

NOBUGS 2022

py-ISPyB

A new implementation of a LIMS for experiments in structural biology



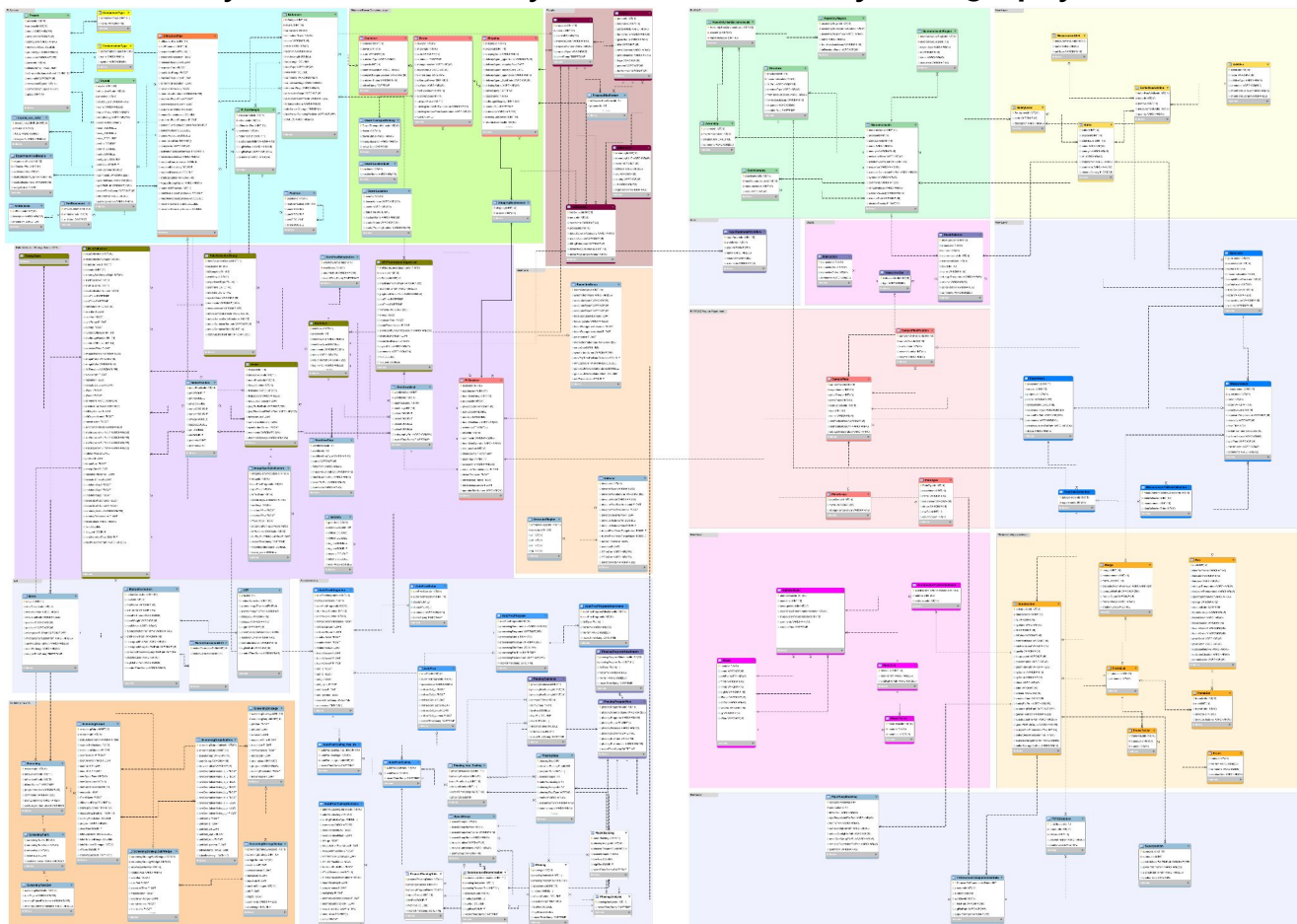
Maël Gaonach

Software Engineer
Data Automation Unit
Software Group ESRF

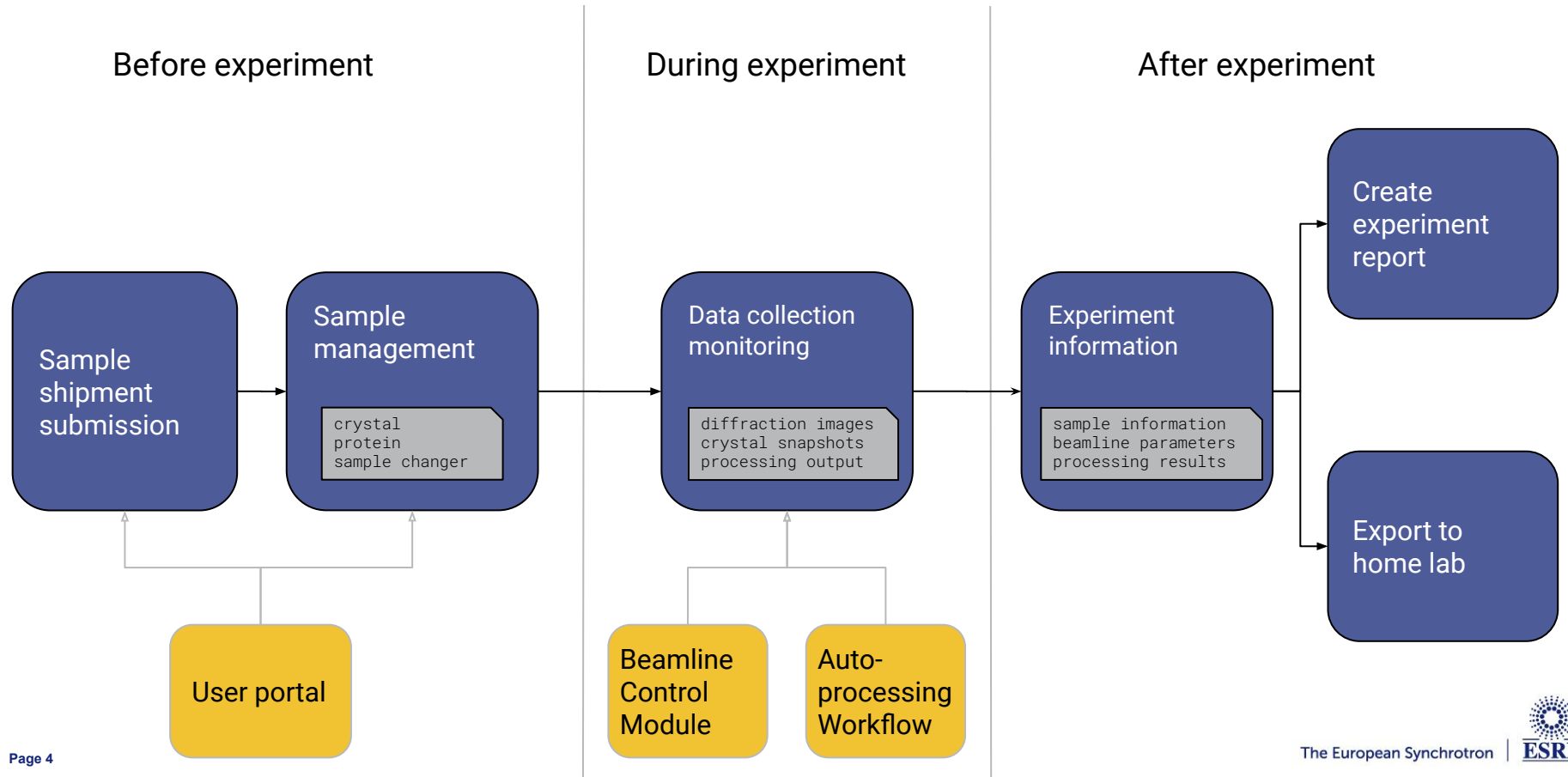


