ExPaNDS

European Open Science Cloud Photon and Neutron Data Services

Technical achievements of ExPaNDS

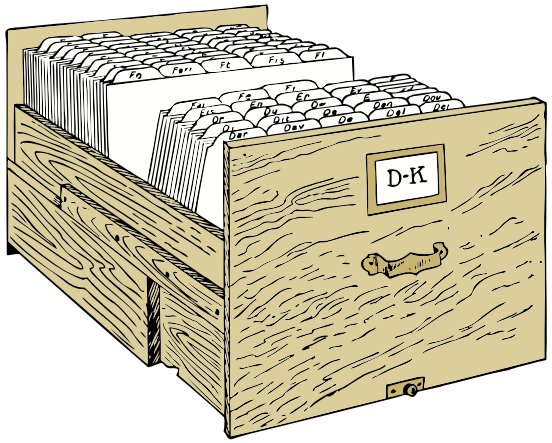
Paul Millar (DESY)
Technical coordinator

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

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WP2: FAIR data principals

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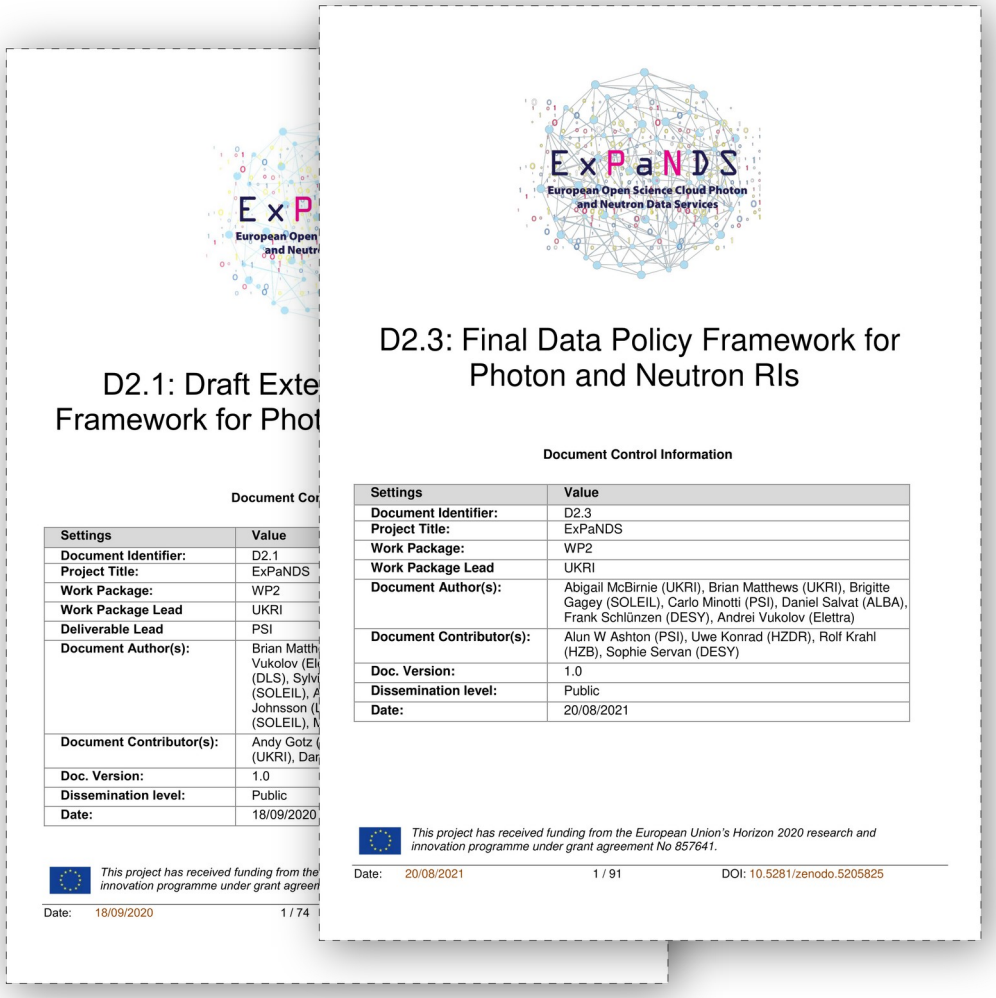
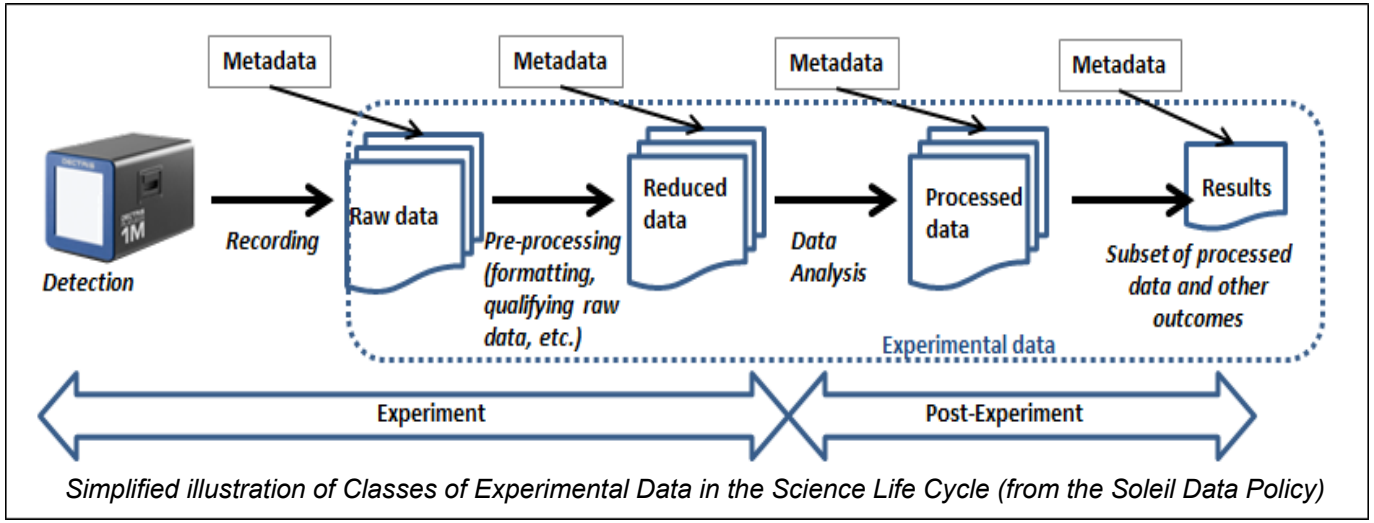
WP2: FAIR data policy framework





