

ExPaNDS

**European Open Science Cloud Photon
and Neutron Data Services**

Technical achievements of ExPaNDS

**Paul Millar (DESY)
Technical coordinator**

2023-01-24

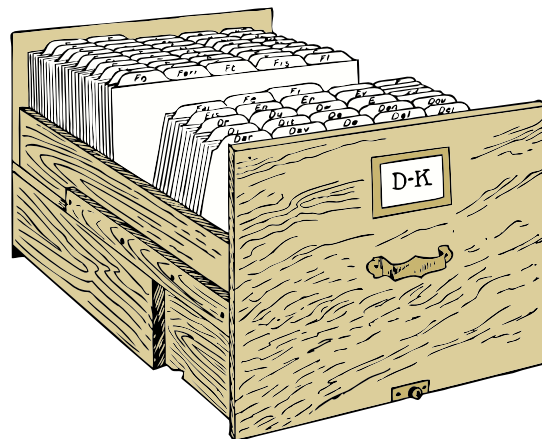


This project receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641

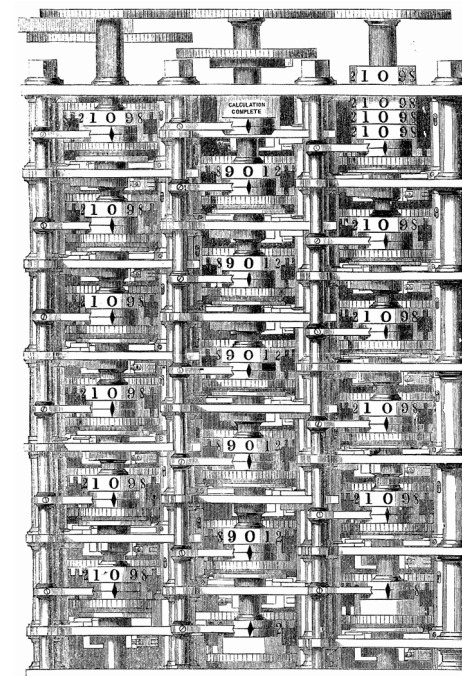
Overview of the technical WPs



WP2: FAIR data principles



WP3: FAIR data catalogues



WP4: FAIR data analysis




WP2: FAIR data principals



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WP2: FAIR data policy framework




D2.1: Draft External Framework for Photon and Neutron RIs

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Document Identifier:	D2.1
Project Title:	ExPaNDS
Work Package:	WP2
Work Package Lead:	UKRI
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Document Contributor(s):	Andy Götze (UKRI), Dan
Doc. Version:	1.0
Dissemination level:	Public
Date:	18/09/2020

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Date: 18/09/2020 1 / 74



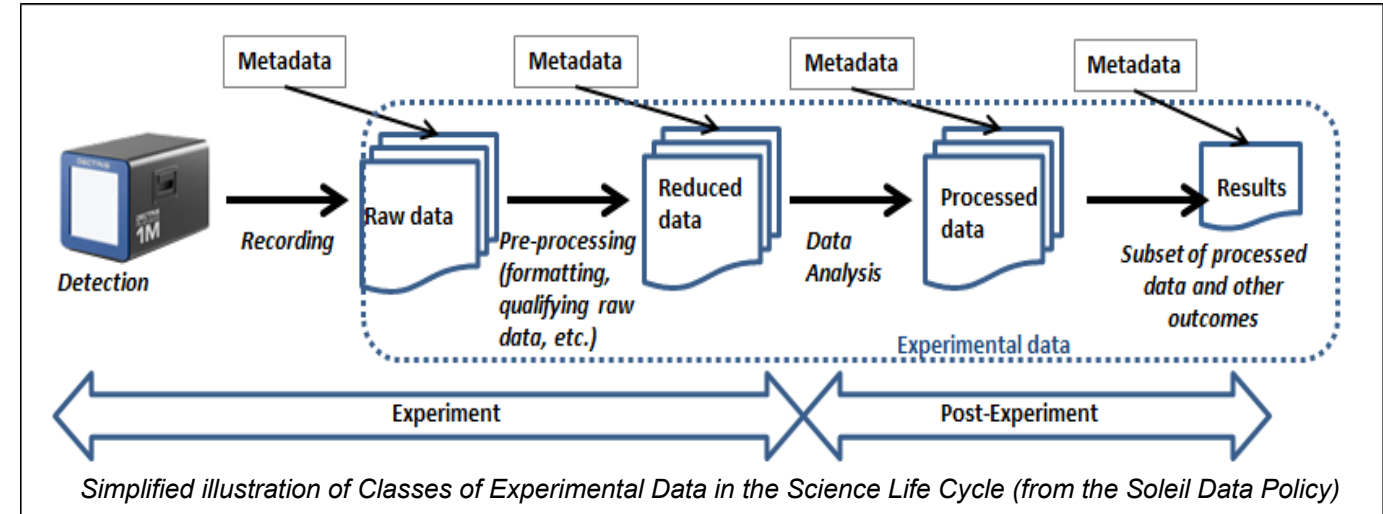
D2.3: Final Data Policy Framework for Photon and Neutron RIs

Document Control Information

Settings	Value
Document Identifier:	D2.3
Project Title:	ExPaNDS
Work Package:	WP2
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Document Author(s):	Abigail McBirnie (UKRI), Brian Matthews (UKRI), Brigitte Gagey (SOLEIL), Carlo Minotti (PSI), Daniel Salvat (ALBA), Frank Schlünzen (DESY), Andrei Vukobratovic (SOLEIL), N. Johnson (SOLEIL), M.
Document Contributor(s):	Alun W Ashton (PSI), Uwe Konrad (HZDR), Rolf Krah (HZB), Sophie Servan (DESY)
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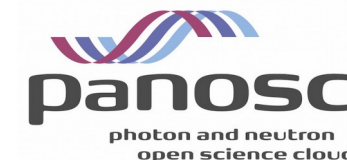
 This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857641.

