

# PaNOSC project Introduction + Overview

16 June 2020

Andy Götz, on behalf of PaNOSC project



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

# Outline

- Motivation → Why
- Overall Concept → What
- Current Status → When
- PaN Commons Vision → Future
- Impact of COVID-19 → Dry Run

# PaNOSC & EOSC : built on Boldness

“

Whatever you can do, or  
dream you can do, begin it.  
Boldness has genius,  
power, and magic in it.  
**BEGIN IT NOW.**

- Goethe



# PaNOSC factsheet

**Call:** Horizon 2020 InfraEOSC-04

**Partners:** ESRF, ILL, XFEL.EU, ESS, CERIC-ERIC, ELI-DC, EGI

**Description:** cluster of ESFRI Photon and Neutron sources

**Observers/non-funded:** GÉANT, EUDAT, national RIs

**Linked 3<sup>rd</sup> parties via EGI:** DESY, STFC, CESNET

**Status:** Started 1/12/2018

**Github:** <https://github.com/panosc-eu>

**Home page:** <https://panosc.eu>

**Twitter:** @PaNOSC\_eu #PaNOSC

**Budget:** 12 M€

**Coordinator:** ESRF

**Started:** 1/12/2018

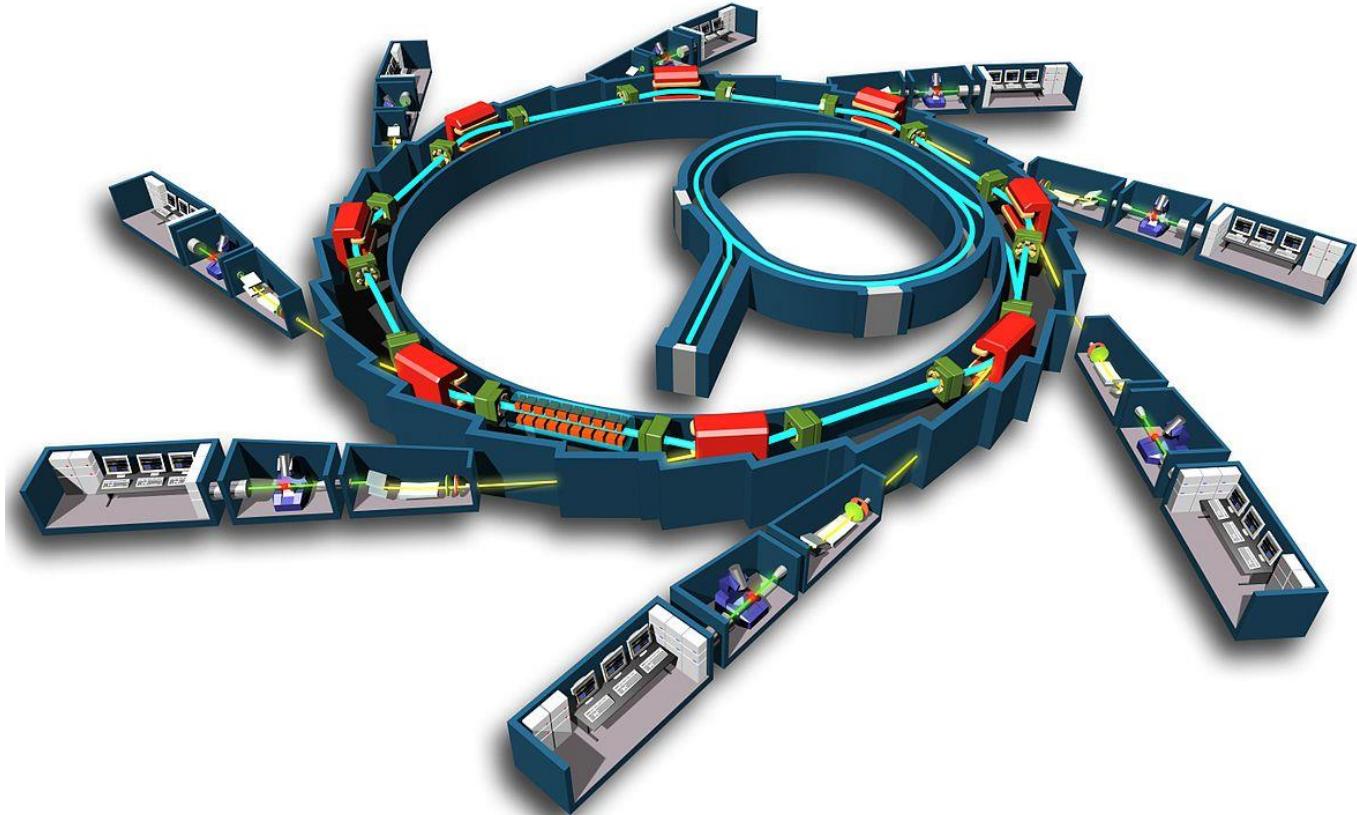
**Duration:** 4 years



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# How do PaN facilities work?

1. User: has an idea / need to study a sample



ability

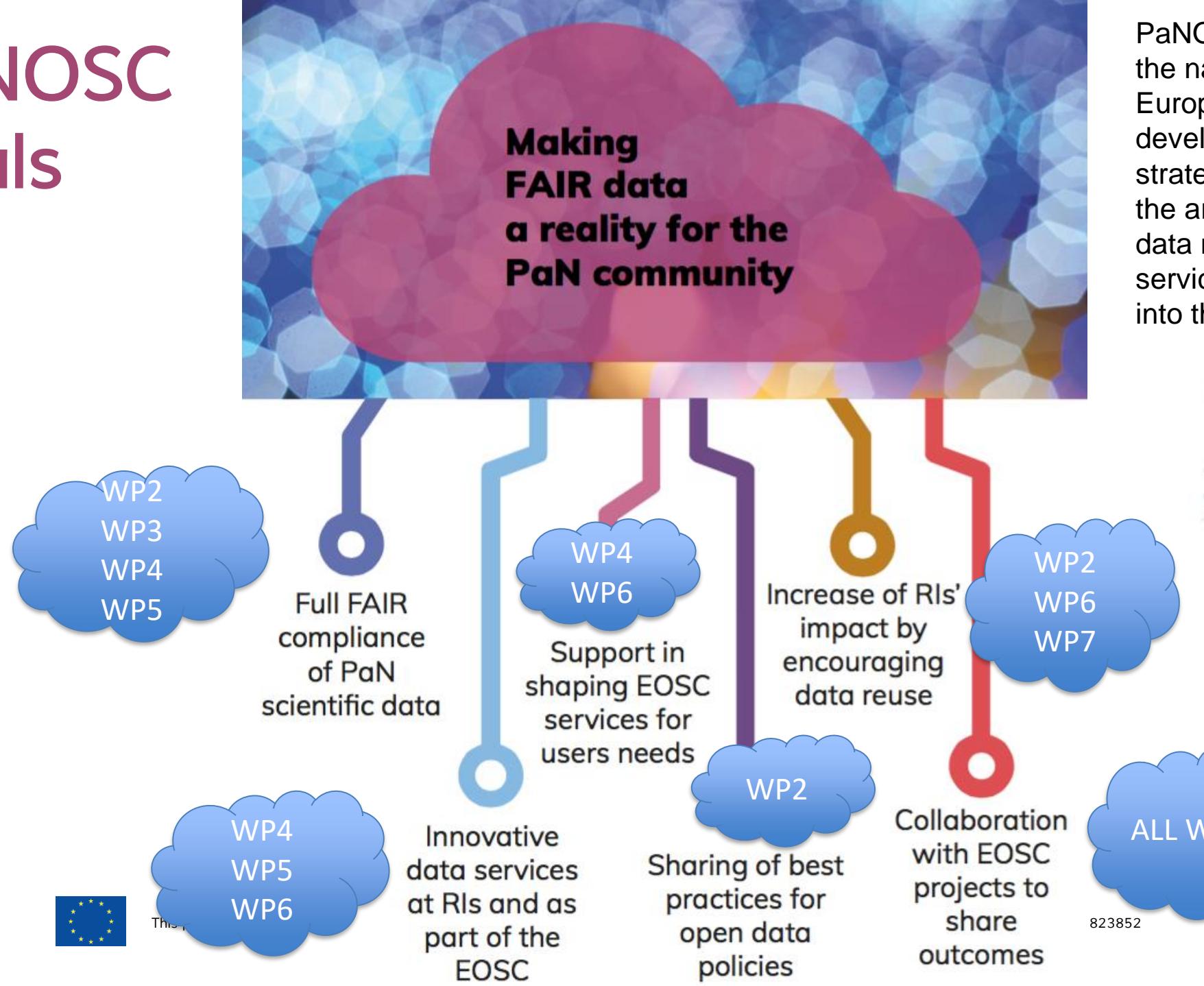
8. Publication: User publishes results (DOI) in peer review journal



