

User Portal, Metadata Catalog and Logbook at European XFEL

19th May, 2021

Luís Maia,
On behalf of European XFEL



Agenda

■ Introduction

- Context

- Purpose

- Landscape & Architecture

■ Governance & Resources

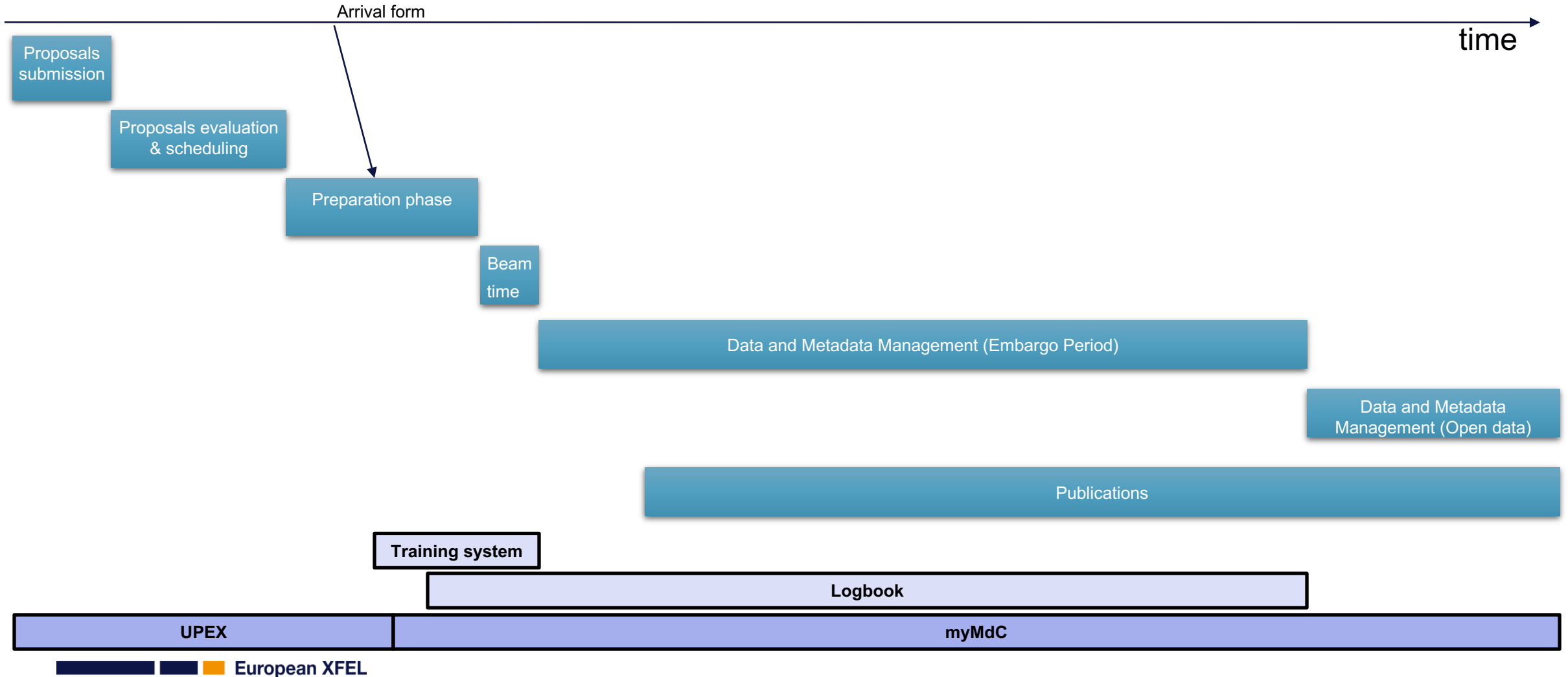
■ myMdC application (**optional**)

- Roles and permissions

- Key features

Context

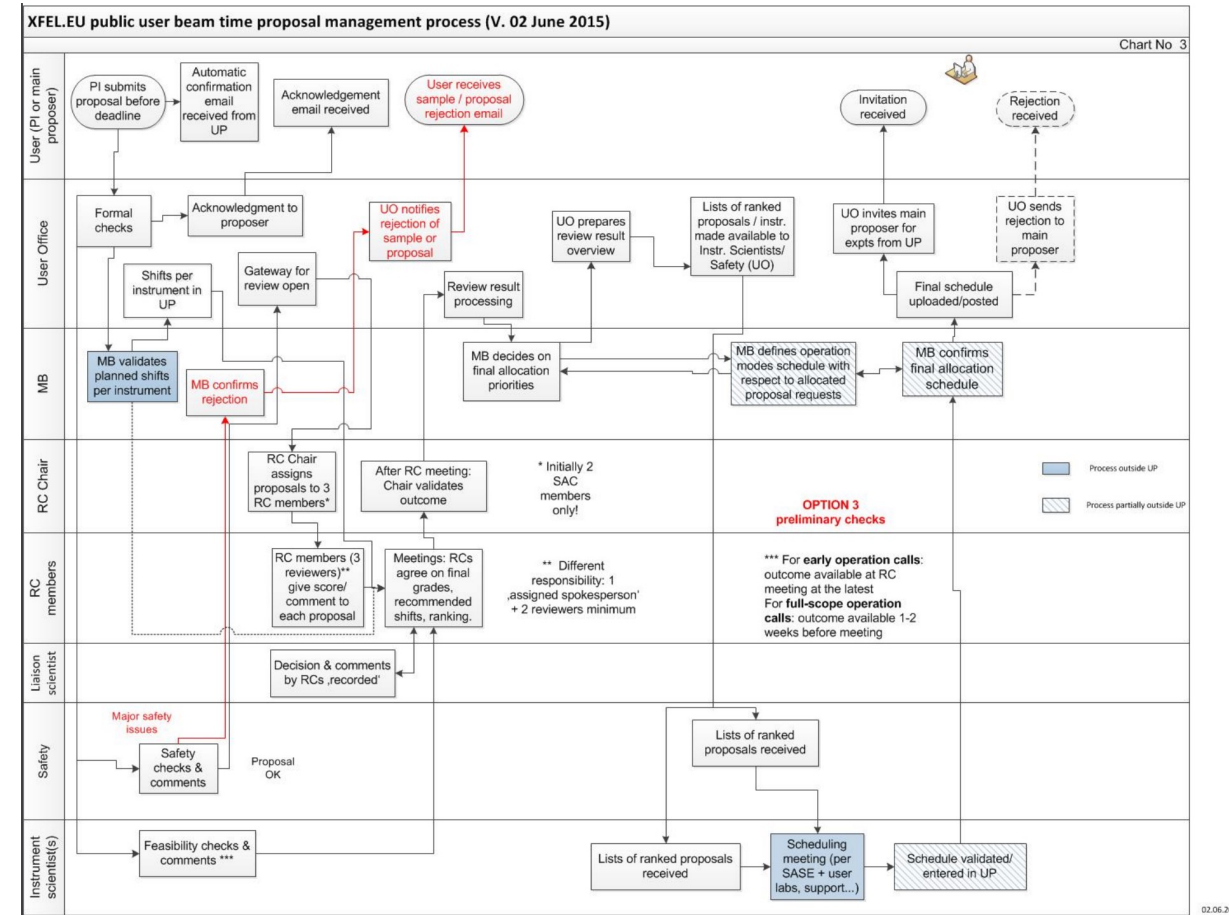
Users support (and Experiments lifecycle)



UPEX Purpose (I)

- First entry point for users
- Handling Policies & Acceptances
- Provide a means to orchestrate the facility user public beam time proposal management process

7/23 operation mode
- Organize and manage users personal data and existing accounts in a coherent way
 - IAM
Personal data
 - Zerberus
Sanction lists
 - Registry
Users accounts password
 - MyMdC
Users and internal proposals
Proposals Experiment team & Samples sheet
 - Training / Access management system



myMdC Purpose (I)

- Provide a means of storing, retrieving and query raw and run based data in an organised way
- Organize and manage data and metadata in a coherent way
- Assist on the execution of the Data Management policies
- Manage data and metadata authorisation and responsibilities (especially during the Embargo period)
- Manage and restrict the GLOBAL unique entities used during data taking
 - Proposal number
 - Proposal path
 - Sample
 - Run type

myMdC Purpose (II)

Glue together different systems and services

UPEX

Users and internal proposals
 Proposals Experiment team & Samples sheet
 Check and sync users accepted data policies
 Trigger proposal team snapshot
[Internal proposals “fast-track”](#)
[Users with access to Labs](#)
 Booked system integration

7/23 operation mode

Registry

Users accounts
 Staff organisational group
 Instrument support groups*

Upgrade Registry 2.0

LDAP

Users Proposal groups

Upgrade to LDAP Gateway 2.0

GPFS

Repository location
 Universal folders management
 Proposal folders creation
 Runs data migration
 Folders removal*

SLURM

[Priority queues reservation for beamtime*](#)

Zoom integration – proposal rooms

European XFEL

Data Audit and reconciliation*

Run Data location
[Number of files, size, migration dates](#)

Elog

Elog logbook config file generation
 Integration with Elog replacement tool

Karabo - DAQ

Universal Run Management
 Run tagging and basic details
[Data Source Groups definition](#)
 Run Data Source Groups

