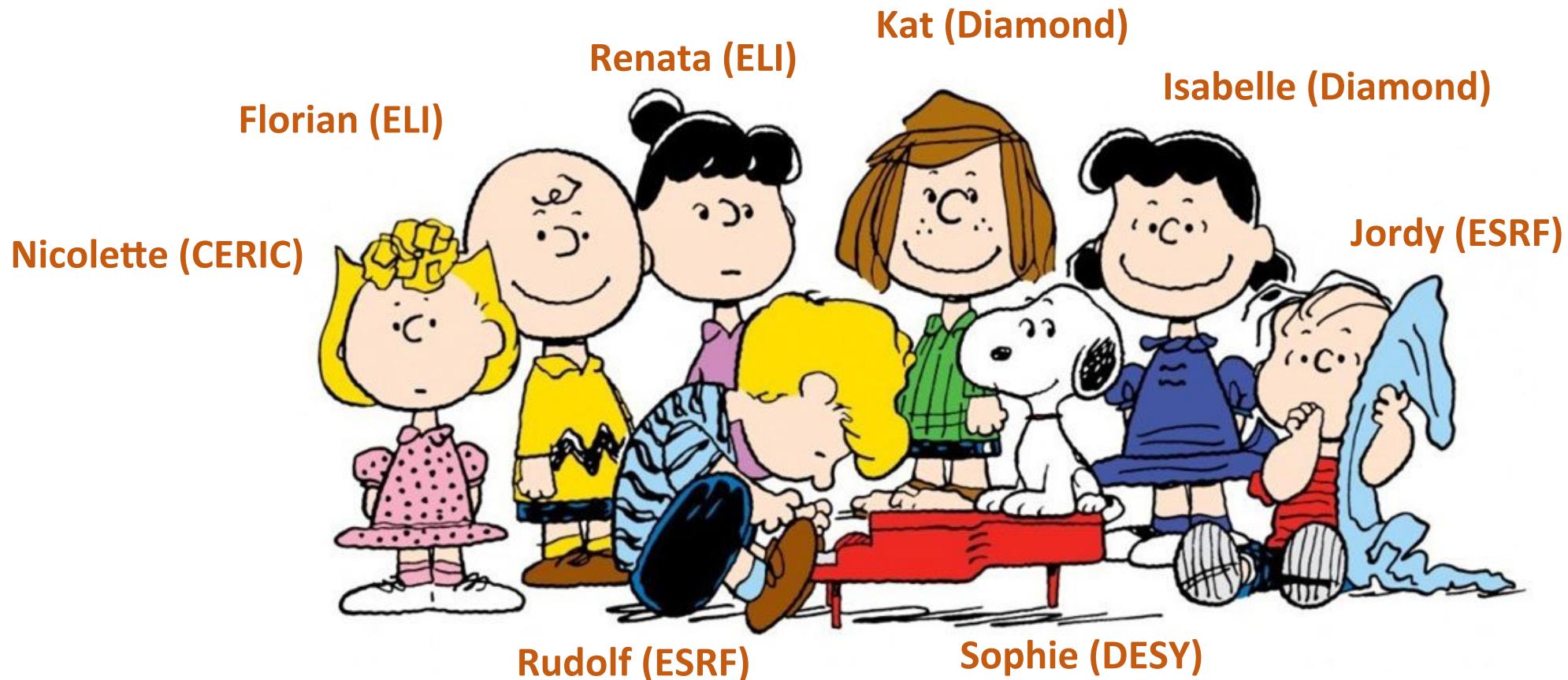
*9<sup>th</sup> of November 2020*

By Andy, Patrick and the PaNOSC and ExPaNDS team.



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.

# The coordinators would like to express their gratitude to the "Annual Meeting" Orga Team!



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# Overview

- What actually is the PaN community?
- PaN facility types and the massive upgrade program.
- What can you do with a PaN beam?
- How do PaNOSC and ExPaNDS relate to this all?
- Bumpy ride through PaN use cases!
- Project work and achievements!
- Next Steps!
- Conclusion

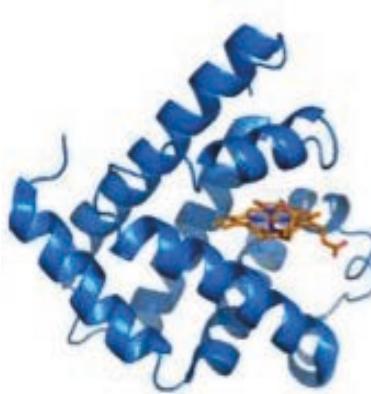
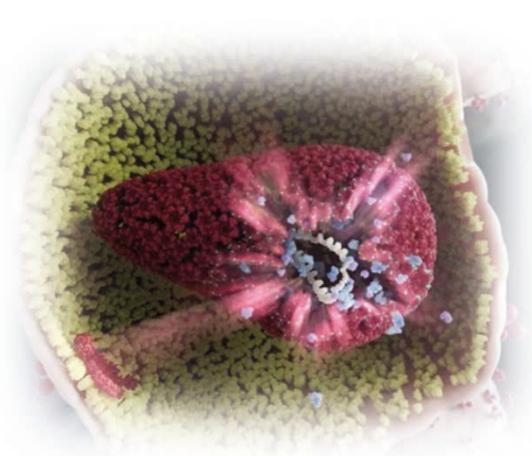


© PNTS

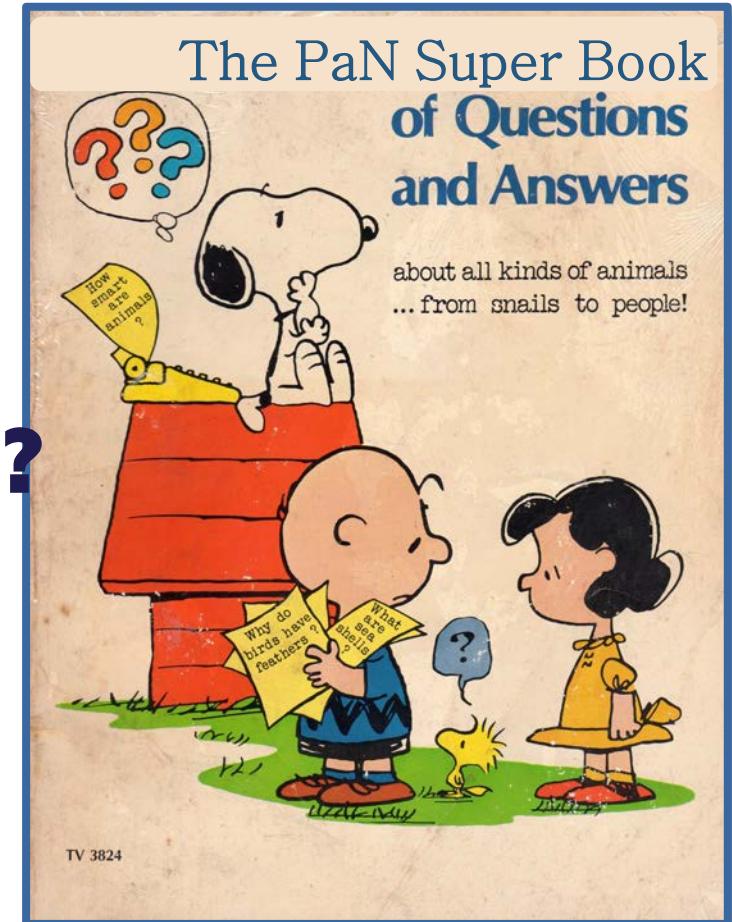
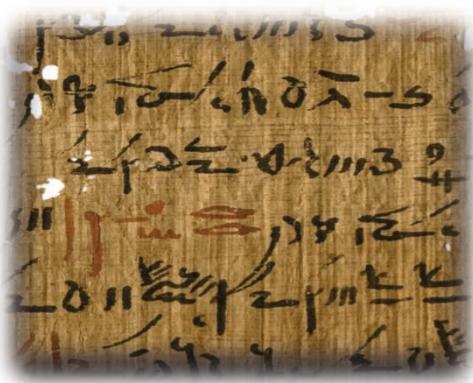


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# What is the PaN community doing?



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# Photon and Neutron Facilities upgrade program!

## Photons

### Synchrotrons



PETRA III

ESRF



### Free Electron Lasers



Eu XFEL

SwissFEL

### Conventional Lasers



ELI

## Neutrons

### Neutron Reactor Sources

ILL



### Spallation Source

ESS



Images borrowed from Facility Webpages @ ESRF, Eu-XFEL, Petra III, SwissFel, ELI, ESS, ILL

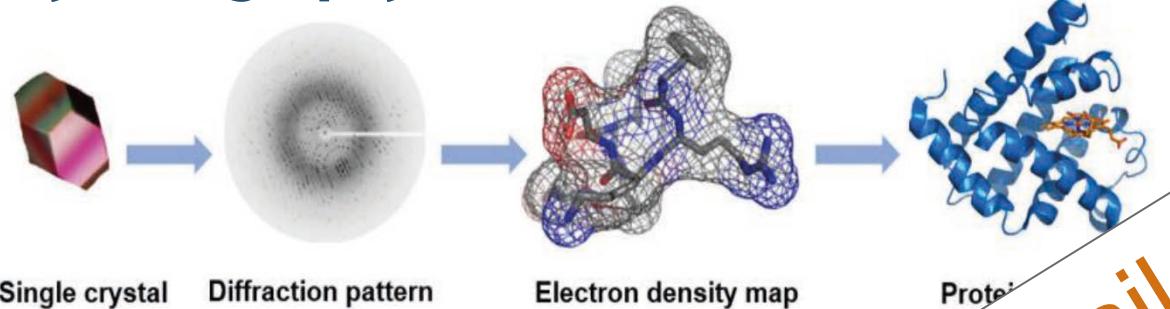


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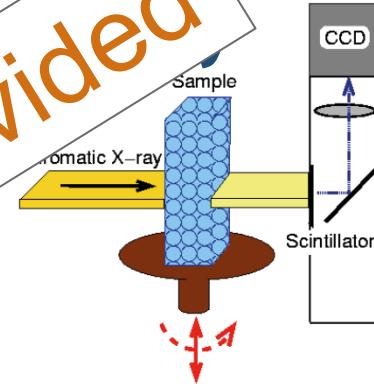


# What can you do with Photon Neutron Beams?

## Conservative Crystallography



## Photon Tomography

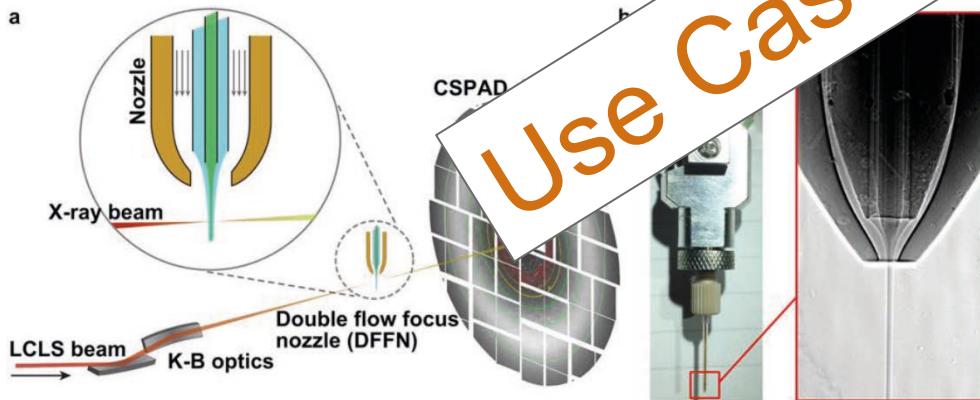


## Neutron Tomography



A new Neutron Radiography / Tomography / Imaging Station DINGO at OPAL

## Serial Crystallography



Thanks to Frank Schünzen for a lecture in PaN Physics

Use Case Details will be provided

## Plasma Physics, Quantum Physics , \*\*\*\*\*

See [Lightsources.org](http://Lightsources.org)



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# What is PaNOSC and ExPaNDS



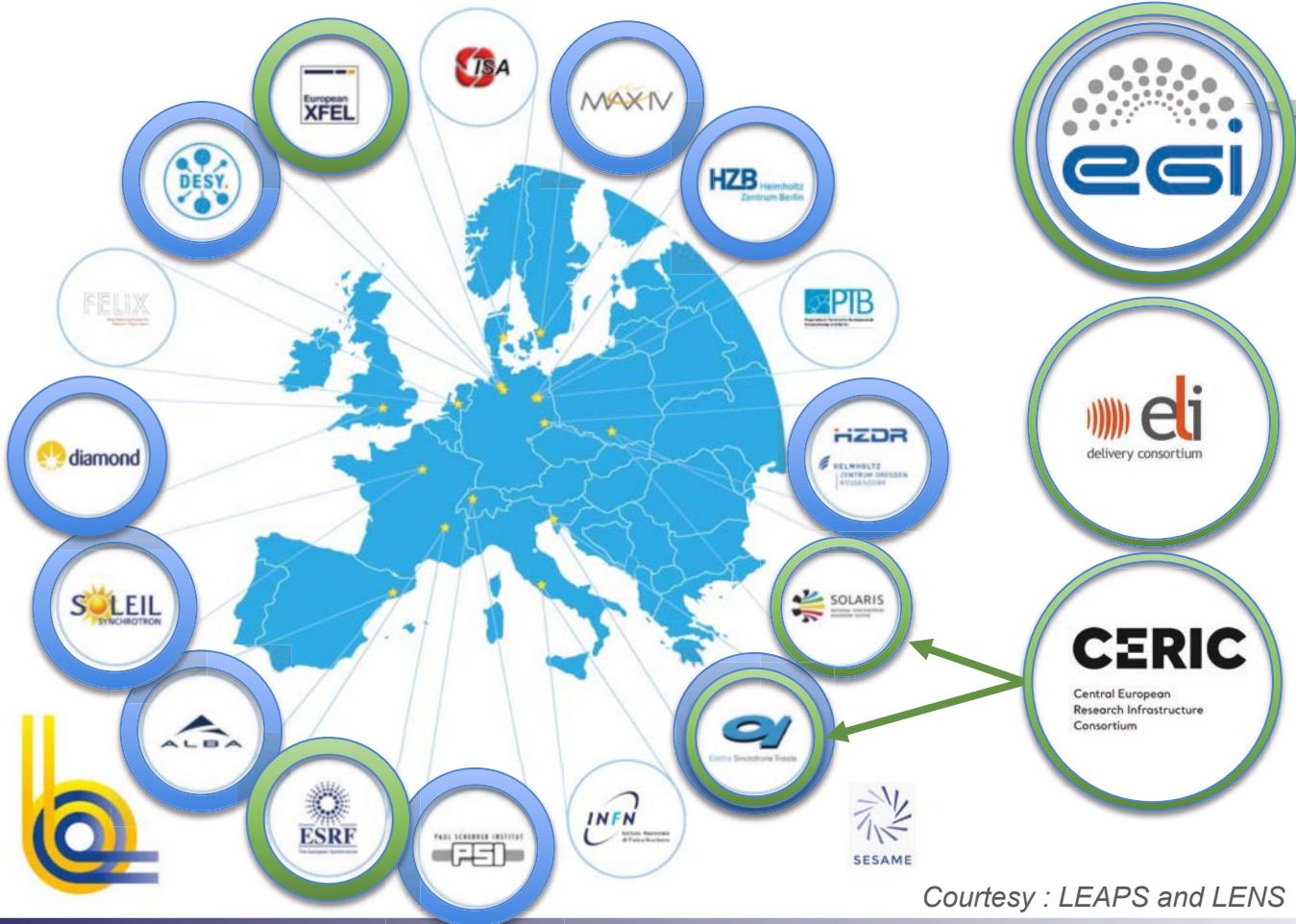
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# What is PaNOSC and ExPaNDS



## Photon (LEAPS)



## Neutron (LENS)



Courtesy : LEAPS and LENS Web Pages



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# Why PaNOSC and ExPaNDS ?

- PaN is only **ONE community**
- Each facility scientist provides a **unique skillset.**
  - So the more the merrier.
- To succeed, it is essential to **work together.**
- Facility users need a **common approach to data**, to be able to work efficiently at their home or across facilities.
- Only PaNOSC and ExPaNDS together reach a Critical Mass in terms of real engagement in Open Science through **Open Data and FAIRness.**
- Involvement of a majority of facilities in Europe avoids the impression of dictatorship, when suggesting or implementing solutions.



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# Why PaNOSC and ExPaNDS ?

- INFRAEOSC-04-2018 call:

*"This topic will ensure the connection of the **research infrastructures identified in the ESFRI Roadmap to the EOSC**. Support to this activity will be provided through **cluster projects gathering ESFRI projects and landmarks** in each of the following large thematic domains .... While the ESFRI infrastructures represent the core component of any cluster, **other relevant world class research infrastructures with a European dimension, established as ERICs or International Organisations, can also be involved in a cluster...**" [1]*

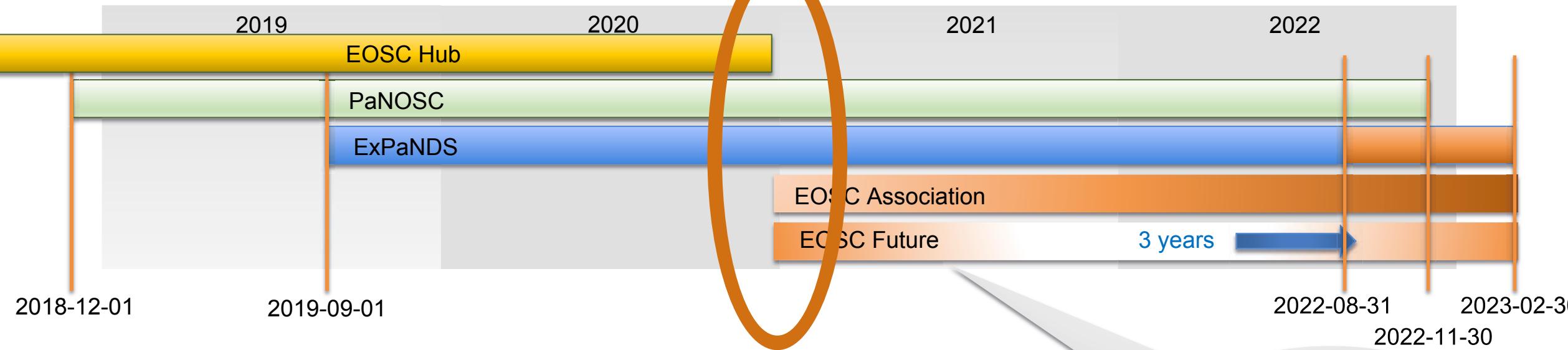
- PaN community are not organized like Elixir, CESSDA , ENVRI.
- **Good news:** PaNOSC and ExPaNDS were funded (thanks EC!).
- PaNOSC + ExPaNDS are a unique opportunity to create a **PaN data Commons** supported by LEAPS and LENS.