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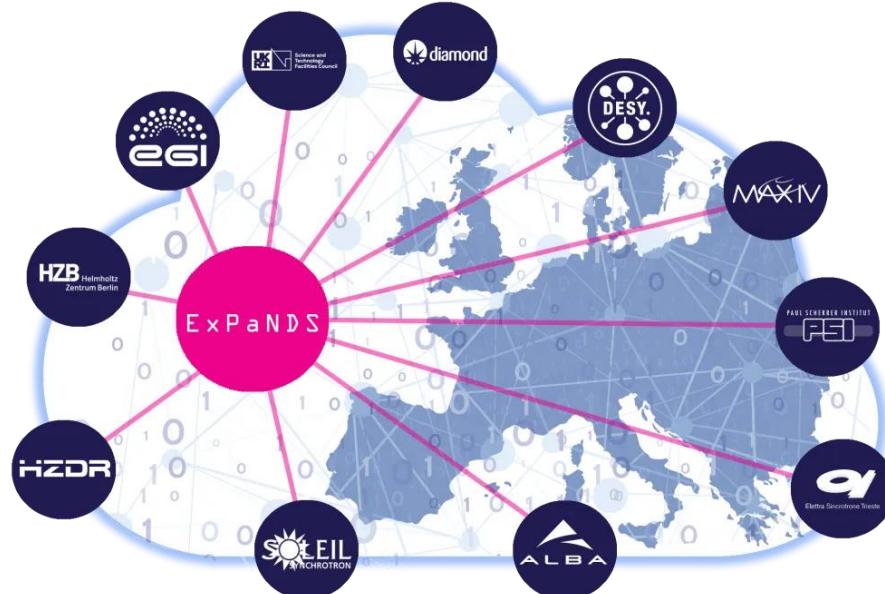
# PaNOSC goals



PaNOSC works closely with the national PaN sources in Europe via ExPaNDS to develop common policies, strategies and solutions in the area of FAIR data policy, data management and data services, integrating them into the EOSC.



# ExPaNDS – Extending Photon and Neutron Data Services



- Together PaNOSC+ExPaNDS represent all photon and neutron sources in Europe
- PaNOSC and ExPaNDS are collaborating closely in all common Work Packages i.e. WP1, WP2, WP3, WP4, WP8, WP9



# COVID-19 : A Dry Run for PaNOSC + EOSC

Definition of 'dry run'

**dry run**

Collins COBUILD



Word forms: plural **dry runs**

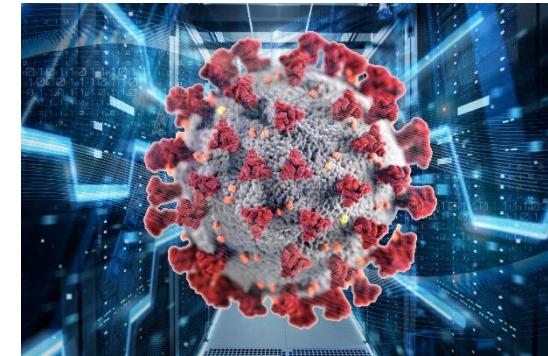
COUNTABLE NOUN

If you have a **dry run**, you practise something to make sure that you are ready to do it properly.

*The competition is planned as a dry run for the World Cup finals.* [+]

for

COBUILD Advanced English Dictionary. Copyright © HarperCollins Publishers



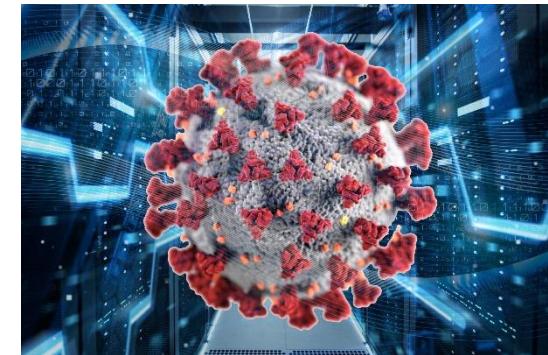
## How ready are PaNOSC + EOSC for the COVID-19 pandemic?



# COVID-19 : a test for PaNOSC and EOSC

- PaNOSC + EOSC should offer:

1. FAIR data
2. Downloadable Metadata & Raw data
3. Software service to browse and analyse raw data
4. Platform as a service to do computations + simulations
5. Common space to share progress and workflows



# PaNOSC KPIs

	ILL	ESRF	CERIC	XFEL	ELI	ESS
Data/year 2018	0.2 PB	8 PB	1 PB	3PB	< 1 PB	0
Data/year 2023	0.6 PB	50 PB	15 PB	100 PB	10 PB	< 1 PB
Data Policy 2018	2011	2010	2014(3/8)	2017	in prog	2017
Data Policy 2023	FAIR	FAIR	FAIR	FAIR	FAIR	FAIR
Metadata catalogue 2018	Local	Icat	Local	myMdC	No	SciCat
Metadata catalogue 2023	Local	Icat	Local	myMdC	[TBD]	SciCat
Metadata definition 2018	Nexus	Nexus	custom	myMdC	?	Nexus
Metadata definition 2023	Nexus	Nexus	Nexus	Nexus	[Nexus]	Nexus
DOI 2018	yes	yes	no	yes	no	yes
DOI 2023	yes	yes	yes	yes	yes	yes



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# PaNOSC is making Data Policies FAIR

This screenshot shows the Zenodo interface with a blue header bar containing the Zenodo logo, a search bar, an upload button, and a communities link. Below the header, the date 'February 11, 2011' is displayed. In the center, there are two buttons: 'Project deliverable' (dark grey) and 'Open Access' (green). The main content area features the title 'Common policy framework on scientific data' and the author 'Dimper, Rudolf'. A detailed text description follows, mentioning the Pan-data project's role in harmonizing data policies across European research facilities. At the bottom, there is a preview section with a large blue arrow pointing right.