Simplified illustration of Classes of Experimental Data in the Science Life Cycle (from the Soleil Data Policy)

"Data should be FAIR when it leaves the Facility"

21 policy principles

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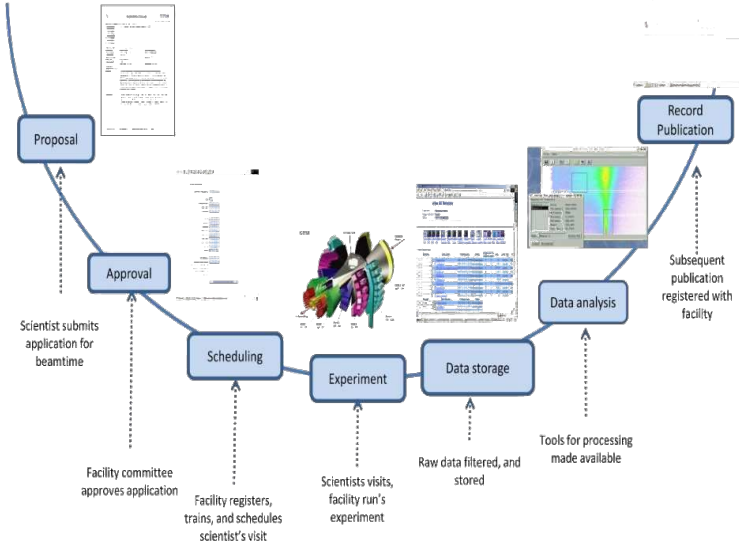
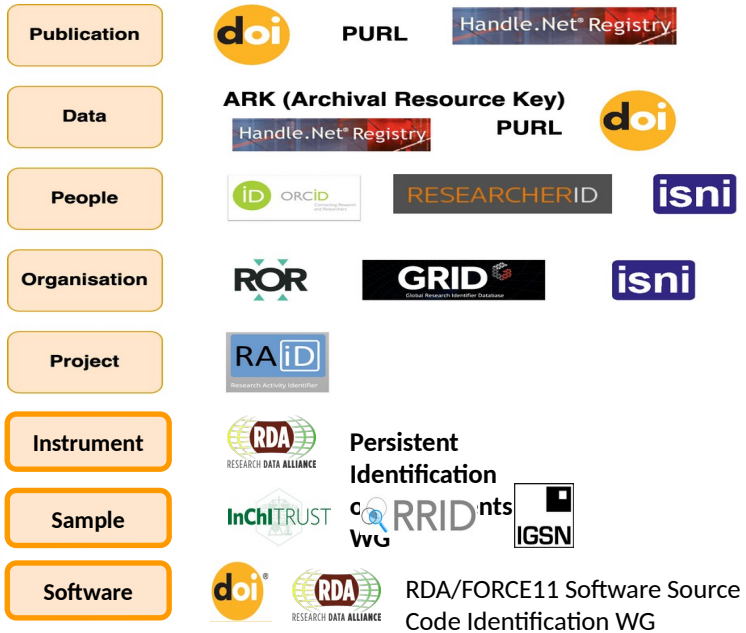
WP2: FAIR data management



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



The PID "zoo"

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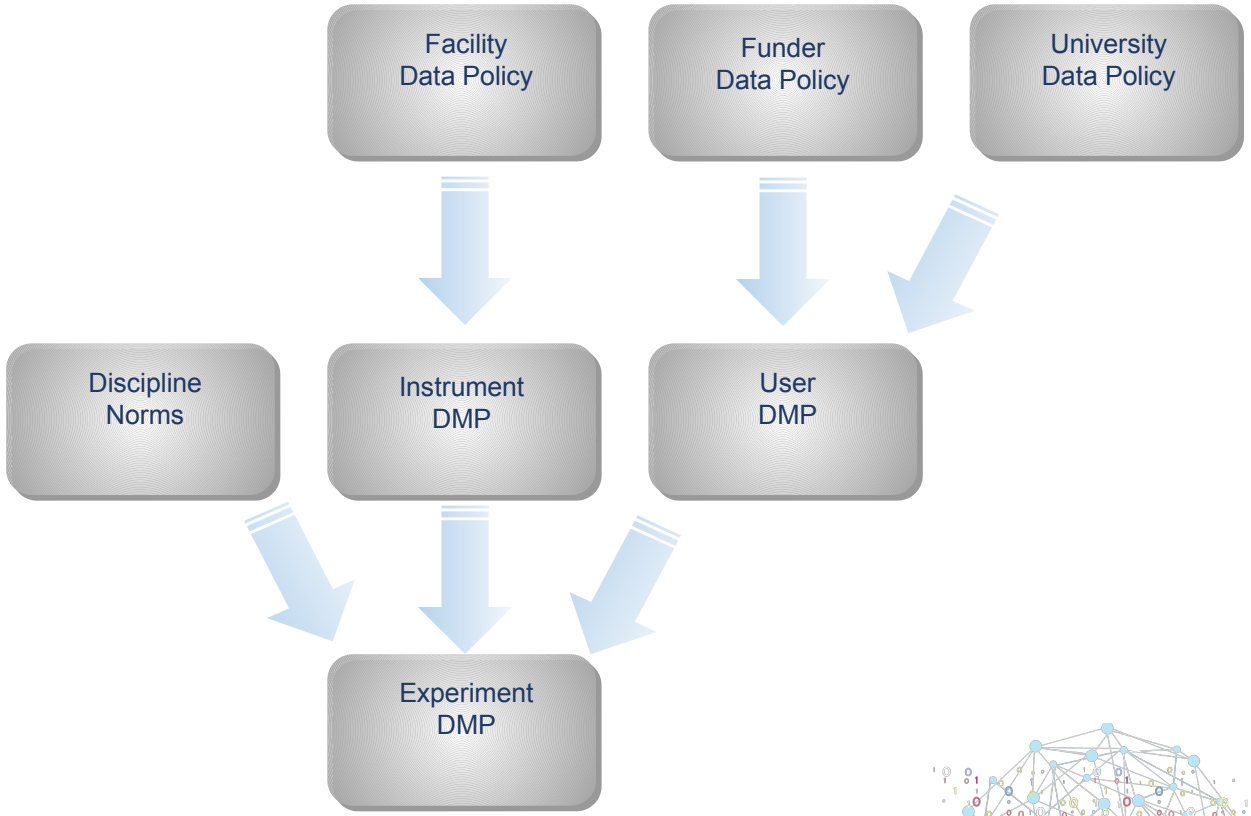
WP2: Data Management Plans