Date: 20/08/2021 1 / 91 DOI: 10.5281/zenodo.5205825




“Data should be FAIR when it leaves the Facility”

21 policy principles



WP2: FAIR data management



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D2.7: Final Recommendations for FAIR Photon and Neutron Data Management

Document Control Information

Settings	Value
Document Identifier:	D2.7
Project Title:	ExPaNDS
Work Package:	WP2
Document Author(s):	Nicolas Soler (ALBA), Abigail McBirnie (UKRI), Alejandra Gonzalez-Beltran (UKRI), Andrey Vukolov (ELETTRA), Carlo Minotti (PSI), Heike Götz (HZB), Krisztian Pozsa (PSI), Darren Spruce (MAX IV), Brian Matthews (UKRI)
Document Reviewer(s):	1.0
Doc. Issue:	Public
Dissemination level:	Public
Date:	07/07/2022

Abstract
This deliverable (D2.7) provides final recommendations for FAIR Photon and Neutron Data Management. It is part of the ExPaNDS project, which aims to develop a European Open Science Cloud for Photon and Neutron Data Services.

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Publication

Data

People


Organisation

Project

Instrument


Sample


Software




doi

PURL







doi




ARK (Archival Resource Key)

PURL







ORCID




RESEARCHERID




isni




ROR




GRID




isni




RAiD




RDA



InChI TRUST



RRID



IGSN

The PID "zoo"

The idealised facilities lifecycle from PaN-data ODI D6.1

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WP2: Data Management Plans

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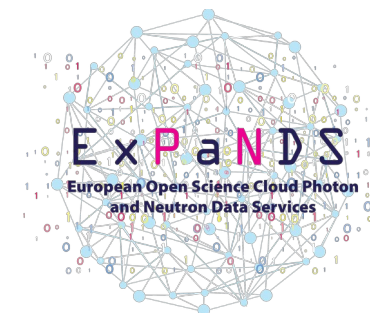
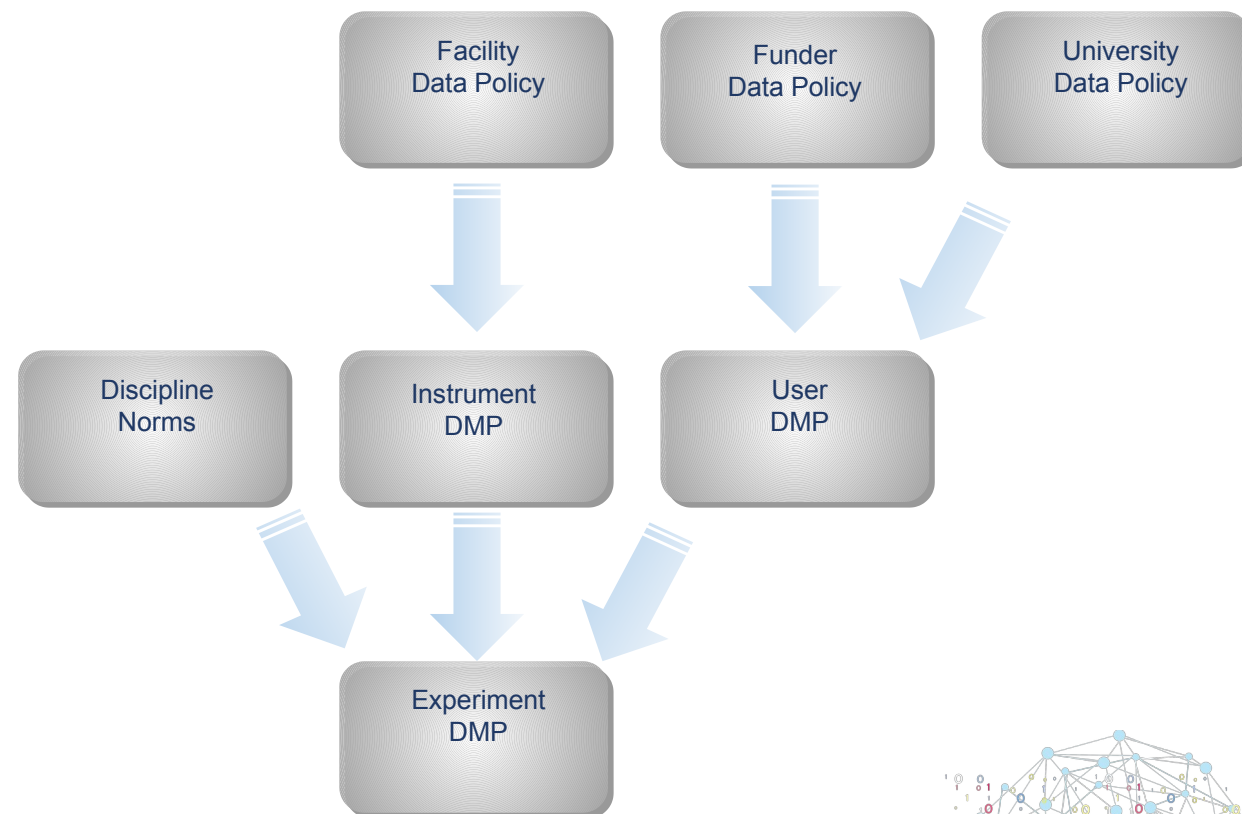
Active DMPs for Photon and Neutron
RIs

D2.4: DMPs for Photon and Neutron RIs

Document Control Information

Settings	Value
Document Identifier:	D2.8 active DMPs for Photon and Neutron RIs
Project Title:	ExPaNDS
Work Package:	WP2
Document Author(s):	Heike Görzig (HZB), Vasily Bunakov (UKRI), Alejandra Gonzalez-Beltran (UKRI), Janusz Malka (EuXFEL), Brian Matthews (UKRI), Abigail McBirnie (UKRI), Nicolas Soler (ALBA), Noel Vizcaino (UKRI), Majid Ounsy (SOLEIL), Others: Marjolaine Bodin (ESRF), Fredrik Bolmsten (ESS), Andrei Vukolov (Elettra)
Document Reviewer(s):	Steve P. Collins (Diamond), Oliver Knodel (HZDR)
Responsible Partner:	HZB
Doc. Issue:	1.0
Dissemination level:	Public
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Date: 20/12/2022 1 / 40 DOI: 10.5281/zenodo.7223438