February 11, 2011

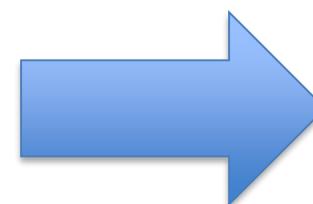
Project deliverable Open Access

## Common policy framework on scientific data

Dimper, Rudolf

The increasingly high profile of issues surrounding preservation and access of research data makes it important to work towards harmonisation of data policies across the research base. PaN-data brings together a significant number of major world class European research infrastructures to lay the foundation for a fully integrated, pan-European, information infrastructure supporting the complete scientific cycle from experiment definition to publications. The participating facilities are used by researchers in universities, publicly funded research entities, and industry. This document describes the common framework for scientific data management at photon and neutron facilities. This document and any future revisions is also available at [pan-data.eu](http://pan-data.eu).

This screenshot displays the first page of the PaN-data Europe deliverable D2.1. It features the Pan-data Europe logo, which includes the 'SEVENTH FRAMEWORK PROGRAMME' logo, the text 'pandata.europa', and the words 'PaN-data Europe' and 'Deliverable D2.1'. Below this, there is a large amount of text about the project's goals and the common policy framework. At the bottom, there is a file download section with a 'Files (352.4 kB)' link and a rating section with three stars.



This screenshot shows the Zenodo interface with a blue header bar containing the Zenodo logo, a search bar, an upload button, and a communities link. Below the header, the date 'May 20, 2020' is displayed. In the center, there are two buttons: 'Project deliverable' (dark grey) and 'Open Access' (green). The main content area features the title 'PaNOSC FAIR Research Data Policy framework' and a list of authors: Gotz, Andy; Perrin, Jean-Francois; Fangohr, Hans; Salvat, Daniel; Gliksohn, Florian; Markvardsen, Anders; McBirnie, Abigail; Gonzalez-Beltran, Alejandra; Taylor, Jonathan; Matthews, Brian. A detailed text description follows, explaining the new photon and neutron research data policy framework based on the previous PaNDATA policy. At the bottom, there is a preview section.

May 20, 2020

Project deliverable Open Access

## PaNOSC FAIR Research Data Policy framework

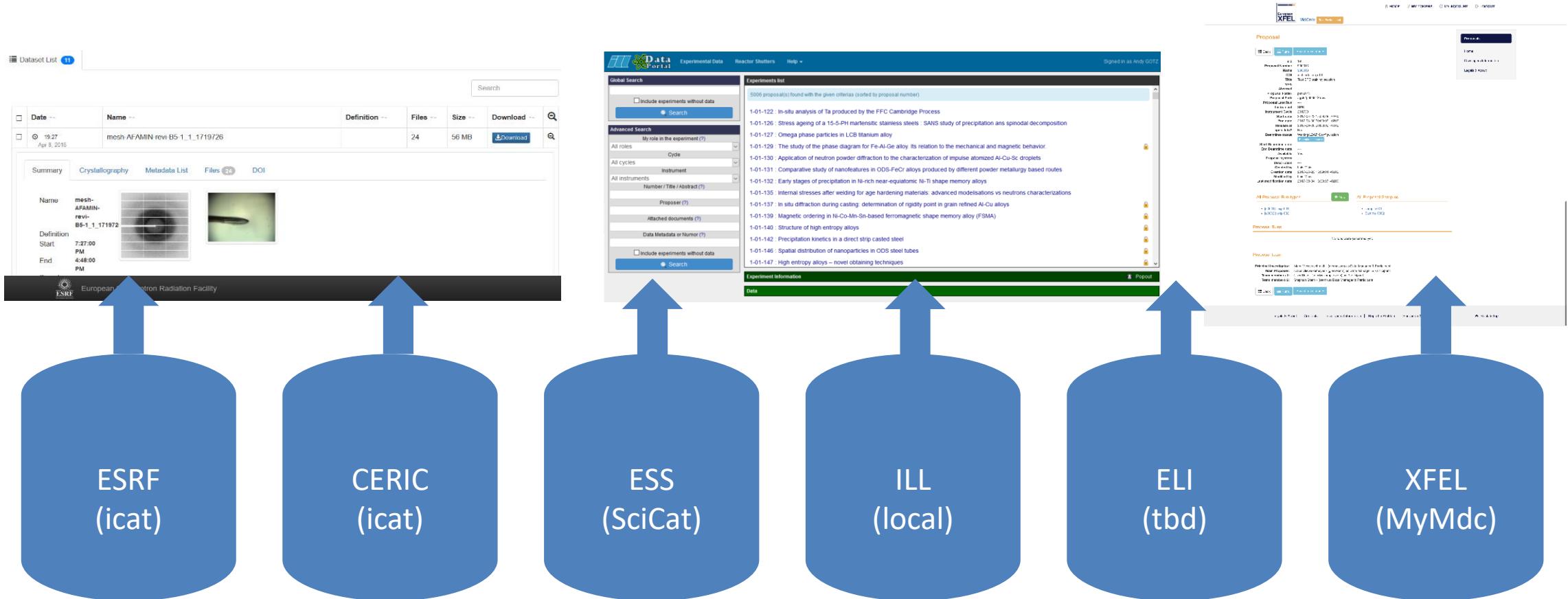
Gotz, Andy; Perrin, Jean-Francois; Fangohr, Hans; Salvat, Daniel; Gliksohn, Florian; Markvardsen, Anders; McBirnie, Abigail; Gonzalez-Beltran, Alejandra; Taylor, Jonathan; Matthews, Brian

This paper presents the new photon and neutron research data policy framework based on the previous PaNDATA policy (<https://doi.org/10.5281/zenodo.3738497>) applicable to all photon and neutron facilities and scientific research data in general. The data policy framework is strongly aligned with the FAIR principles. The aim of the policy is to ensure that the FAIR principles are applied in research data policies. This deliverable has been prepared by the EOSC projects PaNOSC (<https://panosc.eu>) and ExPaNDS (<https://expands.eu>) together to ensure harmonisation of the updated data policies for the photon and neutron communities.