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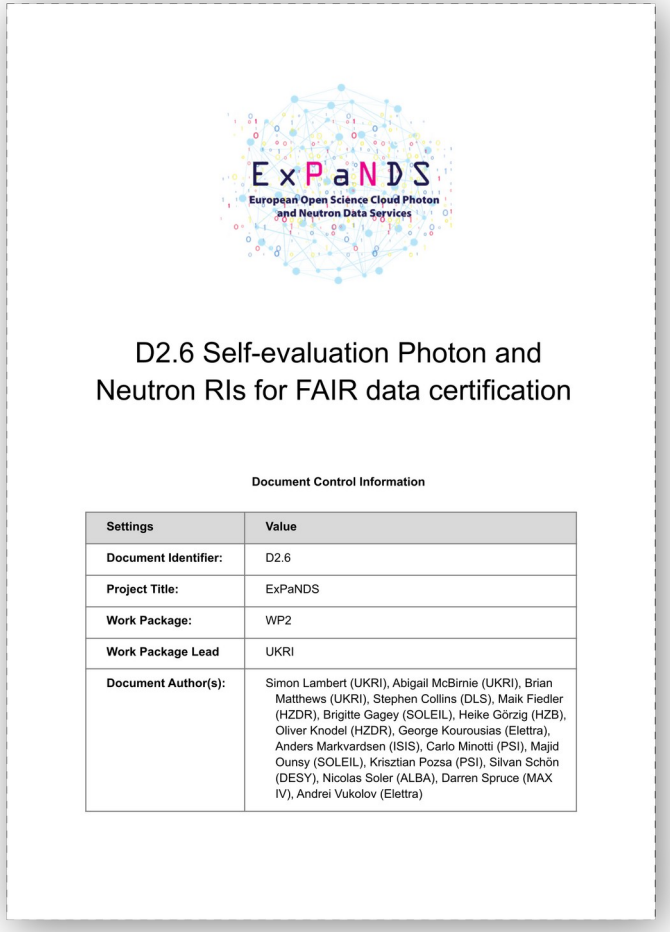
WP2: FAIR self-assessment



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

Document Control Information

Settings	Value
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 Görzig (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

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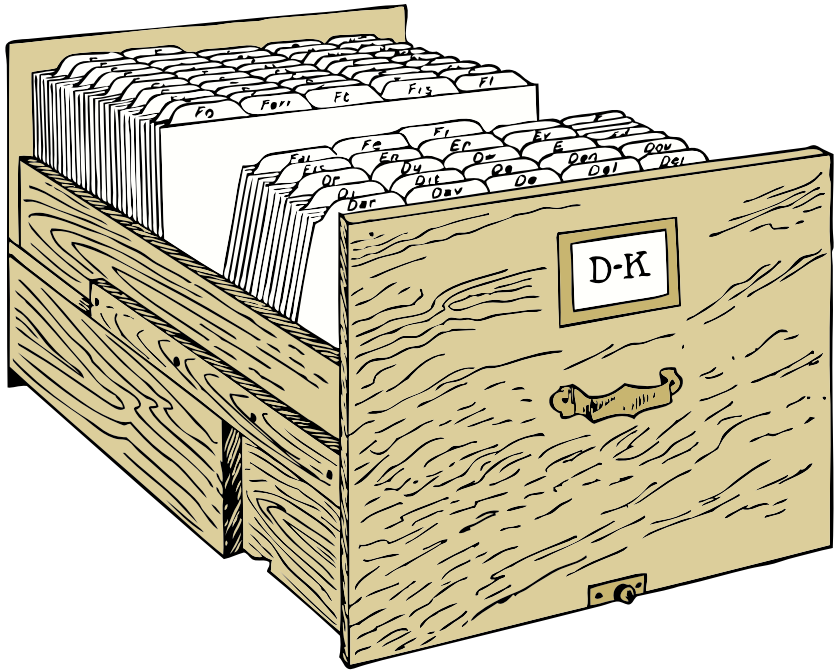
WP3: FAIR data catalogues