WP2: FAIR self-assessment



D2.6 Self-evaluation Photon and Neutron RIs for FAIR data certification

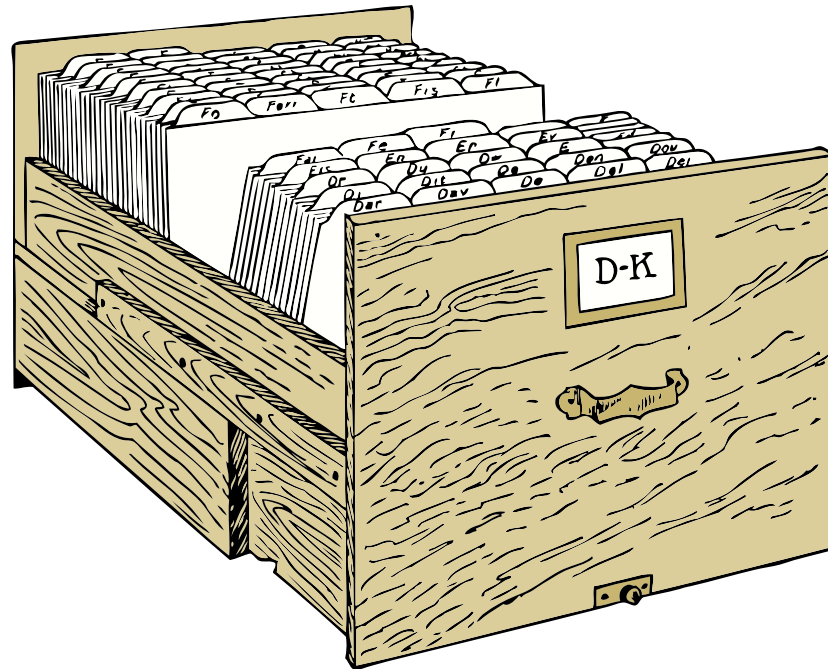
Document Control Information

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Document Identifier:	D2.6
Project Title:	ExPaNDS
Work Package:	WP2
Work Package Lead	UKRI
Document Author(s):	Simon Lambert (UKRI), Abigail McBirnie (UKRI), Brian Matthews (UKRI), Stephen Collins (DLS), Maik Fiedler (HZDR), Brigitte Gagey (SOLEIL), Heike Götzig (HZB), Oliver Knodel (HZDR), George Kourousias (Elettra), Anders Markvardsen (ISIS), Carlo Minotti (PSI), Majid Ounsy (SOLEIL), Krisztian Pozsa (PSI), Silvan Schön (DESY), Nicolas Soler (ALBA), Darren Spruce (MAX IV), Andrei Vukolov (Elettra)

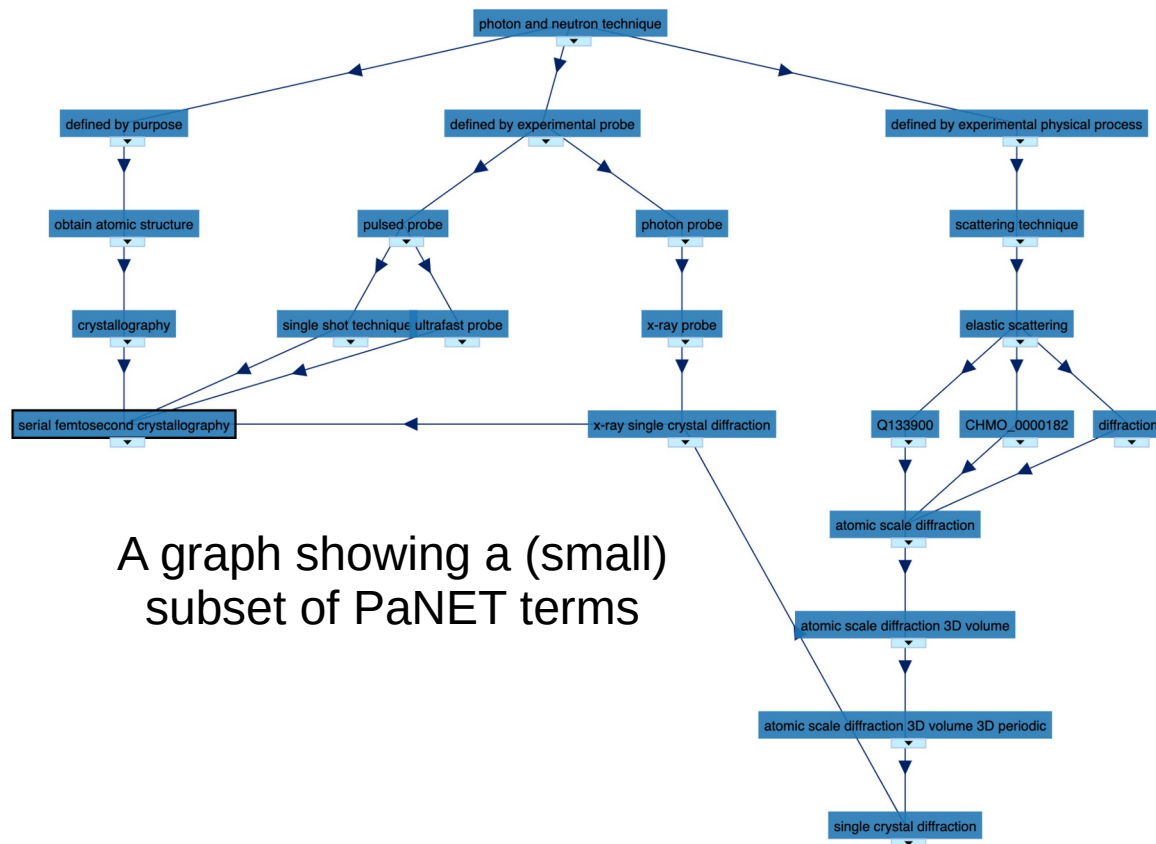
- FAIR Assessment
 - Test your data to see if it satisfies the FAIR Principles
- But we want to be sure that *every* experiment results in FAIR data
 - Test your process to see if it includes the right things to make the data FAIR
- A self assessment method for facilities to ask the questions
 - 29 questions to test the FAIR-Ness of the facility



WP3: FAIR data catalogues



WP3: PaNET ontology



A graph showing a (small) subset of PaNET terms

small angle scattering^C

[back to ToC](#) or [Class ToC](#)

