ExPaNDS

European Open Science Cloud Photon and Neutron Data Services

PaN portal demo

Carlo Minotti::PSI::ExPaNDS closing event::Hamburg 2023

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

European Photon and Neutron Open Data Search Portal

Type a query to search for open data from photon and neutron sources:

diffraction

... or try one of these queries: diffraction, lung

The European Photon and Neutron sources are working together in the PaNOSC and ExPaNDS projects financed by the European Commission to build the **European Open Science Cloud**. One of the main objectives of the EOSC is to make **Open Data** from these facilities FAIR. This portal implements the F(indable) part of FAIR via a **federated search engine** from the following facilities:

- European Synchrotron Radiation Facility
- European Spallation Source
- Institut Laue Langevin
- MAX IV
- Paul Scherrer Institut
- Central European Research Infrastructure Consortium
- European XFEL

Additional facilities will be included in the federated search as their search engines come online locally. The goal is to include all photon and neutron facilites who provide open data by the end of the two projects PaNOSC and ExPaNDS.

The mission of the PaN data search portal is to contribute to the realization of a data commons for Neutron and Photon science. The search results provide a link to the landing page of the data DOIs through which the other data services provided by PaNOSC and ExPaNDS for data downloading, analysis, notebooks and simulation can be accessed. The aim of the portal is to facilitate using data from photon and neutron sources for the many scientists from existing and future disciplines. To achieve this aim, the exchange of know-how and experiences is crucial to driving a change in culture by embracing Open Science among the targeted scientific communities. This is why the project works closely with the national photon and neutron sources in Europe to develop common policies, strategies and solutions in the area of FAIR data policy, data management and data services.

Fundings

This project receives funding from the *European Union's*

Partner Project

ExPaNDS

Get in Touch

Follow us

panosc

femtosecond crystallography

23 documents found

Facility

all

Technique

Select a technique...

Chemical Formula

Incident Wavelength

min max nm

Incident Photon Energy

min max eV

Temperature

min max K

Pressure

min max Pa

10.22003/XFEL.EU-DATA-700000-00 1.000

Example Data

The European XFEL (EuXFEL) example data proposal contains experimental datasets from various original beam-times, currently covering the techniques of serial femtosecond crystallography (SFX), coherent diffraction imaging (single particle imaging, SPI), X-ray powder...

> Details, services ...

Released by **EuXFEL** on January 1st 2018

10.16907/e8effd03-b358-473c-9f66-fa5660b7ffb2 0.995

Advances in long-wavelength native phasing at X-ray free-electron lasers

Long-wavelength pulses from the Swiss X-ray free-electron laser (XFEL) have been used for de novo protein structure determination by native single-wavelength anomalous diffraction (native-SAD) phasing of serial femtosecond crystallography (SFX) data. In this work,...

> Details, services ...

Released by **PSI** on January 1st 2020

10.16907/efb03af6-f28b-414f-8eb1-77b31a035fb7 0.707

Optical excitation of electromagnons in hexaferrite

Understanding ultrafast magnetization dynamics on the microscopic level is of strong current interest due to the potential for applications in information storage. In recent years, the spin-lattice coupling has been recognized to be essential for ultrafast...

> Details, services ...

Released by **PSI** on January 1st 2021

10.16907/808de0df-a9d3-4698-8e9f-d6e091516650 0.707

JUNGFRAU detector for brighter X-ray sources - solutions for IT and data science challenges in macromolecul...

Demonstration dataset collected with JUNGFRAU 4M at X06SA beamline

> Details, services ...

Released by **PSI** on January 1st 2020

10.16907/14c30658-cc0b-41fe-b25b-240a9790d5ec 0.707

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femtosecond crystallography

23 documents found

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all

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Example Data

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Released	1. January 2018
Facility	European XFEL
Type	Proposal

Services

VISA

PaNdata Software Catalogue

10.16907/e8effd03-b358-473c-9f66-fa5660b7ffb2 0.995

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> Details, services ...

