

Open Science and Data at SOLEIL

Brigitte GAGEY Synchrotron SQLEIL – IT Strategy and Quality October 17, 2022







Synchrotron SOLEIL, in a nutshell

A high-technology facility at the service of research, major national challenges and industry



- Decision to build the facility made in 2000
- Open to external users in 2008
- ➤ Overall construction budget ~600 M€
- > Annual budget ~63 M€
- ~450 staff members



- Storage ring 354m, 2.75GeV
- > 29 Beamlines, covering 9 orders of magnitude in energy



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CQD

28%

72%





per year : ~5.000 hours of available beamtime for users ~ 1.200 experiment proposals, <50 % accepted

> 2021 : 3.500 user visits + 650 remote 700 publications

Users (2017-2021)					
Biology and Health	2000				
Energy	650				
Physical sciences and engineering	4300				
Earth science and environment	350				
Human and social sciences	300				
Astrophysics and astrochemistry	300				





Towards an explosion in the data production

- Flyscan acquisition : multi-techniques / multi-detectors, fast, synchronous
- High-rate and high-volume detectors
- More automated Beamlines



Raw Data:

Past and projected data production



2010-2020 : Amount of data stored 2021-2023 : Projection based on BL scientists' responses to a survey

4.5 Petabytes stored until 10 October 2022



Addressing new scientific and societal challenges



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Photon and Neutron Facilities towards Open Science and Data



 $\Rightarrow A \text{ template for Data Policy (<u>https://doi.org/10.5281/zenodo.3738497</u>) establishing common principles, adopted progressively according to the context of each facility$





PaNOSC and ExPaNDS H2020 projects

PaNOSC ExPaNDS		2021 2022 2023 ExPaNDS
	photon and neutron open science cloud	European Open Science Cloud Photon and Neutron Data Services
EU Call	HORIZON 2020 INFRA-EOSC-04	HORIZON 2020 INFRA-EOSC-5B
Description	Cluster of ESFRI PaN Sources	EOSC PaN Data Services
Partners	ESRF, ILL, ESS, EU-XFEL, CERIC-ERIC, ELI-DC, EGI	DESY, ALBA, DLS, ELETTRA, EGI, HZB, HZDDR, MAX IV, PSI, SOLEIL , UKRI
Observers	GEANT EU-DAT National RI's	
Linked 3 rd Party	DESY STFC CESNET	
Start – End (Duration)	2018-12-01 – 2022-11-30 [4 Years]	2019-09-01 – 2023-02-28 [3 1/2 Years]
Coordinators	A. Götz, J. Bodera	P. Fuhrmann, S. Servan
Budget	12 M Euros	6 M Euros
Home Page	PaNOSC.EU	ExPaNDS.EU
Twitter	@PaNOSC_eu #PaNOSC	@ExPaNDS_eu #ExPaNDS
GitHUB	github.com/panosc-eu	Github.com/expands-eu



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

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SOLEIL towards Open Science and Data





SOLEIL Data Management Policy established in consultation with SOLEIL Users and Beamlines' Scientists, with the support of CNRS experts in research data management.

Encouraging and helping SOLEIL Users and Scientists to produce FAIR data *Findable, Accessible, Interoperable, Reusable*

« Open data as possible, closed data as necessary »

- Applicable to data obtained via public research conducted at SOLEIL
- Long-term storage of raw data and metadata up to 5 years (striving for up to 10 years)
- Curated in well-defined formats (HDF5/NeXus)
- With a unique persistent Identifier, DOI
- Access via an online data catalogue
- 3+1+1 years embargo; open access after the embargo
- <u>CC-BY-4.0</u> license



The experimental team has to establish a data management plan (DMP) and to ensure the completeness of the metadata. SOLEIL committed to provide means for the capture of metadata, for the reduction and processing of raw data.