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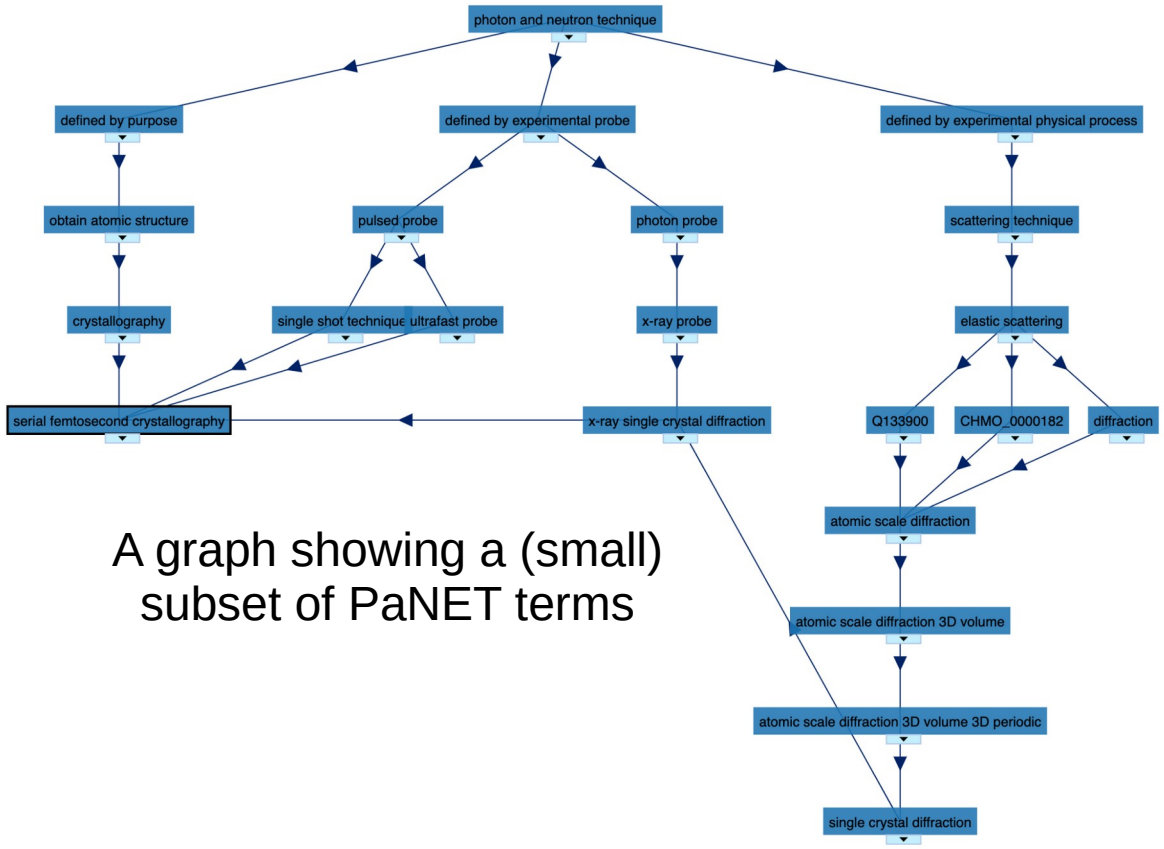
WP3: PaNET ontology



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 scatteringng [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]

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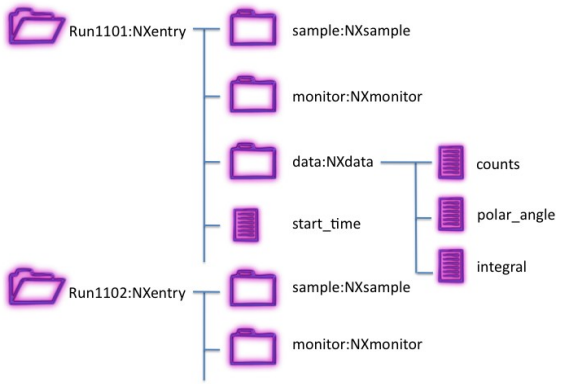
WP3: NeXus ontology