This screenshot displays the first page of the PaNOSC FAIR Research Data Policy framework document. It features the PaNOSC logo, which includes a stylized wave graphic and the text 'panosc' and 'photon and neutron open science cloud'. Below this, there is a large amount of text about the project's goals and the FAIR principles. At the bottom, there is a file download section with a 'Files (352.4 kB)' link and a rating section with three stars.

Deliverable: D2.1 - PaNOSC data policy framework

# PaNOSC has 6 data catalogues with different APIs + UIs <sup>WP3</sup>



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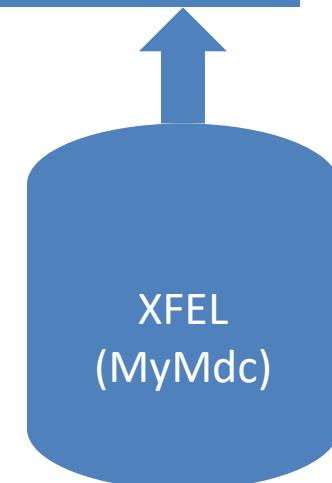
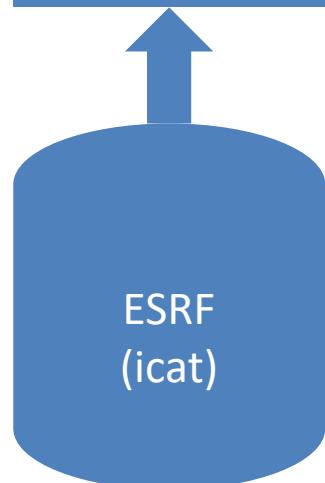
# PaNOSC common API across all sites



Search for Datasets



Common API to search across all PaNOSC catalogues



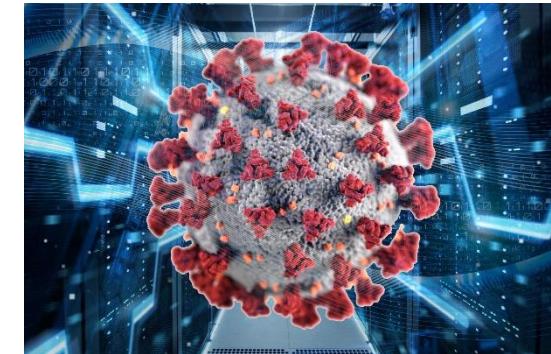
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# COVID-19 : a test for PaNOSC and EOSC

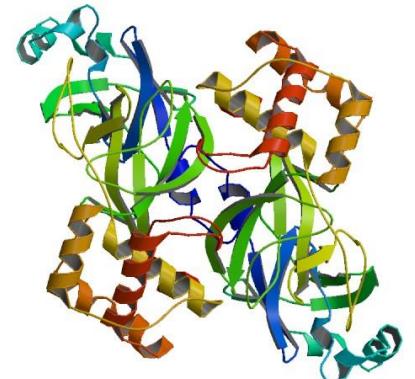
- FAIR data & Downloadable  
Metadata & Raw data : In Progress

→ e.g. ESRF has 15 Coronavirus structures in the Protein Data Bank  
but no raw data ...



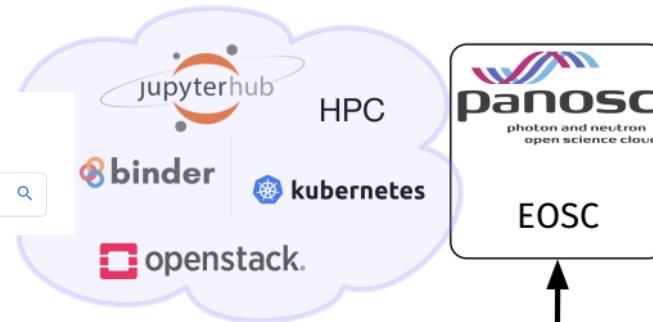
SARS-CoV/2c3s

SARS-CoV/2c3s, SARS-CoV/2beq, SARS-CoV/2bez,  
SARS-CoV/2h85, bovine-coronavirus/3cl4, bovine-  
coronavirus/3cl5, HCoV-OC43/6qfy, MERS-CoV/4ud1,  
MERS-CoV/6g13, murine\_coronavirus/4c7l,  
murine\_coronavirus/4c7w, murine\_coronavirus/5jif,  
murine\_coronavirus/5jil, 2cme, SARS-CoV/2xyr, SARS-CoV/2xyv,  
SARS-CoV/2fav, SARS-CoV/1qz8, SARS-CoV/1uw7





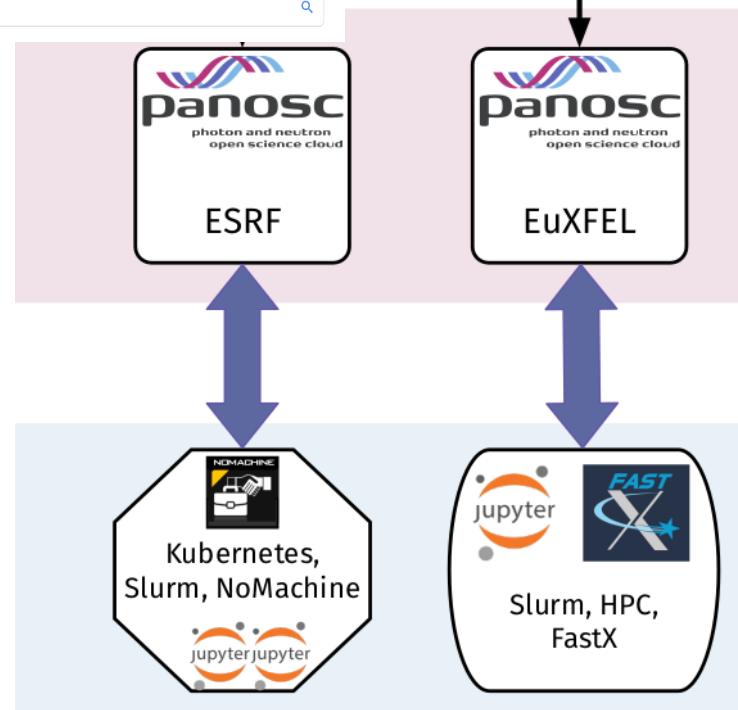
Search for Datasets



## Presentation & Demo – Towards Reproducible Publications with FAIR Data



Search for Datasets



The screenshot shows a presentation slide with the title 'PaNOSC presentation & demo - Towards R...', the PanOSC logo, and the subtitle 'Towards Reproducible Publications with FAIR Data' by Robert Rosca – European XFEL. The slide includes a video player icon and links for 'Watch later' and 'Share'. At the bottom, it states: 'This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852'.