IRI: <http://purl.org/pan-science/PaNET/PaNET01124>

Source

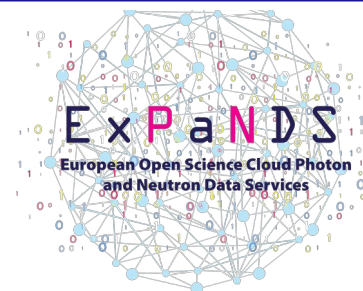
https://en.wikipedia.org/wiki/Small-angle_scattering

has super-classes

[c h m o 0000182](#)^C, [diffraction](#)^C, [low momentum transfer scattering](#)^C, [q133900](#)^C

has sub-classes

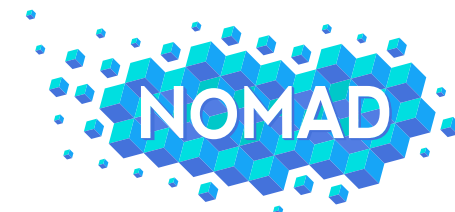
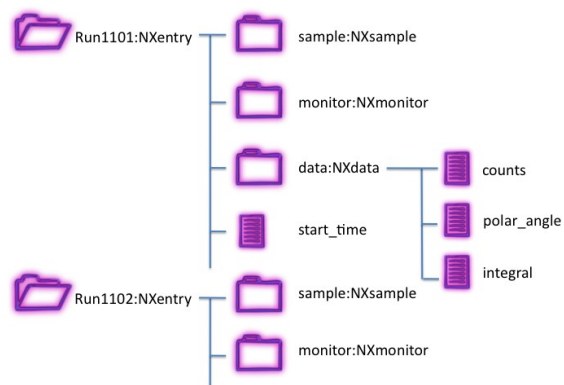
[anomalous small angle x-ray scattering](#)^C, [diffuse small angle scattering](#)^C, [grazing incidence small angle scattering](#)^C, [inelastic small angle scattering](#)^C, [small angle inelastic scattering](#)^C, [small angle neutron scattering](#)^C, [small angle x-ray scattering](#)^C, [spin echo small angle scattering](#)^C, [ultra small angle scattering](#)^C