Calibration Pipeline

Trigger Processed data generation
[Trigger Dark Runs generation and report download](#)

calCat

[Dark Runs CCV integration](#)
 Document used CCV on Process data

Grid-FTP / [Globus](#) / Off-shore data exportation

[Repositories](#)
 Transfer Agent Off-shore data migration

DataCite / Tind.io

[Automatic](#) DOI generation and publish
 Public DOI end point

RESTful APIs

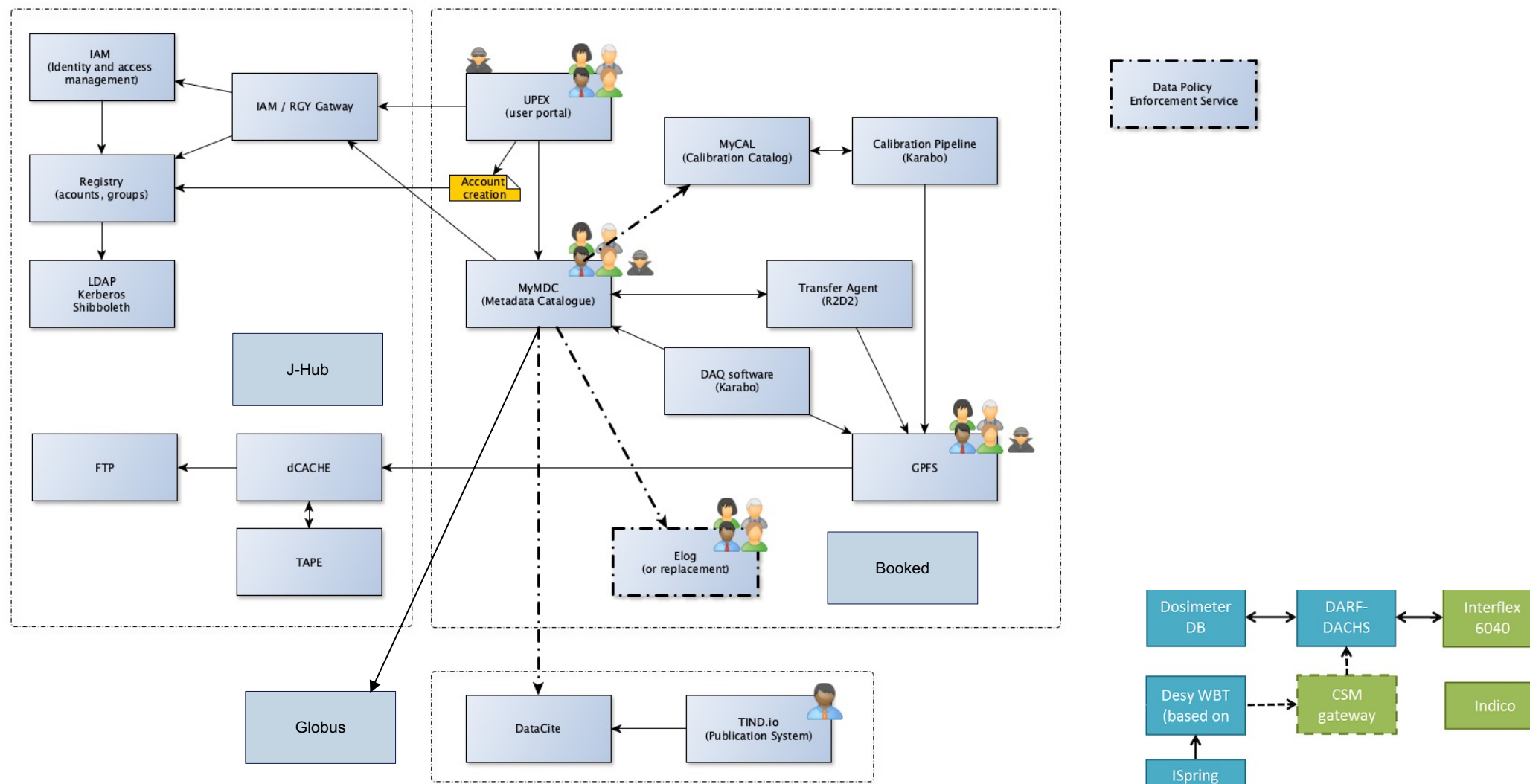
Metadata Client and Metadata Tools python libraries
[Document APIs using Swagger](#)

Notifications*

Statistics

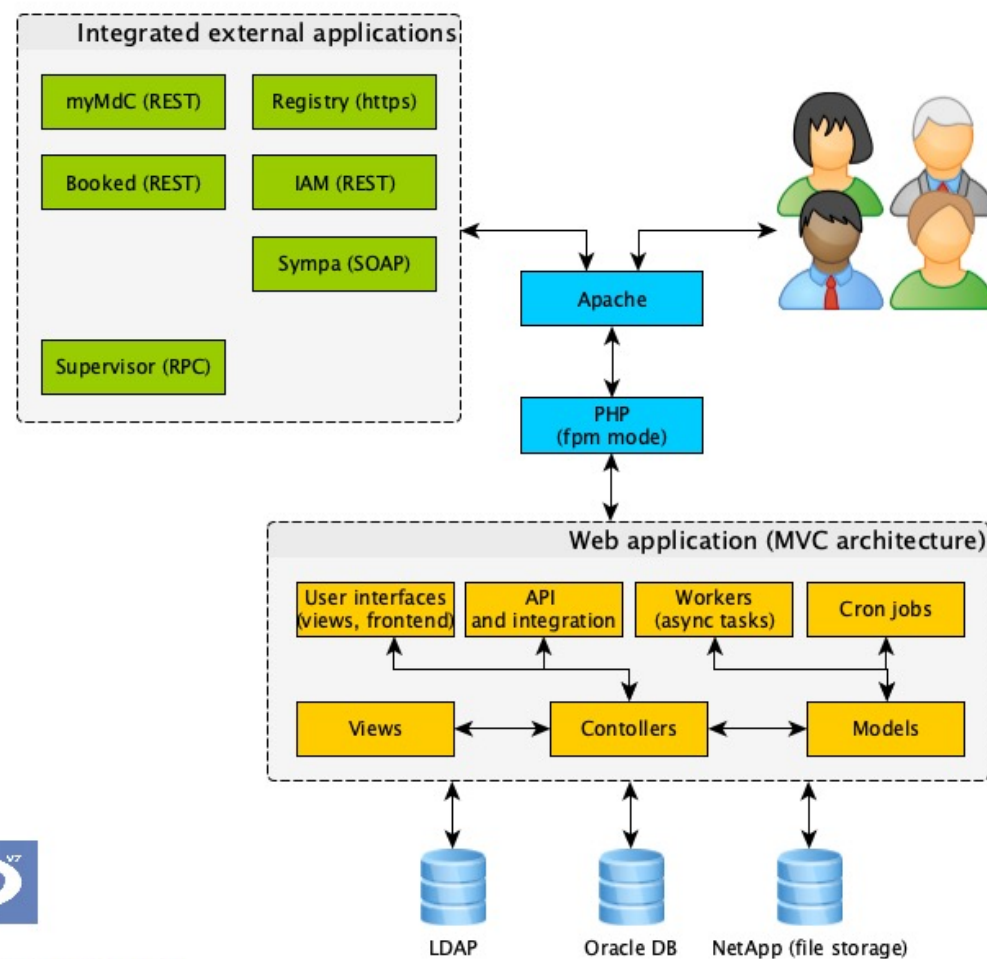
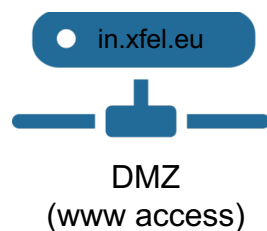
[Leading Scientists assessing delivered shifts](#)

Landscape



UPEX Architecture (I)

Based on DUO instance got from PSI in 2015



ORACLE
DATABASE



Bootstrap 3



jQuery

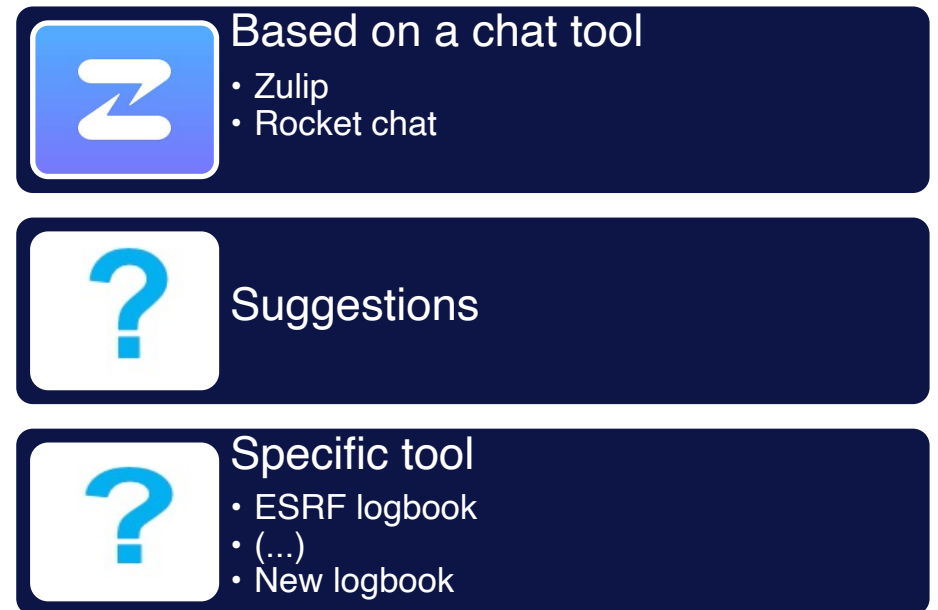
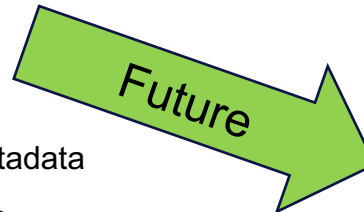
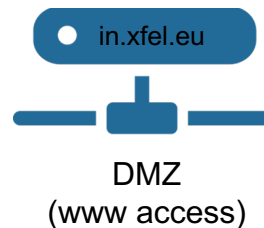


eLog Architecture (I)

