PaNOSC/ExPaNDS

ESFRI Science Clusters long-term commitment to Open Science

11 June 2021

Rudolf Dimper (ESRF-PaNOSC) – **Patrick Fuhrmann** (DESY ExPaNDS)

These projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements No. 823852 and 857641

Photon and Neutron analytical research infrastructures in Europe

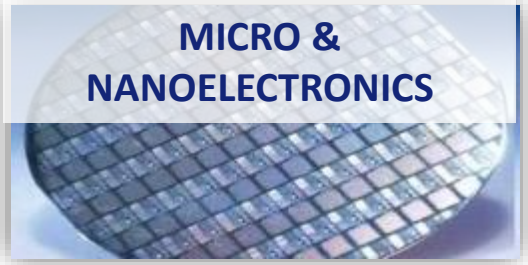
Fundamental, applied and industrial research on atomic structure and dynamics, link function and properties to atomic structure

ENERGY & ENVIRONMENT

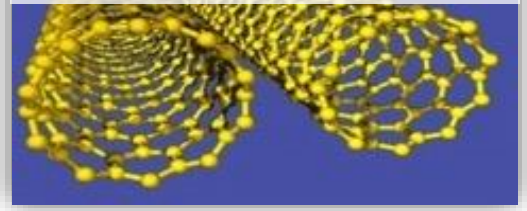
BIOLOGY & HEALTH

FOOD

MICRO & NANOELECTRONICS



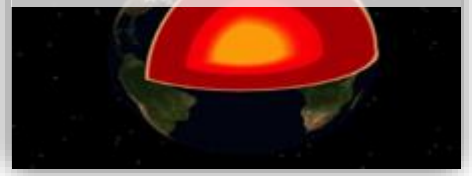
NEW MATERIALS



CHEMISTRY & CATALYSIS

SPACE & TRANSPORT

GEOSCIENCES & EXTREME CONDITIONS



CULTURAL & NATURAL HERITAGE

These projects have received funding from the European Union's Horiz

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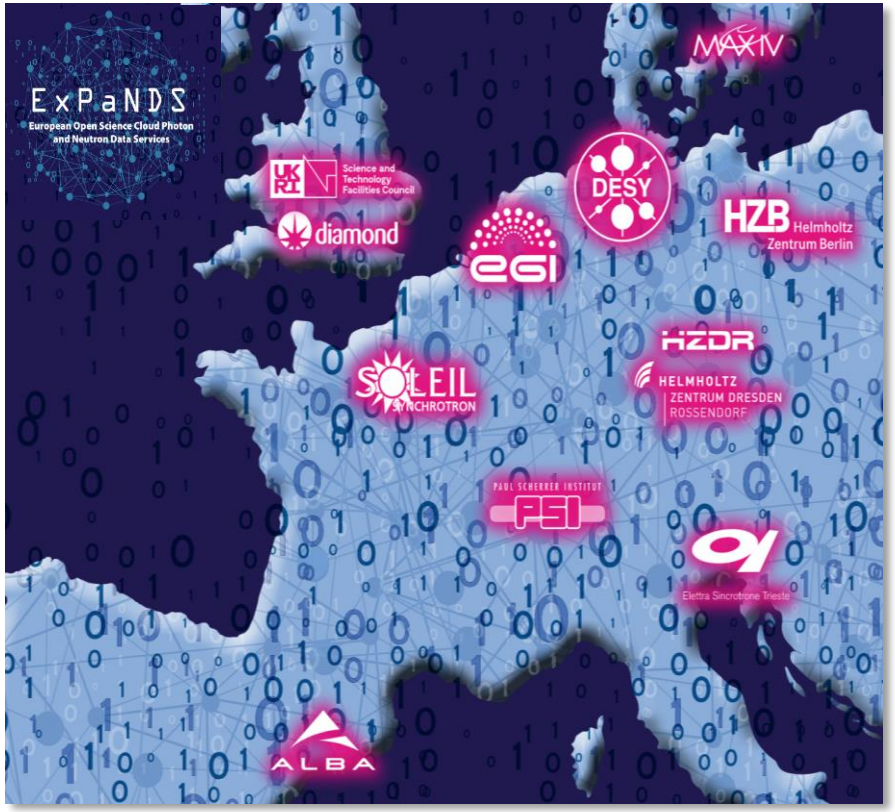
ExPaNDS
European Open Science Cloud Photon and Neutron Data Services