[1] [https://cordis.europa.eu/programme/id/H2020\\_INFRAEOSC-04-2018](https://cordis.europa.eu/programme/id/H2020_INFRAEOSC-04-2018)



# PaNOSC and ExPaNDS cheat sheet

## Timeline



## Core data

|                               | PaNOSC                 | ExPaNDS                 |
|-------------------------------|------------------------|-------------------------|
| Call                          | INFRAEOSC 04           | INFRAEOSC 5B            |
| Budget                        | 12 M Euro              | 6 M Euro                |
| Number of Partners/Facilities | 1 ERIC / 5 ESFRI + EGI | 10 National + EGI       |
| Start                         | 2018-12-01             | 2019-09-01              |
| End                           | 2022-11-30             | 2022-08-31 / 2023-02-30 |

*EOSC Future will unlock the potential of European research through a vision of Open Science for Society.*



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# Engagement with other initiatives and Stakeholders

ESFRI cluster projects



Sharing of  
good  
practices

Promote  
adoption and  
sustainability



E x P a N D S  
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## Task Forces

- Coordination
- Landscaping
- FAIR
- Services
- Policies

INFRAEOSC 5B



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# Making FAIR Data a reality for PaNs

For us, FAIR is not an end in itself, but  
It is the prerequisite for Open Science



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# Making FAIR reality for PaNs



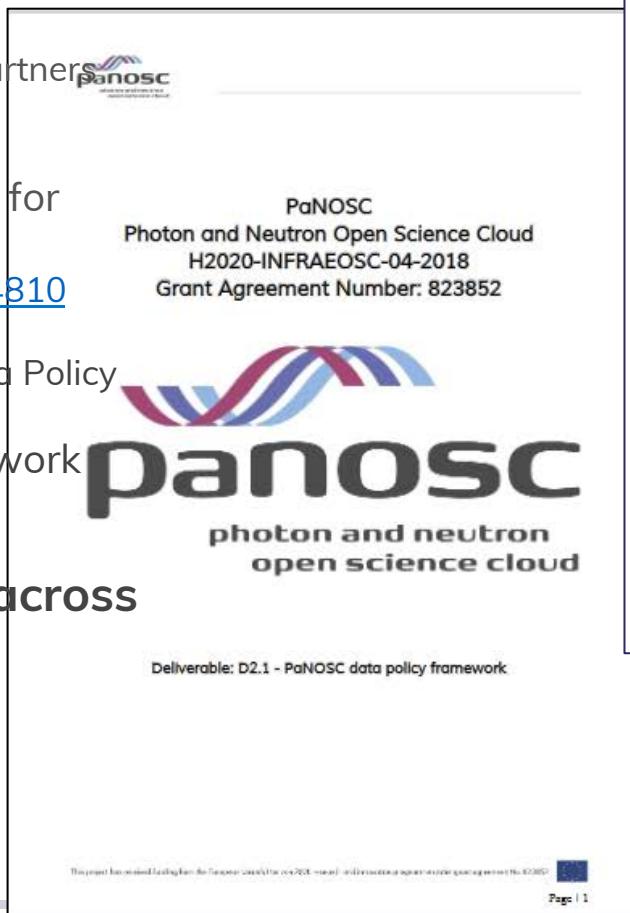
# Towards FAIR policies for Photon and Neutron RIs

- ExPaNDS and PaNOSC have been working together to revise data policies frameworks in the light of FAIR data principles

- PaNOSC D2.1: PaNOSC data policy framework
  - A model policy for adaptation and adoption by PaNOSC Partners
  - [May 2020: https://doi.org/10.5281/zenodo.3826039](https://doi.org/10.5281/zenodo.3826039)
- ExPaNDS D2.1: Draft Extended Data Policy Framework for Photon and Neutron RIs
  - 18<sup>th</sup> September 2020: <https://doi.org/10.5281/zenodo.4014810>
  - Guidance on adopting a FAIR data policy for national RIs
  - Taking into account FAIRsFAIR's recommendations on Data Policy
- Key Policy Elements within a PaN RI Data Policy Framework
  - 30 data policy framework elements

- Aim to have a common approach to data policy across all P&N RIs

- Value in a compatible approach in different facilities
- Easier for users to move around, easier to combine data



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|------------------------------|--|
| Settings                     | Value  |
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Date: 18/09/2020 Page: 1 / 1 DOI: 10.5281/zenodo.4014810

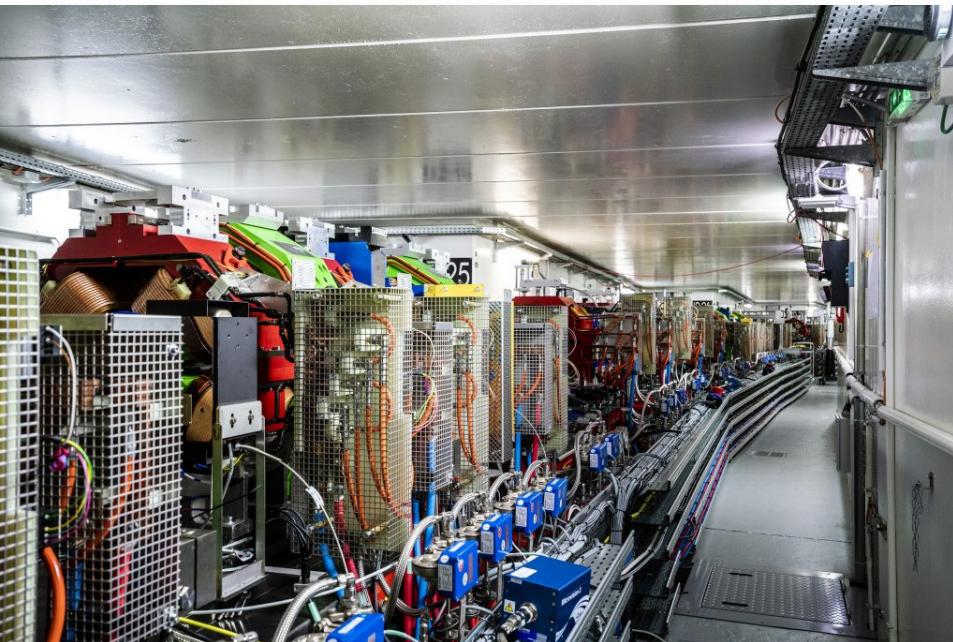


# New sources working to produce FAIR data



## Example ESRF-EBS

*"A new data policy is a big part of the return to user service mode at the upgraded ESRF-EBS, with big implications for users."*



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## INSIGHT

### New dawn, new data

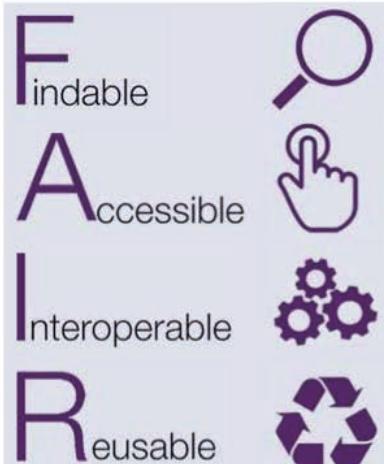
A new data policy is a big part of the return to user service mode at the upgraded ESRF-EBS, with big implications for users.

#### Why is there a data policy?

In short, because there is a lot of data out there. In the early 1990s, when user experiments began, the ESRF was generating tens of gigabytes of data a year; today, it generates some 30 terabytes every single day. Meanwhile, like the rest of the world, the ESRF has been caught up in a digital revolution, in which it has become possible to store, share and search vast quantities of data much more easily than ever before. Both these trends have given rise to the thinking that data can be analysed profitably not just by the experimenters who first record it, but also by other researchers, with faster and more rigorous scientific developments as a result. Indeed, many researchers and collaborations have already been sharing data in this way for some time: data policies such as the ESRF's are merely a way of doing so consistently and according to collectively agreed principles.

#### What are those principles?

Back in 2007, when large research infrastructures were first exploring the best ways to share data, the Organization for Economic Co-operation and Development named 13 underlying concepts, ranging from openness and transparency to security and sustainability. By 2016, however, more than 50 scientists had come together to distil these into just four "FAIR" principles: Findability, Accessibility, Interoperability, and Reusability. Very simply, "findable" means that data are accompanied by a set of universal metadata that both humans and computers can easily understand; "accessible" means that there must be well-defined terms dictating when, and for whom, a data repository is opened; "interoperable" means that data are written in a broadly understood language to make them reusable; and "reusable" itself means that data are presented in such a way as to help scientists apply them in different settings, or to replicate them.



FAIR principles are at the heart of the new ESRF data policy.

#### So the ESRF's data policy is FAIR?

In fact, the formulation of the ESRF's data policy began back in 2008, when European photon and neutron facilities grouped to discuss the thorny issues at the heart of data sharing and management. In 2015, five years after that project was complete, the ESRF became the first light source in Europe to adopt a definite data policy based on principles today recognisable as FAIR – even though FAIR itself would come a year later. After the adoption, the ESRF software group spent a further two years identifying the technologies necessary to back up the policy – the use of ICAT as a database for metadata, for example – before steadily implementing them beamline by beamline. Since last month, all the ESRF beamlines have been operating under the new data policy.

#### What does that mean in practice?

The biggest change is that the ESRF is now the official data custodian. In that role, it automatically generates

metadata, which it stores forever, and archives all raw data for 10 years. This is a huge undertaking, and one many believed impossible in early discussions, but has proved possible due to the fast-rising capacities of tape storage. For three years, the experimental group will have sole access to the data that it generates; beyond that embargo period, the data become freely available to anyone via the ICAT portal (online at <https://data.esrf.fr>) by default – unless the experimental group submits a written request to extend the embargo to the ESRF directors of research.

#### How has the new data policy been received?

The FAIR principles have been embraced by much of the scientific community as part of a broader "open science" movement. Likewise, many ESRF users are enthusiastic about a FAIR-aligned ESRF data policy. Shared data could help to restore trust in science, making it easier for scientists to attempt to replicate one another's findings. The policy will also give funders more "bang for buck", pave the way for shared data processing and analysis services, and allow data once thought to be exhausted to be revisited in new contexts. Imagine, for instance, if past data of coronaviruses could have been revisited in light of the current COVID-19 pandemic.

Not everyone is on board. Despite the possibility of extending the embargo period, some researchers feel anxious that their hard-won data will automatically go public before they have published everything they ever intend to in journals. But for Andy Götz, head of the ESRF software group, the question at the heart of it all is one of duty. "Data are the ESRF's primary product," he says. "I've always thought something's missing if we don't curate data properly." ■

**Jon Cartwright**

# Bringing FAIR to the Experiment

## From Data Policies to DMP's

### Advantages of user and experiment DMP's

- **Data Policy** applies at the facilities level
  - This needs to be made happen for each experiment
    - Contract between the facility and the user/experiment.
    - Clear specification of resource usage.
    - Allows planning reliability on both sides.
    - Optionally extends responsibilities beyond the end of the experiment, for
      - ✓ data stewardship
      - ✓ compute resources
        - In case users won't have storage space at home facility.
        - In case data volume doesn't allow relocation (in time)
- **For each experiment**
  - Data/ data, software, metadata to be collected, data storage, connections to derived products like Hard Work!!
  - Sounds like Hard Work!!
    - Allows planning reliability on both sides.
    - Optionally extends responsibilities beyond the end of the experiment, for
      - ✓ data stewardship
      - ✓ compute resources
        - In case users won't have storage space at home facility.
        - In case data volume doesn't allow relocation (in time)
- **DMP for an experiment needs to be done in context:**
  - The DMP for its institution and funder
  - The community or for the discipline
  - The DMP of the user's institution and funder
    - ✓ data stewardship
    - ✓ compute resources
      - In case users won't have storage space at home facility.
      - In case data volume doesn't allow relocation (in time)
- **The DMP should be active during the experiment**
  - Help steer the collection of data
  - Citizen science
    - Help steer the collection of data
    - Work with for example an Electronic Notebook

University  
Data Policy



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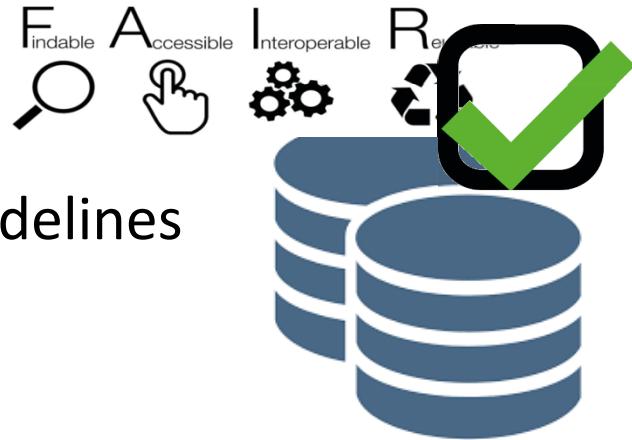
# Verifying FAIR ness of repositories



- Policy work done by RDA
  - FAIR Data Maturity Model: specification and guidelines
  - <https://doi.org/10.15497/RDA00050>
- Fairness engines by EOSC Synergy
  - Not a standalone system but a plug-in for repositories
    - DSpace, DIGITAL.CSIC
  - Open Source Code (available: [https://github.com/EOSC-synergy/FAIR\\_eva](https://github.com/EOSC-synergy/FAIR_eva))
- Fairness engine by EOSC Nordic



Was presented during  
the EOSC Nordic  
Workshop  
Didn't have time to look  
into it yet.



## Machine-actionable FAIR Maturity indicators



| Metric name                   | Principle association | Principle description   |
|-------------------------------|-----------------------|---|
| 1 UNIQUE IDENTIFIER           | F1                    | (Meta)data are assigned a globally unique and persistent identifier |
| 2 IDENTIFIER PERSISTENCE      | F1                    | (Meta)data are assigned a globally unique and persistent identifier |
| 3 DATA IDENTIFIER PERSISTENCE | F1                    | (Meta)data are assigned a globally unique and persistent identifier |
| 4 STRUCTURED METADATA         | F2                    | Data are described with rich metadata (defined by R1 below)         |
| 5 GROUNDED METADATA           | F2                    | Data are described with rich metadata (defined by R1 below)         |

# Science Use Cases

- Use Cases – The Template
- [1] Cultural Heritage
- [2] Post azimuthal integration maps
- [3] Carboxysomes
- [4] Parkinson's disease & Brain Map
- [5] Remote Access
- [6] Simulation
- [7] Zeptosecond birth time delay



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# Use Cases - Template

- The success of PaNOSC + ExPaNDS will be judged by the number of scientific use cases served by the projects!
  
- **Proposal:** A template has been developed, which will be used to gather real scientific uses cases from real scientists.
  - [#realscienceusecases](#)

## PaNOSC USE CASE - TEMPLATE

|  |  |
|--|--|
| <b>Title*</b><br>Short description of use case   | <b>Submitted by*</b><br>Who submitted the use case                                   |
| <b>Scientist*</b><br>Names of some scientists (and their affiliations) who have requested and will use the service   | <b>Date*</b><br>DD/MM/YYYY (creation date of use case)                               |
| <b>Objective*</b><br>Longer description of the use case including a description of the scientific objectives of the use case   |  |
| <b>Description of needs *</b><br>Description of what the use case is requesting from PaNOSC  |  |
| <b>Main Contributors*</b><br>Contributor 1<br>...<br>Contributor N   | Description of the contributors, their role in the use case and what they contribute |
| <b>PaNOSC work packages</b> (to be filled in by PaNOSC)<br>WP 1<br>...<br>WP N   |  |
| <b>Use case action flow</b><br>1: Step Name<br>...<br>N: Step Name   |  |
| <b>Impacts from the implementation*</b><br>Description of scientific and technical impacts for users   |  |
| <b>Generalisation of Use Case</b><br>Description of the possible take up of the solution by other PaNOSC or ExPaNDS partners and the scientific community in general. A description of application of the use case to other users. | <b>Partners</b><br>Other partners interested in this use case                        |
| <b>Resources</b><br>Description of software and/or source code repositories to be used.  |  |



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# Use Cases - Example

## ➤ Title

- ✓ Generic Jupyter notebooks for analysing cultural heritage data

## ➤ Description

- ✓ The goal will be to perform 2 $\mu$ XRD maps on painting fragments from various historical paintings.

## ➤ Objectives:

- ✓ To **improve the efficiency of the experiment** (many different users, a possible regular beamtime, remote experiment), I think it **would help a lot to have a dedicated Jupyter notebook for data processing**. It would be a good way:
  - to **save time**,
  - to **record which map has already been processed** and how,
  - and **have a coherent data processing between users and between sessions**, and also for possible users who would like to **reuse data after the embargo period**.