WP3: NeXus ontology



NeXus Definition Language

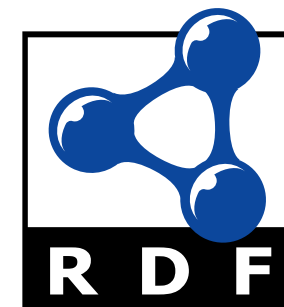


NOVEL MATERIALS DISCOVERY

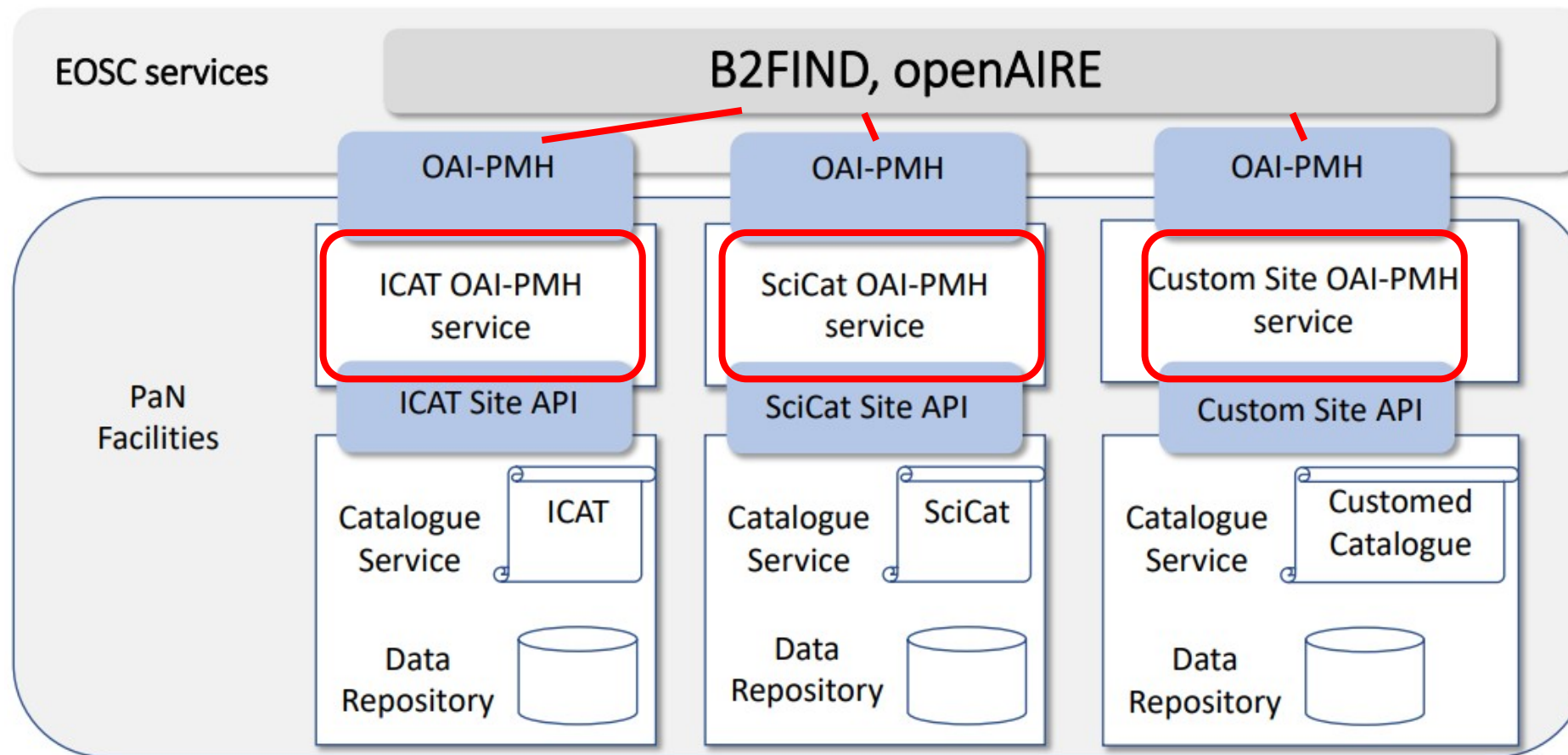


OWL

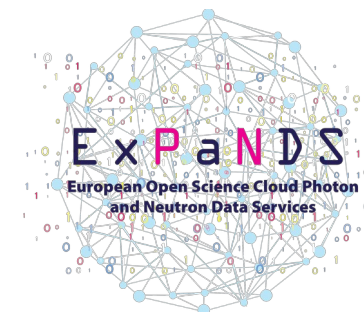
Being adopted and enhanced by NOMAD



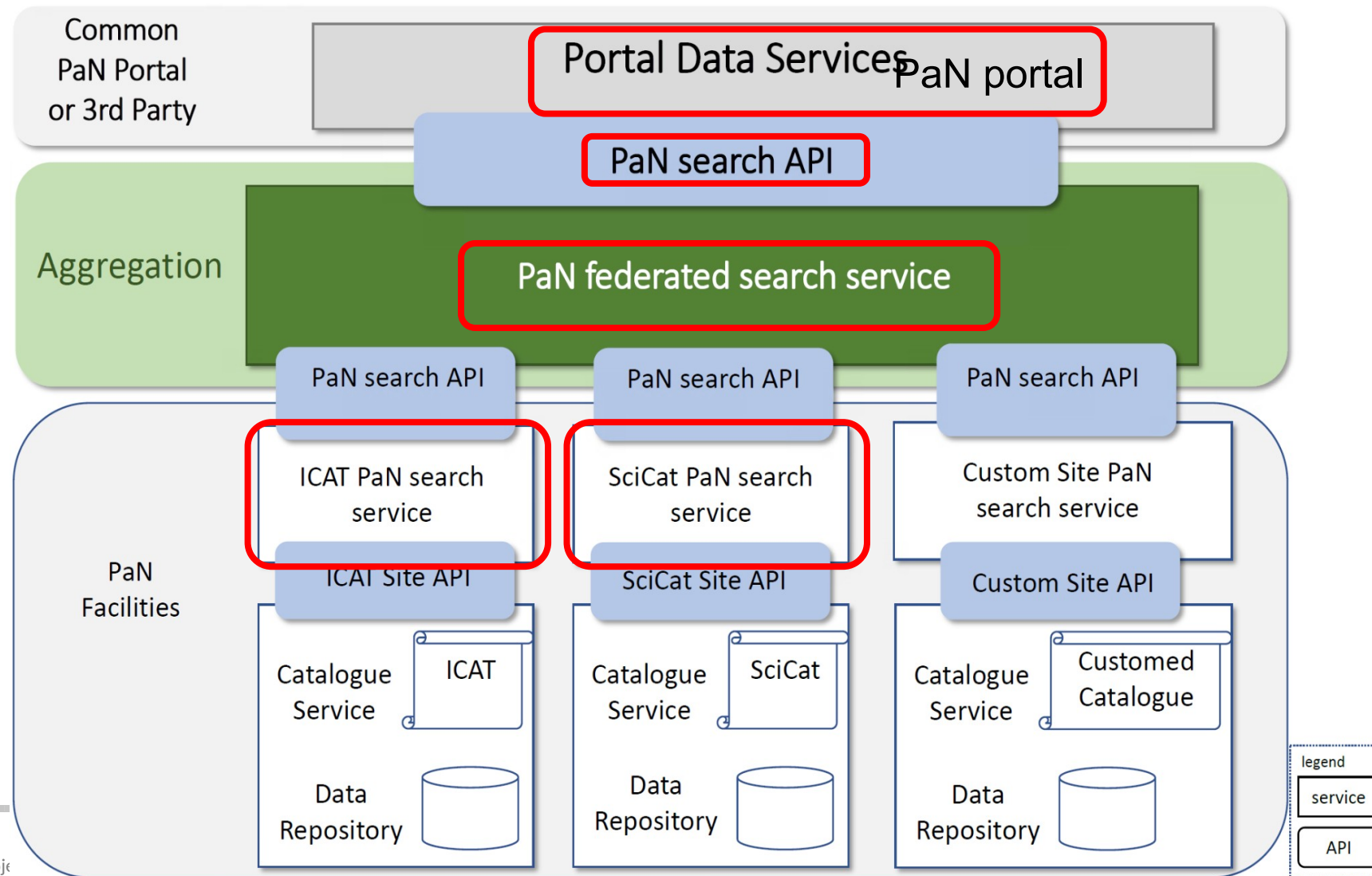
WP3: OAI-PMH