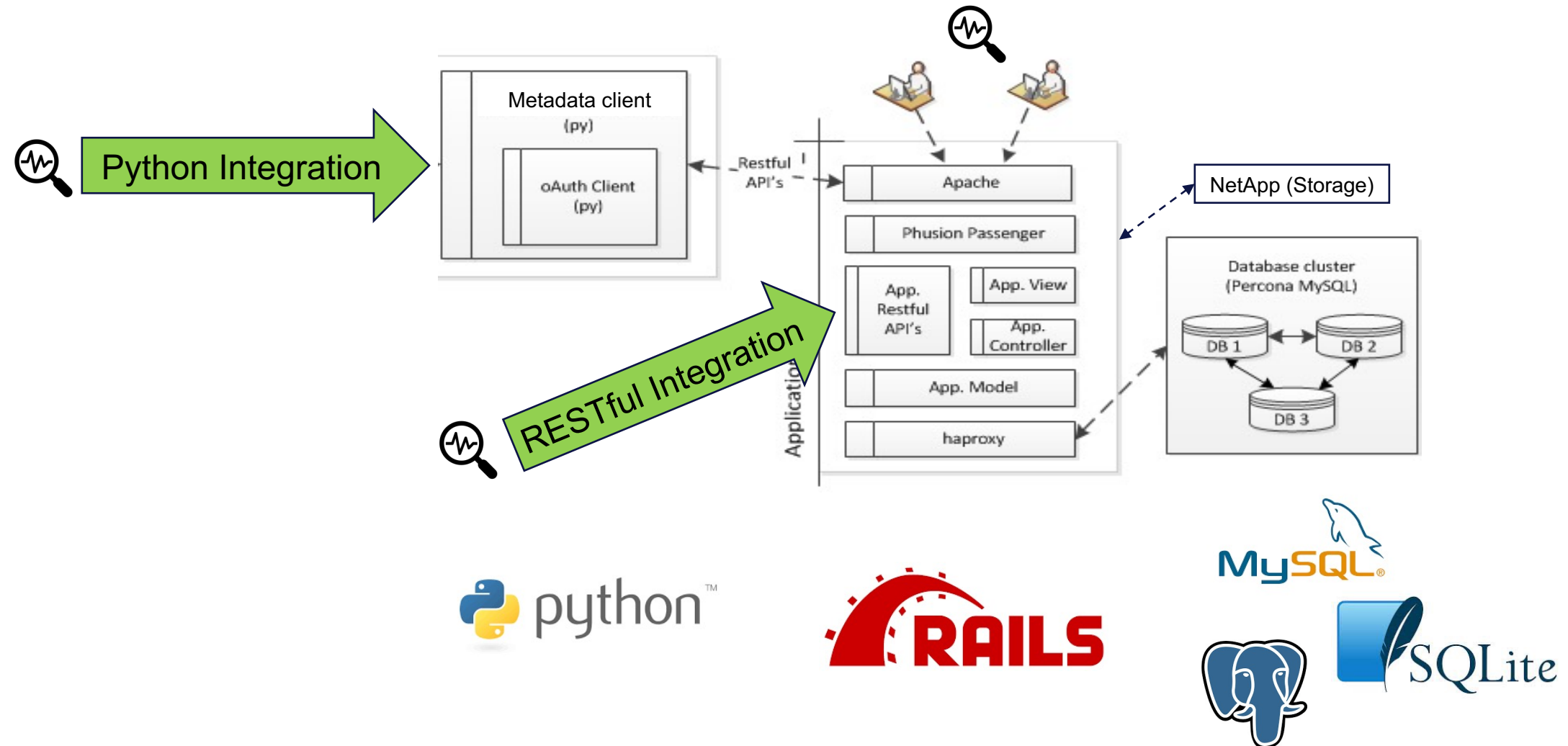
■ PSI Elog (<https://elog.psi.ch/elog/>) , adjusted visually (CSS) and configured for XFEL purposes

■ There is no real integration with anything

- Logbooks and Users created by script manually
- Logbooks permissions managed by instrument experts
- No integration with Control System and/or parameters metadata



myMdC Architecture (I)



myMdC Architecture (II)



Agenda

- Introduction
 - Context
 - Purpose
 - Landscape & Architecture
- **Governance & Resources**
- myMdC application (**optional**)
 - Roles and permissions
 - Key features

Governance & Resources

Product Owner

Several groups

Architecture Owner

Web DevOps

Team Members

Luis Maia* (50%)

Maurizio Manetti (25%)

Illia Derevianko (50%)

Bharathi Vanganuru (75% - 2Y)

Sudhanshu Singh (67% - 3Y)

Varun Singh (40% - 2Y)

Stakeholders

Data Management experts

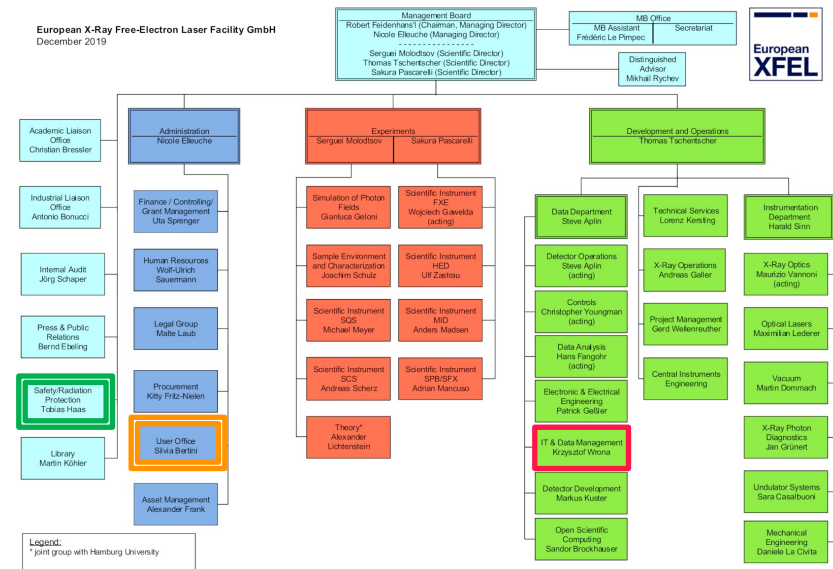
Detector experts

Instrumentation groups

Instruments experts

Users

Administration



Agenda

- Introduction
 - Context
 - Purpose
 - Landscape & Architecture
- Governance & Resources
- myMdC application (optional)
 - Roles and permissions
 - Key features

Roles and permissions (I)

myMdC roles

Administration

- admin** is the role assigned to myMdC administrators and ITDM OCD personnel
- Trusted** is the role assigned to people that needs to access all system information

Users & Staff

- read_only** is the default role for everybody accessing myMdC
- user** is the role granted to users with UPEX account and the latest Data Policy accepted

Systems

- Specific roles to be assign to system integration local users

Dashboard / Roles

List

Export

Filter

Refresh

<input type="checkbox"/>	Id	Name	Flg default
<input type="checkbox"/>	1	admin	0
<input type="checkbox"/>	2	trusted	0
<input type="checkbox"/>	3	user	0
<input type="checkbox"/>	4	read_only	1
<input type="checkbox"/>	6	karabo_sys	0
<input type="checkbox"/>	7	upex_sys	0
<input type="checkbox"/>	8	gpfs_sys	0
<input type="checkbox"/>	9	cal_sys	0
<input type="checkbox"/>	10	panosc_user	1
<input type="checkbox"/>	11	monitoring_sys	1

10 roles

Roles and permissions (II)

Responsibilities in the context of instrument and proposal

■ **LS:** Instrument's Leading Scientist

- Any user in myMdC that is associated as the leading scientist to the Instrument where the given proposal is taking place

■ **BE:** Instrument's Expert

- Any user in myMdC that is associated as an expert user to the Instrument where the given proposal is taking place

■ **SG:** Instrument's Support Group

- Any user in myMdC that is a member of the support group associated with the instrument where the given proposal is taking place (e.g. SPBDATA)