## USE CASE EXAMPLE – Jupyter notebooks for Cultural Heritage @ ESRF

|  |               |
|--|---------------|
| Title*   | Submitted by* |
| Generic Jupyter notebooks for analysing cultural heritage data | A.Götz        |

|   |                             |
|---|-----------------------------|
| Scientist*  | Date*                       |
| M.Cotte (ESRF), M.Burghammer (ESRF), V.Gonzalez (Rijks Museum), C.Rivard (SOLEIL) | 05/11/2020<br>(of use case) |

|   |
|---|
| Description*  |
| The goal will be to perform 2 $\mu$ XRD maps on painting fragments from various historical paintings. |

|   |
|---|
| Objective(s)*   |
| To improve the efficiency of the experiment (many different users, a possible regular beamtime, remote experiment), I think it would help a lot to have a dedicated Jupyter notebook for data processing. It would be a good way i) to save time, ii) to record which map has already been processed and how, iii) and have a coherent data processing between users and between sessions, and also for possible users who would like to reuse data after the embargo period. |

|  |
|--|
| Request*   |
| Provide users with .hdf5 post azimuthal integration maps, so the Jupyter notebook should mainly take care of PyFAI integration of 2D maps.   |
| It would be good as well to preliminary check the integration on the average of the map (on max or mean) (for example to check that there is no sudden modification of the set-up, such as energy, distances...) |
| To be discussed if the calibration of the set-up (obtaining the .poni file) should also be included or be available on a separate file (this will probably be of interest for many experiments at ID13).         |

|                    |   |
|--------------------|---|
| Main Contributors* |   |
| L.Huder            | Scientific software developer will develop python scripts + notebooks + HDF5    |
| J.Kieffer          | Scientific software developer author and expert in pyFAI and parallel computing |
| W.de Nolf          | Expert in 2 $\mu$ XRD data analysis and HDF5                                    |

|                      |  |
|----------------------|--|
| PaNOSC work packages |  |
| WP 3                 | Metadata definitions, HDF5 + Nexus formats     |
| WP 4                 | Data analysis services using Jupyter notebooks |

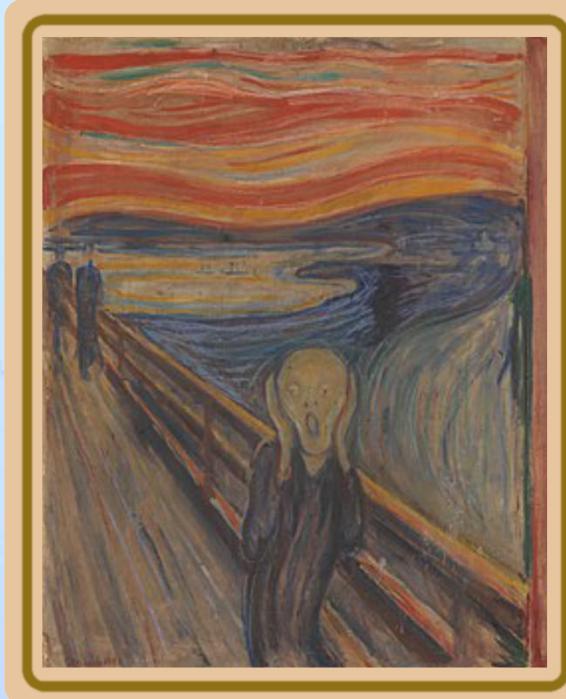
|                       |  |
|-----------------------|--|
| Use case action flow  |  |
| 1: Extract data       | Write python scripts to extract data from raw data files                   |
| 2: Radial integration | Write python scripts to call pyFAI in highly optimised way                 |
| 3: Combine maps       | Stitch integrated data together to make 2D/3D maps and output an HDF5 file |

|  |
|--|
| Impacts from the implementation*   |
| The goal will be to perform 2 $\mu$ XRD maps on painting fragments from various historical paintings |



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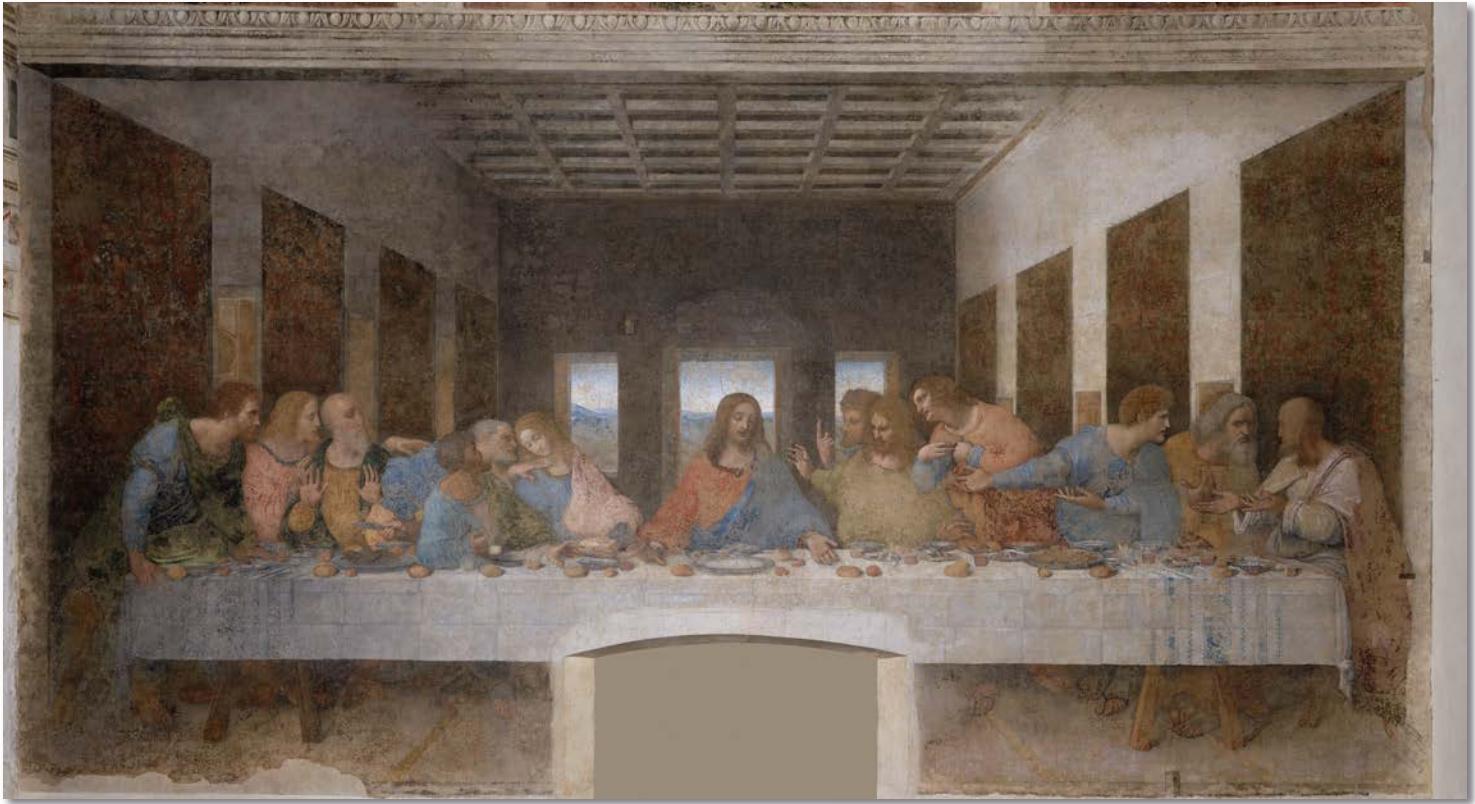
# Use Case 1 Cultural Heritage



# Cultural Heritage

## Cultural Heritage

- **Institutes:**
  - ✓ ESRF, SOLEIL
- **Scientists**
  - ✓ M. Cotte, C.Rivard
- **Objective**
  - ✓ Conservation of old paintings e.g. Last Supper by L. Da Vinci
- **Request:**
  - Prepare data reduction scripts as Jupyter notebooks for non-expert users.

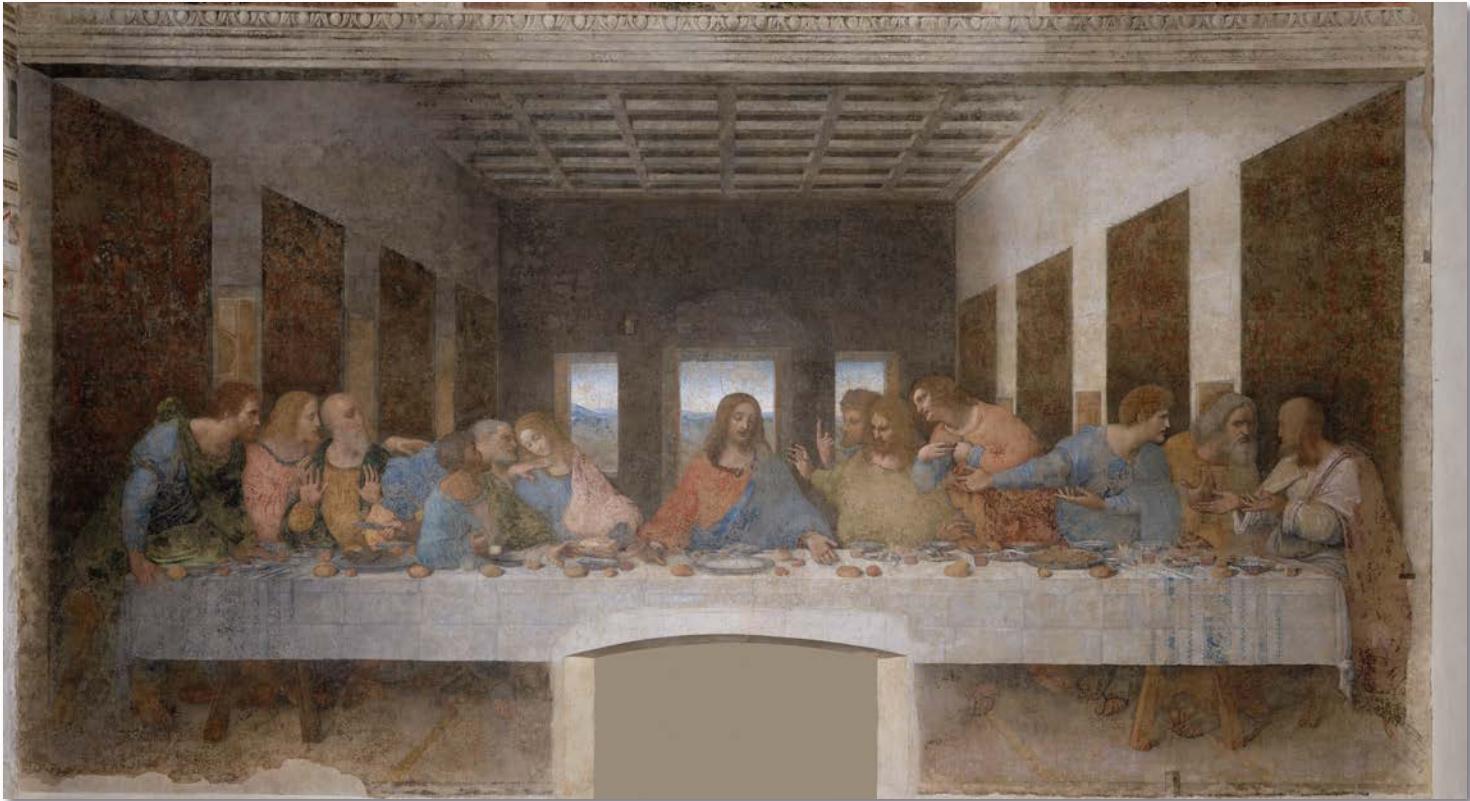


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# Cultural Heritage (cont.)

- **Demonstrates**
  - Jupyter notebooks,
  - Data portal
  - HDF5 data format
  - Software Catalogue
- **Work packages**
  - WP3, WP4, WP6
- **Beneficial to**
  - Any user community which needs standard data reduction scripts in a standard data format
- **Potential**
  - 100s experiments, 1000s users



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.



## Use Case 2

# Post azimuthal integration maps!



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# “Post azimuthal integration maps”

## ➤ Motivation

- “... improve the efficiency of the experiment (many different users, a possible regular beamtime, remote experiment),

*I think it would help a lot to have a dedicated Jupyter notebook for data processing. It would be a good way i) to save time, ii) to record which map has already been processed and how, iii) and have a coherent data processing between users and between sessions, and also for possible users who would like to reuse data after the embargo period.” Scientist*

## ➤ Use Case

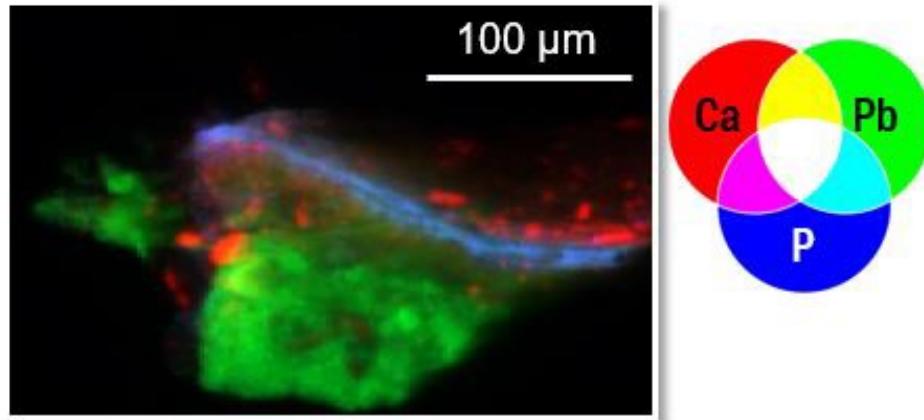
- Provide users with post azimuthal integration maps in HDF5, with Jupyter notebooks taking care of PyFAI integration of 2D maps.

## ➤ Users

- Scientists doing experiments in cultural heritage.

## ➤ Contacts

- Loic + Scientist



*Fig.1 : SR- $\mu$ -XRF map (ID21) revealing the presence of a leadfosphate compound in the stratigraphy of a sample from a Leonardo da Vinci painting. SR- $\mu$ XRD (ID13) analysis revealed the compound to be phosphohedyphane,*



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## Use Case 3

# Carboxysomes

### Carboxysomes

**WIKIPEDIA**  
The Free Encyclopedia

are bacterial microcompartments (BMCs) consisting of polyhedral protein shells filled with the enzymes ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO)—the predominant enzyme in carbon fixation and the rate limiting enzyme in the Calvin cycle—and carbonic anhydrase.

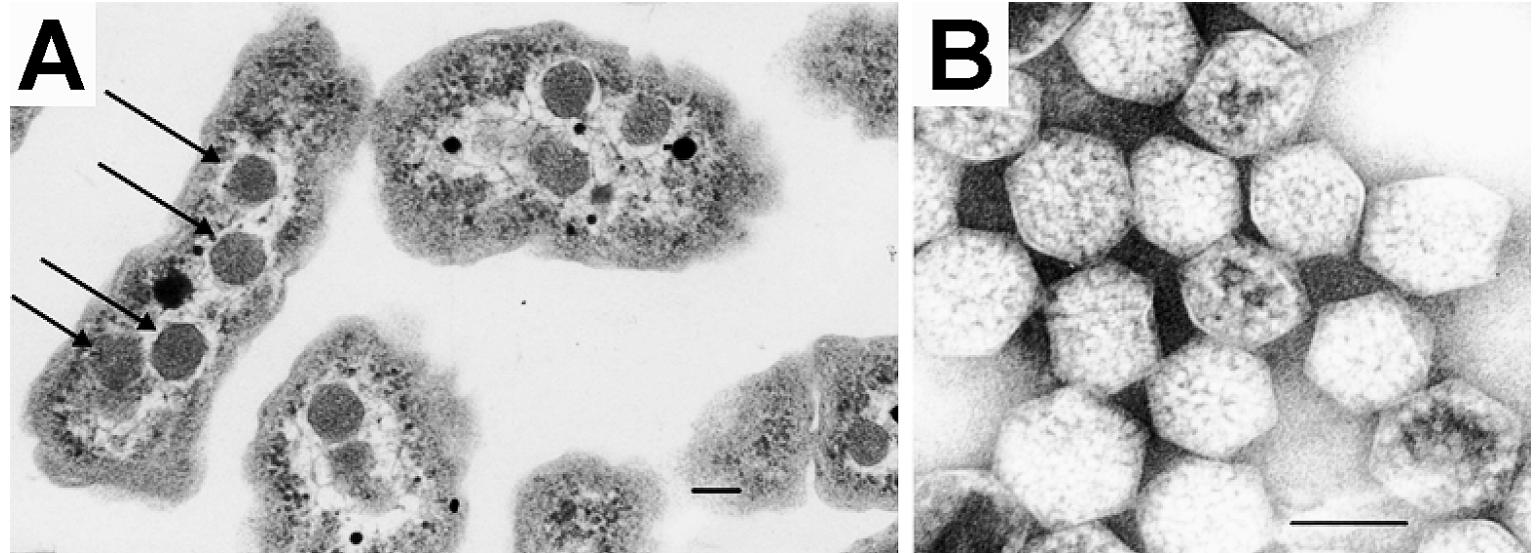


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# Use case: Carboxysomes

- **Institutes:**
  - ELI, XFEL, DESY
- **Scientist:**
  - M.Hantke, J.Hajdu, F.Maia, A.Barty et al.
- **Objective:**
  - publish results as Open Data
- **Request:**
  - data published in CXIDB but should be possible via institute repository in the future

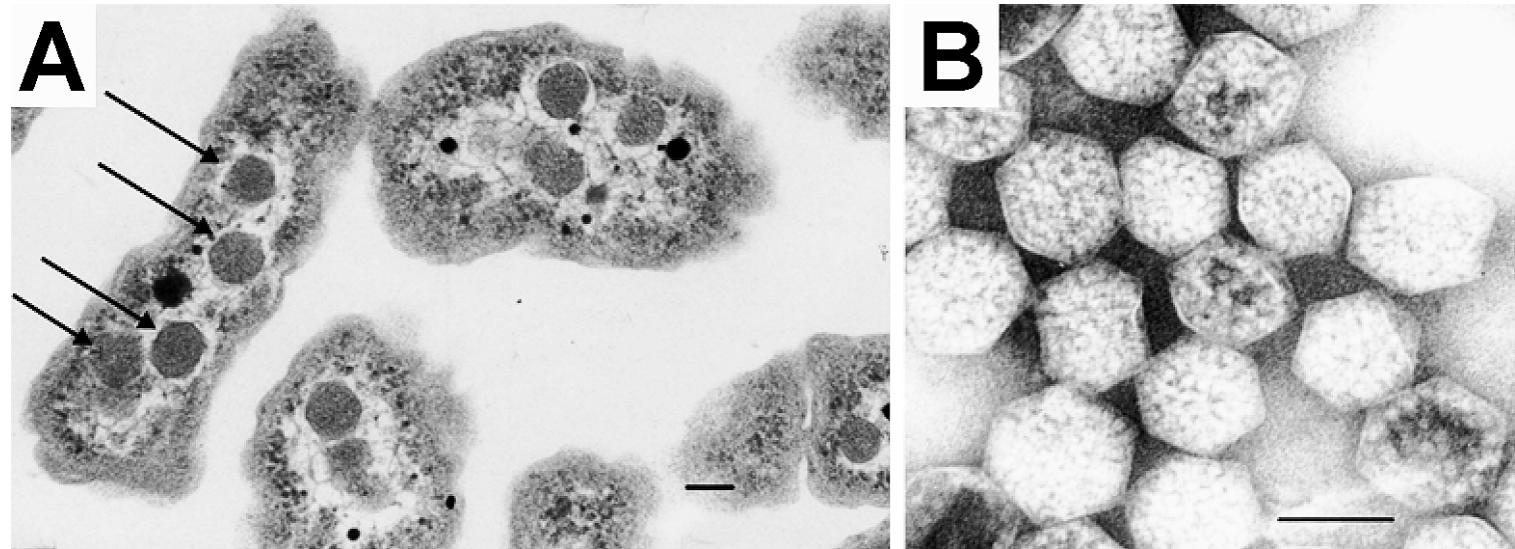


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# Use Case: Carboxysomes (Cont.)