Released by **PSI** on January 1st 2021

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VISA

Home

Help

Data Analysis, in the cloud

VISA (Virtual Infrastructure for Scientific Analysis) makes it simple to create compute instances on the data analysis infrastructure to analyse your experimental data using just your web browser

Sign in with your user account

Analyse your data

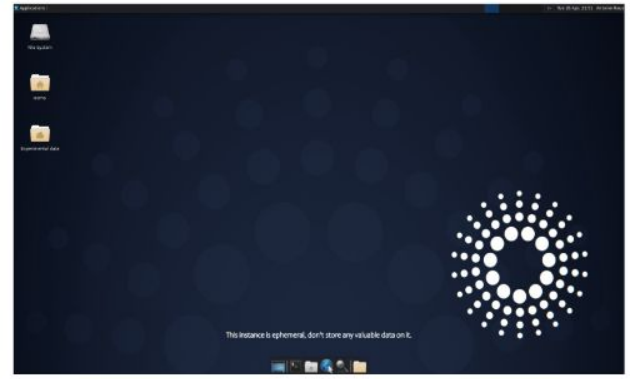
Create a new compute instance and use your web browser to access a Remote Desktop or JupyterLab to start analysing your experimental data

Collaborate with your team

Share your compute instance with other members of your team to collaborate together in real time

No need to install software

The compute instances come with pre-installed data analysis software so you can start analysing your experimental data immediately



panosc

serial crystallographic structure

50+ documents found

Facility

all

Technique

Select a technique...

Chemical Formula

Incident Wavelength

min max nm

Incident Photon Energy

min max eV

Temperature

min max K

Pressure

min max Pa

10.11577/1598270 0.950

Evaluation of serial crystallographic structure determination within megahertz pulse trains

All 'hits' in hdf5 files (Cheetah slab format) together with geometries and all CrystFEL .stream files, .hkl files and .mtz files. Also all Phenix .pdb files together with log files. All scripts needed to reproduce the result are also included.

> Details, services ...

Released by **PSI** on January 1st 2020

10.16907/e8effd03-b358-473c-9f66-fa5660b7ffb2 0.816

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Long-wavelength pulses from the Swiss X-ray free-electron laser (XFEL) have been used for de novo protein structure determination by native single-wavelength anomalous diffraction (native-SAD) phasing of serial femtosecond crystallography (SFX) data. In this work,...

> Details, services ...

Released by **PSI** on January 1st 2020

10.5291/ILL-DATA.5-14-231 0.815

Interplay of structure and electronic properties in rubrene single crystals

Rubrene (5,6,11,12-tetraphenyltetracene) has recently attracted attention for applications in organic field effect transistors, due to its high carrier mobility at room temperature. This mobility decreases dramatically below 175 K and differential scanning calorimetry revea...

> Details, services ...

Released by **ILL** on May 16th 2018

10.5291/ILL-DATA.5-12-315 0.815

Neutron diffraction study on hydrogen-bonded systems: 1,2:3,4:5,6-tri-O-isopropylidene-D-chiro-inositol (1).

The chemical structure of 1,2:3,4:5,6-Tri-O-isopropylidene-D-Chiro-inositol (1) seems unusual when analyzed by single-crystal X-ray diffraction. Compound 1 is a cyclohexyl cyclitol derivative protected with an isopropylidene protection group. The cyclohexane ring of 1...

> Details, services ...

Released by **ILL** on November 23rd 2020

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Facility
all

Technique
Select a technique...

Chemical Formula

Incident Wavelength
min max nm

Incident Photon Energy
min max eV

Temperature
min max K

Pressure
min max Pa

10.11577/1598270 0.950

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Released	1. January 2020
Facility	Paul Scherrer Institut
Type	publication

Services

Remote Desktop Service

Jupyter Hub (PSI Network only)

PaNdata Software Catalogue

Members

Oleksandr Yefanov

Techniques

serial femtosecond crystallography

Parameters

incident_photon_energy	9.3 keV
beamlineParameters.Sample	Lysozyme
beamlineParameters.Lightsource	European XFEL
beamlineParameters.Beamline	SPB/SFX

10.16907/e8effd03-b358-473c-9f66-fa5660b7ffb2 0.816

Advances in long-wavelength native phasing at X-ray free-electron lasers

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{?}

serial femtosecond crystallography[C]

back to ToC or Class ToC

IRI: http://purl.org/pan-science/PaNET/PaNET01168

Source
https://en.wikipedia.org/wiki/Serial_femtosecond_crystallography

has super-classes
crystallography [C], single shot technique [C], ultrafast probe [C], x-ray single crystal diffraction [C]

has sub-classes
time resolved serial femtosecond crystallography [C]

serial synchrotron crystallography[C]

back to ToC or Class ToC

IRI: http://purl.org/pan-science/PaNET/PaNET01169

has super-classes
crystallography [C], pulsed probe [C], single shot technique [C], x-ray single crystal diffraction [C]