Together PaNOSC+ExPaNDS represent almost all Photon and Neutron sources in Europe



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ExPaNDS
European Open Science Cloud Photon and Neutron Data Services

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 3rd 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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ExPaNDS
European Open Science Cloud Photon and Neutron Data Services

ExPaNDS factsheet

Call: Horizon 2020 INFRAEOSC 5B

Partners: EGI, DESY, Max IV, Soleil, ALBA, HZB, HZDR, UKRI, Diamond, Elettra, PSI

Description: National Photon and Neutron sources

Status: Started 1/12/2018

Github: https://github.com/ExPaNDS-eu/ExPaNDS

Home page: https://expands.eu

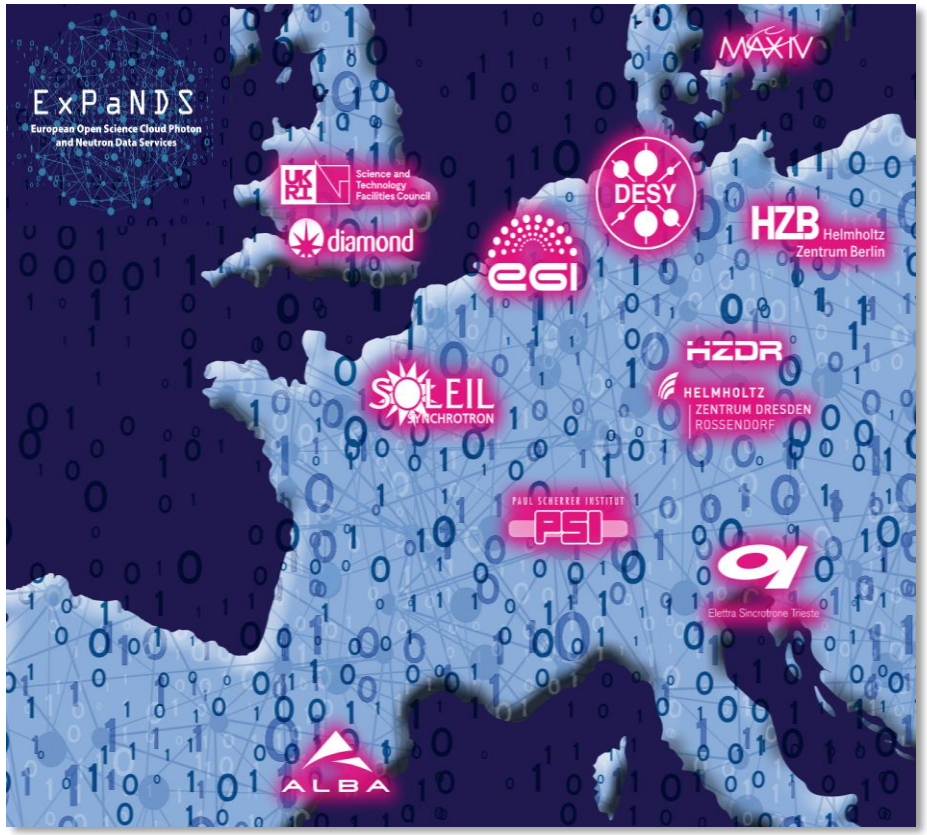
Twitter: https://twitter.com/ExPaNDs_EU

Budget: 6 M€

Coordinator: DESY

Started: 1/09/2019

Duration: 3 1/2 years



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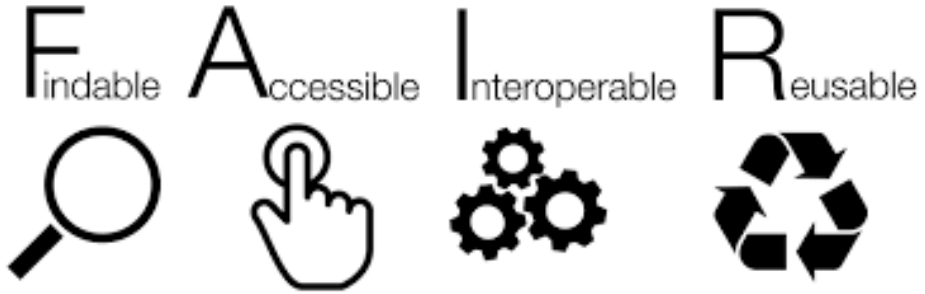
Some of the PaN Research Infrastructures

PaNOSC/ExPaNDS + EOSC: building data services on FAIR data



= DATA + SERVICES

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Where is the DATA?