- **Demonstrates**
  - Open Data,
  - Data portal,
  - HDF5 data format
  - Search API
- **Work packages**
  - WP2, WP3, WP4,
- **Beneficial:**
  - Any user community which needs to publish open data and make it FAIR for their community and/or search for data
- **Potential:**
  - 10000s of users



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# Use Case: Carboxysomes (Cont.)

## ➤ Demonstrates

- Open Data,
- Data portal,
- HDF5 data format
- Search API

## ➤ Work packages

- WP2, WP3, WP4,

## ➤ Beneficial:

- Any user community which needs to publish open data and make it FAIR for their community and/or search for data

## ➤ Potential:

- 10000s of users

The screenshot shows the CXIDB website interface. At the top, there is a logo for "CXIDB Coherent X-ray Imaging Data Bank" featuring stylized orange and blue squares. Below the logo is a navigation bar with links: Home, Mission, CXI File Format, Browse Data, Resources, Sponsors, and Contact Us. The main content area displays a dataset page for "CXIDB ID 25". The page has three main sections: "Deposition Summary", "Publication Details", and "Experimental Conditions".

**Deposition Summary**

|                  |   |
|------------------|---|
| Depositor:       | Max F. Hantke   |
| Contact:         | han...@xray.bmc.uu.se   |
| Deposition date: | 2014-11-17  |
| Last modified:   | 2016-07-28  |
| DOI:             | <a href="https://doi.org/10.11577/1169545">10.11577/1169545</a> |

**Publication Details**

|          |   |
|----------|---|
| Title:   | High-throughput imaging of heterogeneous cell organelles with an X-ray laser    |
| Authors: | Max F. Hantke et al.  |
| Journal: | Nature Photonics  |
| Year:    | 2014  |
| DOI:     | <a href="https://doi.org/10.1038/nphoton.2014.270">10.1038/nphoton.2014.270</a> |

**Experimental Conditions**

**Description**

Preprocessed detector images that were used for the paper "High-throughput imaging of heterogeneous cell organelles with an X-ray laser". The CXI file contains the entire recorded data - including both hits and blanks. It also includes down-sampled images and LCLS machine parameters. Additionally, the Cheetah configuration file is attached that was used to create the pre-processed data.

This dataset is part of the [Scientific Data XFEL Biodata collection](#).

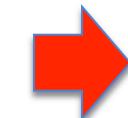


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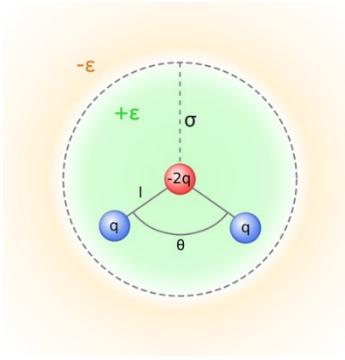


# Reusability of data example

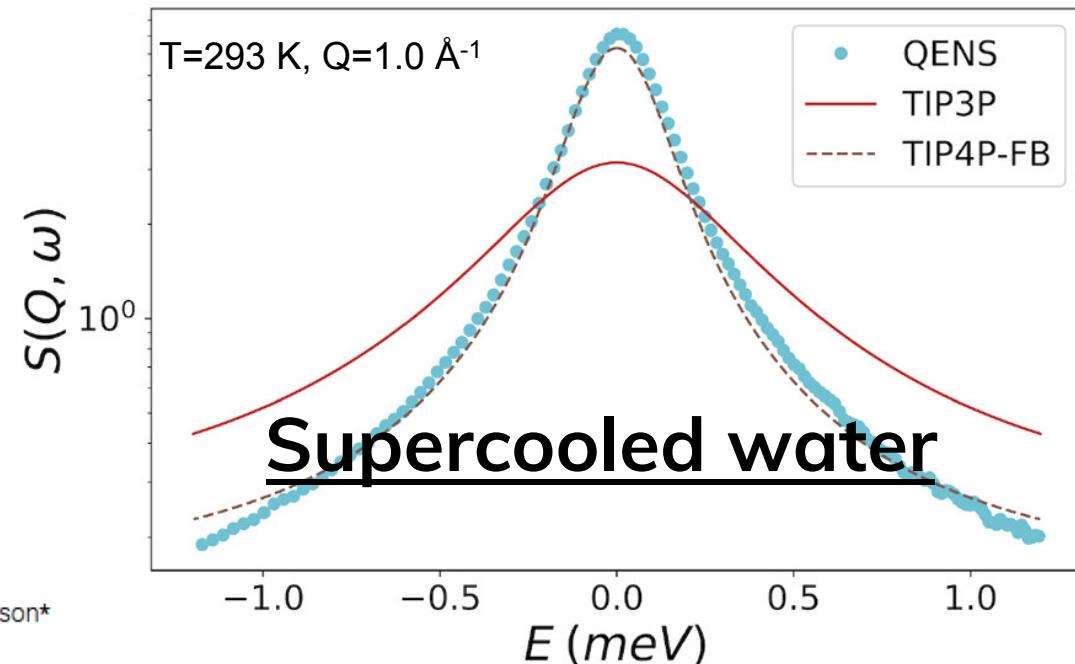
QENS data published in 2011  
(Qvist, Schober & Halle, JCP 2011)



Raw data was not publicly available ...



Reused in 2020 by different group of scientists for evaluating water models



RETURN TO ISSUE | < PREV PHYSICAL INSIGHTS IN... NEXT >

## Dynamical Accuracy of Water Models on Supercooling

Thomas O. Farmer\*, Anders J. Markvardsen, Thomas H. Rod, Heloisa N. Bordallo, and Jan Swenson\*

Cite this: *J. Phys. Chem. Lett.* 2020, 11, 18, 7469–7475

Publication Date: August 11, 2020

<https://doi.org/10.1021/acs.jpclett.0c02158>

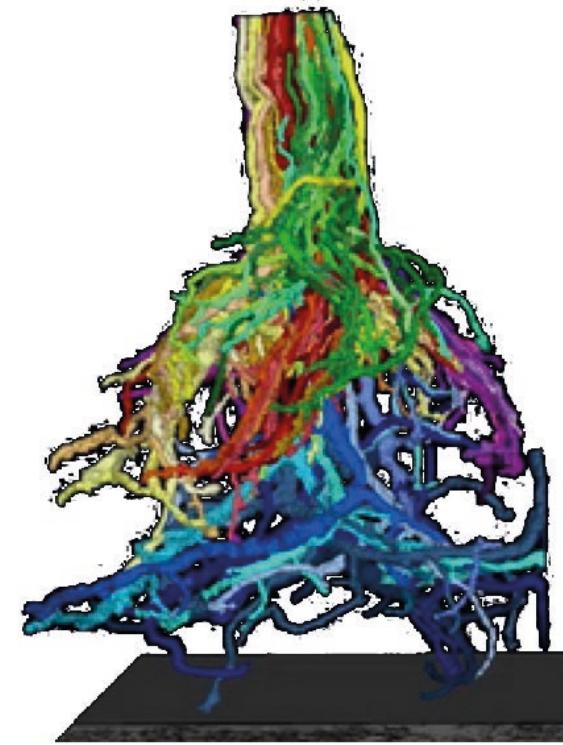
Copyright © 2020 American Chemical Society

[RIGHTS & PERMISSIONS](#)

Article Views 200 | Altmetric 1 | Citations -  
[LEARN ABOUT THESE METRICS](#)

credits – Thomas Rod

## Use Case 4



## Parkinson's disease & Mapping the brain



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# Use Case: Parkinson's disease & Mapping the brain

➤ **Parkinson's disease**

➤ **Institute:**

➤ CERIC-ERIC, ESRF

➤ **Scientist**

➤ L.Casalis et al.

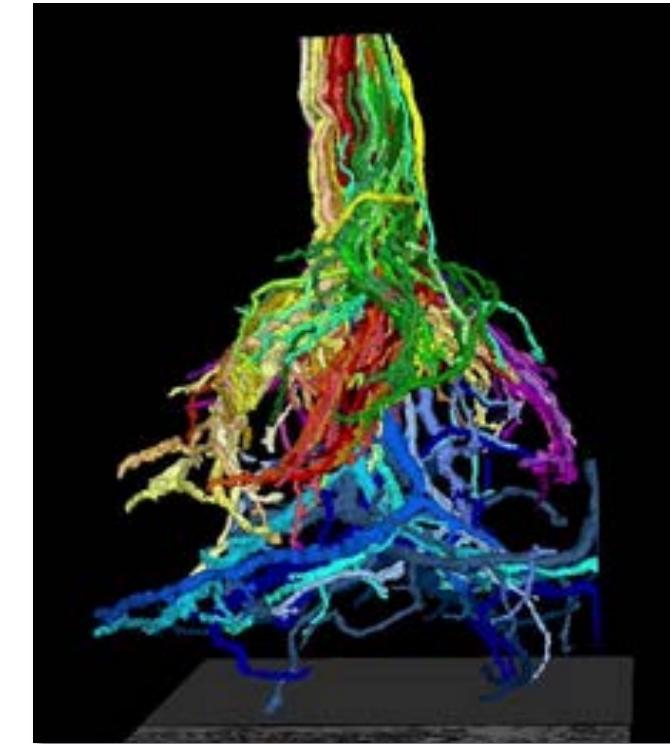
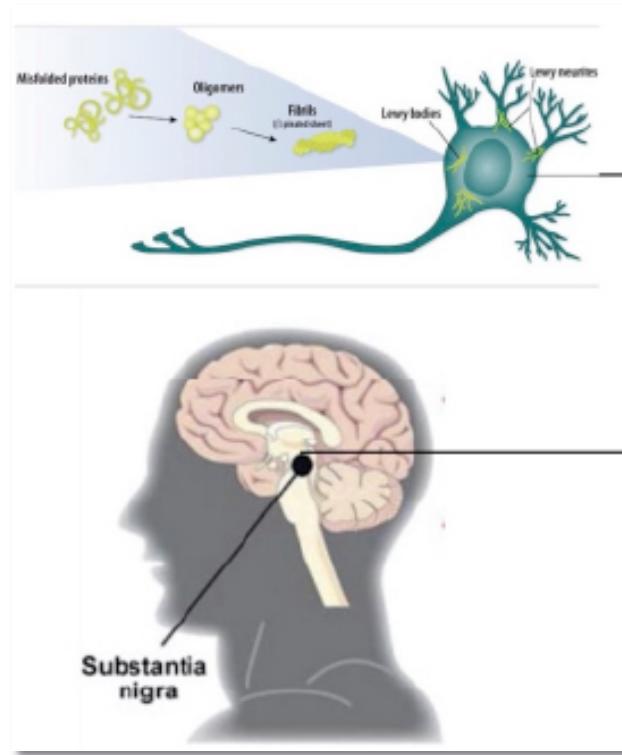
➤ A.Pacureanu et al.

➤ **Objective:**

➤ Mapping of neurons in 2d and 3d

➤ **Request**

➤ Make large data volumes available as Open Data



<https://doi.org/10.1039/D0NR00287A>

Original Title : *Parkinson research sheds lights on the iron-mediated interaction between alpha-synuclein and membrane models*

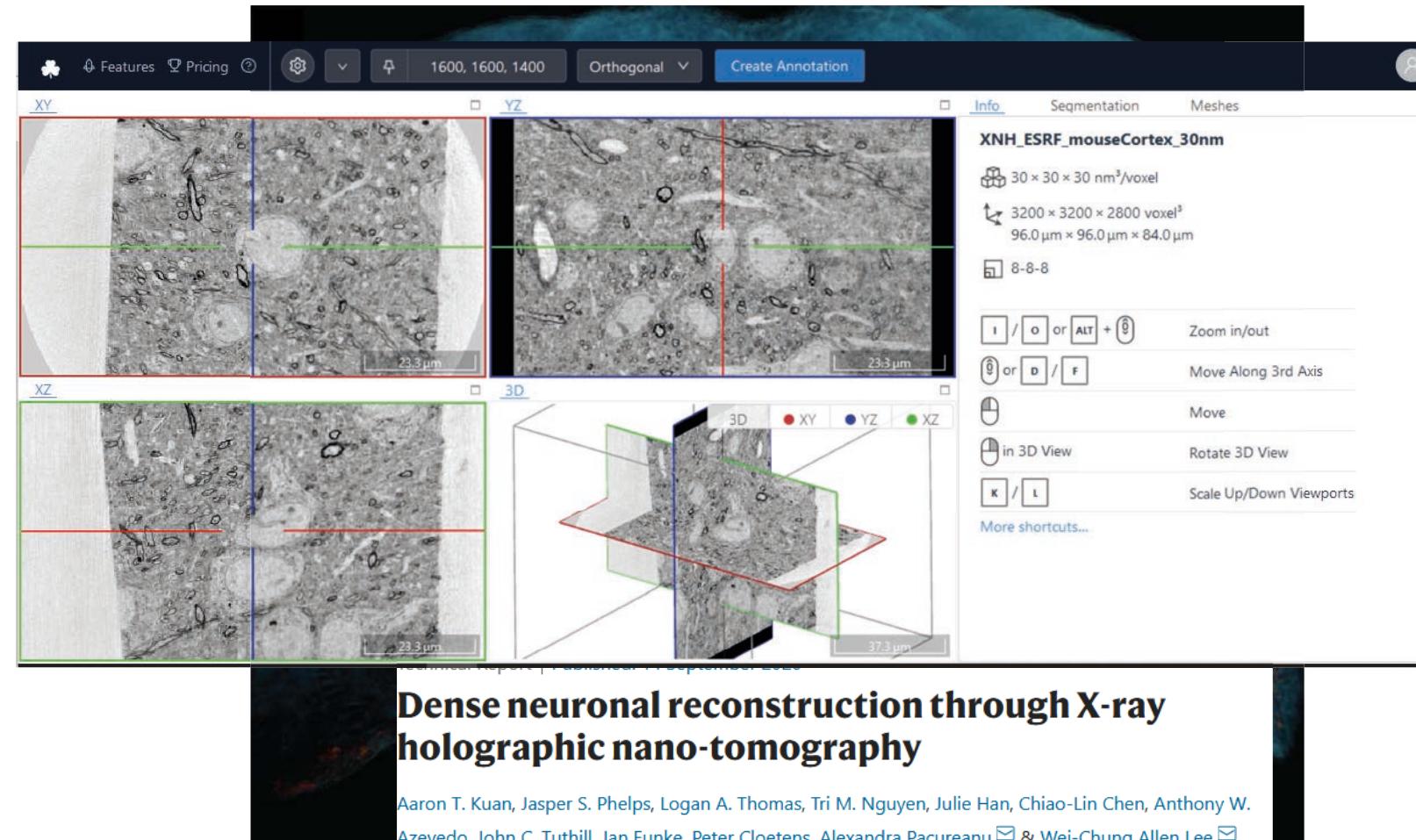


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# Use Case: Mapping the brain (cont.)

- **Demonstrates**
  - Open data, big data download, data portal, HDF5 data format, search API
- **Work packages**
  - WP2, WP3, WP4, WP6
- **Beneficial**
  - Any user community which needs to publish open data and make it FAIR for their community
- **Potential**
  - All users



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# Use Case 5

## Remote access



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# Use Case: Remote Access

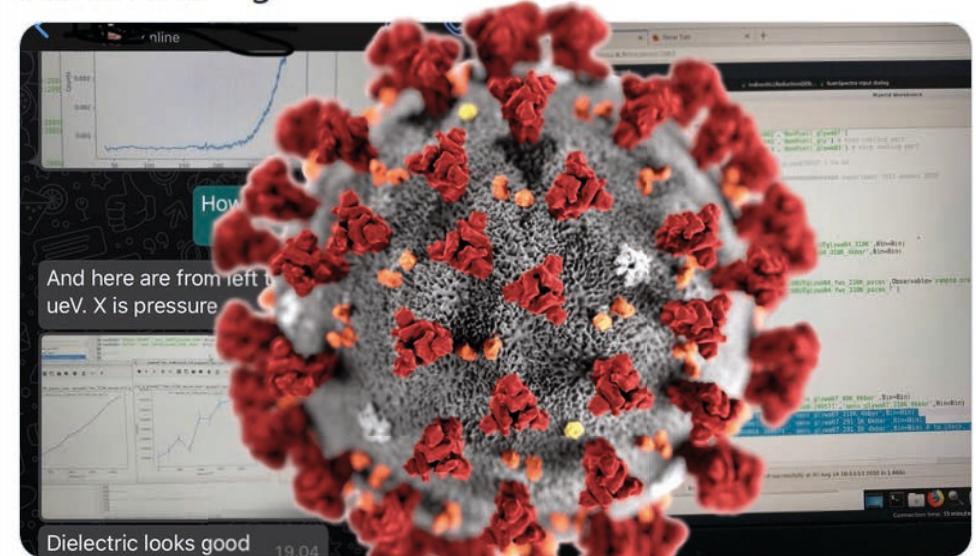
- **Remote Access**
- **Institute**
  - ILL (VISA), CERIC-ERIC + ELETTRA (RAFEC), ESRF (ICAT+Guacamole)
- **Scientist**
  - All remote users
- **Objective**
  - Run experiments remotely without coming on site!
- **Request**
  - Make all data services remote!