has sub-classes
fixed target serial synchrotron crystallography [C], lipidic cubic phase serial synchrotron crystallography [C], time resolved serial synchrotron crystallography [C]

single crystal diffraction[C]

back to ToC or Class ToC

IRI: http://purl.org/pan-science/PaNET/PaNET01029

has super-classes
atomic scale diffraction 3D volume 3D periodic [C]

has sub-classes
borrmann effect [C], high pressure single crystal diffraction [C], macromolecular crystallography [C], neutron single crystal diffraction [C], photo crystallography [C], small molecule diffraction [C], x-ray single crystal diffraction [C]

has members
mySingleCrystalDiffractionTechnique [ni]

single shot technique[C]

back to ToC or Class ToC

IRI: http://purl.org/pan-science/PaNET/PaNET01003

has super-classes
pulsed probe [C]

has sub-classes
serial femtosecond crystallography [C], serial synchrotron crystallography [C], single-shot imaging [C]

single wavelength anomalous diffraction[C]

back to ToC or Class ToC

crystallography[C]

back to ToC or Class ToC

IRI: http://purl.org/pan-science/PaNET/PaNET01082

Source
https://en.wikipedia.org/wiki/Crystallography

has super-classes
obtain atomic structure [C]

has sub-classes
macromolecular crystallography [C], photo crystallography [C], serial femtosecond crystallography [C], serial synchrotron crystallography [C]

dataset[C]

back to ToC or Class ToC

IRI: PaNET:dataset

A dataset in the domain of neutron, muon and accelerator-based light sources

has super-classes
thing [C]

has members
my_ARPES_data [ni], my_microfocus_spectrosopy_data [ni], my_neutron_powder_diffraction_diffraction_data_55 [ni], my_single_crystal_x-ray_diffraction_data_123 [ni]

defined by experimental physical process[C]

back to ToC or Class ToC

IRI: http://purl.org/pan-science/PaNET/PaNET00003

A technique defined by a physical process

has super-classes
photon and neutron technique [C]

has sub-classes
absorption technique [C], dispersive technique [C], emission technique [C], force measurement [C], interferometry technique [C], magnetism technique [C], nonlinear interaction [C], propagation technique [C], reflection technique [C], refraction technique [C], resonance phenomenon [C], scattering technique [C]

has members
myARPEStechnique [ni], myHighResNeutronPowderDiffractionTechnique [ni], myMicrofocusX-rayAbsorptionSpectroscopyTechnique [ni], mySingleCrystalDiffractionTechnique [ni]

defined by experimental probe[C]

back to ToC or Class ToC

IRI: http://purl.org/pan-science/PaNET/PaNET00002

A technique defined by its experimental probe type

has super-classes
photon and neutron technique [C]

has sub-classes

panosc | serial crystallographic structure | 3 documents found

Facility
all

Technique
crystallography

Chemical Formula

Incident Wavelength
min | max | nm

Incident Photon Energy
min | max | eV

Temperature
min | max | K

Pressure
min | max | Pa

10.11577/1598270 0.950

Evaluation of serial crystallographic structure determination within megahertz pulse trains

All 'hits' in hdf5 files (Cheetah slab format) together with geometries and all CrystFEL .stream files, .hkl files and .mtz files. Also all Phenix .pdb files together with log files. All scripts needed to reproduce the result are also included.

> Details, services ...

Released by **PSI** on January 1st 2020

10.16907/14c30658-cc0b-41fe-b25b-240a9790d5ec 0.780

Dynamics and mechanism of a light-driven chloride pump - datasets collected with 13.7 keV X-ray energy

Chloride transport by microbial rhodopsins is an essential process of which the molecular details have remained elusive, such as the mechanisms that convert light energy to drive ion pumping and ensure the unidirectionality of the transport. We combined time-resolved serial crystallography with time-resolved spectroscopy and multiscale simulations to elucidate the molecular mechanism of a chloride pumping rhodopsin and the structural dynamics throughout the transport cycle. We traced transient anion binding sites, obtained evidence for how light energy is used in the pumping mechanism, and identified steric and electrostatic molecular gates ensuring unidirectional transport. An interaction with the π-electron system of the retinal supports transient chloride ion binding across a major bottleneck in the transport pathway. These results allow us to propose key mechanistic features enabling finely controlled chloride transport across the cell membrane in this light powered chloride ion pump.