NOMAD
NOVEL MATERIALS DISCOVERY

NeXus

NeXus Definition Language



OWL

Being adopted and enhanced by NOMAD

RDF

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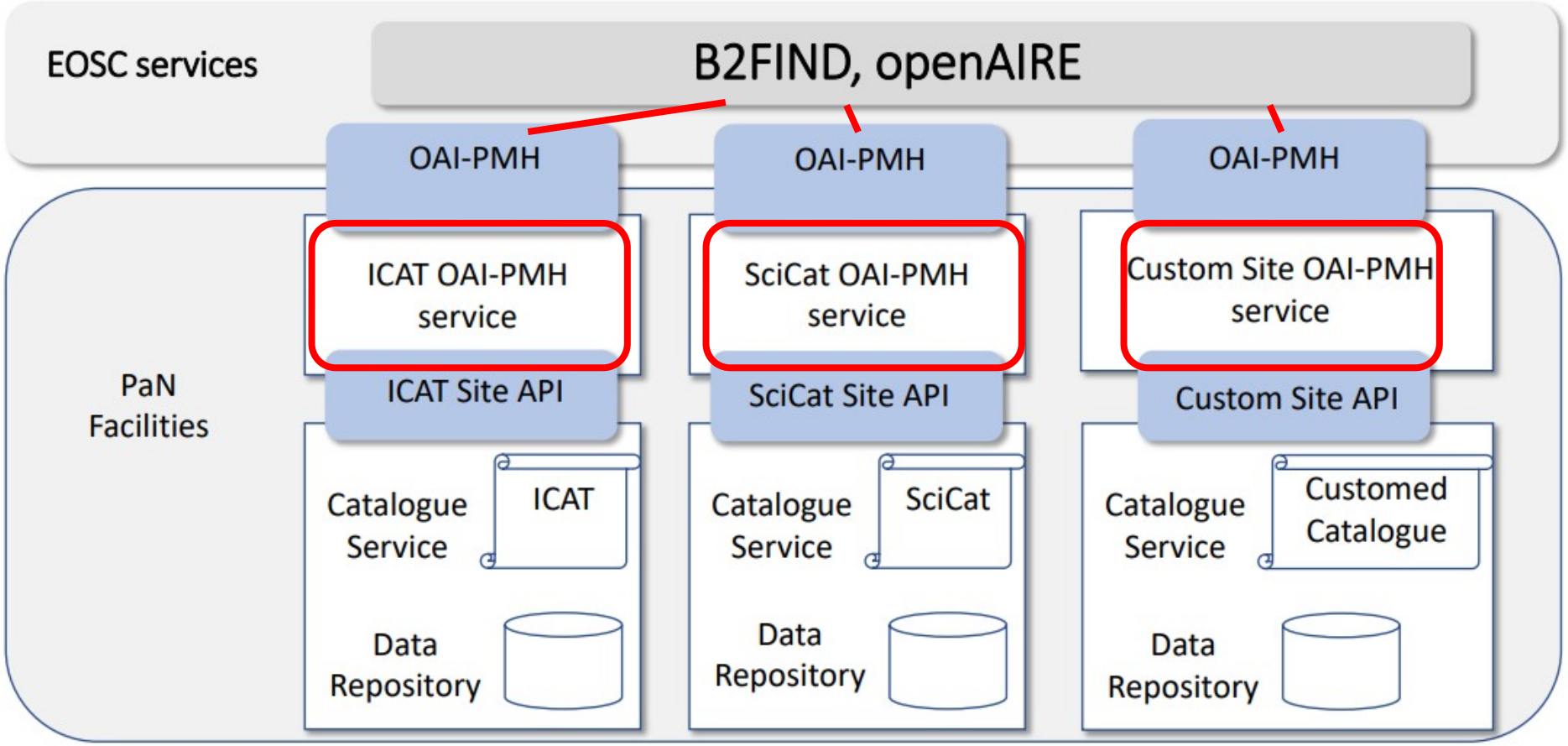
WP3: OAI-PMH