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



# Simulation services - ViNYL

- Virtual Neutron and x-ray Laboratory (**ViNYL**) will:
- Offer services for simulation and modelling of photon and neutron instruments, as well as start-to-end simulations to describe entire experiments at photon and neutron facilities
- Make simulation data services inter-operable among the involved partners, such as **OASYS**, **McSTAS** and **SIMEX**
- Enable RIs to seamlessly link this experiment simulation services to their in-house data reduction, analysis, and visualization infrastructures.
- **SIMEX** is responsible for photon experiment simulations

PaNOSC demo – Simulating and analysing serial crystallography data in Jupyter Notebooks



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# PaNOSC KPIs

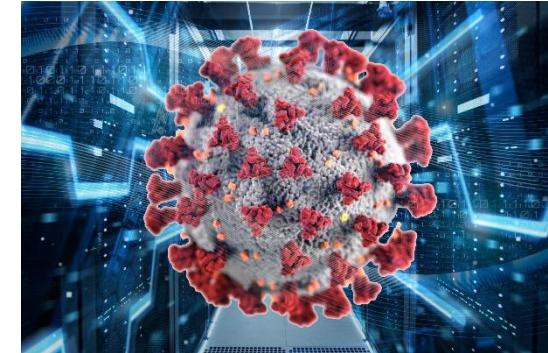
	ILL	ESRF	CERIC	XFEL	ELI	ESS
<b>Open Data 2018</b>	100s	2	0	10s	0	0
<b>Open Data 2023</b>	1000s	1000s	100s	1000s	100s	10s
<b>Data Services 2018</b>	Pilot	In progress	Remote	In progress	?	In progress
<b>Data Services 2023</b>	Desktop Jupyter	Jupyter Desktop	Jupyter Desktop	Jupyter Desktop	Desktop Jupyter	Jupyter Desktop
<b>Common data API 2018</b>	No	No	No	No	No	No
<b>Common data API 2023</b>	Yes	Yes	Yes	Yes	Yes	Yes
<b>User training 2018</b>	No	No	No	No	No	No
<b>User training 2023</b>	Yes	Yes	Yes	Yes	Yes	Yes



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# COVID-19 : a test for PaNOSC and EOSC

- Software & Platform service to browse and analyse raw data :  
In Production and/or In Test



→ EuXFEL, ILL, ESRF, CERIC-ERIC, ESS, ELI provide remote analysis services :

Jupyter → EuXFEL, ILL, ESRF, CERIC-ERIC, EGI in production,  
ESS + ELI in test

Desktop → EuXFEL, ILL, ESRF, CERIC-ERIC, EGI in production  
But not scalable to all users

HPC → EuXFEL, ILL, ESRF, EGI in production for local users  
But not scalable to all users

Server Options

Simple      Advanced

Architecture

Intel (x86\_64)      IBM Power (ppc64le)  
Intel Xeon      IBM POWER9

CPUs

Minimum      Medium      Maximum  
1 core(s)      14 core(s)      Entire node

Job duration 1 hour

List of available resources:

Current Status		
Partition	# nodes	# avail
nice	41	12
p9gpu	4	2
deb9-fast-io	1	0
deb9-gpu	1	1
id16a	2	1

Start

# EOSC Integration – Data transfer

- **3 uses cases :**
  - User driven data transfer of GB to TBs (**Globus Online**)
  - Data archiving for RIs (**STFC as the archive center**)
  - Transfer from RIs to compute facilities on behalf of users (i.e. based on the scenario where users perform analysis on a different infra than the one of the RI where the data have been produced). Currently exploring **OneData**.
- **Pilots with EGI Support of Use Case 2 &3, evaluating :**
  - Integration with the existing RI IT infra
  - AAI interoperability
  - Limit of the model in terms of data volume

# PaNOSC & EOSC – Experience

- EOSC is under development :
  - 4 Working Groups
  - 40+ EOSC-related projects
  - Hundreds of potential collaborators
  - Many meetings + reports to read / comment on
  - EOSC is like the internet – there are many views
- Pros :
  - Clusters are getting together + sharing know-how
  - Working with e-infrastructures EGI + GÉANT is beneficial
- Future : EOSC will improve reproducibility and boost Open Science + Open Data