■ **PI:** Principal Investigator

- Any user in myMdC

■ **MP:** Main Proposer

- Any user in myMdC

■ **LC:** Local Contact

- Any user in myMdC that is a Instrument Expert

■ **T_Part:** Execution team Participant

- Any user in myMdC

■ **T_DM:** Execution team Data Manager

- Any user in myMdC

■ **T_UL:** Execution team User Lab

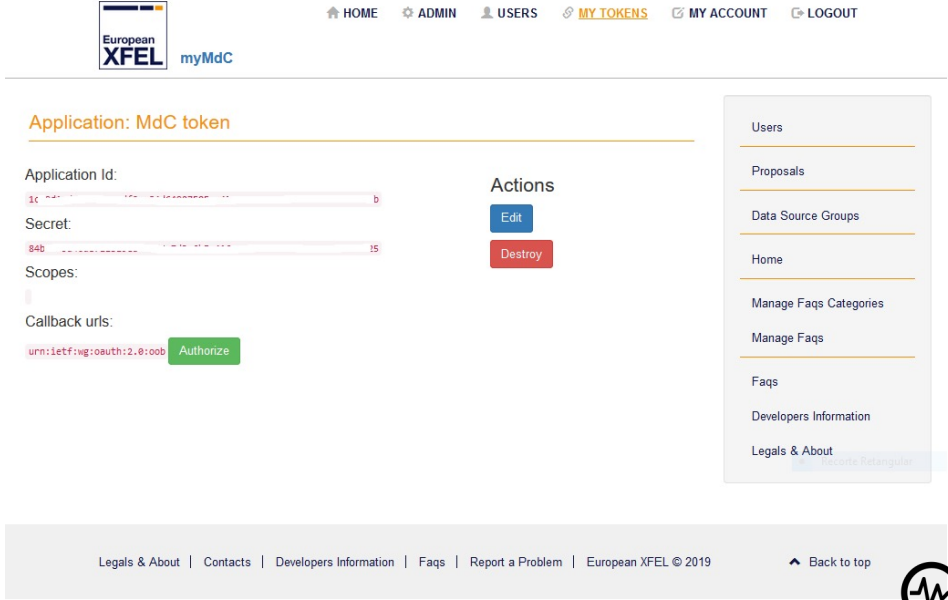
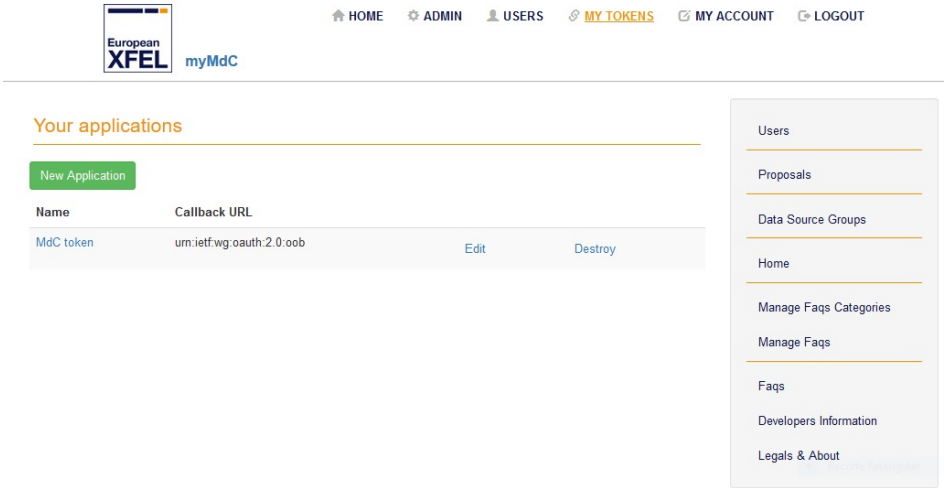
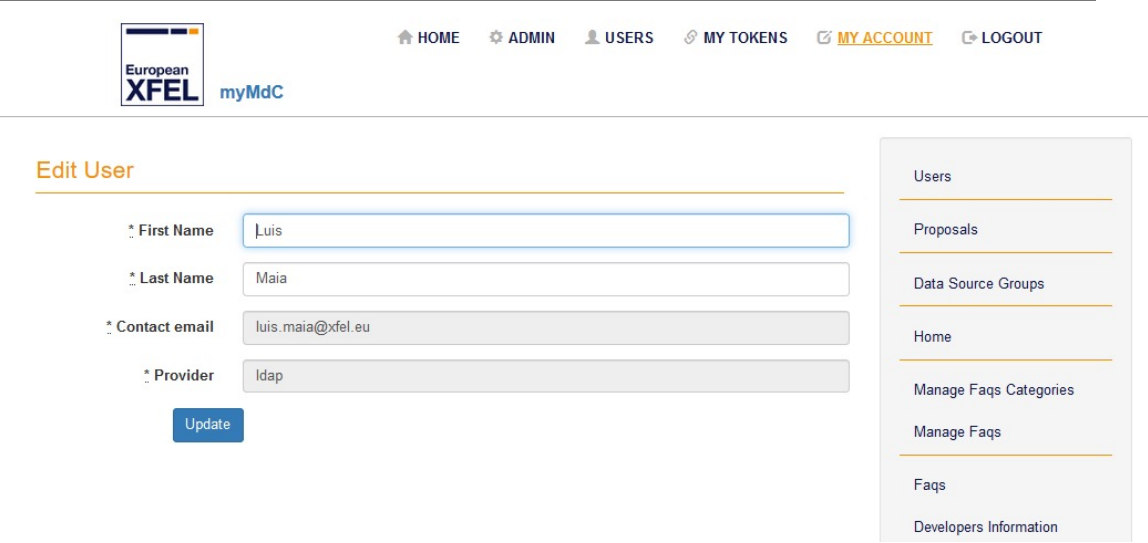
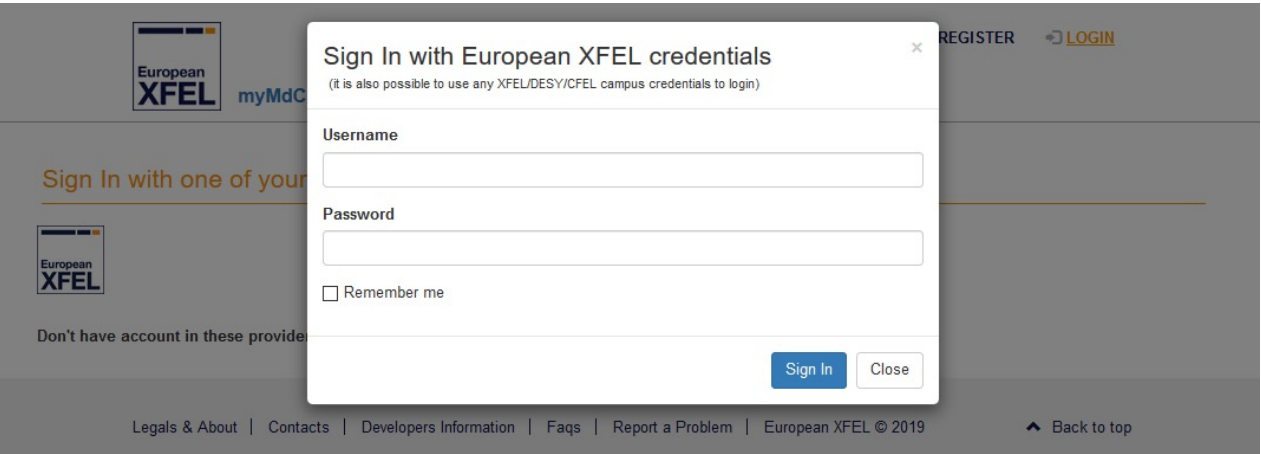
- Any user in the execution team

■ **Others:** Non users or non members

- Any user in myMdC not having any responsibility on the proposal and not being Administrator

Key Features

Authentication



Key Features

Application Layout & Responsiveness

The screenshot shows the myMdc application interface. At the top, there is a navigation bar with the European XFEL logo, the text 'myMdc', and a 'MENU' icon. Below this, a horizontal menu contains links: HOME, ADMIN, USERS, MY TOKENS, MY ACCOUNT, and LOGOUT. A blue banner below the menu says 'Signed in!'. The main content area has a 'Welcome to the myMdc' heading, a subheading 'The Data Management portal for European XFEL users', and a 'Quick Introductory Tour' button. A note below the button states: 'Please Note, that you should use your XFEL/DESY/CFEL campus credentials to login in this system.' A red arrow points from the 'ADMIN' link to the 'Users' menu item in the sidebar. Another red arrow points from the 'USERS' link to the 'Users' menu item. A third red arrow points from the 'ADMIN' link to the 'Proposals' menu item. A fourth red arrow points from the 'ADMIN' link to the 'Data Source Groups' menu item. A fifth red arrow points from the 'ADMIN' link to the 'Manage Faqs Categories' menu item. A sixth red arrow points from the 'ADMIN' link to the 'Manage Faqs' menu item. A red text label 'Administrators Only!' is positioned below the arrows. The sidebar menu includes: Users, Proposals, Data Source Groups, Manage Faqs Categories, Manage Faqs, Faqs, Developers Information, and Legals & About. The footer contains links: Legals & About, Contacts, Developers Information, Faqs, Report a Problem, European XFEL © 2019, and a 'Back to top' button.

European XFEL myMdc

HOME ADMIN USERS MY TOKENS MY ACCOUNT LOGOUT

Signed in!

Welcome to the myMdc

The Data Management portal for European XFEL users

Quick Introductory Tour

Please Note, that you should use your XFEL/DESY/CFEL campus credentials to login in this system.

Administrators Only!

Users

Proposals

Data Source Groups

Manage Faqs Categories

Manage Faqs

Faqs

Developers Information

Legals & About

Legals & About | Contacts | Developers Information | Faqs | Report a Problem | European XFEL © 2019

Back to top



myMdc

MENU

Welcome to the myMdc

The Data Management portal for European XFEL users

Quick Introductory Tour

Please Note, that you should use your XFEL/DESY/CFEL campus credentials to login in this system.

Users

Proposals

Data Source Groups

Manage Faqs Categories

Manage Faqs

Faqs

Developers Information

Legals & About

Legals & About | Contacts

Back to top

Developers Information | Faqs

Report a Problem

European XFEL © 2019

Show	10	▼	entries	○ Search anywhere:	<input type="text"/>	🔍 Search by column	Copy	Print	Export
Number	Title	Instrument	Beamtime status	Start date					
<input type="text" value="Filter"/>	<input type="text" value="Filter"/>	<input type="text" value="TSTSA2"/>	<input type="text" value="Filter"/>	<input type="text" value="Filter"/>					
900054	TST SASE2 DAQ tests	TSTSA2	Closed	2018-09-24 22:00:01 UTC	🔗 📄 🗑️				
900058	TST SASE2 DAQ tests	TSTSA2	Finished and Reviewed	2019-01-20 23:00:01 UTC	🔗 📄 🗑️				
900083	TST SASE2 DAQ tests	TSTSA2	Finished and Reviewed	2019-06-14 22:00:01 UTC	🔗 📄 🗑️				
900116	TST SASE2 DAQ tests	TSTSA2	Finished and Reviewed	2020-01-17 09:04:50 UTC	🔗 📄 🗑️				
900165	TST SASE2 DAQ tests	TSTSA2	Finished (Beamtime)	2020-06-30 22:00:02 UTC	🔗 📄 🗑️				
900190	TST SASE2 DAQ tests	TSTSA2	Active	2020-12-31 23:00:02 UTC	🔗 📄 🗑️				

Showing 1 to 6 of 6 entries (filtered from 431 total entries)

+ New

HIDE

MENU 

General Public Information Runs Team **Repositories** **Beta!** **Calibration Constants** **Beta!** History

 globu

All Proposal Run types

+ New

All Proposal Samples

- [e0001]: Test DAQ

- No Sample

[Back](#)
[Edit](#)
[Clone](#)
[+ Add another](#)
[Runs](#)
[Delete](#)
[Beamtime status ▾](#)