Slide thanks to
Carlo Minotti

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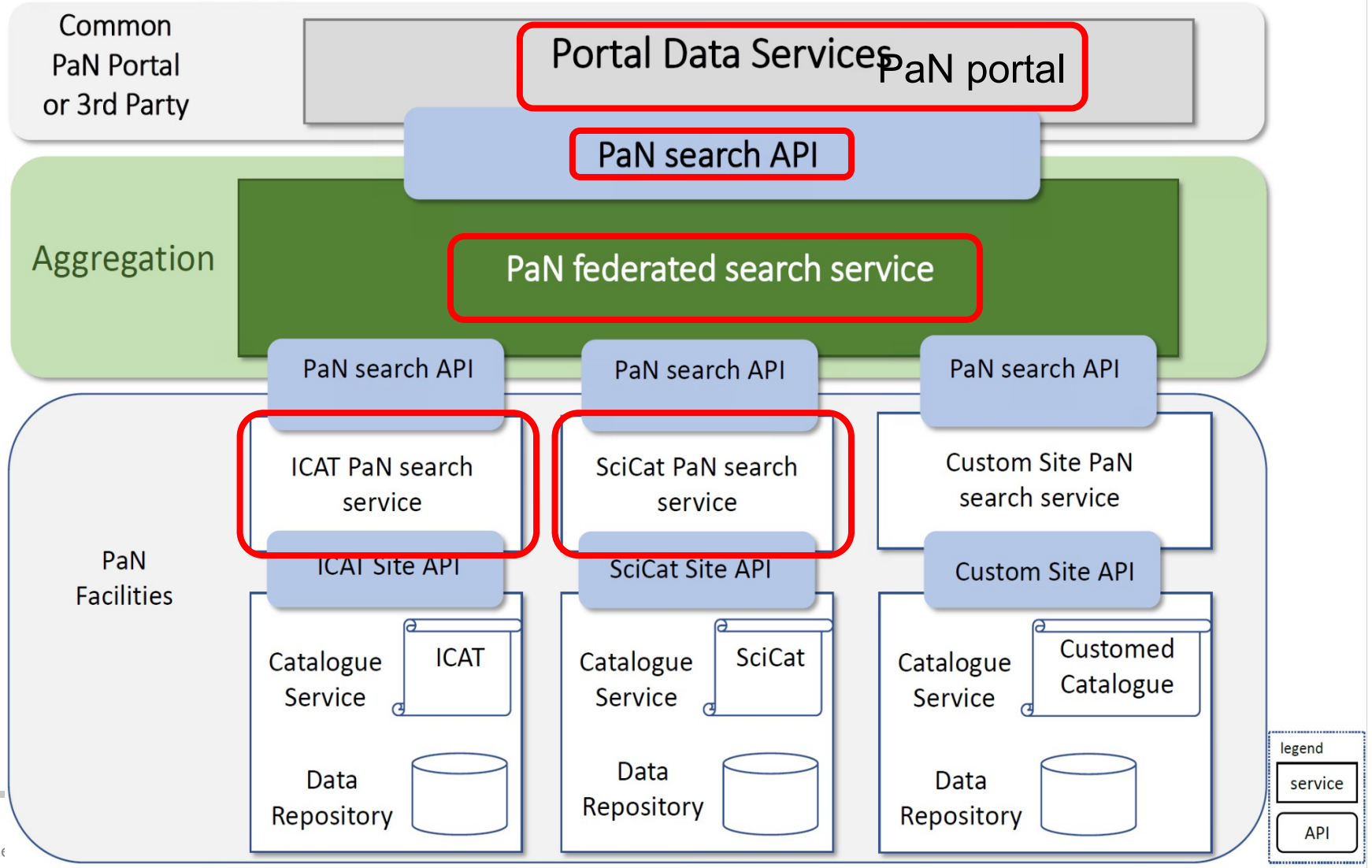
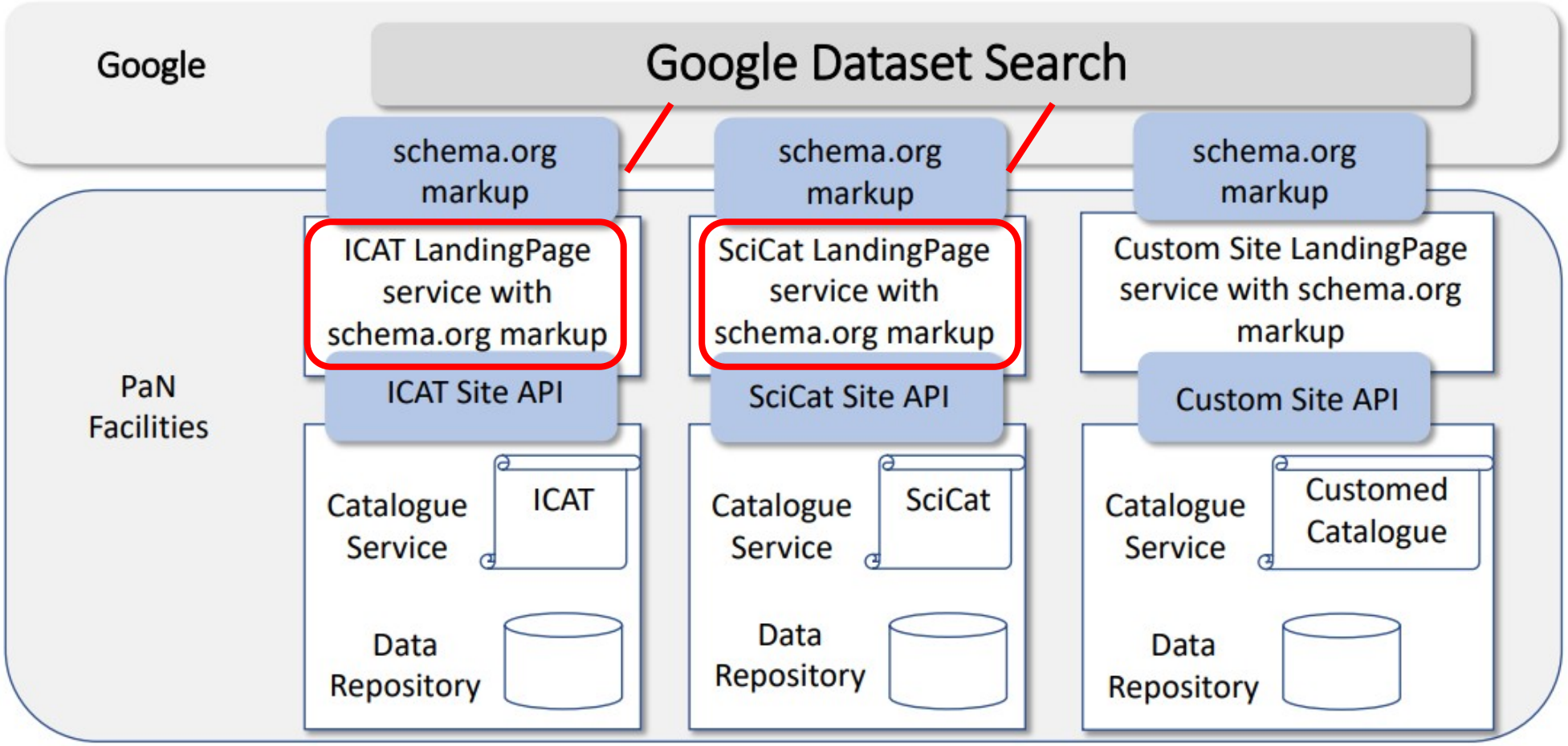
WP3: PaN Search API