**EUROPEAN OPEN  
SCIENCE CLOUD**

**Progress on Open Science:  
Towards a Shared Research  
Knowledge System**

Final Report of the Open Science Policy Platform



WP3

WP4

WP5

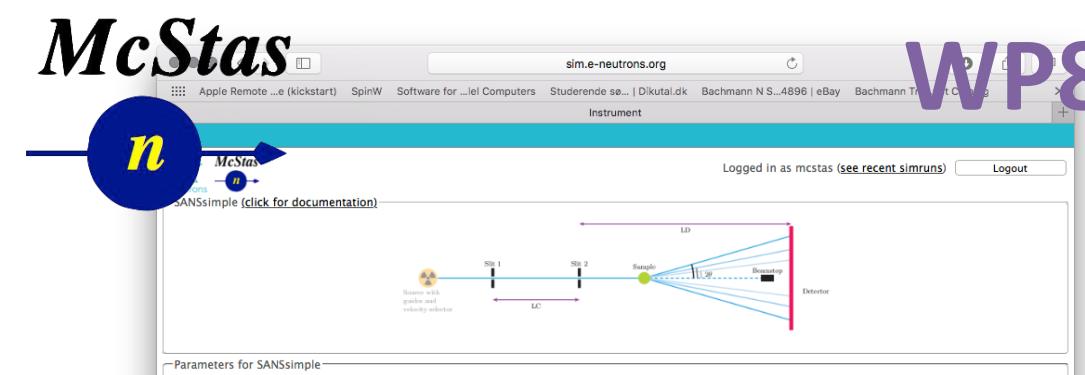
WP8

# Outreach Events & Developments

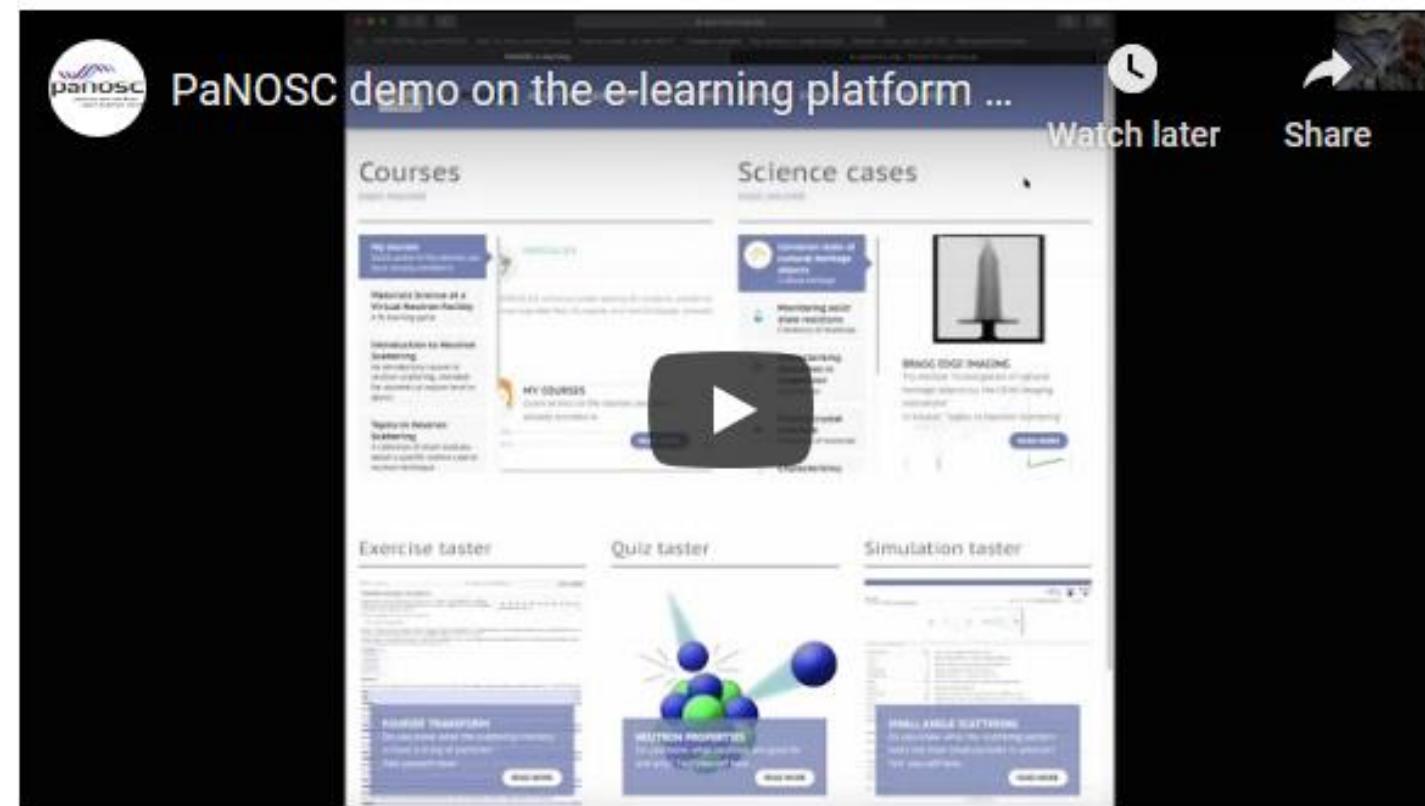
- **1<sup>st</sup> PaNOSC OASYS School**, 14-16 May 2019, Grenoble – France
- **HDF5 European Workshop for Science and Industry**, 17-18 September 2019, @ESRF, Grenoble
- **h5py code camp**, 19-20 September 2019, @ESRF, Grenoble 
- **Nexus data format** – extend for synchrotron, FELs + lasers, generalize use of Nexus in PaN community
- **hdf5 – h5py** python library for manipulating hdf5 files + **h5web** web viewer of hdf5 
- **Jupyter notebooks** – integrate batch schedulers + integrate h5web viewer, provide notebooks for use cases
- **Data portal** – develop a PaN portal for generic services + remote desktop
- **Pan-learning** – integrate jupyter notebooks into moodle

# e-learning on Neutrons and Photons

- e-neutrons.org
  - Wiki with neutron scattering theory
  - Web instrument simulation using McStas
  - Quizzes using both theory and simulation
- Migration to ESS servers underway
- Extensions:
  - Support for Jupyter Notebooks
  - Integrate WP 4 data analysis services
  - Integrate WP 5 simulation services



Demo on the e-learning platform [www.pan-learning.org](http://www.pan-learning.org)



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Now, we utilize a rather intuitive identity from quantum mechanics, valid when  $\lambda$  is an eigenstate of the Hamiltonian  $H$  with eigenvalue  $E_\lambda$ :  
 (4) 
$$\exp(-\lambda H) = \exp(-\lambda H) \exp(\lambda H) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \exp\left(-\frac{E - \lambda}{\hbar}\right) \exp(-iE_\lambda t) dE.$$
  
 (5) 
$$\exp\left(\frac{i}{\hbar} \lambda H\right) = \exp\left(\frac{i}{\hbar} \lambda H\right).$$



# e-learning on Open Science

WP8

- Train young scientists + PhDs on how to do Open Science and make Data Open and FAIR
- Team up with Eurodoc<sup>1</sup> Hercules school, local universities<sup>2</sup>, FAIRsFAIR, EOSC, etc.

<sup>1</sup> <http://eurodoc.net/>

<sup>2</sup> <https://www.datacc.org/>

The slide is titled "How to be an Open Scientist at University of Camerino". It features a hand holding a magnifying glass over a green circular graphic, symbolizing research and discovery. The slide is divided into several sections:

- Open Data Management**:
  - Why?**
    - Real-time collaboration
    - Immediate results
    - Increased sharing
  - How?**
    - Uniform data management
    - Open data repositories
    - Intelligent access & interoperability
- Open Source Code**:
  - Why?**
    - Personal benefit
    - Agile development
    - Real-time evaluation
  - How?**
    - Community networking
    - Open source code repositories
- Involving the Public**:
  - Why?**
    - Mutual learning (science <-> public)
    - Civic empowerment
    - Recognition of other perspectives
  - How?**
    - Citizen Science
    - Social Media/Blogs/Apps
    - Public Speaking
- Sharing Results with Colleagues**:
  - Why?**
    - Support wide-spread of information
    - Creating broader networks
  - How?**
    - Open access publishing
    - Pre-print servers
    - University repositories
- Sharing Results with Public**:
  - Why?**
    - Keep shareholders informed
    - Informed public = informed policy
    - Avoid misinformation
  - How?**
    - Traditional/Social media
    - Public speaking
    - Science Cafés, Open Museum nights
- Collaborating with Researchers**:
  - Why?**
    - "Two heads are better than one"
  - How?**
    - Enhanced scope of project
    - Avoid potential bias