Released	1. January 2022
Facility	Paul Scherrer Institut
Type	publication

Services

Remote Desktop Service

Jupyter Hub (PSI Network only)

PaNdata Software Catalogue

Members

Przemyslaw Nogly

Techniques

macromolecular crystallography

{?}

panosc | serial crystallographic structure | 1 document found

Facility
all

Technique
crystallography

Chemical Formula

Incident Wavelength
min | max | nm

Incident Photon Energy
9000 | max | eV

Temperature
min | max | K

Pressure
min | max | Pa

10.11577/1598270 0.950

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PaNdata Software Catalogue

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Oleksandr Yefanov

Techniques

serial femtosecond crystallography

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incident_photon_energy	9.3 keV
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beamlineParameters.Lightsource	European XFEL
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Facility
all

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crystallography

Chemical Formula

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10.11577/1598270

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PaNdata Software Catalogue

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Oleksandr Yefanov

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serial femtosecond crystallography

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beamlineParameters.Lightsource	European XFEL
beamlineParameters.Beamline	SPB/SFX

PSI Remote Desktop Service

PSI Remote Desktop Service

Beamline console and HPC cluster access

Organisation: **Paul Scherrer Institute**

(0.0 /5) 0 reviews Add to comparison Add to favourites

Access the resource

ORDER REQUIRED

Webpage | Helpdesk e-mail | Manual

Ask a question about this resource?

ABOUT | DETAILS | REVIEWS (0)

The purpose of this service is to offer PSI and external users convenient access to compute resources, in particular to the beamline consoles and the Ra offline data analysis cluster. The NoMachine software provides a full graphical user interface to the resources. Users of the service need to have a PSI_account and can access only those services, to which they are explicitly entitled.

SCIENTIFIC CATEGORISATION

Generic

- Generic
  - Generic

CATEGORISATION

- Compute
  - Other

CXIDB ID 98

Deposition Summary	
Depositor:	Oleksandr Yefanov
Contact:	oleks...@desy.de
Deposition date:	2020-02-07
Last modified:	2020-02-07
DOI:	10.11577/1598270

Publication Details	
Title:	Evaluation of serial crystallographic structure determination within megahertz pulse trains
Authors:	Oleksandr Yefanov et al.
Journal:	Structural Dynamics
Year:	2019
DOI:	10.1063/1.5124387

Experimental Conditions	
Method:	Serial Femtosecond Crystallography
Sample:	Lysozyme
Wavelength:	1.33 Å (9.30 keV)
Lightsource:	European XFEL
Beamline:	SPB/SFX

Data Files		
Raw Data:	cheetah/	(4 KB)
Indexing:	indexing/	(4 KB)
Auxiliary Files		
Phenix Files:	phenix_r0051-r0151.tar.gz	(262.6 MB)

Description

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Open • Submitted: 14 August 2019 • Accepted: 21 October 2019 • Published Online: 04 December 2019

Evaluation of serial crystallographic structure determination within megahertz pulse trains

Structural Dynamics 6, 064702 (2019); https://doi.org/10.1063/1.5124387

Oleksandr Yefanov[1], Dominik Oberthür[1], Richard Bean[2], Max O. Wiedorn[1,3], Juraj Knoska[1], Gisel Pena[1], Salah Awel[1], Lars Gumprecht[1], Martin Domaracky[1], Iosifina Sarrou[1], P. Lourdu Xavier[1], Markus Metz[1], Saša Bajt[4], Valerio Mariani[1], Yaroslav Gevorkov[1,5], Thomas A. White[1], Aleksandra Tolstikova[1], Pablo Villanueva-Perez[1], Carolin Seuring[1], Steve Aplin[1], Armando D. Estillore[1], Jochen Küpper[1,3,6], Alexander Klyuev[4], Manuela Kuhn[4], Torsten Laurus[4], Heinz Graafsma[4], Diana C. F.
more...

View Affiliations View Contributors

ABSTRACT

The new European X-ray Free-Electron Laser (European XFEL) is the first X-ray free-electron laser capable of delivering intense X-ray pulses with a megahertz interpulse spacing