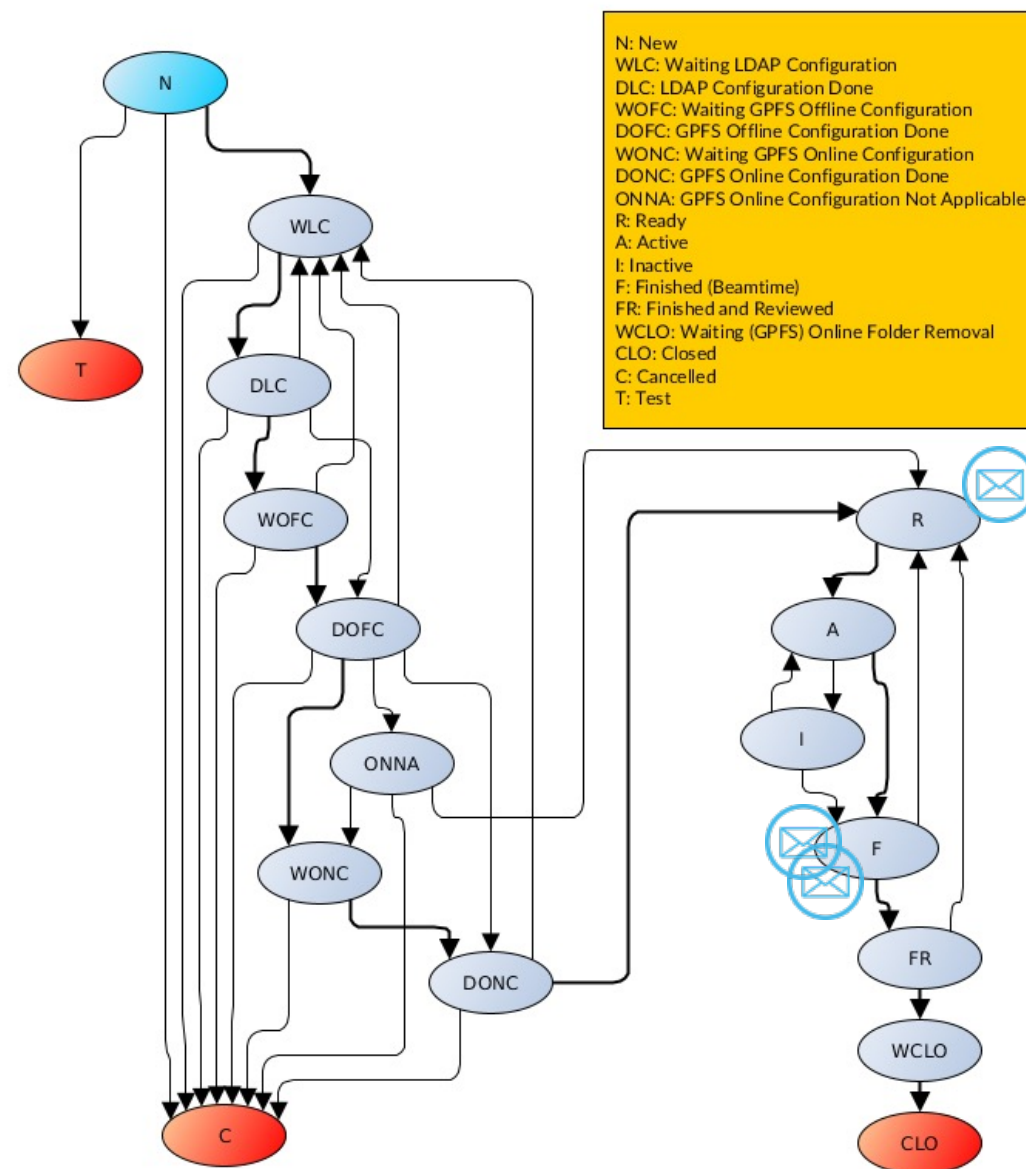
Key Features

Proposal workflow and notifications

no. delivered shots: ---
 Beamtime 1: 2019-01-21 00:00:01 +0100 - 2019-06-30 23:59:58 +0200
 Release at: 2022-12-31 23:59:58 +0100
 open data?: No
 Beamtime status: Ready
 Start Beamtime date:
 End Beamtime date:
 Proposal system: ---
 Description:
 Created by: Luis Maia

no. delivered shots: ---
 Beamtime 1: 2018-09-25 00:00:01 +0200 - 2018-12-31 23:59:58 +0100
 Release at: 2021-12-31 23:59:59 +0100
 open data?: No
 Beamtime status: Finished (Beamtime)
 Start Beamtime date:
 End Beamtime date:
 Proposal system:
 Description:
 Created by: Janusz Malka
 Creation date: 2018-09-25 10:47:10 +0200
 Modified by: System

myMdc Proposals' Beamline status workflow



Key Features

Proposal DOIs integration

Proposal no. 900058

Back Edit Clone Add another Runs Delete Beamtime status

General Public Information Runs Team Repositories **Beta** Calibration Constants **Beta** History

Public Information

DOI: 10.22003/XFEL.EU-DATA-900058-00 Internal Only: DOI not searchable in Metadata

Publish DOI

Proposal Number: 900058
Name: p900058
Title: TST SASE2 DAQ tests
Beamtime 1: 2019-01-21 00:00:01 +0100 - 2019-06-30 23:59:58 +0200
Instrument: Test SASE2
Instrument Cycle: 201930
Principal Investigator: Djelloul Boukhelef

Proposal no. 002012

Back Edit Clone Add another Runs Delete Beamtime status

General Public Information Runs Team Repositories **Beta** Calibration Constants **Beta** History

Public Information

DOI: 10.22003/XFEL.EU-DATA-002012-00 DOI Published

Hide DOI Metadata

Proposal Number: 002012
Name: p002012
Title: Serial Femtosecond Crystallography at MHz repetition rates
Abstract: This community proposal arising out of the SFX-SPB workshop held in December 2016 directly addresses the key issue of high throughput structure determination for maximising the science output from EuXFEL.
We will:
(1) Establish sample delivery methods suitable for the MHz repetition rates;
(2) Exploit these techniques to establish high throughput serial crystallography; and
(3) Obtain the first new structure(s) of biological interest using the EuXFEL.
Beamtime 1: 2017-09-14 20:00:00 +0200 - 2017-09-19 08:00:00 +0200
Beamtime 2: 2018-03-29 20:00:00 +0200 - 2018-04-02 08:00:00 +0200
Instrument: SPB/SFX SASE1
Instrument Cycle: 201701
Principal Investigator: Ready User
Main Proposer: Anton Barty
Local Contact: Beamline Expert User
Release at: 2021-04-02 08:00:00 +0200
open data?: No

This proposal data is open

Would you like to get access to this proposal datasets?

Please contact us through the open.data@xfel.eu email address.

Thank you for visiting!

Back Edit Clone Add another Runs Delete Beamtime status

doi

HOME | HANDBOOK | FACTSHEETS | FAQs | RESOURCES | REGISTRATION AGENCIES | NEWS | MEMBERS AREA

The DOI® System

ISO 26324

Resolve a DOI Name

Type or paste a DOI name, e.g., 10.1000/xyz123, into the text box below. (Be sure to enter all of the characters before and after the slash. Do not include extra characters, or sentence punctuation marks.)

[REGISTER](#) [LOGIN](#)

Proposal no. 002012

DOI: 10.22003/XFEL.EU-DATA-002012-00

Proposal Number: 002012
Name: p002012
Title: Serial Femtosecond Crystallography at MHz repetition rates
Abstract: This community proposal arising out of the SFX-SPB workshop held in December 2016 directly addresses the key issue of high throughput structure determination for maximising the science output from EuXFEL.
We will:
(1) Establish sample delivery methods suitable for the MHz repetition rates;
(2) Exploit these techniques to establish high throughput serial crystallography; and
(3) Obtain the first new structure(s) of biological interest using the EuXFEL.
Participation is open to anyone who wishes to contribute, results will be shared openly with the community.
Beamtime 1: 2017-09-14 20:00:00 +0200 - 2017-09-19 08:00:00 +0200
Beamtime 2: 2018-03-29 20:00:00 +0200 - 2018-04-02 08:00:00 +0200
Instrument: SPB/SFX SASE1
Instrument Cycle: 201701
Principal Investigator: Henry Chapman
Main Proposer: Anton Barty
Local Contact: Richard Bean
Release at: 2021-04-02 08:00:00 +0200
open data?: No

This proposal data is open

Would you like to get access to this proposal datasets?

Please contact us through the open.data@xfel.eu email address.

Thank you for visiting!

Key Features

Proposal runs (data) management

Proposal no. 900054

Back Edit Clone Add another Runs Delete Beamtime status

General Public Information Runs Team History

Proposal Runs

Run Number (alias)	Run type	Sample Name	Start date	Run status	Data Assessment	Calibration	Run Comment	Edit
0082	Test DAQ	No Sample	2019-01-23 14:20:18 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0081	Test DAQ	No Sample	2019-01-23 12:10:47 +0100	Closed	Run Quality	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0080	Test DAQ	No Sample	2019-01-23 03:13:08 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0079	Test DAQ	No Sample	2019-01-22 14:29:27 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0078	Test DAQ	No Sample	2019-01-22 14:16:09 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0077	Test DAQ	No Sample	2019-01-22 14:07:09 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>

Good (migrate data to Maxwell)
Unclear (migrate data to Maxwell)
Not interesting (data won't be migrated to Maxwell)

Proposal no. 900054

Back Edit Clone Add another Runs Delete Beamtime status

General Public Information Runs Team History

Proposal Runs

Run Number (alias)	Run type	Sample Name	Start date	Run status	Data Assessment	Calibration	Run Comment	Edit
0082	Test DAQ	No Sample	2019-01-23 14:20:18 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0081	Test DAQ	No Sample	2019-01-23 12:10:47 +0100	Closed	Run Quality	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0080	Test DAQ	No Sample	2019-01-23 03:13:08 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0079	Test DAQ	No Sample	2019-01-22 14:29:27 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>
0078	Test DAQ	No Sample	2019-01-22 14:16:09 +0100	Closed	Unknown/Unclear	<input type="button" value="Calibration"/>	<input type="button" value="Comment"/> <input type="button" value="Share"/>	<input type="button" value="Edit"/>

Proposal no. 900054 > Edit Run no. 79

* Run Number: 79

Run Alias:

* Run type: Test DAQ

Sample: No Sample

Run Status: Closed

Run Quality: Unclear (migrate data to Maxwell)

Description:

Audit fields

Created by: KARABO Migrator

Created by: 2019-01-22 14:29:27 +0100

Modified by: Luis Maia

Last modification date: 2019-04-02 04:15:18 +0200

Back Save Save and add another Cancel

Key Features

Proposal team and History

Proposal no. 900054

Back

Edit

Clone

Add another

Runs

Delete

Beamtime status

GeneralPublic InformationRunsTeamHistory

Experiment Team

- Principal Investigator: Djelloul Boukhelef - (boukhele) as Data Manager & Participant
- Main Proposer: Nasser Al-Qudami - (alqudami) as Data Manager & Participant
- Team members 1: Luis Maia - (maia) as Participant
- Team members 2: Jolanta Sztuk-Dambietz - (jsztuk) as Data Manager & Participant
- Team members 3: Maurizio Manetti - (manettim) as Participant
- Team members 4: Krzysztof Wrona - (wrona) as Data Manager & Participant
- Team members 5: Peter Zalden - (zaldenp) as Data Manager & Participant
- Team members 6: Janusz Malka - (jmalka) as Data Manager & Participant
- Team members 7: Juergen Hannappel - (hannappj) as Participant

Download:

CSV

JSON

Eleg format

Back

Edit

Clone

Add another

Runs

Delete

Beamtime status

Team members

* User

Luis Maia

Data access

Participant



* User

Luis Maia

Data access

Participant

* Lab Access

☐ Yes

☒ No



* User

Djelloul Boukhelef

Data access

Data Manager &



* User

Karen Appel

Data access

Data Manager & Participant

* Lab Access

☐ Yes

☒ No



* User

Jolanta Sztuk-Dambietz

Data access

Data Manager &



* User

Djelloul Boukhelef

Data access

Data Manager & Participant

* Lab Access

☐ Yes

☒ No



* User

Maurizio Manetti

Data access

Participant



* User

Data access

* Lab Access

* User

Krzysztof Wrona

Data acc

Data Ma

Proposal no. 900054

Back

Edit

Clone

Add another

Runs

Delete

Beamtime status

GeneralPublic InformationRunsTeamHistory

History

2019-02-14 15:27:59 +0100 – ## System ##			
Preferred data output	Processed	⇒	Raw
2019-01-29 18:23:55 +0100 – ## System ##			
Repository	---	⇒	XFEL_GPFS_ONLINE_SASE_2
2019-01-29 03:41:47 +0100 – Luis Maia			
Beamtime status	Active	⇒	Finished (Beamtime)
2019-01-23 16:24:10 +0100 – Janusz Malka			
Team changes	---	⇒	Juergen Hannappel (Participant)
2018-10-19 16:39:06 +0200 – Janusz Malka			
Beamtime status	Ready	⇒	Active
2018-09-27 16:38:46 +0200 – Janusz Malka			
Team changes	---	⇒	Janusz Malka (Data Manager & Participant)
2018-09-25 17:30:09 +0200 – Luis Maia			
Beamtime status	GPFS Online Configuration Done	⇒	Ready
2018-09-25 17:28:04 +0200 – Luis Maia			
Beamtime status	GPFS Offline Configuration Done	⇒	GPFS Online Configuration Done

Audit fields

Created by Janusz Malka

+ add member

Key Features

Proposal Repositories

Proposal no. 900190

MENU

BackEditCloneAdd anotherRunsDeleteBeamtime status

GeneralPublic InformationRunsTeamRepositoriesBetaCalibration ConstantsBetaHistory

Repositories

Beta warning!

Yes, this feature is in beta!

We are testing and developing actively this feature. Currently some information may not be 100% accurate, especially for old proposals and runs.

Thanks for noticing!

Request the Copy of Raw Data to available Remote repositories

No remote repositories are available.

Raw data availability per run and repository

Run Number (full)	Data Group	Run Quality	XFEL GPFs Raw online for SASE 1	XFEL GPFs online for SASE 2	XFEL GPFs online for SASE 3	XFEL GPFs online for SASE DET	XFEL GPFs online Raw data in DESY CC	XFEL GPFs online Raw data in DESY CC	XFEL GPFs online Raw data in DESY CC
0011	raw_e0001_n0011	To be evaluated							
0010	raw_e0001_n0010	To be evaluated							
0009	raw_e0001_n0009	To be evaluated							
0008	raw_e0001_n0008	To be evaluated							
0007	raw_e0001_n0007	To be evaluated							
0006	raw_e0001_n0006	To be evaluated							
0005	raw_e0001_n0005	To be evaluated							
0004	raw_e0001_n0004	To be evaluated							
0003	raw_e0001_n0003	Unknown/Unclear							
0002	raw_e0001_n0002	Unknown/Unclear							
0001	raw_e0001_n0001	Unknown/Unclear							

BackEditCloneAdd anotherRunsRunsDeleteBeamtime status

Proposal no. 900190 > Run no. 3

MENU

BackEditCloneAdd anotherDelete

#id: 89110

Proposal Number: 900190

Run Number: 3

Run Alias:

Run Folder: r0003

Run type: Test DAQ

Sample Name: No Sample

Start date: 2021-02-03 16:28:49 +0100

End date: 2021-02-03 16:30:29 +0100

First Train: 976049117

Last Train: 976050119

Size (Bytes): 1484032

No. files: 1

Available: Yes

Run Quality: Unknown/Unclear

Run Status: Closed

Original Format: ---

DAQ system message: ---

Calibrated Process data status: Not Available

Calibration: Binomial auto-Breaks

Migration requested at: 2021-03-04 09:48:33 +0100

Migration begin at: 2021-03-04 09:48:40 +0100

Migration end at: 2021-03-04 09:49:11 +0100

No. Calibration Requests: 0

Calibration last request at: ---

Calibration last begin at: ---

Calibration last end at: ---

Description: ---

Created by: KARABO Migrator

Creation date: 2021-02-03 16:28:49 +0100

Modified by: GPFs Migrator

Last modification date: 2021-03-04 09:49:11 +0100

Data Groups

Expand all | Collapse all

raw_e0001_n0003

RAW-R0003-DA04-S00000.h5 (relative_path ==> 0003/)



File Manager

Panels

Collection: euxfel#euxfel

Path: /gpfs/exfel/exp/TSTSA2/202130/p900190/raw/r0003/

Bookmark

view

Share

Transfer or Sync to...

New Folder

Rename

Delete Selected

Download

Open

Upload

Get Link

Show Hidden Items

Manage Activation

NAME

LAST MODIFIED

SIZE

RAW-R0003-DA04-S00000.h5

2/3/2021, 4:30 PM

1.51 GB

Key Features

Proposal Calibration

Proposal no. 900204

Back

Edit

Clone

Add another

Runs

Delete

Beamtime status

General

Public Information

Runs

Team

Repositories

Beta! Calibration Constants

History

Calibration Constants

Request Dark Run Calibration

Detector

SPB_IRDA_JF4M

Detector Units

JNGFR01

JNGFR02

JNGFR03

JNGFR04

JNGFR05

JNGFR06

JNGFR07

JNGFR08

Select All Unselect All

Operation Mode

Adaptive Gain

Operation Mode Description

Standard operation mode for AGIPD and Jungfrau detectors with 3 gain stages used. To be able to process calibration constants from dark data, the data should be taken for each gain stage in separate runs. Therefore, the run number for each gain stage has to be specified in the following order #1- high (HG/G0) #2-medium (MG/G1) #3 - low (LG/G2)

Run Number(s)

Run #1

98

Run #2

99

Run #3

100

Description

Request

Dark runs requests

Status	Last Updated at	Detector	Detector Units	Operation Mode	Run Number(s)	External resources
Finished	2021-03-23 12:04:54 +0100	SPB_IRDA_JF4M	JNGFR01, JNGFR02, JNGFR03, JNGFR04, JNGFR05, JNGFR...	Adaptive Gain	98, 99, 100	(VPN required)
Finished	2021-03-18 11:51:13 +0100	SPB_IRDA_JF4M	JNGFR01, JNGFR02, JNGFR03, JNGFR04, JNGFR05, JNGFR...	Adaptive Gain	145, 146, 147	(VPN required)
Finished	2021-03-14 10:38:40 +0100	SPB_IRDA_JF4M	JNGFR01, JNGFR02, JNGFR03, JNGFR04, JNGFR05, JNGFR...	Adaptive Gain	132, 133, 134	(VPN required)
Finished	2021-03-14 09:37:31 +0100	SPB_IRDA_JF4M	JNGFR01, JNGFR02, JNGFR03, JNGFR04, JNGFR05, JNGFR...	Adaptive Gain	129, 130, 131	(VPN required)
Finished	2021-03-14 09:19:27 +0100	SPB_DET_AGIPD1M-1	AGIPD00 (Q1M1), AGIPD01	Adaptive Gain	129, 130,	(VPN required)

European XFEL

European XFEL

CalCat

Test Environment

HOME

ADMIN

USERS

MY TOKENS

MY ACCOUNT

LOGOUT

MENU

Report

#id: 13

Name: dark_900113_r9985_r9984_r9983_210211_122050.pdf

File path: /gdfs/exfel/d/cal_tst/caldb_store/xfel/reports/CALLAB/HED_DET_AGIPD500K2G/dark/dark_900113_r9985_r9984_r9983_210211_122050.pdf

Download:

Available: Yes

Description: ---

Created by: Admin User

Creation date: 2021-02-11T12:27:19+0100

Modified by: Admin User

Last modification date: 2021-02-11T12:27:19+0100

Associated Calibration Constant Versions

Deploy all versions

Warning In the table below, Karabo DA and Detector of the associated Physical Detector Unit are shown as they were at the moment of the calibration constant version's creation date and time

Name	Deployed	Good quality	Start date	Validity start	Creation date	Calibration Constant	Physical Detector Unit	Detector
20210211_112807_slidx=0	false	true	2020-09-23 13:26:59	2020-09-23 13:26:59	2021-02-11 12:28:08	AGIPD-Type_BadPixelsDark_AGIPD DefG7npSmbfU	AGIPD_SIV1_AGIPDV11_M 116IN (AGIPD00)	HED_DET_AGIPD500K2G
20210211_112811_slidx=0	false	true	2020-09-23 13:26:59	2020-09-23 13:26:59	2021-02-11 12:28:11	AGIPD-Type_BadPixelsDark_AGIPD DefHfH5zPJV7	AGIPD_SIV1_AGIPDV11_M 117IN (AGIPD02)	HED_DET_AGIPD500K2G
20210211_112811_slidx=0	false	true	2020-09-23 13:26:59	2020-09-23 13:26:59	2021-02-11 12:28:11	AGIPD-Type_BadPixelsDark_AGIPD DefD+RLqcU6Vg	AGIPD_SIV1_AGIPDV11_M 117OUT (AGIPD03)	HED_DET_AGIPD500K2G

dark_900204_r145_r146_r147_210318_111538.pdf

1 / 1173

100%

+

-

1

2

3

Jungfrau Dark Image Characterization

European XFEL

Detector group

Based on data sample: /gdfs/exfel/exp/SPB/202130/p900204/raw

Release : 3.1.0-hotfix4

March 18, 2021

Key Features

Integration with data acquisition

MID_RUN_CONTROL_GLOBAL_STATE

MID Run Controller

Data Source Groups

source	type	behavior	monitored	access
AGIPD1M_XTDF				
BEAM_COND_3				
MID_AGIPD1M_CTRL				
MID_AGIPD1M_POWER_HV				
MID_AGIPD1M_TEMP				
MID_AGIPD1M_TSYS				
MID_AGIPD1M_MOTION				
MID_OPT_ATT				
SA2_COND_1				
BEAM_COND_1				
BEAM_COND_2				
JF500K_CTRL				
JF500K_M1				
JF500K_M2				
MID_ANDOR_CAM				
MID_AUXT2_IMGPI				
MID_AUXT3_PAM				
MID_AUXT3_PAM_CAM1				
MID_AUXT3_PAM_CAM2				
MID_BAM				
MID_DES_GOTTHARD				
MID_DOC_ADHOC				
MID_ENERGY				
MID_EXP_DES				
MID_EXP_DES_CAM1				
MID_EXP_DES_CAM2				
MID_EXP_DES_CAM3				
MID_EXP_EPIX-1				
MID_EXP_EPIX-2				
MID_EXP_FASTADC				