Slide thanks to
Carlo Minotti

This proje

WP3: Google dataset search



Slide thanks to **Carlo Minotti**

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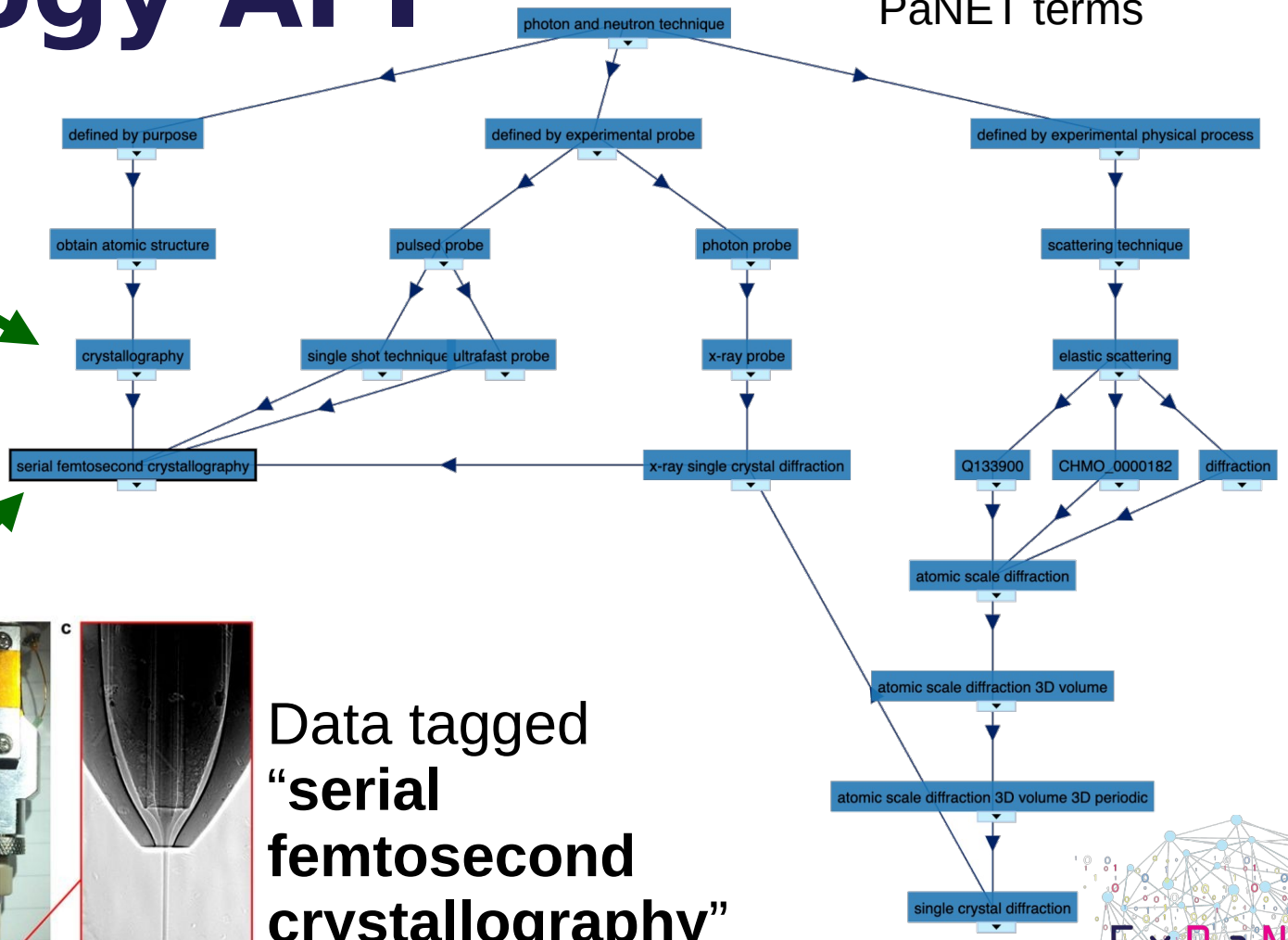
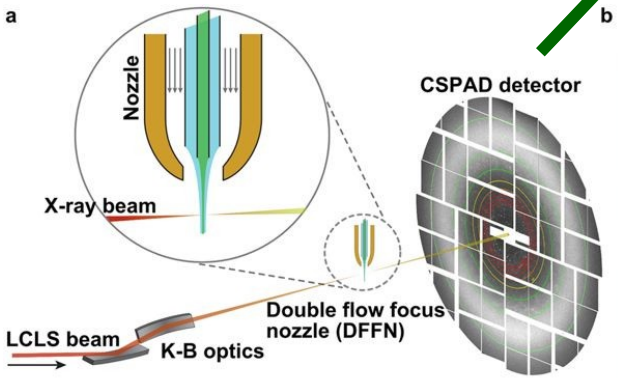
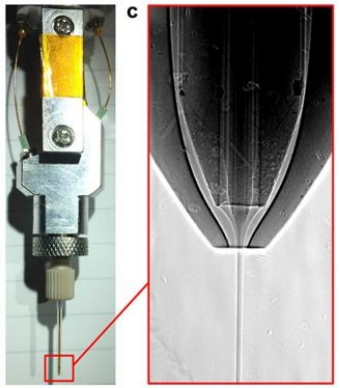
WP3: Ontology API

A graph showing a (small) subset of PaNET terms

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







Data tagged “**serial femtosecond crystallography**”

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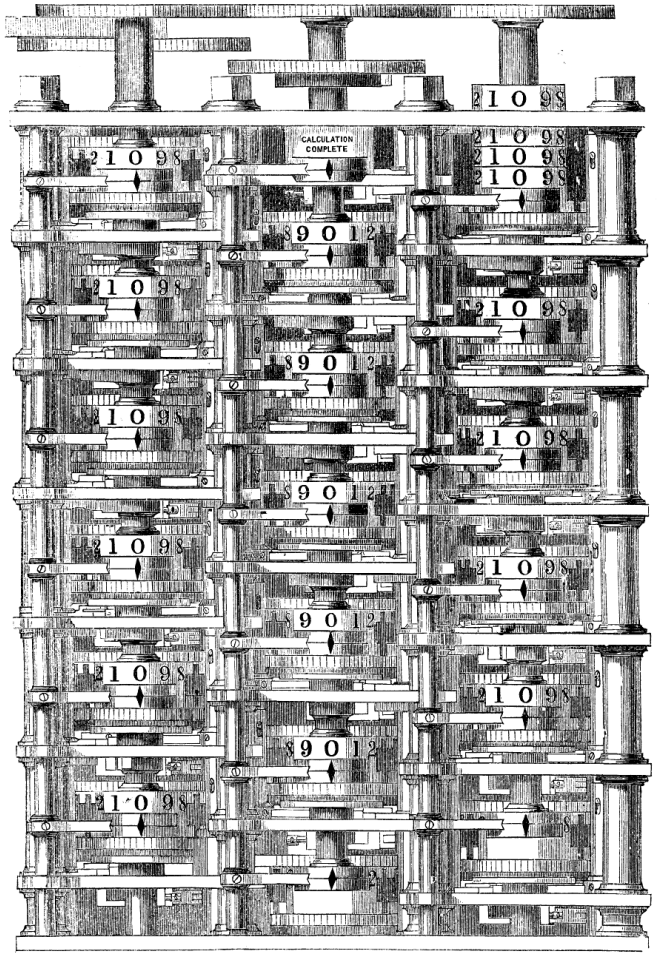
WP4: FAIR data analysis