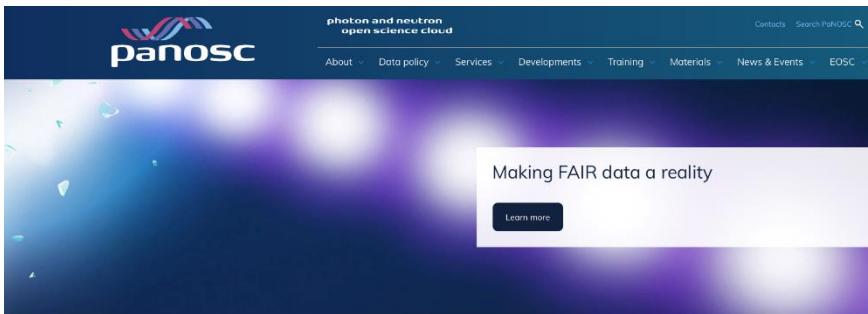
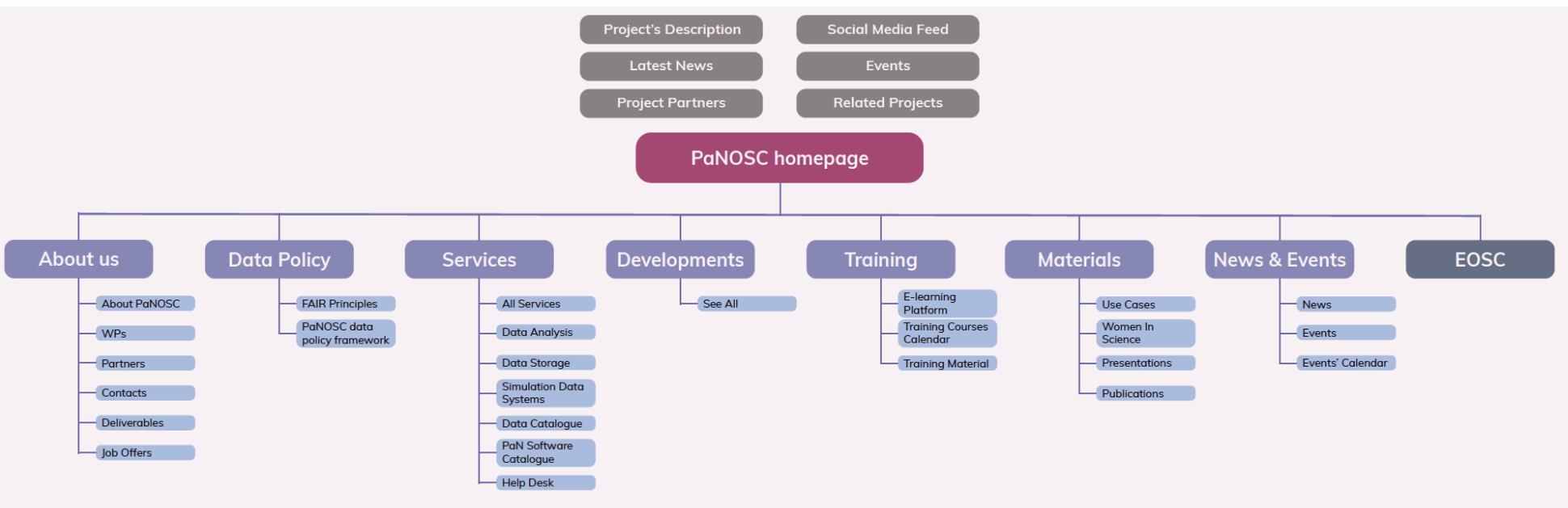
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<http://eurodoc.net/news/2018/handbook-on-how-to-be-an-open-scientist-for-early-career-researchers>

PanOSC

# PaNOSC website – <https://panosc.eu>

WP9



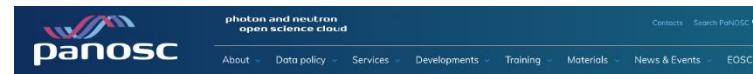
## The Photon and Neutron Open Science Cloud (PaNOSC)

The Photon and Neutron Open Science Cloud (PaNOSC) is a European project (financed by the INFRAEOSC-04 call) for making FAIR data a reality in 6 European Research Infrastructures (RIs), developing and providing services for scientific data and connecting these to the European Open Science Cloud (EOSC).

## Objectives

### Tweets by @Panosc\_eu

PaNOSC will be at the joint CNECT-RTD project meeting & workshop on 9-10 September in Brussels. The workshop aims to increase the visibility of EOSC-related projects, explore their progress and discuss issues on next steps towards building the #EOSC >>[bit.ly/2m1M1hV](https://bit.ly/2m1M1hV)



## News



Published on 7 August 2019  
Reproducible science discussed at the Jupyter for Science workshop

Jupyter is the "Google Docs" of data science. It provides that some kind of easy-to-use ecosystem, but for interactive data exploration, modelling, and analysis. However, some work still needs to be done to make Jupyter the best interactive and practical tool for big science. Doing this right will take a community: New collaborations between core [...]

Read →



Published on 18 July 2019  
Kick-off meeting of PaNOSC WP4 hosted at EuXFEL

The kick-off meeting of PaNOSC work package 4 – Data Analysis Services, took place from 25 to 27 June at EuXFEL in Schenfeld, Germany, with the goal of better coordinating the people involved in the WP and the future operational steps. After an overview of PaNOSC by the project coordinator, Andri Goltz, Prof. Hans Fongler, [...]

Read →



Published on 8 July 2019  
EOSC projects gathered at the EOSC jam session in Turin

On 6-7 June 2019 in Turin, Italy, EOSC Secretariat held its first of a series of events titled "EOSC Jam Session", which gathered all Call-5 and EOSC ESRF Cluster projects, including PaNOSC, with the goal of bringing all EOSC projects together, also involving stakeholders, in support of the EOSC governance in its goal to co-create the EOSC [...]

Read →



## Events

04/11/19

PaNOSC 1st Annual Meeting

The 1st Annual Meeting of the Photon and Neutron Open Science Cloud project (PaNOSC) will take place on 4-5 November 2019 in Trieste, Italy. The meeting will bring together PaNOSC project partners and other EOSC clusters, with the aim of sharing information and increasing collaboration among different parts. Project partners will present the status and progress of [...]

More info →

18/09/19

PaNOSC WP3 workshop at ILL

The ILL will host a PaNOSC WP3 workshop from Wednesday 18th September to Thursday 19th September 2019 in Grenoble, France. The workshop will bring together PaNOSC project partners and other EOSC clusters, with the aim of sharing information and increasing collaboration among different parts. Project partners will present the status and progress of [...]

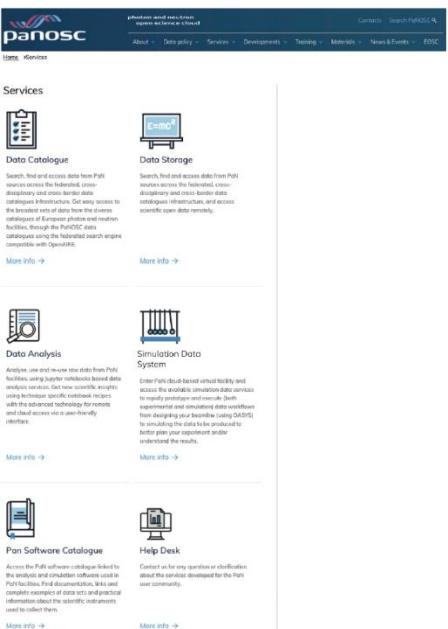
More info →

17/09/19

Register now to the HDF5 European Workshop for Science and Industry

The ESRF, in the frame of PaNOSC and in collaboration with HDF Group, is organizing the HDF5 European Workshop for Science and Industry, taking place at the ESRF headquarters in Grenoble - France, on 17-18 September 2019. The aim of the workshop is to highlight the use of HDF in science and industry, to discuss use [...]