Group to Data Aggregator Mapping

	Data source	Alias	Data aggregator
0	@MID_AGIPD1...	AGIPD1MCTRL00	MID_DAQ_DATA/AGIPD1MCTRL/0
1	@MID_AGIPD1...	AGIPD1MCTRL00	MID_DAQ_DATA/AGIPD1MCTRL/0
2	@MID_AGIPD1...	AGIPD1MCTRL01	MID_DAQ_DATA/AGIPD1MCTRL/1
3	@MID_AGIPD1...	AGIPD1MCTRL01	MID_DAQ_DATA/AGIPD1MCTRL/1
4	@MID_AGIPD...	DA02	MID_DAQ_DATA/DA/2
5	@BEAM_COND...	DA03	MID_DAQ_DATA/DA/3
6	@SA2_COND_1	DA03	MID_DAQ_DATA/DA/3
7	@MID_OPT_ATT	DA04	MID_DAQ_DATA/DA/4
8	MID_DET_AGL...	AGIPD00	MID_DET_AGIPD1M-1/DET/0CH0
9	MID_DET_AGL...	AGIPD10	MID_DET_AGIPD1M-1/DET/10CH0
10	MID_DET_AGL...	AGIPD11	MID_DET_AGIPD1M-1/DET/11CH0
11	MID_DET_AGL...	AGIPD12	MID_DET_AGIPD1M-1/DET/12CH0
12	MID_DET_AGL...	AGIPD13	MID_DET_AGIPD1M-1/DET/13CH0
13	MID_DET_AGL...	AGIPD14	MID_DET_AGIPD1M-1/DET/14CH0
14	MID_DET_AGL...	AGIPD15	MID_DET_AGIPD1M-1/DET/15CH0
15	MID_DET_AGL...	AGIPD01	MID_DET_AGIPD1M-1/DET/1CH0
16	MID_DET_AGL...	AGIPD02	MID_DET_AGIPD1M-1/DET/2CH0

Data Aggregator Status

Device (Alias)	State	
RunController	MONITORING	no_load_
AGIPD00	MONITORING	1/21
AGIPD01	MONITORING	1/21
AGIPD02	MONITORING	1/21
AGIPD03	MONITORING	1/21
AGIPD04	MONITORING	1/21
AGIPD05	MONITORING	1/21
AGIPD06	MONITORING	1/21
AGIPD07	MONITORING	1/21
AGIPD08	MONITORING	1/21
AGIPD09	MONITORING	1/21
AGIPD10	MONITORING	1/21
AGIPD11	MONITORING	1/21
AGIPD12	MONITORING	1/21
AGIPD13	MONITORING	1/21
AGIPD14	MONITORING	1/21
AGIPD15	MONITORING	1/21

Preparation

Proposal number 2929 2929

Retrieve proposal Push to DAQ Apply configuration Monitor data

Ignore data Clear configuration

[16:07:45]: Run closed successfully

Proposal ☒

Data source ☒

Assign ☒

Configure ☒

Monitor ☒

Progress 100%

Global state

Recording

Run Type scattering scattering

Sample Vycor Vycor

Train id 1031309315 Previous run

Start run Stop run

Proposal no. 002929

MENU

Back Edit Clone Add another Runs Delete Beamtime status

General Public Information Runs Team Repositories Calibration Constants History

Proposal Runs


Run Number (alias)	Run type	Sample Name	Start date	Run status	Data Assessment	Calibration	Run Comment	Edit
0020	scattering	Vycor	2021-04-08 18:12:14 +0200	Closed	Run Quality			
0019	scattering	Vycor	2021-04-08 18:10:29 +0200	Closed	Run Quality			
0018	scattering	Vycor	2021-04-08 18:08:30 +0200	Closed	Run Quality			
0017	scattering	Vycor	2021-04-08 18:06:44 +0200	Closed	Run Quality			
0016	scattering	Vycor	2021-04-08 18:01:40 +0200	Closed	Run Quality			
0015	scattering	Vycor	2021-04-08 17:59:05 +0200	Closed	Run Quality			
0014	scattering	Vycor	2021-04-08 16:07:20 +0200	Closed				
0013	scattering	Vycor	2021-04-08 16:05:18 +0200	Closed				
0012	scattering	Vycor	2021-04-08 16:04:04 +0200	Closed	Good			
0011	scattering	Vycor	2021-04-08 16:03:12 +0200	Closed	Good			
0010	scattering	Vycor	2021-04-08 16:01:47 +0200	Closed	Good			
0009	scattering	Vycor	2021-04-08 16:01:05 +0200	Closed	Good			
0008	scattering	Vycor	2021-04-08 16:00:00 +0200	Closed	Good			

Good (migrate data to Maxwell)
Unclear (migrate data to Maxwell)
Not interesting (data won't be migrated to Maxwell)

European XFEL

Key Features

RESTful API's



Swagger
Supported by SMARTBEAR

Select a definitionmyMdc API Docs

metadata APIs

1.0.0OAS3

v1/swagger.yaml

This is the myMdc api documentaion

Contact the developer

Servers

https://in.xfel.eu/metadata/api - Production server (uses live data)

Authorize

facilities

Operations about the facilities

GET

/facilities

Get all the facilities

POST

/facilities

Create facility

GET

/facilities/{id}

Get facility by ID

PUT

/facilities/{id}

Update facility by ID

DELETE

/facilities/{id}

Delete facility by ID

API docs: <https://in.xfel.eu/metadata/api-docs/index.html>

GET

/proposals/by_number/{number}

Get proposal by number

For valid response provide valid proposal number

Parameters

Cancel

Name	Description
number <small>required</small>	Unique number of a given proposal that needs to be fetched
<small>integer(\$int64)</small>	
<small>(path)</small>	
<input type="text" value="900184"/>	
<div>Execute</div>	<div>Clear</div>

Responses

Curl

curl -X GET "https://in.xfel.eu/metadata/api/proposals/by_number/900184" -H "accept: application/json; version=1" -H "X-USER-EMAIL: ..."

Request URL

https://in.xfel.eu/metadata/api/proposals/by_number/900184

Server response

Code	Details
200	<div><div>Response body</div><div><pre>{ "id": 412, "number": 900184, "title": "SASE3 Photon Beam Measurements", "abstract": "", "proposal_folder": "p900184", "def_proposal_path": "/gpps/exfel/exp/SA3/202130/p900184/raw", "doi": "10.22003/XFEL-EU-DATA-900184-00", "url": "", "instrument_id": 106, "instrument_cycle_id": 165, "principal_investigator_id": 223, "main_proposer_id": 131, "local_contact_id": 223, "orig_repository_id": 3, "last_run": "", "begin_at": "2021-01-01T00:00:00.000+01:00", "end_at": "2021-06-30T23:59:58.000+02:00", "release_at": "2024-06-30T23:59:58.000+02:00", "num_delivered_shifts": null, "num_preparation_shifts": null, "flag_public": false, "flag_proposal_system": null, "flag_nonfargod_data_output": "no" }</pre></div><div>Download</div></div> <div><div>Response headers</div><div><pre>cache-control: max-age=0,private,must-revalidate connection: Keep-Alive content-type: application/json; charset=utf-8 date: Thu, 08 Apr 2021 22:48:17 GMT etag: W/"bc3a1efcf37a11b0abbc0391a08606" keep-alive: timeout=5,max=100 referrer-policy: strict-origin-when-cross-origin server: Apache status: 200 OK strict-transport-security: max-age=16070400; includeSubDomains transfer-encoding: chunked vary: Origin x-content-type-options: nosniff x-download-options: noopen x-frame-options: SAMEORIGIN x-permitted-cross-domain-policies: none x-powered-by: Phusion Passenger 6.0.7 x-request-id: 3e21d8c-a7ce-43bd-b7a5-dcb3cfc6547c x-runtime: 0.035170 x-xss-protection: 1; mode=block</pre></div></div>

Code	Description	Links
200	successful operation	No links

Media type

Key Features

Python client to myMdC RESTful API's

```
exflqr17747:metadata_client mail$ python3 mail.py
{'success': True, 'info': 'Got proposal successfully', 'app_info': {}, 'data': {'id': 85,
'number': 900054, 'title': 'TST SASE2 DAQ tests', 'abstract': '', 'proposal_folder': 'p900
054', 'def_proposal_path': '/gpfs/xfel/exp/TSTSA2/201831/p900054/raw', 'doi': '10.22003/X
FEL.EU-DATA-900054-00', 'url': '', 'instrument_id': 110, 'instrument_cycle_id': 31, 'princ
ipal_investigator_id': 51, 'main_proposer_id': 411, 'local_contact_id': None, 'orig_reposi
tory_id': 2, 'last_run': 82, 'begin_at': '2018-09-25T00:00:01.000+02:00', 'end_at': '2018-
12-31T23:59:58.000+01:00', 'release_at': '2021-12-31T23:59:59.000+01:00', 'num_delivered_s
hifts': None, 'flg_public': False, 'flg_proposal_system': None, 'flg_preferred_data_output
': 'R', 'flg_available': True, 'flg_beamtime_status': 'F', 'beamtime_start_at': None, 'bea
mtime_end_at': None, 'description': '', 'beamtimes': [{'id': 73, 'begin_at': '2018-09-25T0
0:00:01.000+02:00', 'end_at': '2018-12-31T23:59:58.000+01:00', 'flg_available': True, 'des
cription': None}], 'team': [{'id': 1674, 'user_id': 51, 'data_access_role': 1}, {'id': 167
5, 'user_id': 170, 'data_access_role': 1}, {'id': 1677, 'user_id': 391, 'data_access_role'
: 1}, {'id': 1678, 'user_id': 399, 'data_access_role': 1}, {'id': 1679, 'user_id': 411, 'd
ata_access_role': 1}, {'id': 1697, 'user_id': 665, 'data_access_role': 1}, {'id': 1673, 'u
ser_id': 1, 'data_access_role': 2}, {'id': 1676, 'user_id': 231, 'data_access_role': 2}, {
'id': 1959, 'user_id': 1131, 'data_access_role': 2}], 'users_ids': [[51, 'boukhele'], [170
, 'jsztuk'], [391, 'wrona'], [399, 'zaldenp'], [411, 'alqudami'], [665, 'jmalka'], [1, 'ma
ial'], [231, 'manettim'], [1131, 'hannappj']]]}
exflqr17747:metadata_client mail$
exflqr17747:metadata_client mail$
```