← Tweet



Kristine Niss  
@KristineNiss

Combining the @ILLGrenoble remote solution with chat and video conferencing with my onsite PhD student and dedicated local collaborator. Makes me miss the beamtime thrill - but it so much better than nothing. Thx for making it work!



8:36 PM · Aug 14, 2020 from Copenhagen, Denmark · Twitter for iPhone

1 Retweet and comment 5 Likes



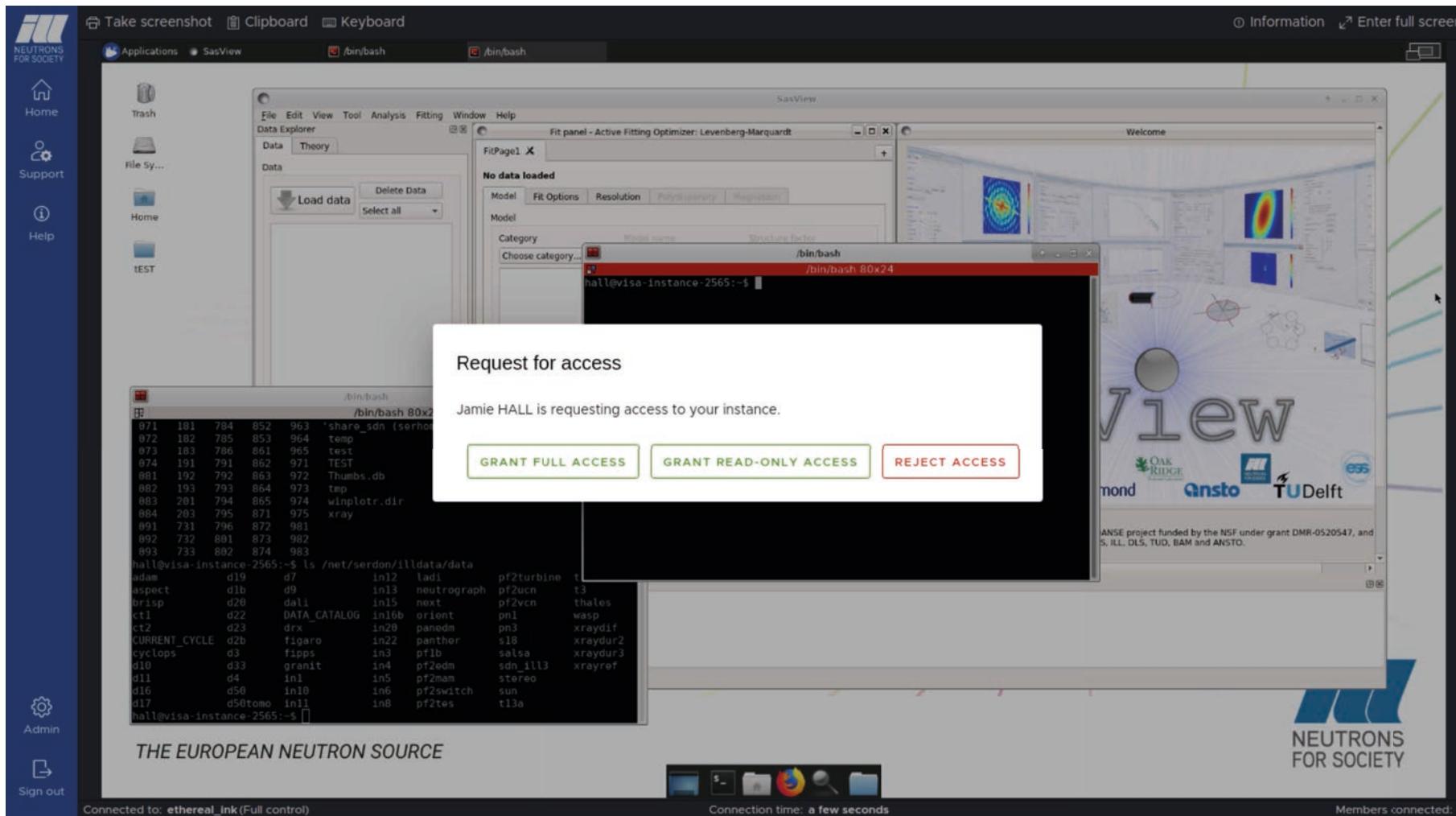
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# Use Case: Remote Access (cont.)

## VISA Remote Access @ ILL

- Developed for experiments post-COVID-19
- In production
- Multiple features will be re-used in PaNOSC portal



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# Use Case: Remote Access (cont.)

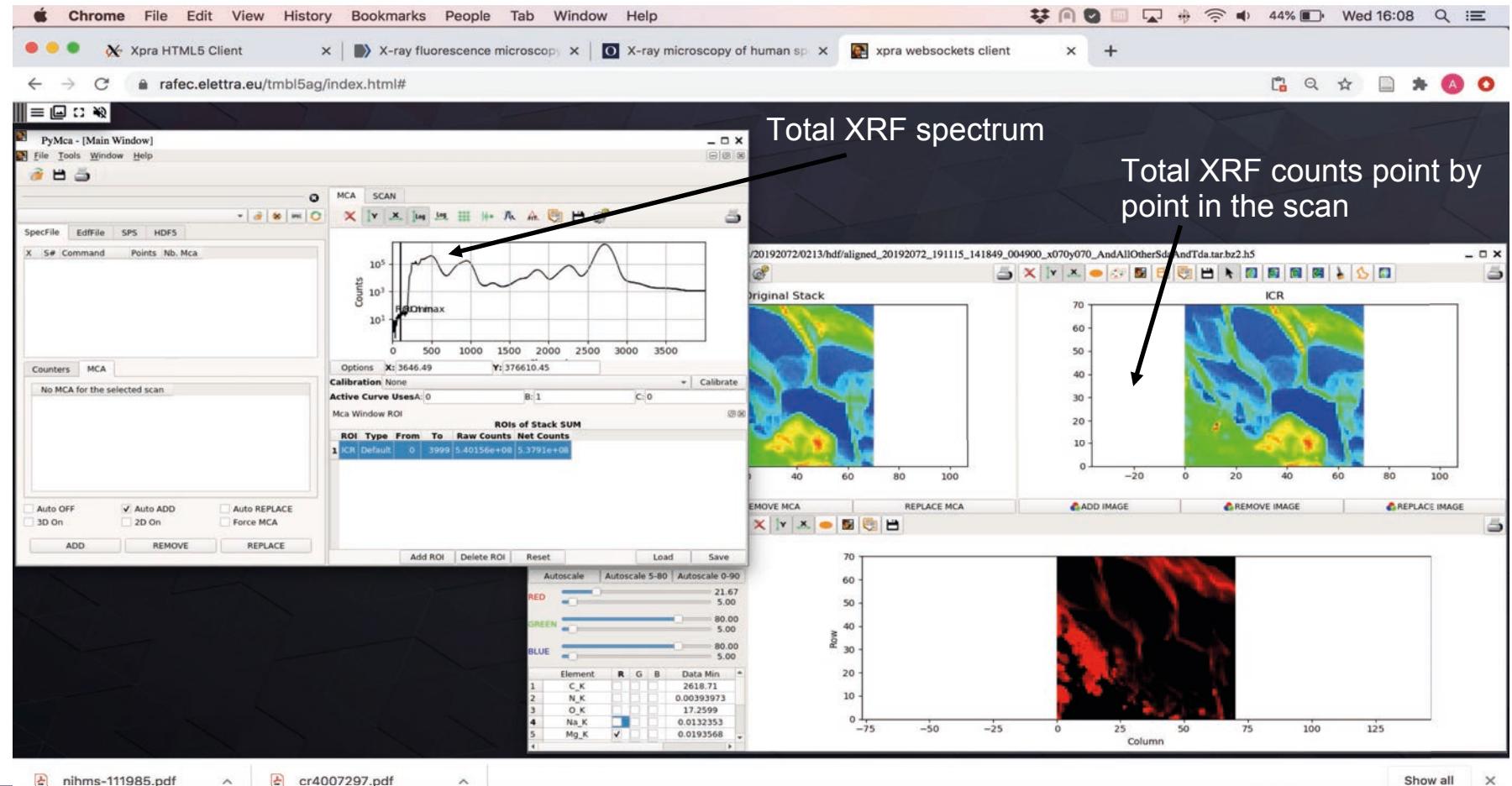
TwinMic @ Elettra synchrotron (CERIC-ERIC)  
Visualisation of XRF maps by PyMCA software

Both beamline scientists  
and the users can access  
the data, launch the data  
analysis, and post-  
process data, remotely



- More rapid analysis
- Users can work in parallel, analysing different datasets

*Impact of Zn excess on biomineralization processes in Juncus acutus grown in mine polluted sites*, Medas D., De Giudici G., Pusceddu C., Casu M.A., Birarda G., Vaccari L., Gianoncelli A., Meneghini C., Journal of Hazardous Materials, 2019, published online, DOI: <https://doi.org/10.1016/j.jhazmat.2017.08.031>



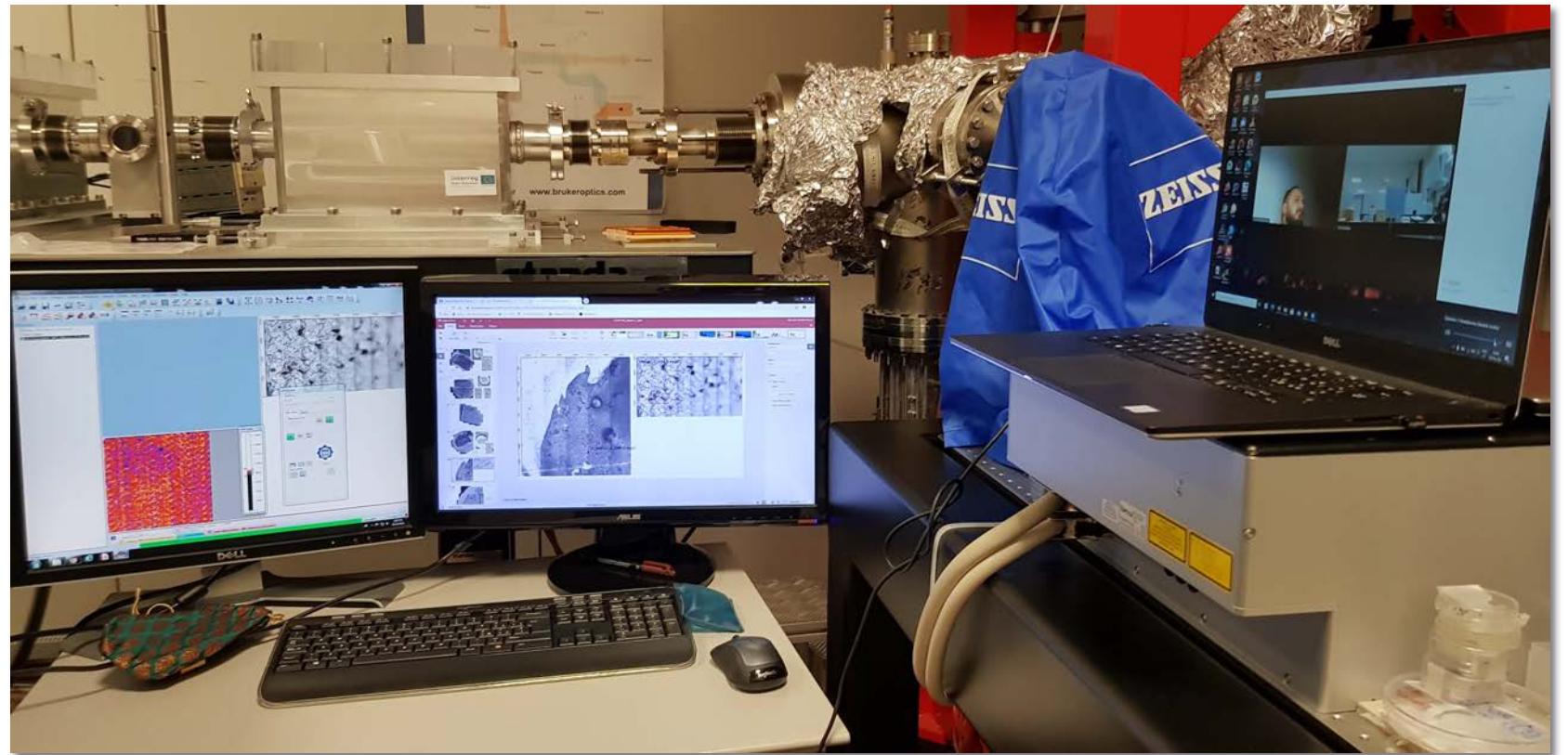
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# Use Case: Remote Access (cont.)

## Remote access to Synchrotron Infrared Source for Spectroscopy and Imaging - SISSI @Elettra synchrotron (CERIC-ERIC)

Remote connection of the user with the SISSI beamline staff and data analysis software, using RAFEC



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# Use Case 6    Simulation



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# Use Case: Simulation

## Simulation

### ➤ Institutes

- EuXFEL, ESS, CERIC-ERIC,  
CERIC-ERIC, ELI, ESRF

### ➤ Scientist

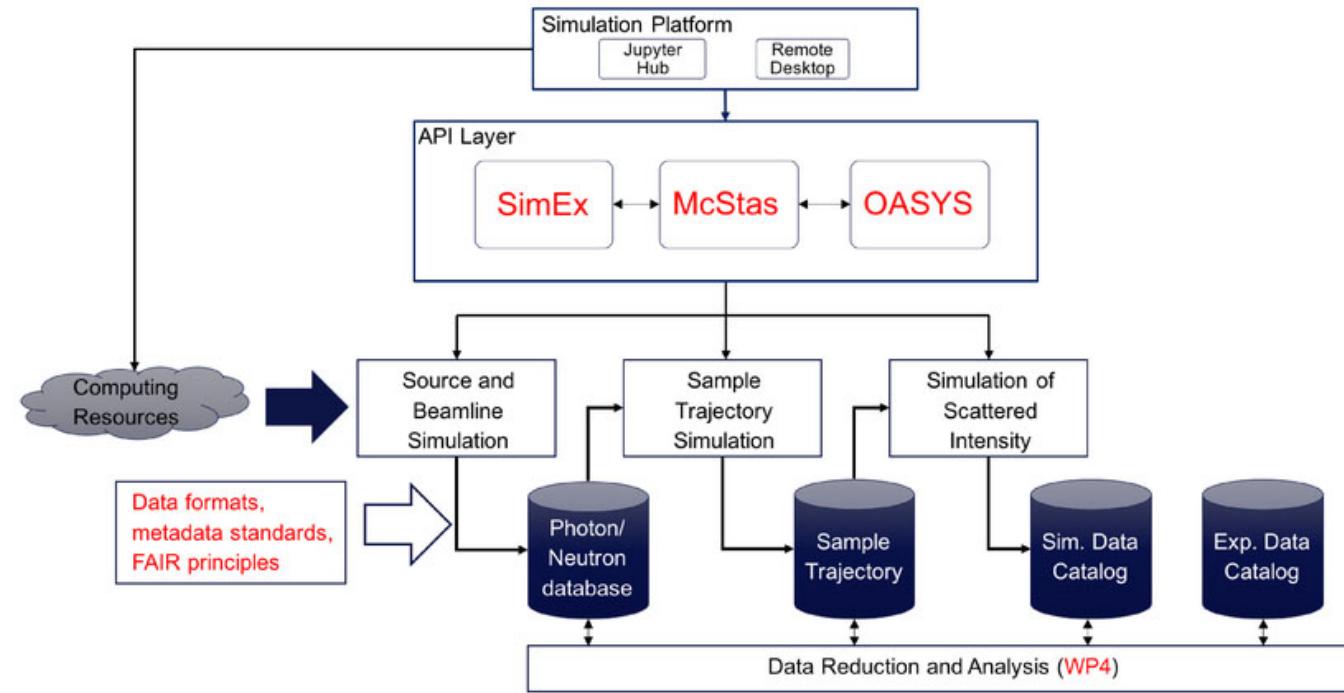
- All beamline scientists + users  
who need data simulation

### ➤ Objective

- Design beamlines and simulate  
data before and after  
experiments

### ➤ Request

- Make all simulation data  
services available via Jupyter  
and WP4 + EOSC!