More info →



# COVID-19 : a test for PaNOSC and EOSC

## Common space to share open science workflows : Work in Progress

→ e.g. EuXFEL OSCOVIDA example of citizen science Jupyter notebooks

oscovida: Open Science COVID Analysis

Home <https://oscovida.github.io/>

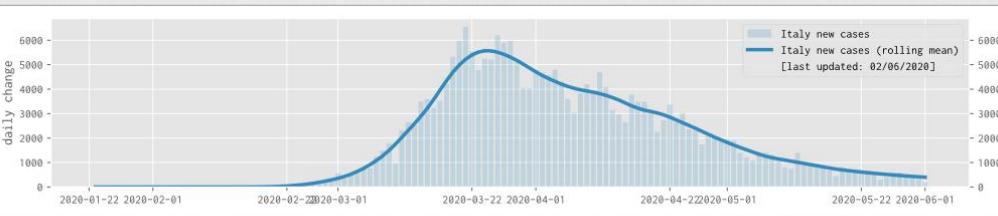
Welcome to the Open Science COVID19 Analysis page! Read about our [motivation](#), [data sources](#), [team](#). Use our analysis plots of COVID19 cases and

science COVID Analysis Home All regions Countries Germany US Articles Analysis About

We provide a standard set of analysis plots (explained here) for different regions:

- List of all regions, countries and US states
- Overview for each country in the world (Johns Hopkins data)
- States in the US (Johns Hopkins data)
- Counties (Landkreise) in Germany (Robert Koch Institute data)

Occasionally, we try to put COVID19 numbers reported in the news into context.



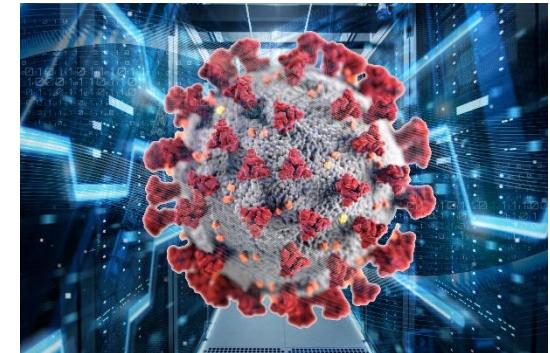
A line chart showing daily new COVID-19 cases in Italy from January 22 to June 1, 2020. The y-axis represents 'daily change' from 0 to 6000. The x-axis shows dates from 2020-01-22 to 2020-06-01. The chart features two data series: 'Italy new cases' (blue bars) and 'Italy new cases (rolling mean)' (blue line). The data shows a sharp increase starting in late February, peaking around 5500 cases on March 22, followed by a gradual decline to near zero by June 1.

If you want to contribute, please get in touch. Ideas, suggestions and error reports, are welcome at our [feedback issue tracker](#).

Future → provide a catalogue of notebooks and workflows for analyzing data from different experimental techniques e.g. like the PANGEON project does ([https://pangeo.io/use\\_cases/index.html](https://pangeo.io/use_cases/index.html))

We are developing a collection of Jupyter Notebooks that demonstrate real science use cases enabled using Pangeo. If you have a use case that you would like to submit, please raise an issue on the [Pangeo GitHub issue tracker](#) to propose your idea.

- Physical Oceanography
  - Sea Surface Altimetry Data Analysis
    - Initialize Dataset
    - Examine Metadata
    - Create and Connect to Dask Distributed Cluster
    - Visually Examine Some of the Data
    - Timeseries of Global Mean Sea Level
    - Sea Level Variability



# PaN Commons

- **Vision** – create a common space for PaNOSC and ExPaNDS facilities where petabytes of PaN data, analysis software, notebooks, analysis software, workflows, and training material can be **Found**, **Accessed** (downloaded and/or executed), **Re-Used** + **Improved** i.e. **FAIR**
- **Remote access** – the PaN commons will be accessible remotely while being executed locally (close to the data) or on 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**)

**HIGH PRIORITY**



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



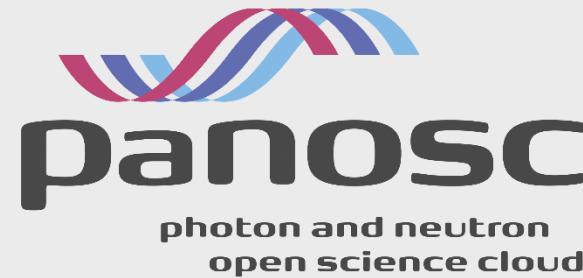
# Conclusion

- **Priority** –PaNOSC priority has increased significantly due to increased need for remote access (post-COVID-19). **COVID-19 demonstrated the need for PaNOSC and that we (PaNOSC + EOSC) are not ready for the next pandemic.**
- **EOSC** – interacting with the EOSC remains a challenge but we hope that in 2021 with the legal entity being created the EOSC will stabilise and be easier to interact
- **Collaboration** – with ExPaNDS is essential and is working well; collaboration with INFRAEOSC-04 clusters is increasing; **with Users during remaining 30 months of project is key to the success of the project**
- **Progress** – Objectives and outcomes of PanNOSC are aligned with the needs of all partner sites; all work packages are progressing well



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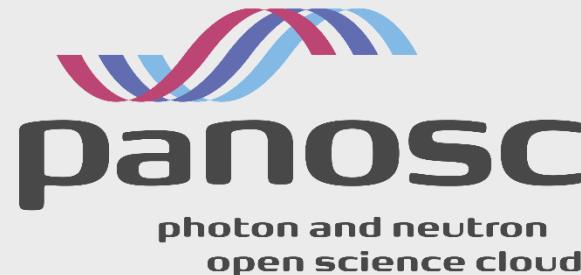


**Thank you to all PaNOSC project  
members for their contributions !**

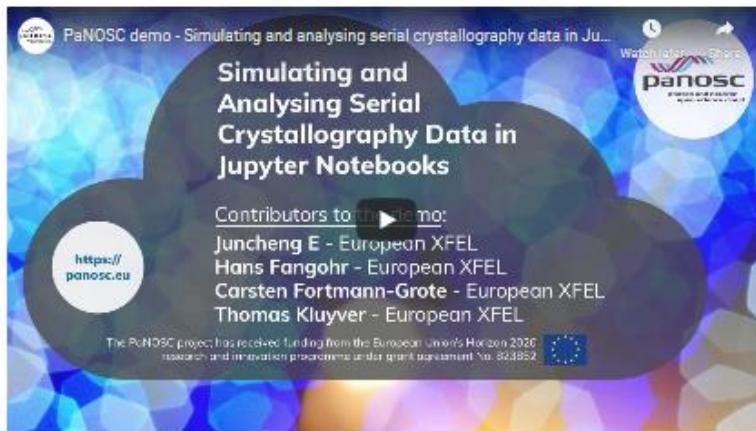
[andy.gotz@esrf.fr](mailto:andy.gotz@esrf.fr)



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PaNOSC demo – Simulating and analysing serial crystallography data in Jupyter Notebooks



Presentation & Demo – Towards Reproducible Publications with FAIR Data

Towards Reproducible Publications with FAIR Data  
Robert Rosca – European XFEL

Demo on the e-learning platform [www.pan-learning.org](http://www.pan-learning.org)



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