- How do I find them?
- How do I get them?
- How do I look at them?
- What does they mean?
- Are they correct?

REDUCING THE BOTTLENECK EFFECT:

"What we're trying to do here is **expedite the time to discovery.** Scientists should be able to **focus on their science** without having to become experts in data management."

—Shawn McKee
research scientist in physics

454 | NATURE | VOL 533 | 26 MAY 2016

How can I:

- download TBs of raw data?
- search, view and process data remotely?
- access a Jupyter notebook to process my data?
- make my data open and get a DOI to cite?
- get credentials to login and use these services?

credits – Jon Taylor (ESS)

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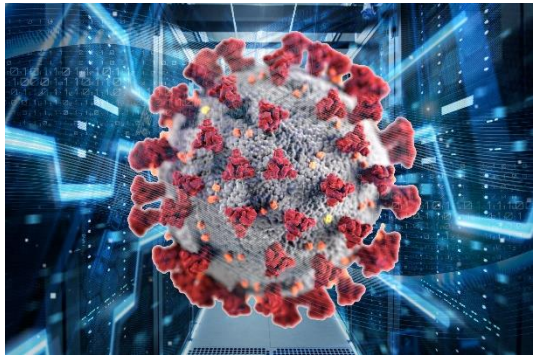
PaNOSC + EOSC should offer:

1. Remote acces to analytical facilities
2. Downloadable metadata & raw data
3. Software services to browse and analyse raw data
4. Platform as a service to do computations + simulations
5. Common space to share progress and workflows
6. Long-term data archive beyond the RI data policies



= is amplifying the needs and making them urgent

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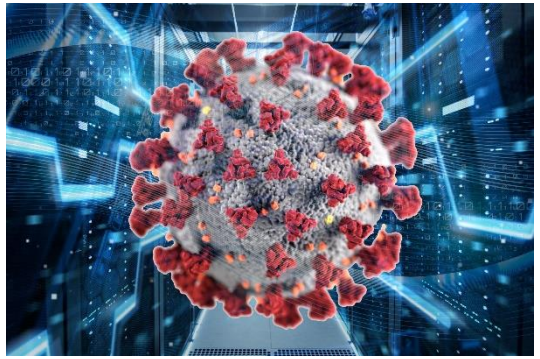
VISA = remote access during COVID-19 and beyond

- **Provide remote data analysis services with access to**
  - Experimental data
  - Analysis software
  - Compute infrastructure
  - Support (IT and Scientific)
- **Make access as simple as possible using a web browser**
- **Allow scientific collaborations**
- **Enable remote experiments**



credits – Jamie Hall (ILL) + Stuart Caunt (ILL)

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PaNOSC and ExPaNDS will provide by 2022

- ✓ Data policy framework
- ✓ Persistent identifiers (DOIs) for data
- ✓ Data management plans
- ✓ Standard metadata
- ✓ Nexus/HDF5
- ✓ Electronic logbooks
- ✓ Open data
- ✓ Data search API
- ✓ Data portal
- ✓ Jupyter notebook service
- ✓ Remote access desktops
- ✓ Data simulation services
- ✓ Data transfer service
- ✓ Persistent user identities (AAI)
- ✓ Scientific software catalogue
- ✓ e-training platform + material