21 August 2020

## VINYL: The Virtual Neutron and x-ray Laboratory and its applications

J. C. E, A. Hafner, T. Kluyver, M. Bertelsen, M. Upadhyay Kahaly, Z. Lecz, S. Nourbakhsh, A. P. Mancuso, C. Fortmann-Grote

Author Affiliations +

Proceedings Volume 11493, Advances in Computational Methods for X-Ray Optics V; 114930Z (2020)

<https://doi.org/10.1117/12.2570378>

Event: SPIE Optical Engineering + Applications, 2020, Online Only

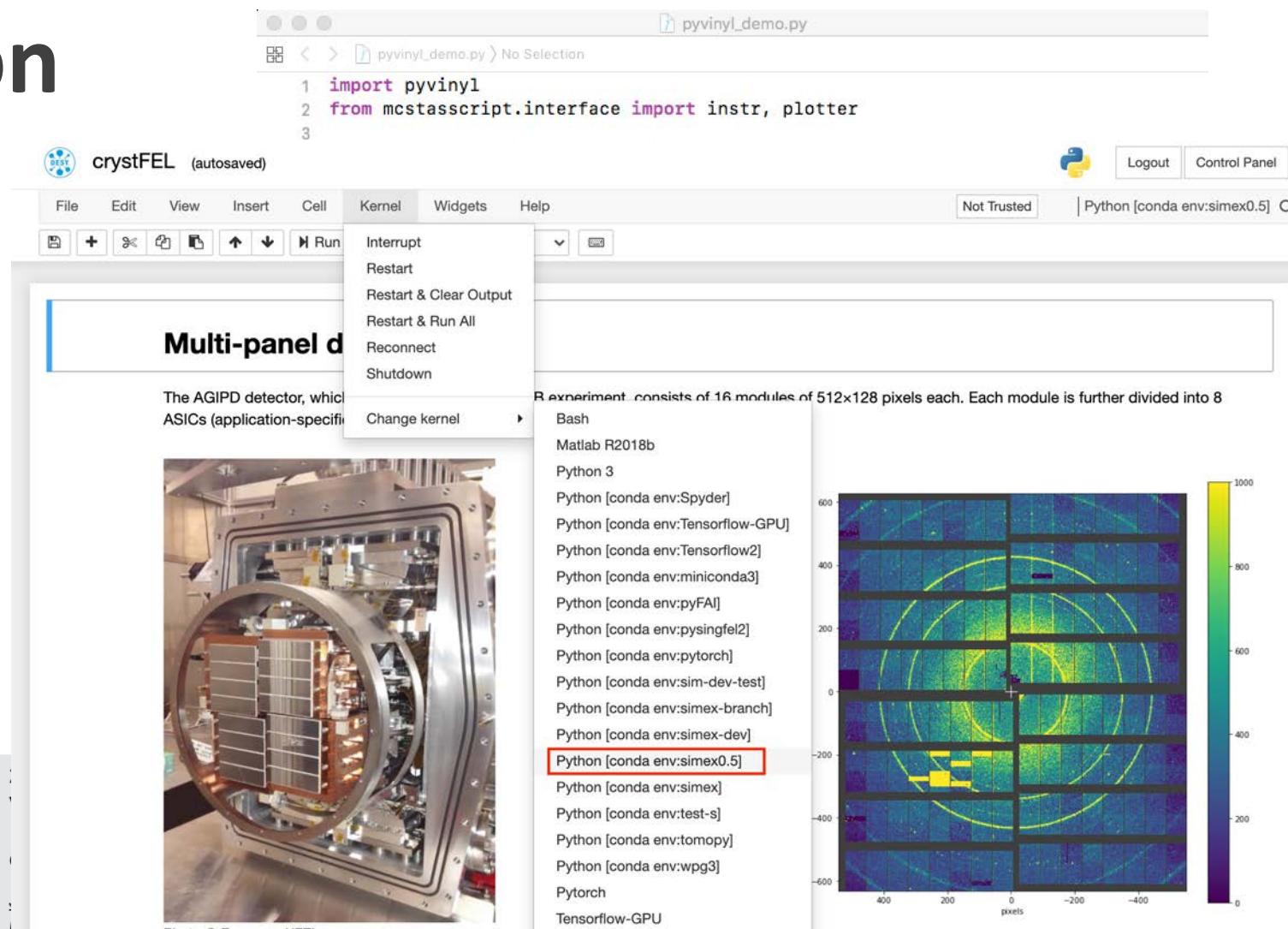


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# Use Case: Simulation

- **Demonstrates**
  - Simulation, analysis portal, open data
- **Work packages**
  - WP2, WP3, WP4, WP5, WP6
- **Beneficial**
  - Any user community which needs to simulate data
- **Potential**
  - All users



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# Use Case: Simulation

## ➤ Demonstrates

- Simulation, analysis portal, beamline design, remote access

## ➤ Work packages

- WP4, WP5, WP6

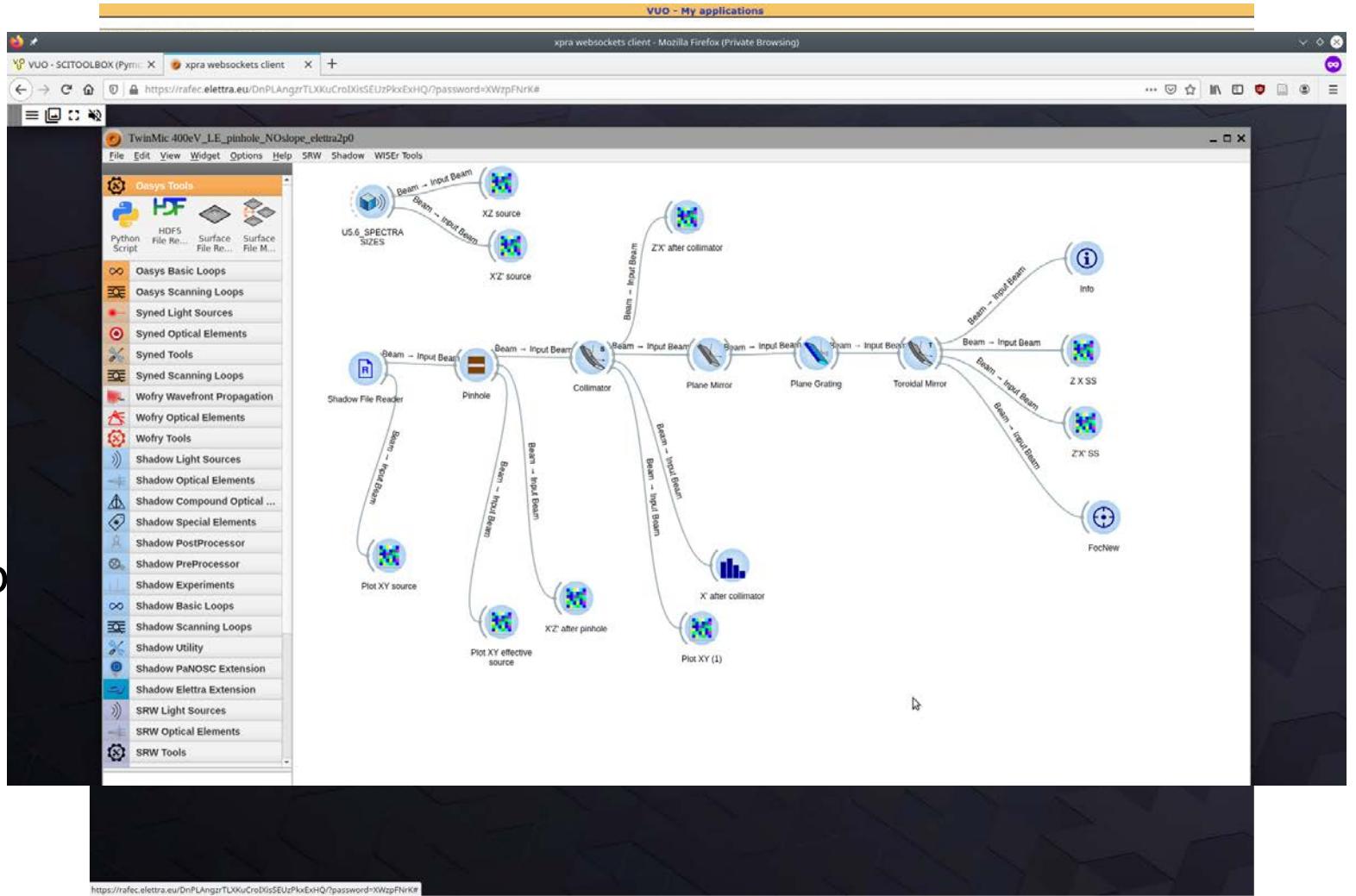
## ➤ Beneficial A

- Any beamline scientist community who needs to design their beamline

## ➤ Potential

- All beamline scientists

Selection of an analysis environment (RAFEC @ CERIC-ERIC)

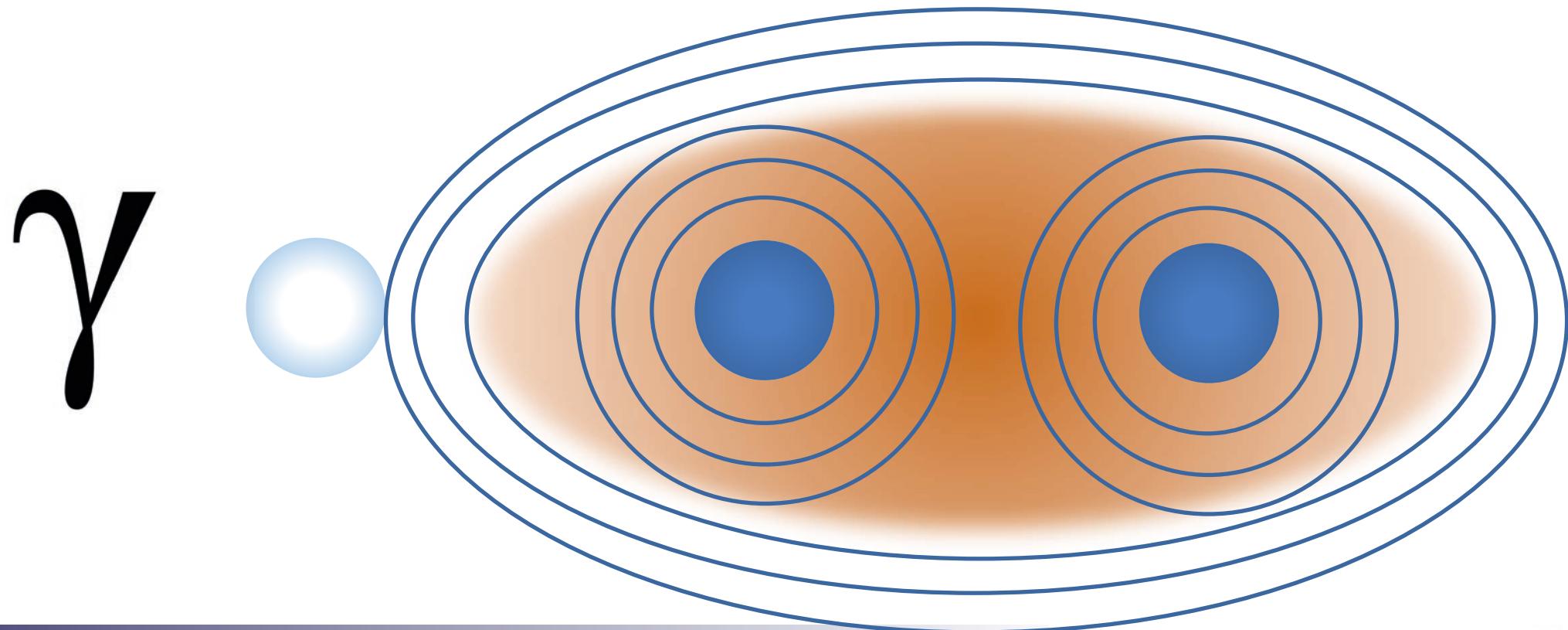


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# Use Case 7

## Physics : Electron Birth time delay



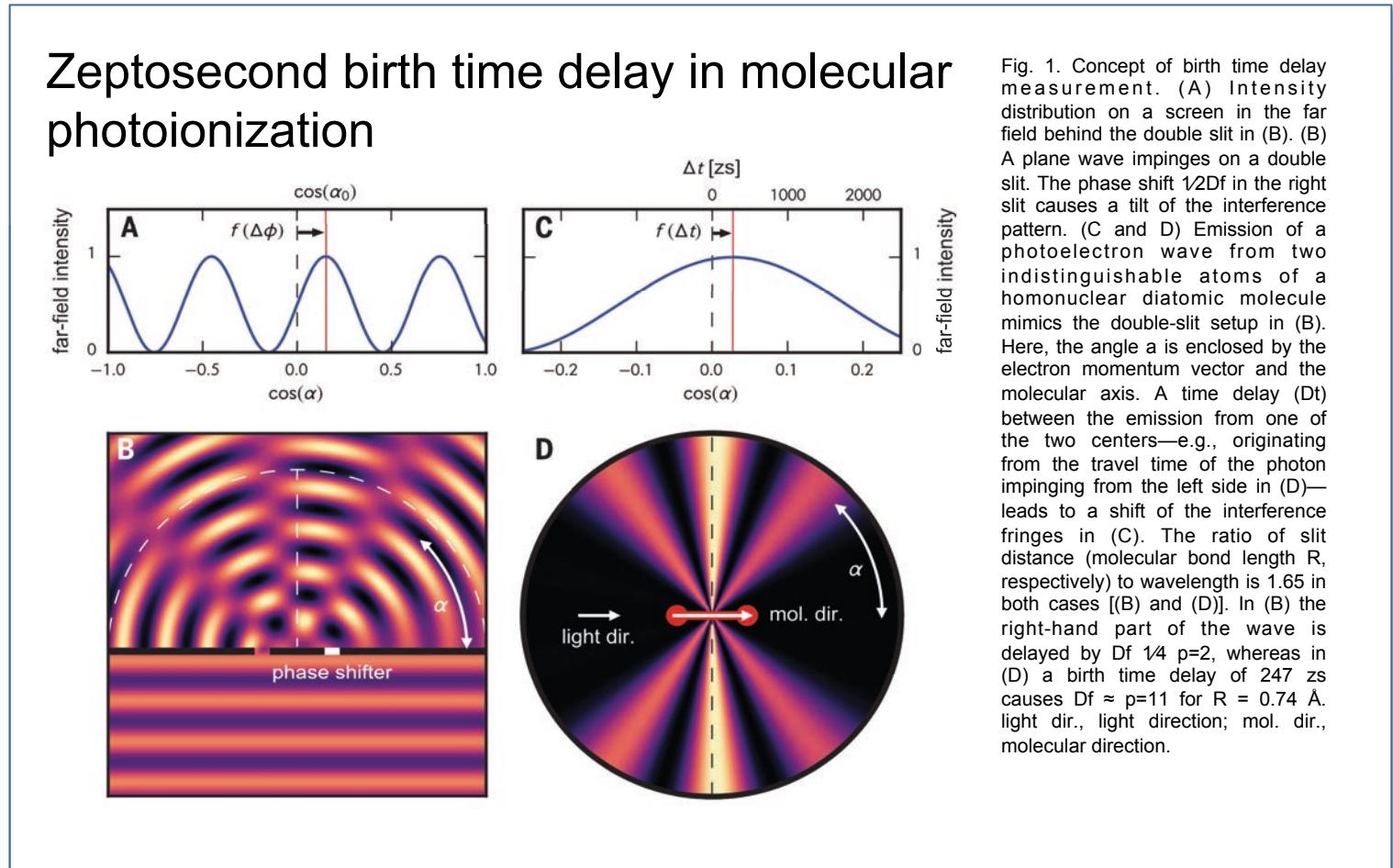
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# Use case: Zeptosecond birth time delay

Zeptosecond birth time delay in molecular photoionization, Sven Grundmann, ...., Florian Trinter et al.

- Physics
- Institute
  - ✓ PETRAIII, UNI Frankfurt
- Scientist:
  - ✓ Grundmann et al.
- Objective
  - ✓ Measuring birth time delay
- Request:
  - ✓ Providing local persistent data repository.
  - ✓ Automated Indexing
  - ✓ DOI generation



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# Use case: Zeptosecond birth time delay

Zeptosecond birth time delay in molecular photoionization, Sven Grundmann (UNI Frankfurt), ...., Florian Trinter (DESY) et al.

Interview with PI, Sven Grundmann (Nov 6, 2020)

- Good example of ‘REUSABLE’.
  - ✓ They found the effect in data not taken for that purpose.
- Sven never heard about the FAIR principles!
- He published the data because it’s a condition when publishing in “SCIENCE”
- But he said, that “I like the idea to make data available for others”.
- “*The ‘proposal portal’ should indicate FAIR options!*”
- “*I would have appreciated if there would have been a mechanism at PETRA III to automatically*”:
  - ✓ Store the data in a local repository (sustainably),
  - ✓ Index the data in (one or more) catalogues,
  - ✓ provide DOIs

The screenshot shows a dataset page on OpenAIRE. At the top, it displays the publication date as June 18, 2020, and indicates 'Dataset' and 'Open Access'. Below this, the title 'Zeptosecond Birth Time Delay in Molecular Photoionization' is shown, along with the author's name, Sven Grundmann. A note states that these datasets are supplements to the publication of the same title. A table lists two files: 'Fig2\_data.txt' (257.8 kB) and 'Fig3\_data.txt' (26.6 kB), each with a download button. To the right, there are statistics: 121 views and 42 downloads. Below the table, the OpenAIRE logo is visible. Further down, the dataset is categorized as 'Research Data . Dataset . 2020' and titled 'Zeptosecond Birth Time Delay in Molecular Photoionization'. It includes author information ('Grundmann, Sven'), an 'OPEN ACCESS' button, and publication details ('Published: 18 Jun 2020', 'Publisher: Zenodo'). On the far right, there are links for 'See more details...', 'Indexed in OpenAIRE', 'Publication date: June 18, 2020', 'DOI: 10.5281/zenodo.3899920', and 'License (for files)'.



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# Dissemination



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# Video Releases - ExPaNDS



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# Video Release



Partners / Projects / Initiatives involved:



Watch the video:  
<https://youtu.be/ekn0qicVFJM>



LINKED ACTIVITIES:

- New mailing lists for queries on DOIs: [pan-data-doi@panosc.eu](mailto:pan-data-doi@panosc.eu)
- Action advocating sci journals to include data DOIs in their published articles



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# Dissemination activities on PaNOSC achievements

Interview on the work carried out in the frame of **PaNOSC WP6** – EOSC integration, towards the set-up of a federated authorization and authentication infrastructure (AAI) for the users of photon and neutron sources, which will allow a seamless access to data and data services.