Slide thanks to
Carlo Minotti



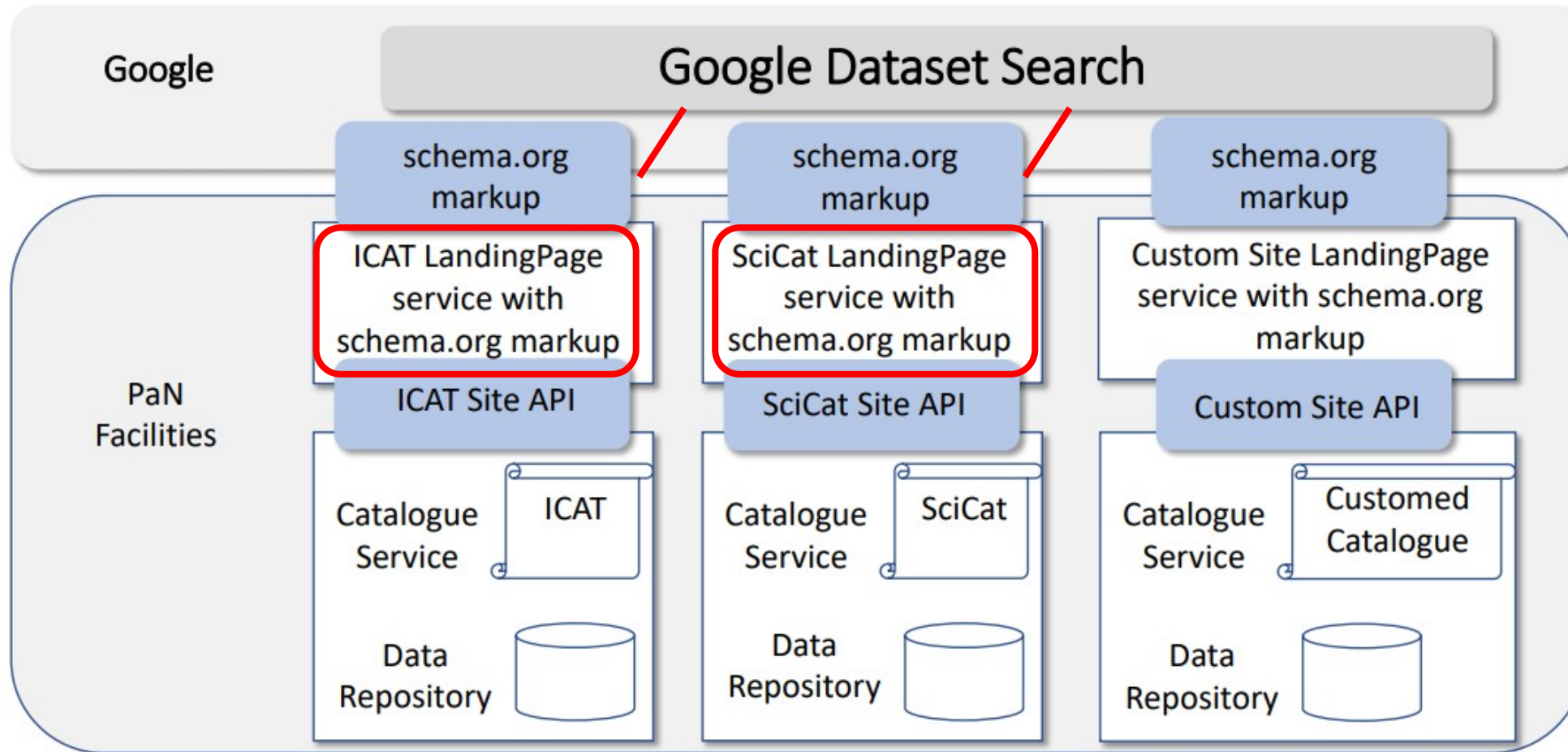
WP3: PaN Search API



Slide thanks to
Carlo Minotti



WP3: Google dataset search



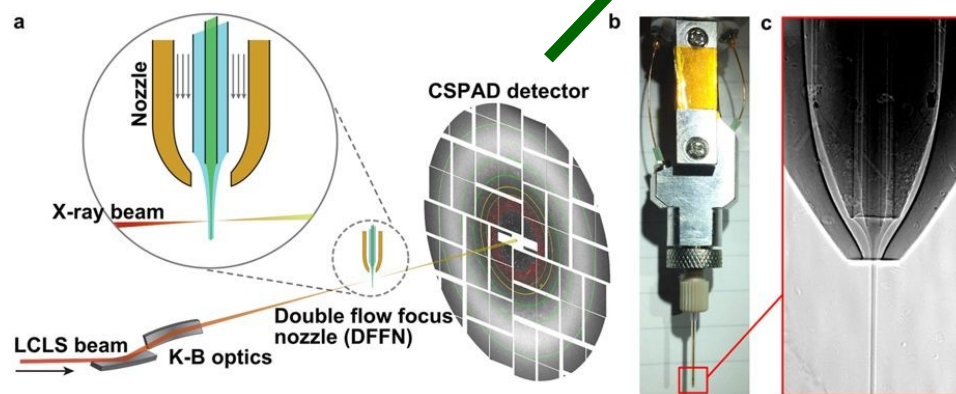
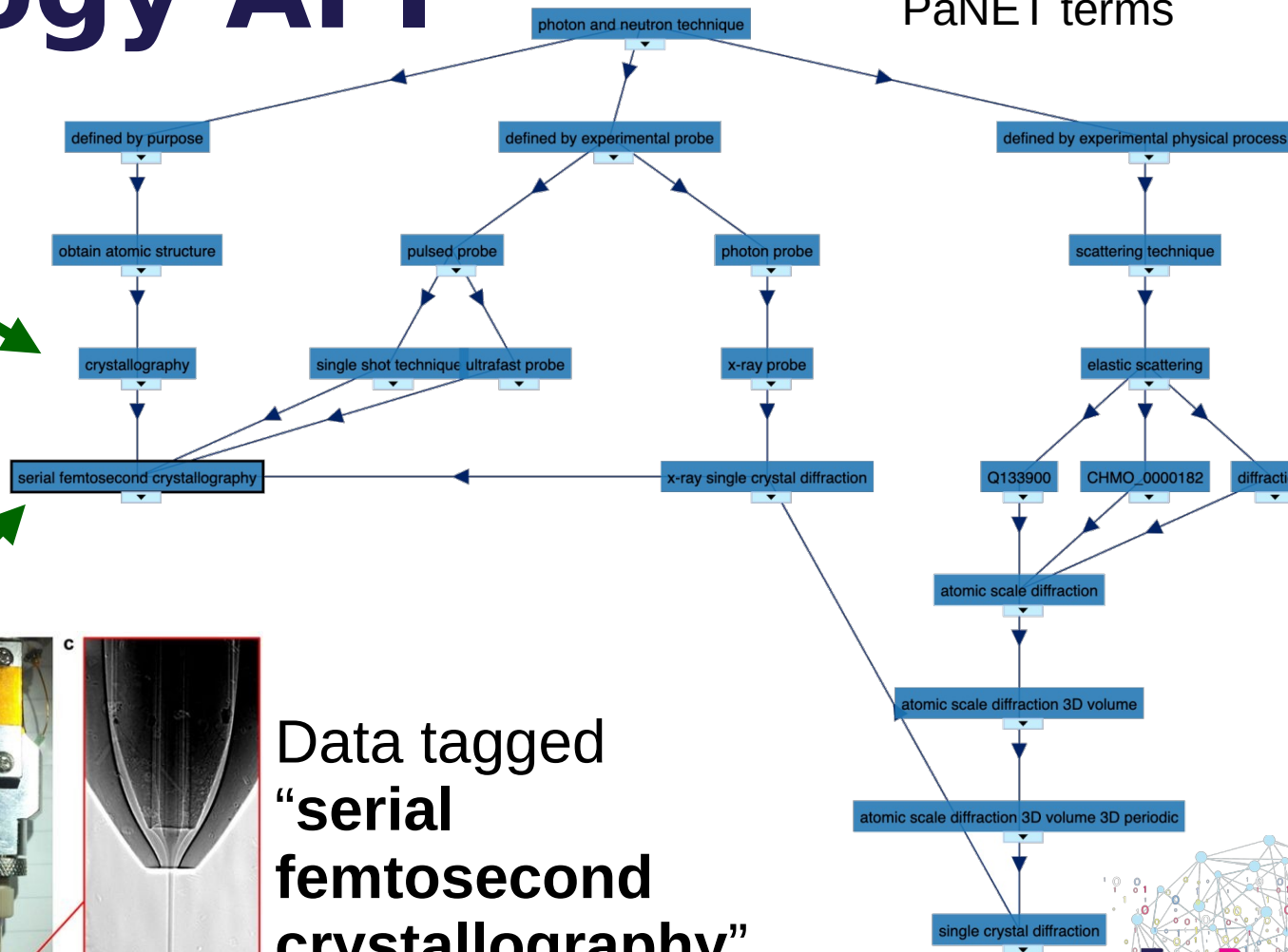
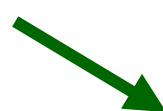
Slide thanks to
Carlo Minotti