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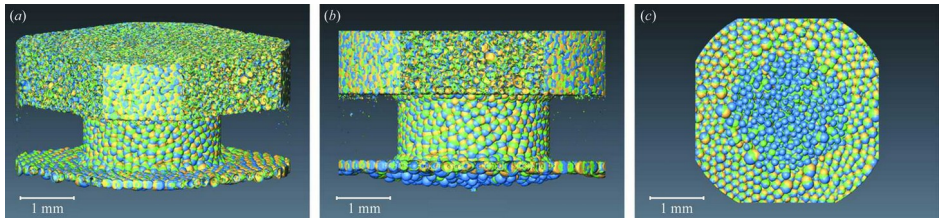
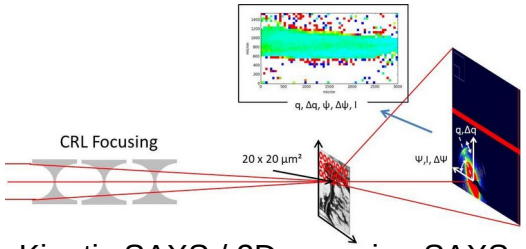
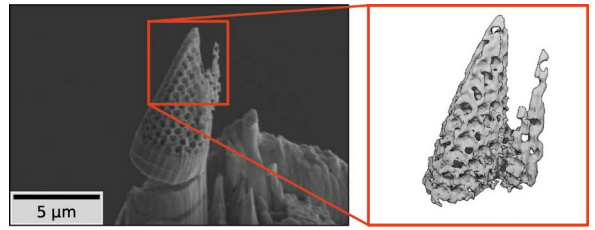
WP4: nine reference datasets



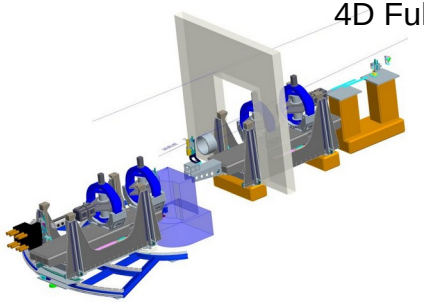
4D Full field tomography (MAX IV)



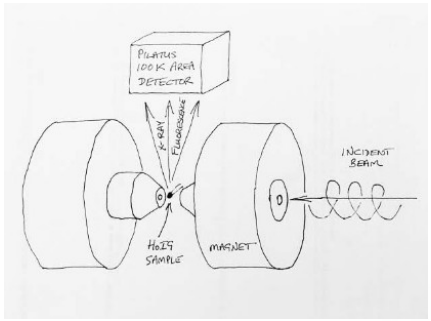
Kinetic SAXS / 2D scanning SAXS (Soleil)



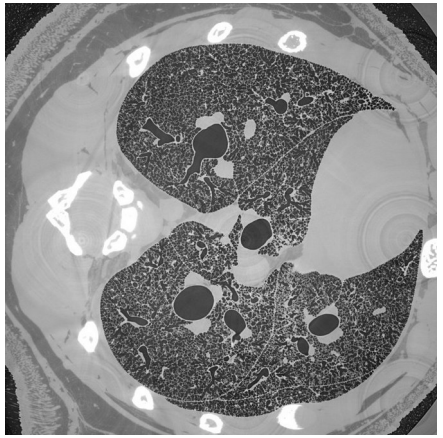
Ptychography / Pty. X-ray CT (MAX IV)



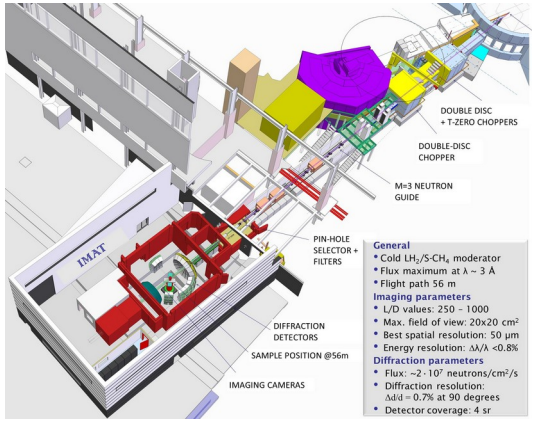
Neutron Reflectometry (UKRI/ISIS)



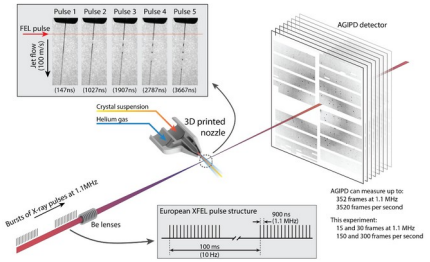
Single crystal X-ray diffraction (Diamond)



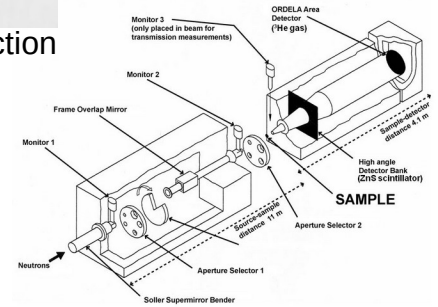
Full field tomography (PSI)



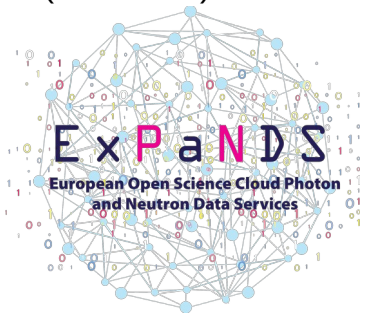
Neutron Imaging / Tomography (UKRI/ISIS)



Serial crystallography (DESY)



Neutron Small Angle Scattering (UKRI/ISIS)



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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

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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.

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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

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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

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