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Management

Data



 Currently : Collected by different tools depending on the Exp. Lifecycle Stages; SOLEIL naming use

ExPaNDS

European Open Science Cloud Photo

and Neutron Data Services

D2.7 deliverable

- ✓ Standardization of PaN MetaData at each Exp. Lifecycle Stage
- PaN Standardized Metadata to be implemented and gathered in the SOLEIL Data Catalog





Format

Data

NeXus/HDF5 recommended since SOLEIL opening Used systematically at 15 SOLEIL Beamlines; depending on the context (instrument, etc.) at the other ones • Now widely adopted at PaN facilities, and supported by anosc ٠

SciCat under implementation at SOLEIL

SciCat Open Source Project



open science cloud



View Public Data (without authentication) \checkmark

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Find, Filter, Generate DOI (after authentication) \checkmark

and Neutron Data Servi

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noton and neutror open science clou



Services

Data Analysis

Remote

4- Data Exploitation

VISA Platform originally developed by ILL



Photon and neutron open science cloud Photon and neutron open science cloud E x P a N D S European Open Science Cloud Photo and Neutron Data Services Providing remote data analysis services in a web browser with access to :

- Experimental data, Analysis software, Compute infrastructure, Support (IT & scientific)

Users can :

- create their own virtual working environment simply by using a web browser;
- access datasets and benefit from the same computing resources as if working on site;
- have the latest version of the analysis program without having to install it, download it, ...
- Jupyter notebook environment

Team members can also :

join a secure work environment, provide support and enjoy real-time collaboration.



https://bit.ly/VISA-video

→ Being installed for SOLEIL Data Analysis Services



Testing SOLEIL (<u>SAMBA Beamline</u>) XAFS data analysis software on a VISA instance

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5- Communication



Communicating, Training, Learning



3- Data Curation

making dissemination and enhancement and processing storage, data for available, Infrastructure data

✓ CNRS & GENCI

✓ Equipex+ / PIA3

FITS Project

- ✓ Started in June 2021
- ✓ 2022, in "pre-FITS" phase SOLEIL Data > 3 years :
- - Copy 🗲 IDRIS
 - Secure archive \rightarrow CC-IN2P3

LEAPS-INNOV project \rightarrow new strategies for data reduction and compression

LEAPS-INNOV has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 101004728

- Implementation of a distributed infrastructure hosted in low carbon environmental conditions
- \rightarrow Federate the services and know-how of the 2 CNRS computing centres (IDRIS and CC-IN2P3)





SOLEIL and EOSC

✓ EOSC portal (<u>https://eosc-portal.eu/</u>) :

SOLEIL registered as a **potential service provider**

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Scientific Domains		Categories						≡
Medical & Health Sciences	Engineering & Technology	Natural Scier	Synchrotron SOLEIL			All resource	s 🗸	۹
Generic	Humanities	Agricultural Sc		Sole IL				
Social Sciences	Other		Ask this provider a question	→ Website	Legal status : Private Company Operational	Life cycle :		

- ➔ SOLEIL data services to be available at the EOSC Portal, in the example of other PaN facilities
- ✓ EOSC Association (<u>https://eosc.eu/</u>) : SOLEIL observer
- ✓ EOSC-France College : SOLEIL member



Examples of Data Services of PaN facilities available at the EOSC portal



- ✓ A long road since the first discussions to establish a SOLEIL experimental data policy
- \checkmark Involving Users, Scientists and IT staff at the early stages.
- An action plan based on international and national collaborations, projects and shared services, and in coherence with European and national initiatives :

not reinventing what is done elsewhere and building on joint efforts

Next Steps :

- Make SOLEIL Experimental Data Policy a reality at all Beamlines
- Deploy SOLEIL Data Services at all Beamlines
- Make SOLEIL Data Services available via the EOSC portal
- Upcoming MoUs to continue the collaborative works
- Sustainability of PaN Data Commons could be managed within LEAPS (the League of European Accelerator-based Photon Sources) and LENS (the League of European Neutron Sources) frameworks
- With EOSC support in the Open Science and Data process
- Data Repository certification under consideration



Thank you for your attention !