Gitlab: <https://in.xfel.eu/gitlab/ITDM/metadata> client

PyPi: <https://pypi.org/project/metadata-client/>



```
metadata_client — spbdaq@exflpc01n0:~ — vim maial_py.py — 92x44
```

```
#!/usr/bin/python3  
from metadata_client.metadata_client import MetadataClient  
  
# Necessary configuration variables to establish a connection  
user_id = '1d[REDACTED]ab'  
user_secret = '84b[REDACTED]25'  
user_email = 'luis.maia@xfel.eu'  
#  
metadata_web_app_url = 'https://in.xfel.eu/metadata/  
token_url = 'https://in.xfel.eu/metadata/oauth/token'  
refresh_url = 'https://in.xfel.eu/metadata/oauth/token'  
auth_url = 'https://in.xfel.eu/metadata/oauth/authorize'  
scope = ''  
base_api_url = 'https://in.xfel.eu/metadata/api/'  
  
proposal_number = 900054  
  
# Generate the connection  
client_conn = MetadataClient(client_id=user_id,  
                             client_secret=user_secret,  
                             user_email=user_email,  
                             token_url=token_url,  
                             refresh_url=refresh_url,  
                             auth_url=auth_url,  
                             scope=scope,  
                             base_api_url=base_api_url)  
  
all_proposal_runs = MetadataClient.get_proposal_info(client_conn, proposal_number)  
#all_proposal_runs = MetadataClient.get_proposal_runs(client_conn, proposal_number)  
print(all_proposal_runs)
```

```
"maial_py.py" 31L, 1268C
```


Key Features

Open data (PaNOSC & EOSC)

The main outcomes of other PaNOSC work packages were also presented. In particular, in [WP3 – Data Catalogue Services](#), the activities carried out since the project's start include:

- Development of an Application Programmers Interface (API) for searching for FAIR data;
- **Integration of a search API into the EOSC portal;**
- Use of Nexus/HDF5 standard format for metadata;
- Automation of metadata collection on beamlines;
- **Use of e-logbook to make data FAIRer;**
- Long-term storage (hundreds of Petabytes).

Source: www.panosc.eu/news

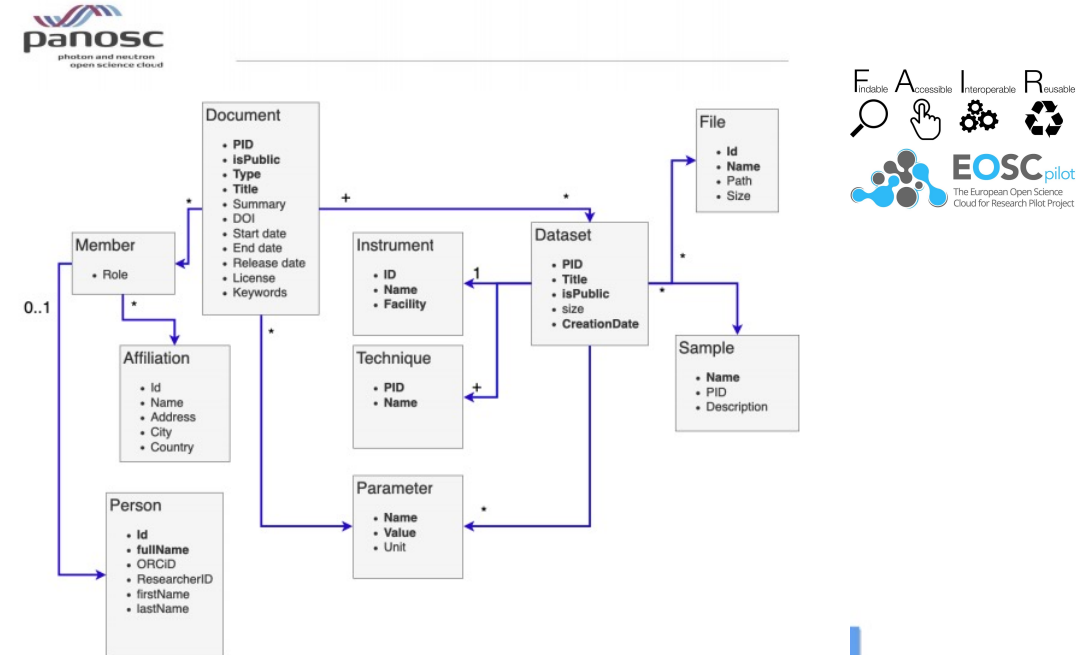


Figure 2: Search API data model

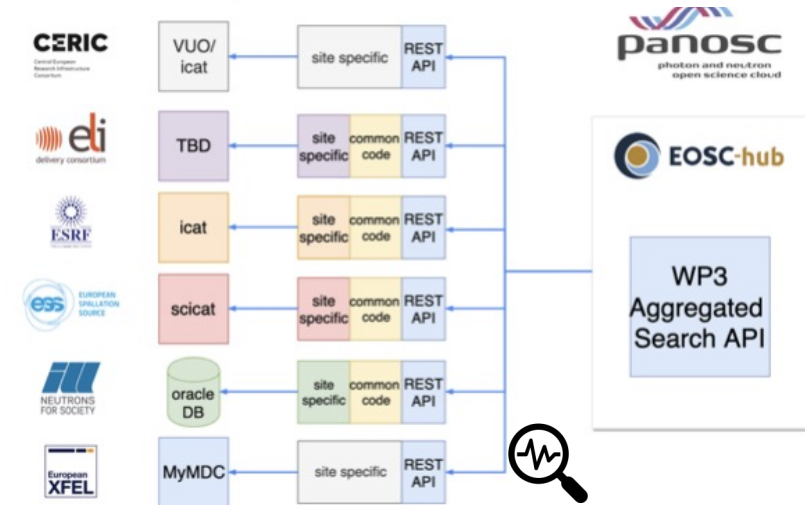


Figure 1: Overview of targeted deployment at partner sites and use of search API.

Key Features Statistics

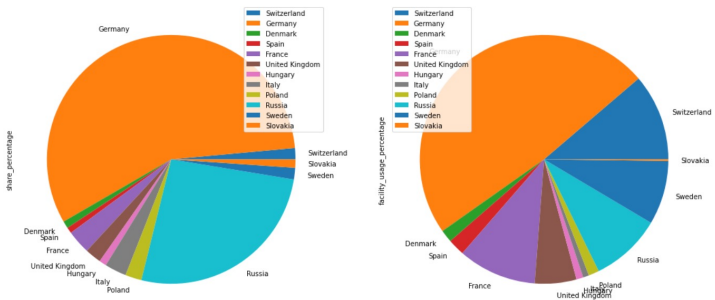
	Mar. 2019	Jan. 2020	Mar. 2021
Users	1296	1886	2196
Groups	346	662	948

	Mar. 2019	Jan. 2020	Mar. 2021
Instruments	15	20	20
Instrument Cycles	59	115	176
Repositories	11	12	12

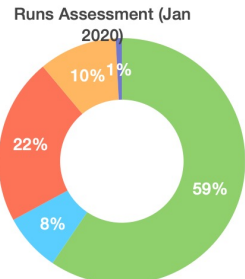
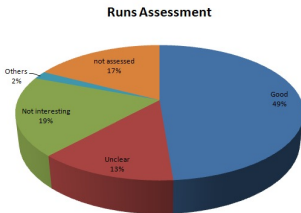
	Mar. 2019	Jan. 2020	Mar. 2021
Proposals	144	287	431
Proposals with published DOI	3	4	13
Samples in all proposals	540	1238	1955
Run Types in all proposals	488	1136	1829
Users in all proposals	2833	6039	8886
Runs in all proposals	29736	64596	91139
Runs migrated to Maxwell	18304	43341	65579
Runs Calibrated (via myMdC)	463	8018	12323
Requested Dark Runs			147
Number of Delivered Shifts			

European XFEL Shareholders Scientific Usage Statistics

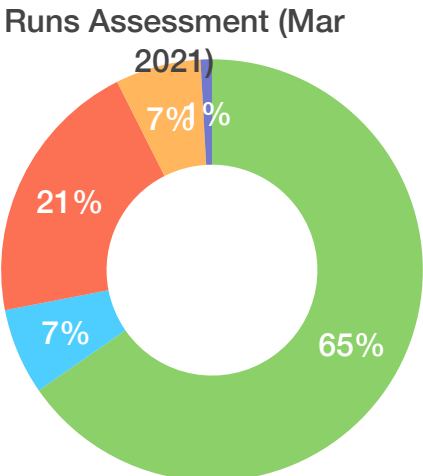
Scope: Calendar Year 2020 (Facility Run no.5 & Facility Run no.6)
Period: from 2020-01-01 till 2020-12-31
Total number of delivered shifts: 159
Statistics calculated with proposal experiment teams grouped by: Laboratories/Departments
Final statistics calculation weighted by: Affiliation



RUNS ASSESSMENT (MAR. 2021)	
Good	59.545
Unclear	6.034
Not interesting	18.790
Not assessed	5.977
Others	793
TOTAL RUNS	91.139



Good
Not interesting
Unclear
Not assessed
Others



Good
Unclear
Not interesting
Not assessed
Others



[This Photo](#) by Unknown Author is licensed under [CC BY-NC-ND](#)

Thank you!

Special thank you to all the people that contributed to the project