Full interview: <http://bit.ly/36ghSwJ>

Interview with prof. Hans Fangohr (leader of **PaNOSC WP4**) on OSCOVIDA, the Open Science COVID Analysis website (<http://oscovida.github.io>) that collects and shows analysis plots of COVID19 cases and deaths to better understand the time development of the pandemic and the measures taken in all countries worldwide.



Full interview: <https://bit.ly/2Xm07Lj>

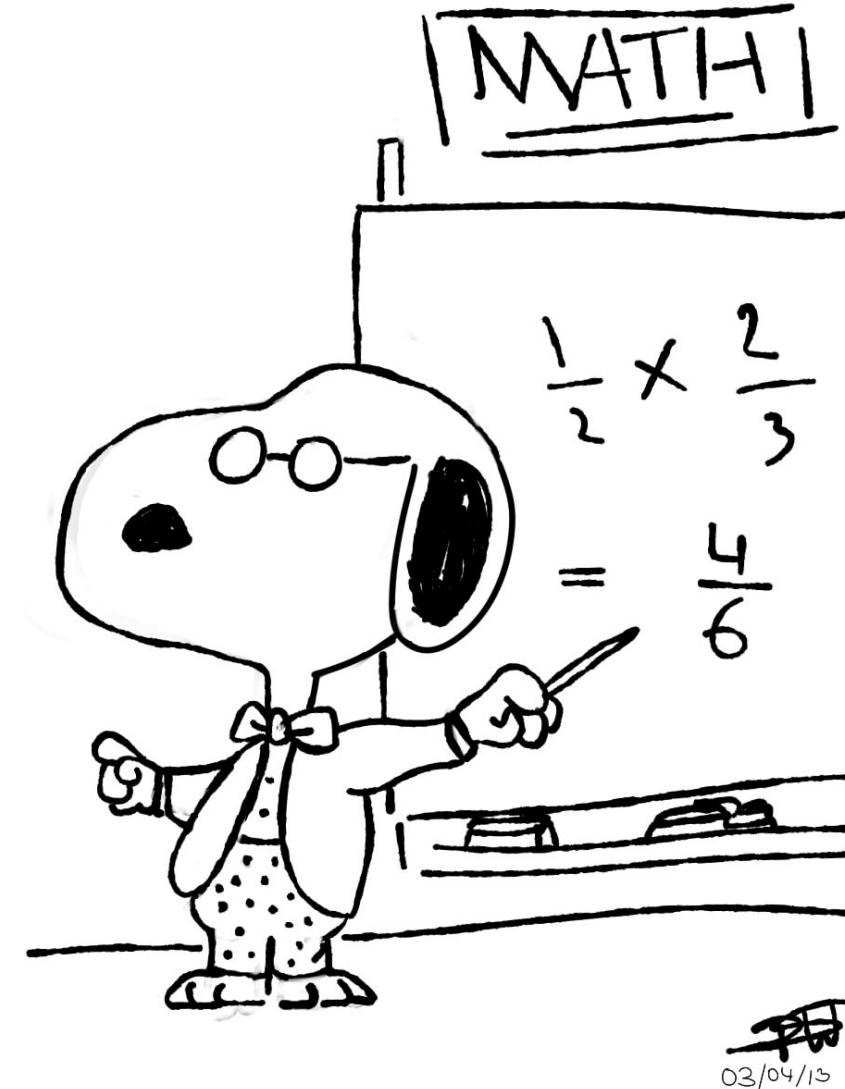
Articles and interviews were published on the PaNOSC website and distributed to the PaNOSC network, via direct email and social media.



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# Teaching and Training



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## External Provider Repositories



# The PaN Training Portal

## Scientific content manager



### Training Events

**Catalogue of training events** of interest for the PaN community  
(Online and F2F events)

- Workshops
- MOOCs
- Summer schools
- Users' meetings



### Training Material

**Catalogue of training materials** of interest for the PaN community

- External links to content provider's website or repositories
- Github
  - Zenodo,
  - Open Aire



## E-Learning Platform

**Tool available to create and store training material**

- Moodle
- Simulation tools
- MediaWiki
- Notebook Integration in preparation



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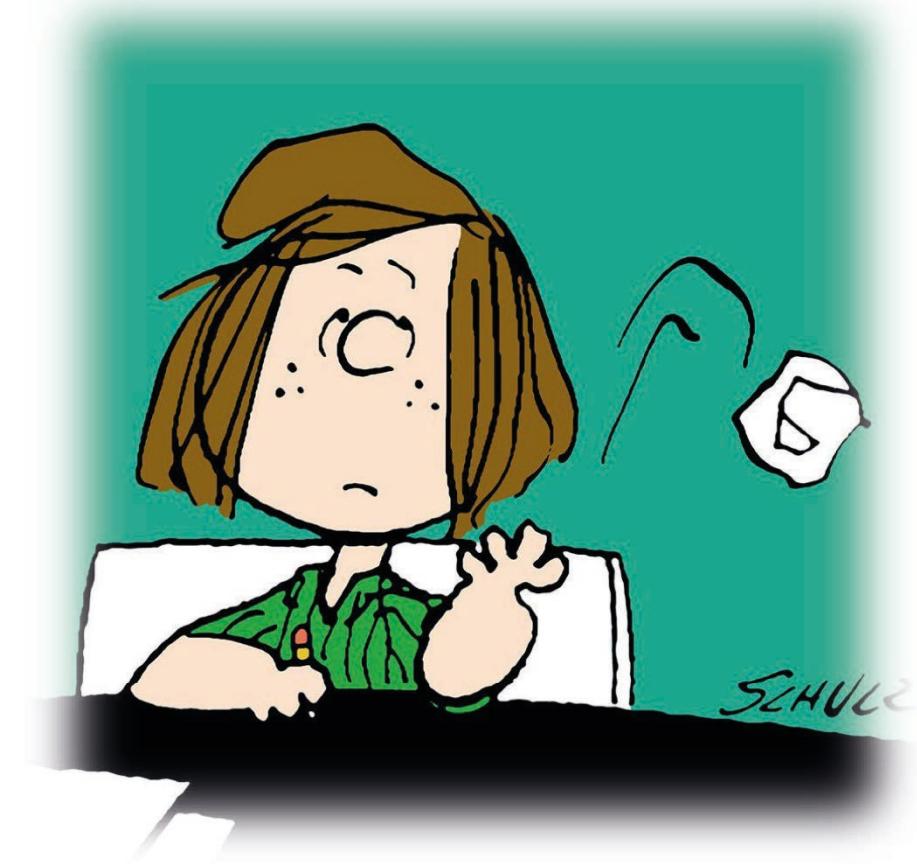


# Unified access to facility resources

DevOps

Data Management

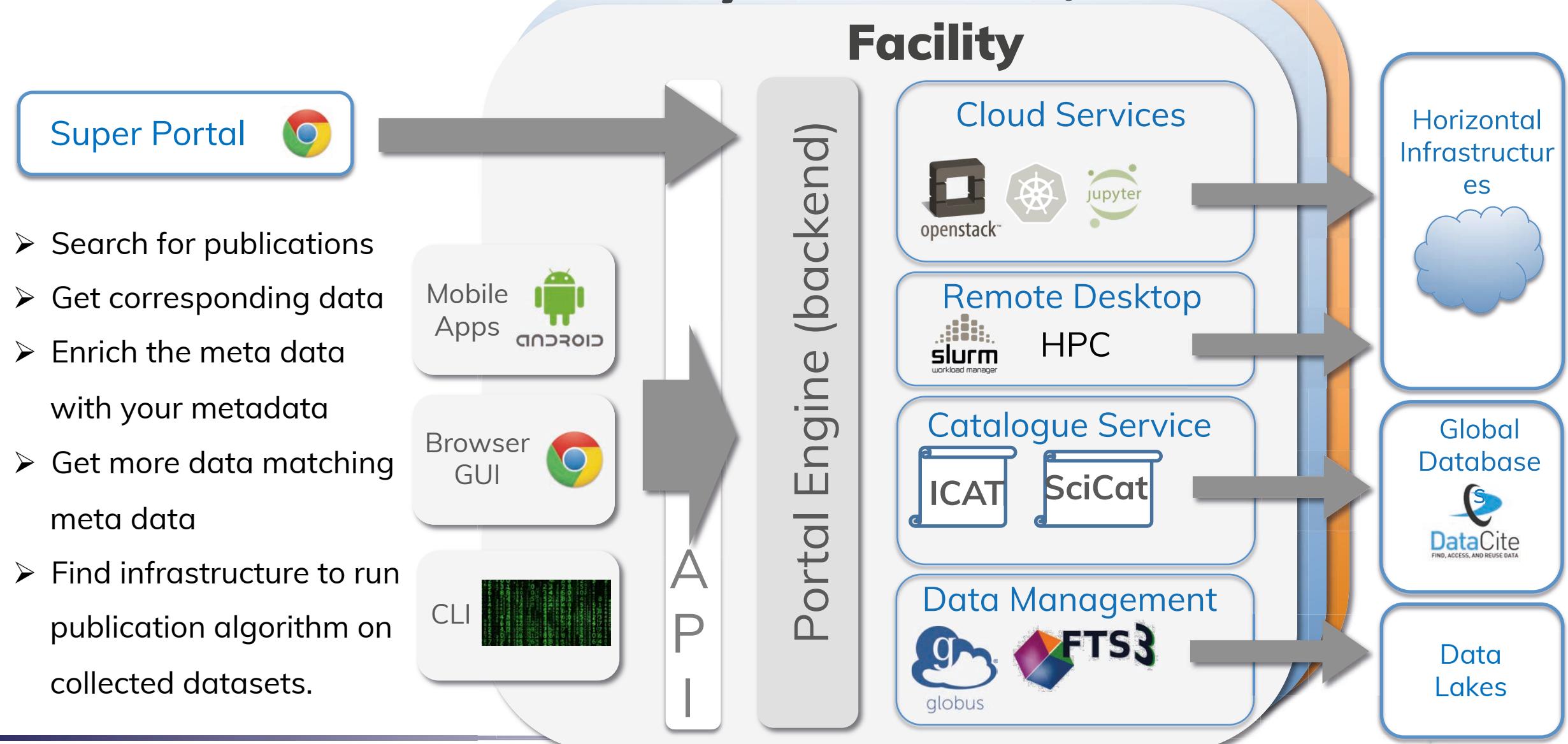
AAI



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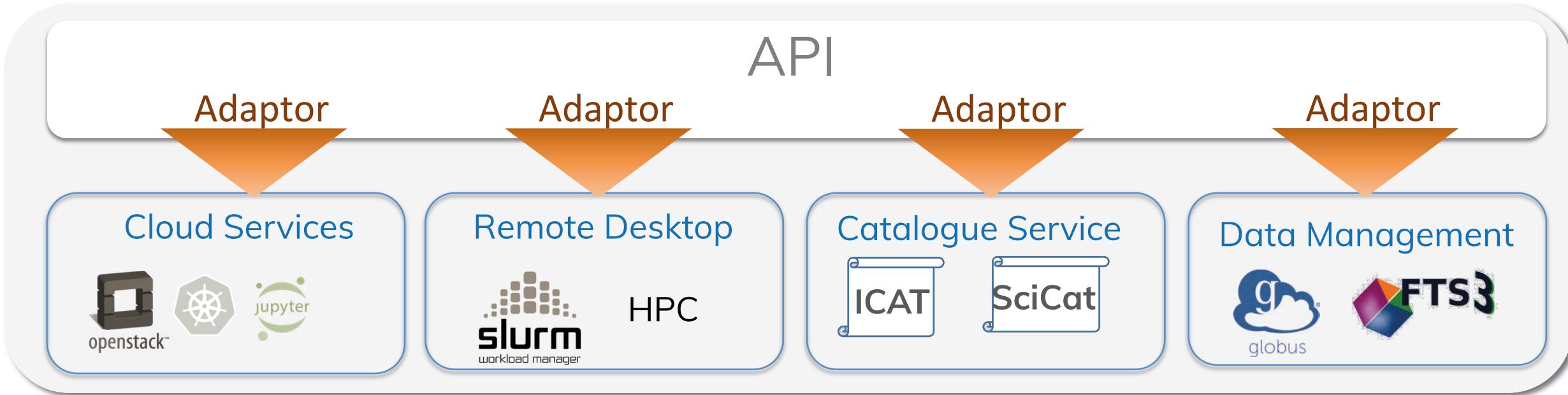
# Unified access to facility resources, The Portal



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# BUT : This only works if facilities play along.



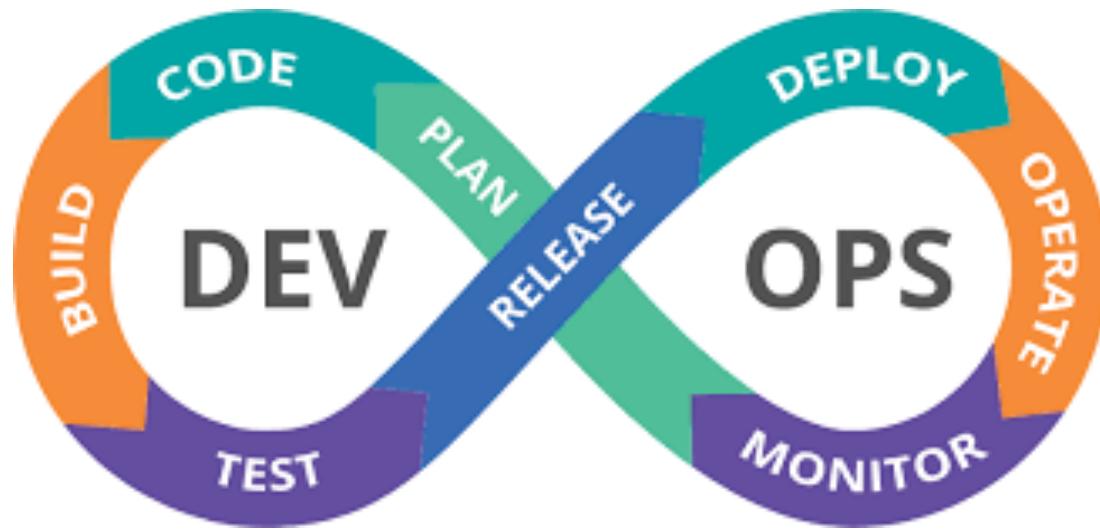
- Facilities have to provide adapters to their services!
- Facilities have to revisit their security/firewall policies!
- Facilities have to open their data to Cloud Mechanisms!
- Facilities have to spend the money they get from PaNOSC and ExPaNDS for ICT integration work!
- This might be the last chance that we get those efforts paid by the EC.



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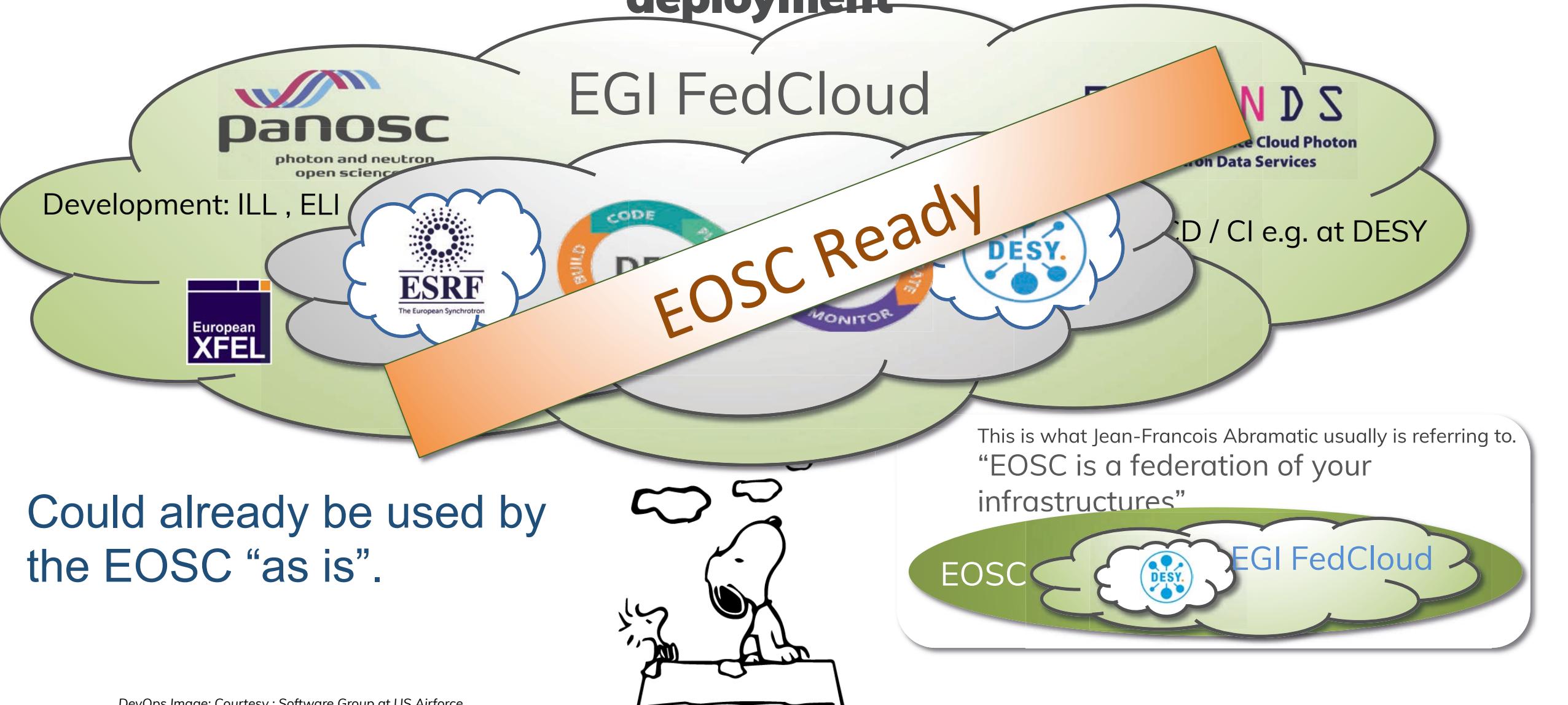
# Common DevOps on a horizontal infrastructure