For enabling Open Data + Open Science

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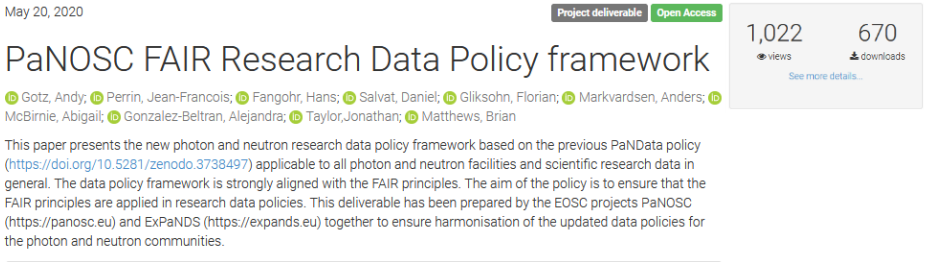
Mid-term achievements of PaNOSC/ExPaNDS

- ✓ Enhancing the PaN software catalogue
- ✓ Designed and developing search data catalogue search API
- ✓ Simulation software APIs released
- ✓ Developed python MacStasScript for McStas, integrated in pan-learning
- ✓ Deployed e-learning platform pan-learning.org supports PaNOSC AAI
- ✓ 2 EOSC services published
- ✓ Support for HDF5 + NeXus
- ✓ Developing PaNOSC portal
- ✓ AAI integrated into eduTEAMS
- ✓ Deployed Jupyter at all partner sites

and also

- ✓ FAIR research data policy framework
- ✓ Working on DMP templates
- ✓ Open call for Use Cases from scientists
- ✓ Provided publications and feedback to EOSC Working Groups
- ✓ Organised with ExPaNDS the PaN EOSC symposium
  - 199 participants, 09/11/2020
- ✓ Many videos promoting Open Science and data management practices


May 20, 2020

Project deliverable | Open Access

1,022 views | 670 downloads

See more details...

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.

Video promoting DOIs + contacted publishers together LEAPS + LENS

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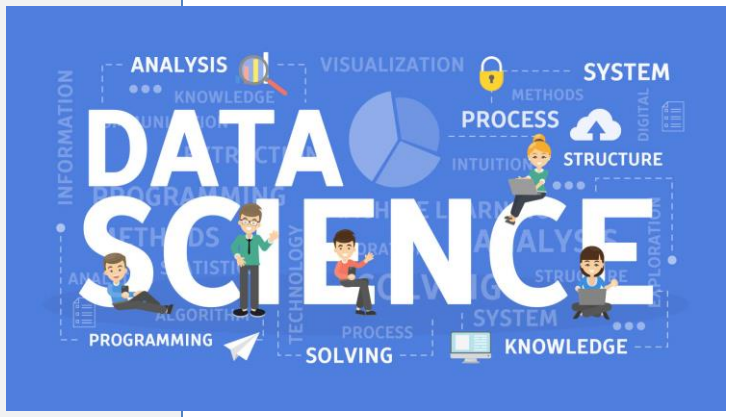
ExPaNDS
European Open Science Cloud Photon and Neutron Data Services

Sustainability of PaNOSC/ExPaNDS

Services to be sustained after the projects:

- AAI
- Data transfer service (RI-RI, RI-HPC-centre, RI-User)
- Helpdesk
- Data catalogue search engine + API
- Software catalogue
- Data visualization service
- Jupyter notebook services + data analysis as a service (DAaaS)
- Simulation services
- E-learning platform



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PaN RIs in PaNOSC/ExPaNDS are coming together in LEAPS & LENS

Photons

(LEAPS – League of European Accelerator based Photon Sources)