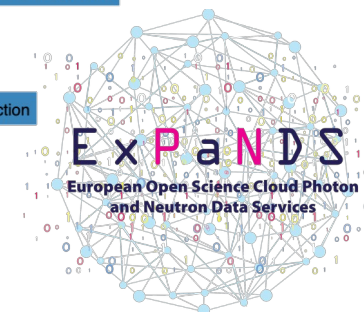
WP3: Ontology API

A graph showing a (small) subset of PaNET terms

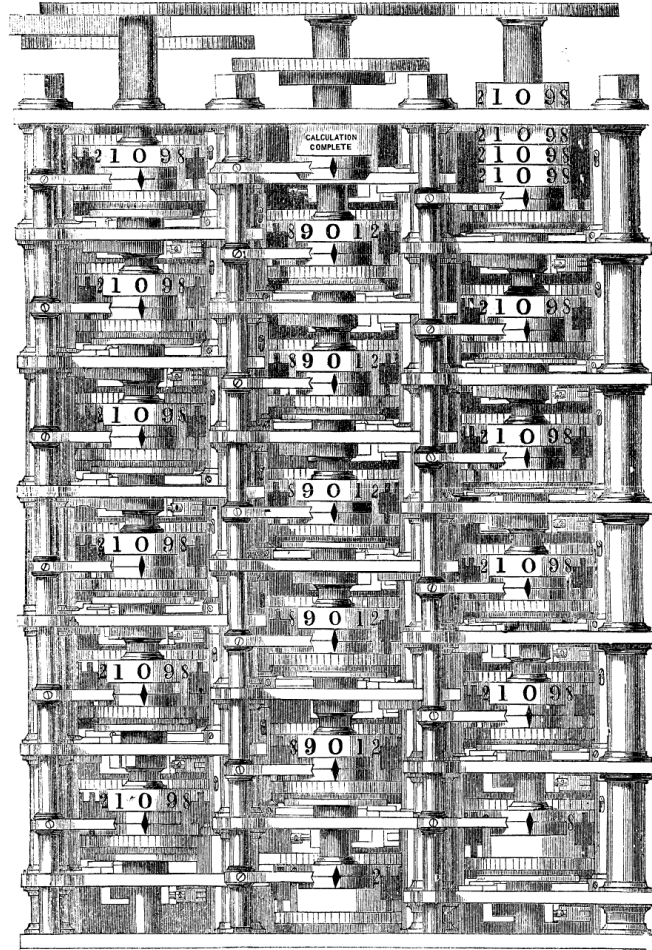
Researcher is searching for
“**crystallography**” data



Data tagged
“**serial
femtosecond
crystallography**”

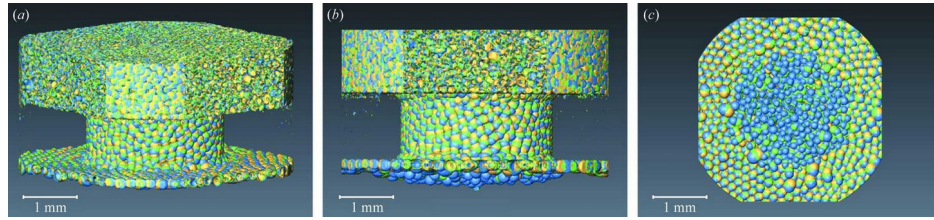


WP4: FAIR data analysis

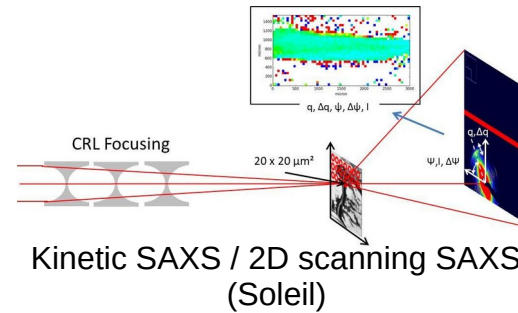


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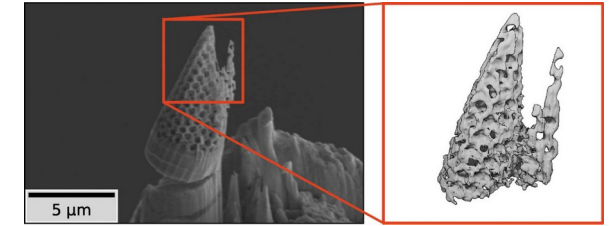
WP4: nine reference datasets



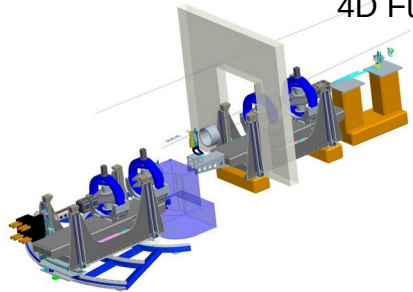
4D Full field tomography (MAX IV)