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# ExPaNDS and PaNOSC contributing to horizontal infrastructure deployment



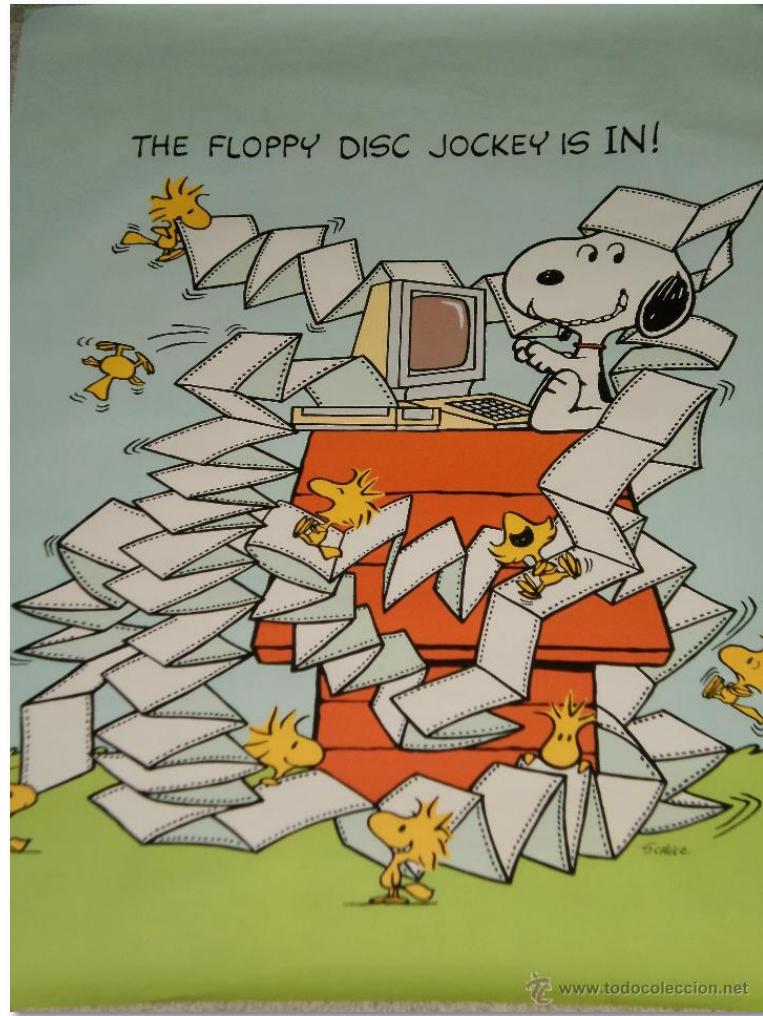
DevOps Image: Courtesy : Software Group at US Airforce



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# Data Management



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# The challenge : PaN RI typical environment

- Large user community (50 000 users/18 Months) with heterogenous profile :
  - Scientific field : Biology, Material science, chemistry ... Archaeology, nuclear physic, HEP.
  - Academic and Industrial users
  - Quite often very limited IT support in the users' home organisation
  - Data analysis to publication takes years due to a lack (pile up of unused space)
- Datasets volume vary from 10s GB to 100s TB
- Yearly data production form 300TB to 10s of PB.
- Data are openly accessible after 3 years of non disclosure period.
- Relatively small IT teams, mainly focus on data production (i.e. experiment) support and integration of existing solutions.



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# Three main use cases

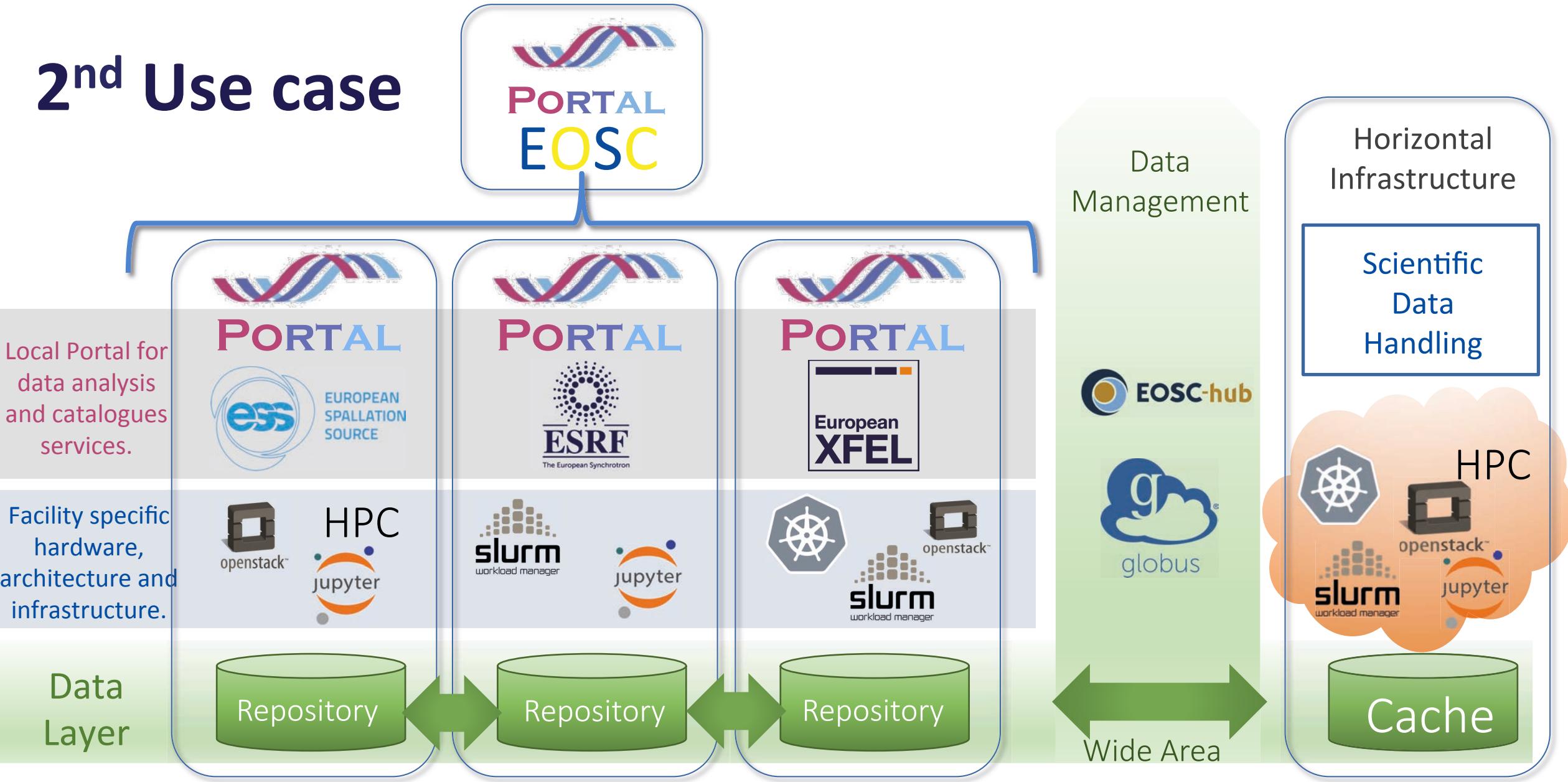
1. An RI wants to archive its experimental data in a remote data centre. Cold backup
2. A user wants to access a data analysis service, data has to be available “transparently”.
3. A facility user wants to transfer a large dataset from an RI’s archive to a remote compute center or her/his home PC.



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# 2<sup>nd</sup> Use case



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# Alternatively .... The ESCAPE Data Lake

Courtesy : ESCAPE

Data Infrastructure

Compute Infrastructure

ESCAPE WP2 (DIOS) already operates an impressive data lake prototype with large European contributors.

It handles

- Data Transfers
- Data Orchestration and
- Caching

It is definitely suitable as one tool of the EOSC

Storage Orchestration Services

PAUL SCHERRER INSTITUTE

ESRF

The European Synchrotron

Facility

HPC



Compute Provisioning

Mass Storage

Volatile Storage

Storage

Data Transfer Services



Delivery and Caching Services



Cloud

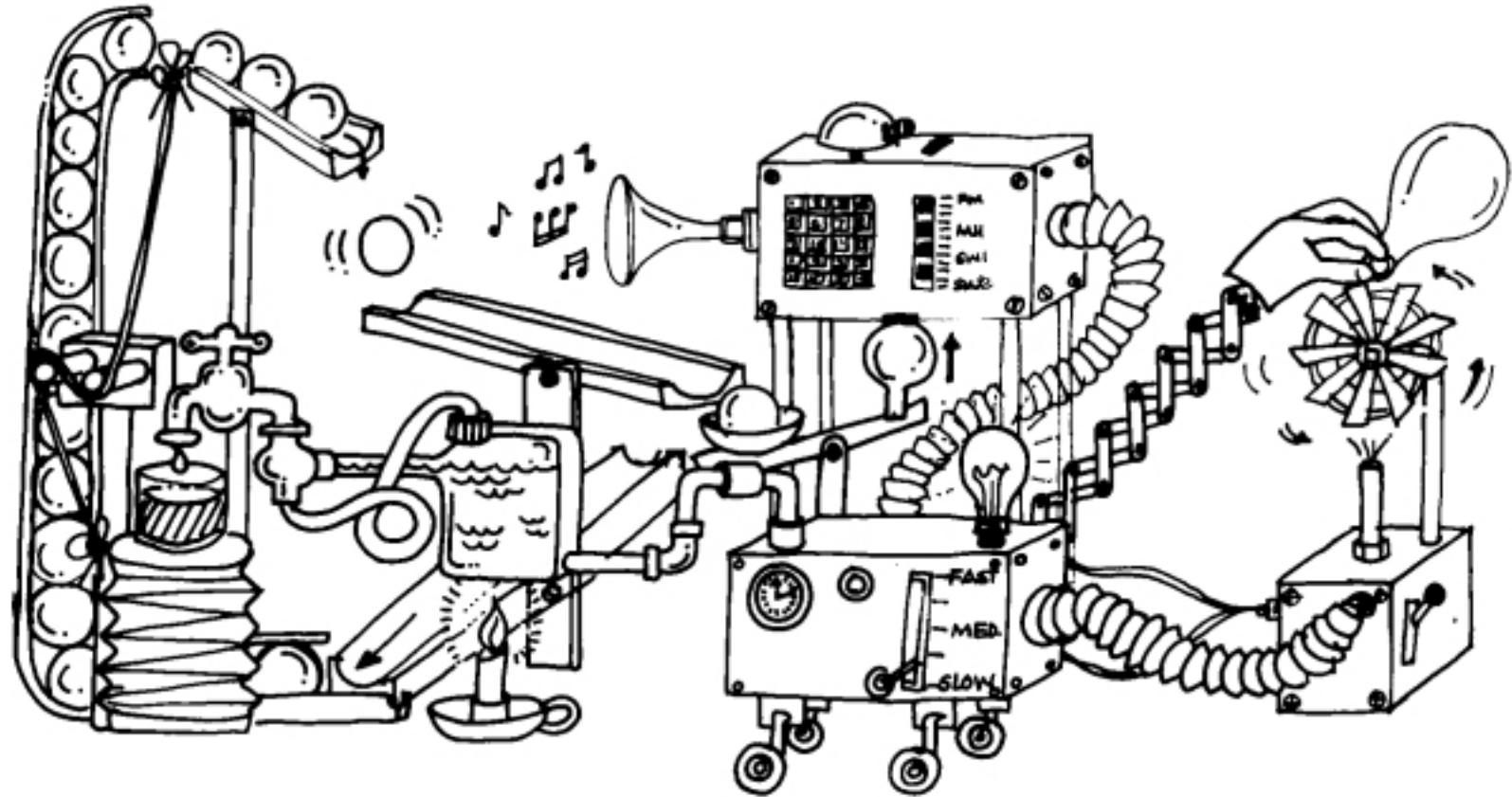
HPC

@HOME



# Progress in AAI

## Reminder

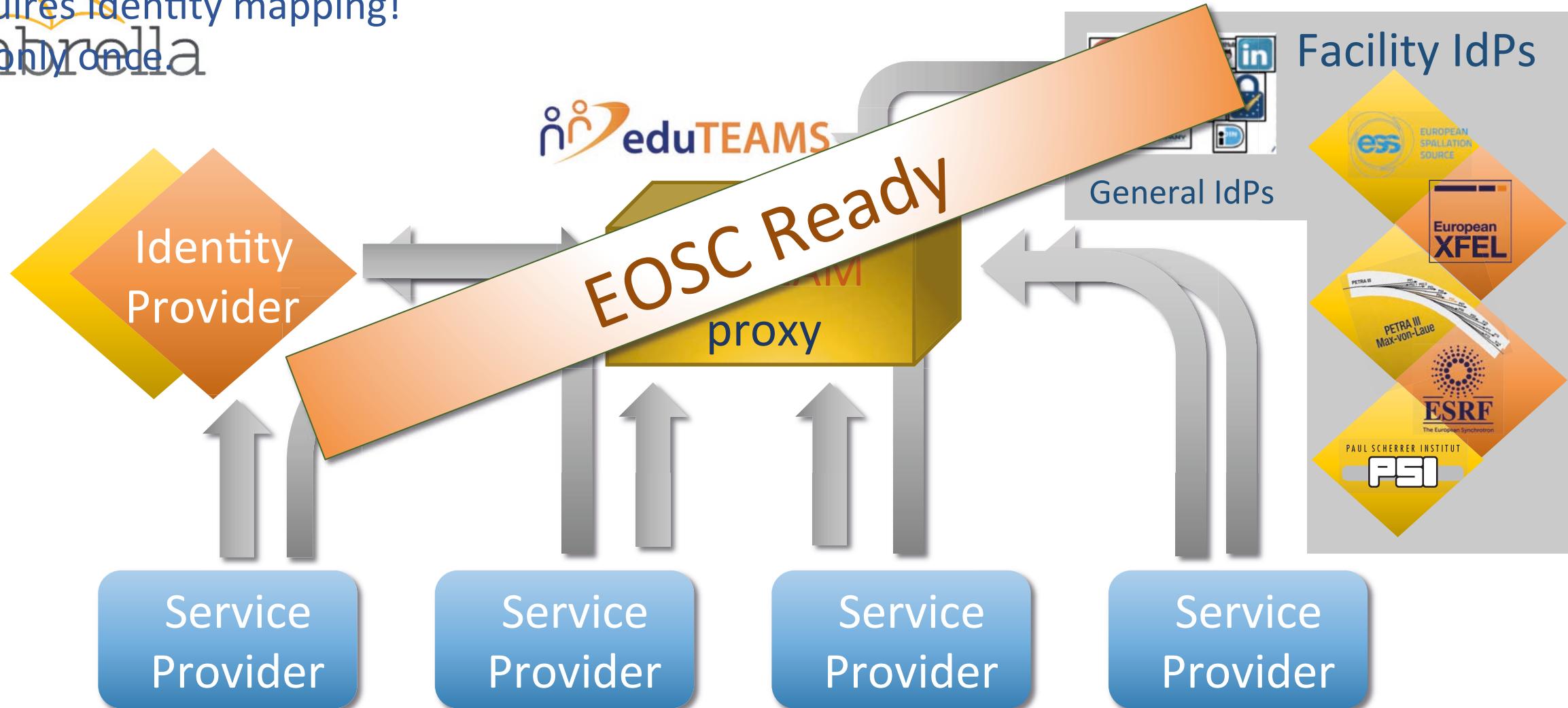


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# Transition from Umbrella to GEANT/eduTEAM

Requires Identity mapping!  
But only once.  
umbrella



# Progress and next steps



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# Progress so far

**PaNOSC and ExPaNDS are working closely together at all levels**

1. Data policies are being made FAIR.
2. A search API is defined and being implemented.
3. Data are being exposed to OpenAIRE.
4. NeXus is being promoted as standard.
5. Standard vocabularies are being defined.
6. Electronic logbooks are being generalized.
7. An alpha version of the data portal is available.
8. Jupyter services are being implemented.
9. HDF5 viewers is developed.
10. Simulation software packages have been aligned and extended.
11. User identity is now EOSC compatible.
12. EOSC compatible Data Transfer mechanisms are being tested and implemented.
13. A training platform is available.
14. Trainings have taken place.
15. Publications and dissemination.
16. Participated in many EOSC events.



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# Next Steps

## Work closely together with **Scientists** on **Use Cases**

- Implement Data Management Plan templates.
- Implement “Search APIs” and deploy them at PaNOSC and ExPaNDS facilities.
- Continue developing data portal and deploy it locally.
- Actively promote the reuse of the simulation developments.
- Deploy Umbrella Id/eduTEAMS at PaNOSC and ExPaNDS facilities.
- Adopt and deploy high speed data transfer solutions.
- Deploy EOSC-compatible e-infrastructure locally.
- Develop training material.
- Continue dissemination at User Meetings.
- Make all of the above sustainable.



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# Conclusion - Where we can help EOSC ?

- Provide real scientific use cases.
- Provide raw and processed data from diverse fields.
- Provide search API and portal to find data.
- Provide data portal and analysis services.
- Help defining and building the EOSC.



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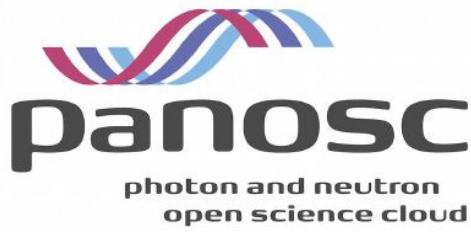
# Conclusion - Where EOSC could help us

- Provide an EOSC wide solution for AAI
- Provide a high speed data transfer service
- Provide a solution for long term data archiving
- Provide compute resources for data simulation
- Create a platform for sharing FAIR guidelines and technical solutions



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*Thanks for listening.*



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