CXIDB
Coherent X-ray Imaging Data Bank

ID 98 Tape Stored Raw Files

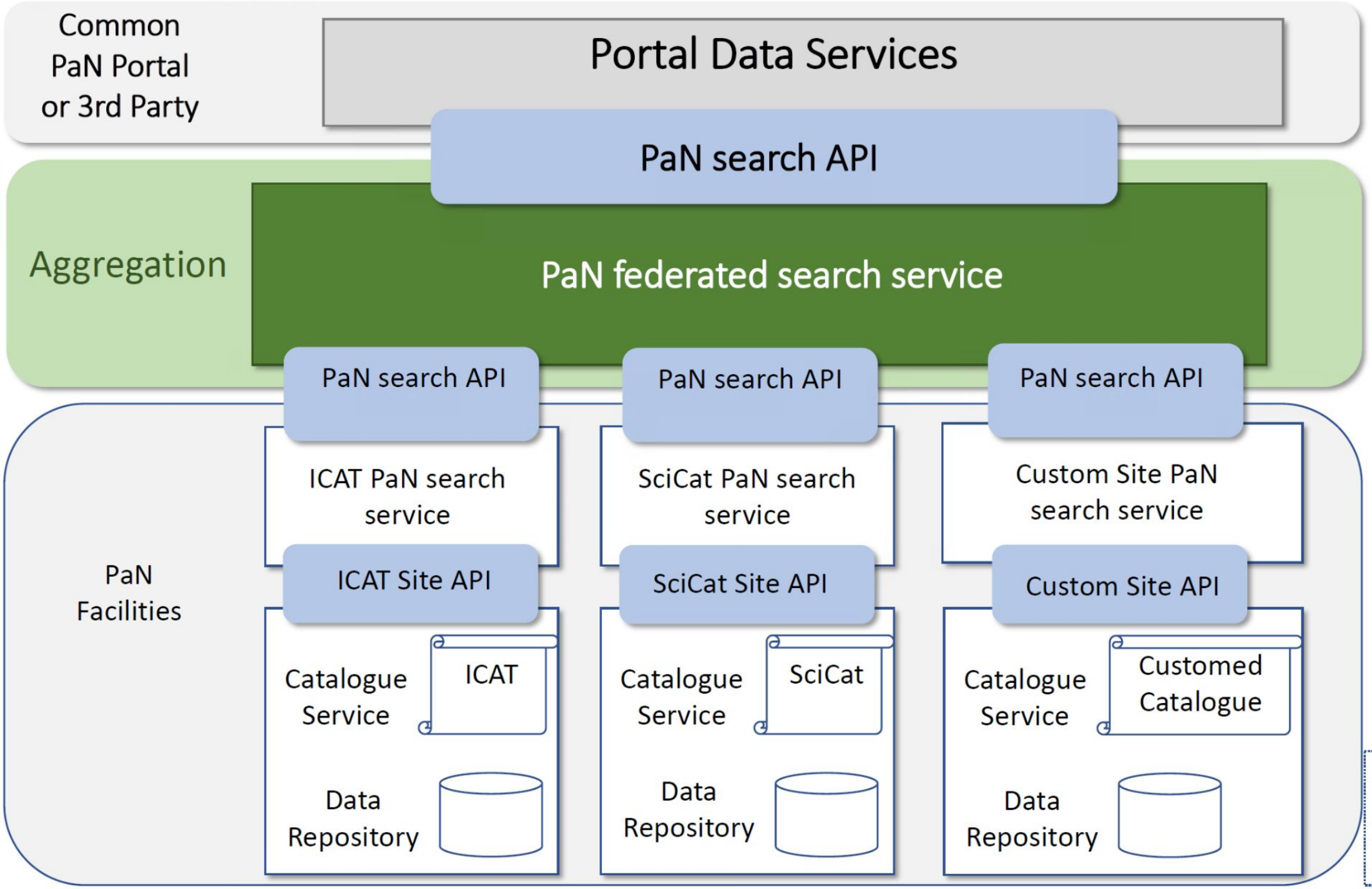
calib/ (directory)
gui/ (directory)
hdf5/ (directory)
indexing/ (directory)
process/ (directory)

Slow server response

These files are located on tape so the links can take several minutes to return something. Using a program such as `wget` is strongly recommended.

A text file with links to all the files can be found here.

MD5 hash of the files.


Common
PaN Portal
or 3rd Party
Portal Data Services
PaN search API
Aggregation
PaN federated search service
PaN search API
PaN search API
PaN search API
ICAT PaN search service
SciCat PaN search service
Custom Site PaN search service
PaN Facilities
ICAT Site API
SciCat Site API
Custom Site API
Catalogue Service
ICAT
Catalogue Service
SciCat
Catalogue Service
Customed Catalogue
Data Repository
Data Repository
Data Repository
legend
service
API

Thanks to all WP3 partners

- ALBA
- DESY
- DLS
- EGI
- ELETTRA
- HZB
- HZDR
- MAXIV
- PSI
- SOLEIL
- UKRI

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