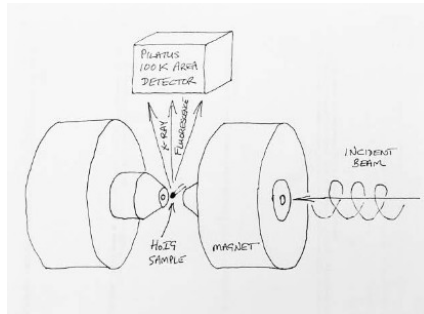
Kinetic SAXS / 2D scanning SAXS (Soleil)



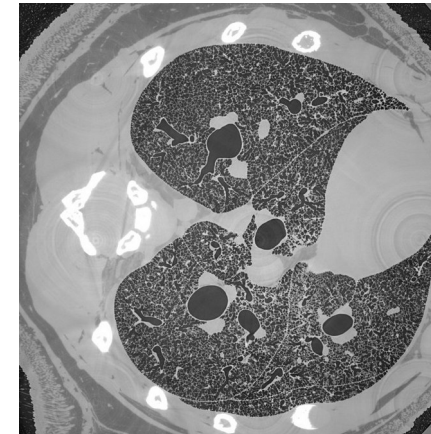
Ptychography / Pty. X-ray CT (MAX IV)



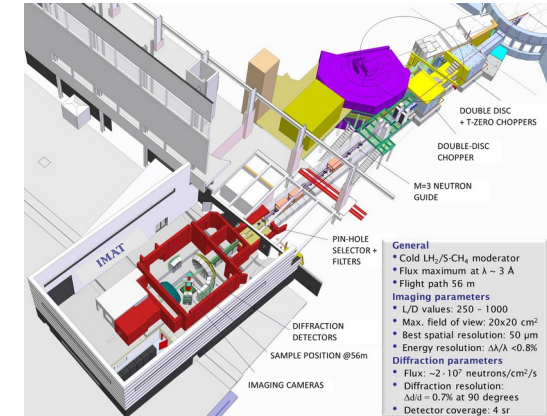
Neutron Reflectometry (UKRI/ISIS)



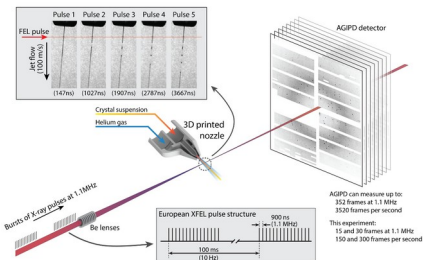
Single crystal X-ray diffraction (Diamond)



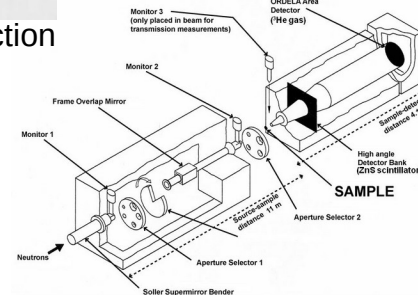
Full field tomography (PSI)



Neutron Imaging / Tomography (UKRI/ISIS)



Serial crystallography (DESY)



Neutron Small Angle Scattering (UKRI/ISIS)



WP4: Working with workflows

- Identified five workflows to act as exemplars:

Serial crystallography, THz Spectroscopy, Full-field Tomography, Ptycho-tomography, Small-Angle Neutron Scattering.

- Packaging workflows to allow execution of workflows outside of facility

Using containers or Jupyter notebooks, as appropriate

- Demonstrating execution of these workflows on multiple infrastructures
- Build a testing and validation framework for CI/CD



WP4: the practical bits....

- On-boarding of (remote) analysis services within EOSC Marketplace
- Helping facilities adopt federated authentication (e.g. Umbrella)
- Work focusing on VISA platform
 - Multiple facilities agreed on adopting VISA.
 - Sharing use-cases with VISA development team.
 - Sharing expertise, within the project, in VISA deployment
 - Site-local VISA integration effort.



Adoption (in October 2022) of PaNOSC+ExPaNDS outcomes

FACILITY	FAIR data policy	DMPs	DOIs	Nexus HDF5	Search API	Open Data Portal	AAI	Jupyter Lab	VISA	VINYL/OASYS/McStas	Pan-learning/training
ALBA	P	P	WIP	WIP	WIP	WIP	P	Y	WIP	N	U
DESY	WIP	WIP	WIP	Y	WIP	P	WIP	Y	U	Y	WIP
CERIC-ERIC	Y	WIP	Y	WIP	Y	Y	Y	Y	Y	Y	Y
DIAMOND											
ELETTRA	Y	WIP	Y	Y	Y	Y	Y	Y	Y	Y	Y
ESRF	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
ELI-ERIC	Y	Y	P	Y	Y	Y	WIP	Y	Y	Y	Y
ESS	Y	Y	Y	Y	Y	Y	Y	WIP	WIP	Y	Y
EuXFEL	Y	WIP	Y	WIP	Y	Y	WIP	Y	WIP	Y	Y
FELIX	Y	P	WIP	U	U	WIP	U	U	N	N	U
HZB	Y	P	WIP	Y	P	Y	P	U	U	U	U
HZDR	Y	WIP	Y	N	U	Y	Y	Y	P	WIP	Y
ILL	Y	WIP	Y	Y	WIP	Y	Y	Y	Y	Y	WIP
MAX-IV	WIP	U	Y	Y	Y	Y	Y	Y	U	U	U
PSI	Y	WIP	Y	WIP	Y	Y	WIP	WIP	N	N	N
PTB	Y	WIP	Y	WIP	N	Y	N	N	N	N	N
SOLARIS											
SOLEIL	Y	WIP	WIP	Y	WIP	WIP	Y	WIP	WIP	U	Y
SESAME	Y	U	P	Y	P	WIP	P	P	N	Y	N

Not Planning to be adopted (N)

Under evaluation (U)

In progress of being adopted (WIP)

open science cloud



Conclusions

- Significant body of work
- Contributions at several areas and levels:
 - Policy and Guidelines
 - Ontologies and knowledge capture
 - Improving and deploying dataset catalogues
 - Building an analysis workflow ecosphere
 - EOSC engagement

ExPaNDS outputs have a strong impact, uptake and sustained contribution