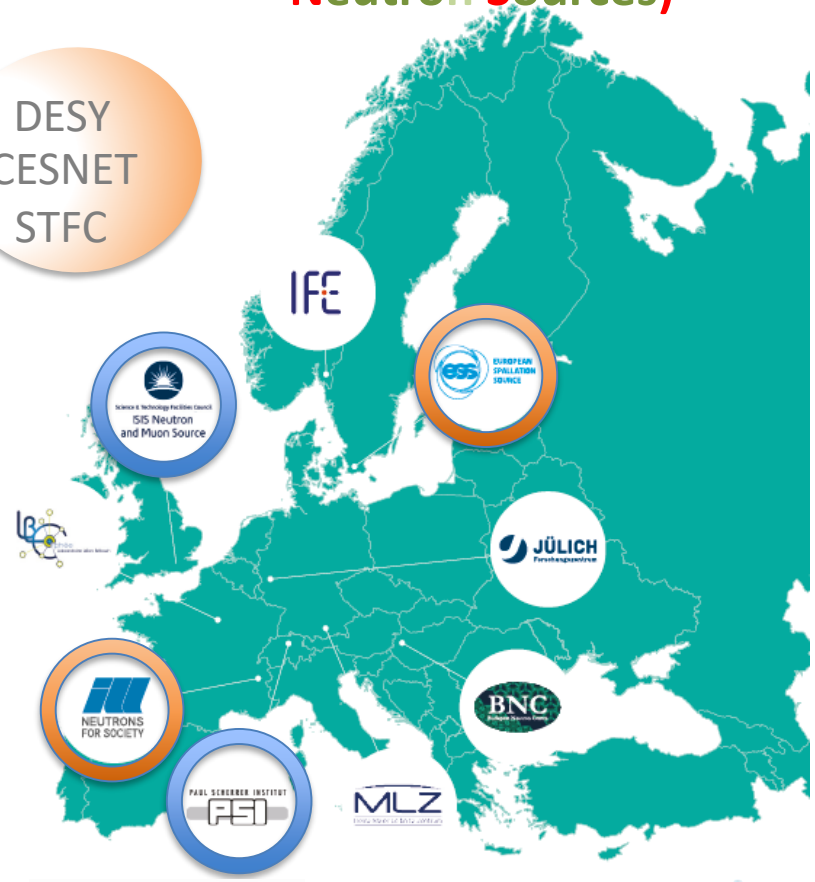
PaNOSC

ExPaNDS

DESY
CESNET
STFC

Neutrons

(LENS – League of European Neutron Sources)



LENS

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European Open Science Cloud Photon and Neutron Data Services

Sustainability of PaNOSC/ExPaNDS via LEAPS & LENS

- ✓ LEAPS & LENS via the RIs in these leagues will share the future sustainability of common services
- ✓ MoUs will define the cost and SLAs for each of the outputs from PaNOSC/ExPaNDS

LEAPS

LENS

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Cross-Cluster activities today and future

- Ontologies – PaNOSC/ExPaNDS + EOSC-Life
- Data stewardship training – PaNOSC/ExPaNDS + EOSC-Life
- Jupyter HDF5 viewver – PaNOSC/ExPaNDS + ESCAPE
- VISA data analysis portal – all clusters and EOSC Future
- HDF5 file format best practices – all clusters
- Data transfer – PaNOSC/ExPaNDS + ESCAPE
- COVID-19 data – PaNOSC/ExPaNDS + EOSC-Life

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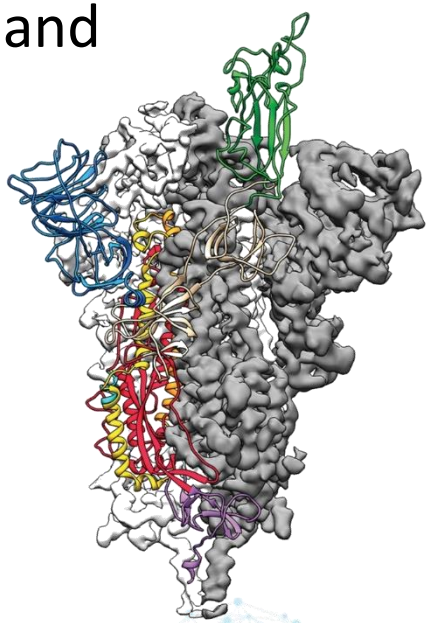
PaNOSC/ExPaNDS in EOSC-Future

- Integrate and exercise the services developed in PaNOSC/ExPaNDS into EOSC
- Apply them to two cross-disciplinary science projects
  - Tracing Bio-Structures
  - Dynamics of biological processes
- Collect feedback, improve services and make them generic, advertise and share results



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Future role of Science Clusters

Science Clusters

- Representing large and divers user communities
- Facing the data challenge – more data, more complex data
- Ensure that time to publication is reduced
- Provide an environment which is user friendly

Desirable common activities

- Cloud procurement of scale
- Use of HPC, access models, accounting
- Workflow tools
- Data compression
- Machine Learning and Artificial Intelligence
- Best practices and knowledge exchange
- Share developments of common interest
- Fostering the Open Science paradigm

ENVRI FAIR

EOSC-Life

ESCAPE

panosc photon and neutron open science cloud

SSHOC

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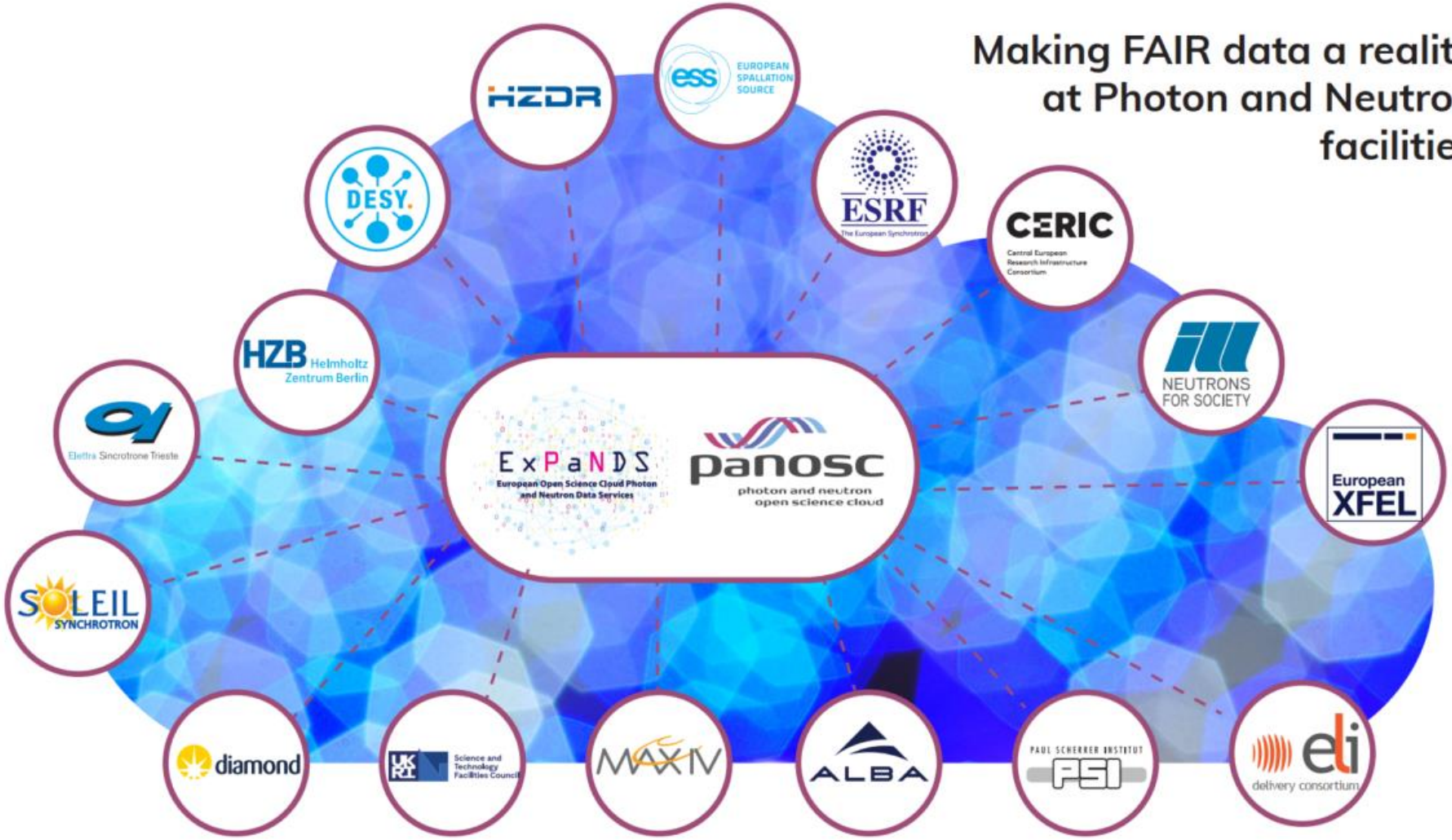

"The scientific communities using the analytical facilities need an EOSC which enables seamless interaction with open data for open science"

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Thank you to all PaNOSC/ExPaNDS project members for their contributions to the project and sharing a common vision!

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