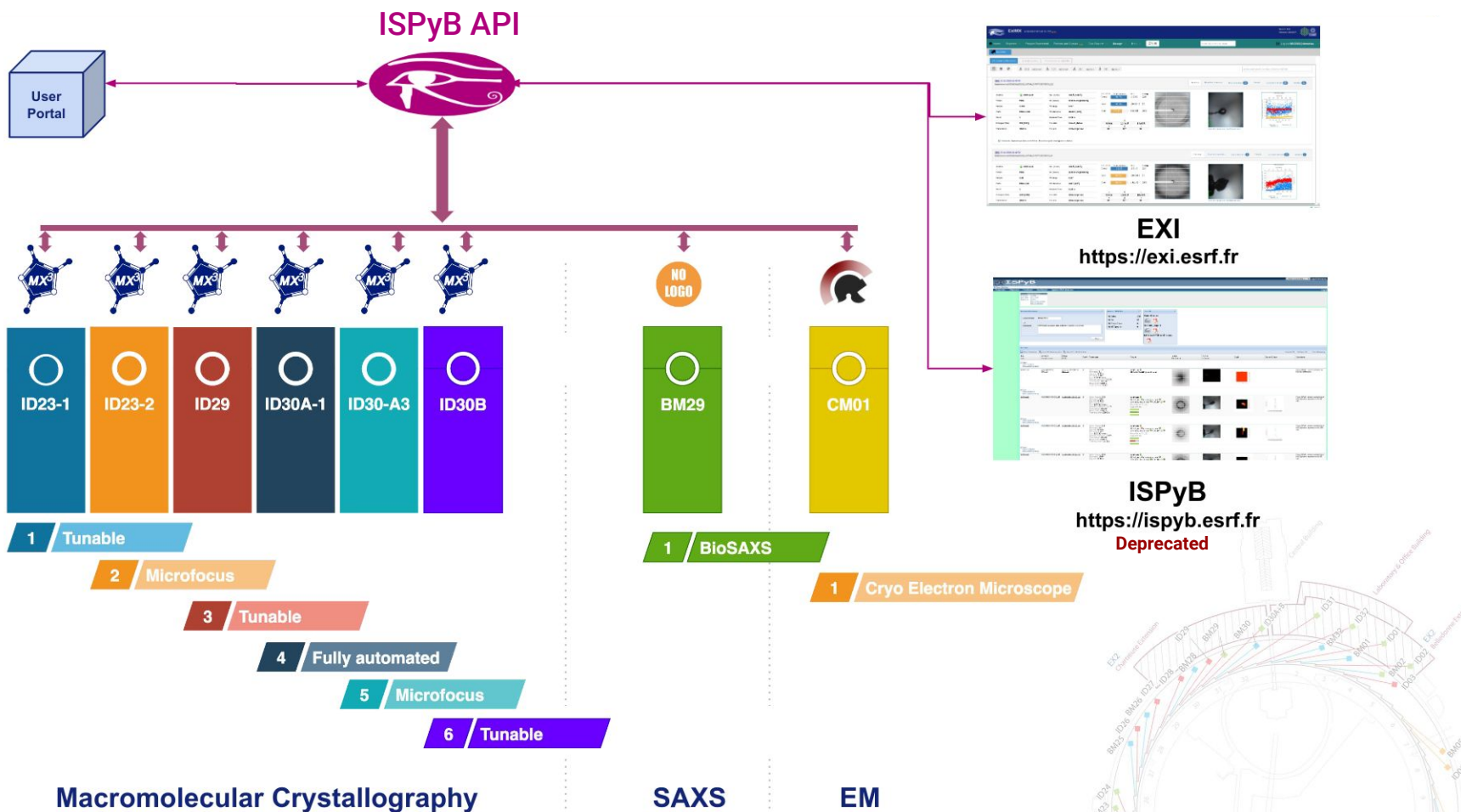
STREAMLINE has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 870313

ISPyB

ISPyB = Information System for Protein crystallography Beamlines

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ISPyB collaboration participants



py-ISPyB

Full-stack collaboration

Server side

- Technical redesign
- Implementation language changed from Java to Python
- Modern API (REST)
- Includes new administrative & scientific requirements
- Backwards compatibility + new features

User interface

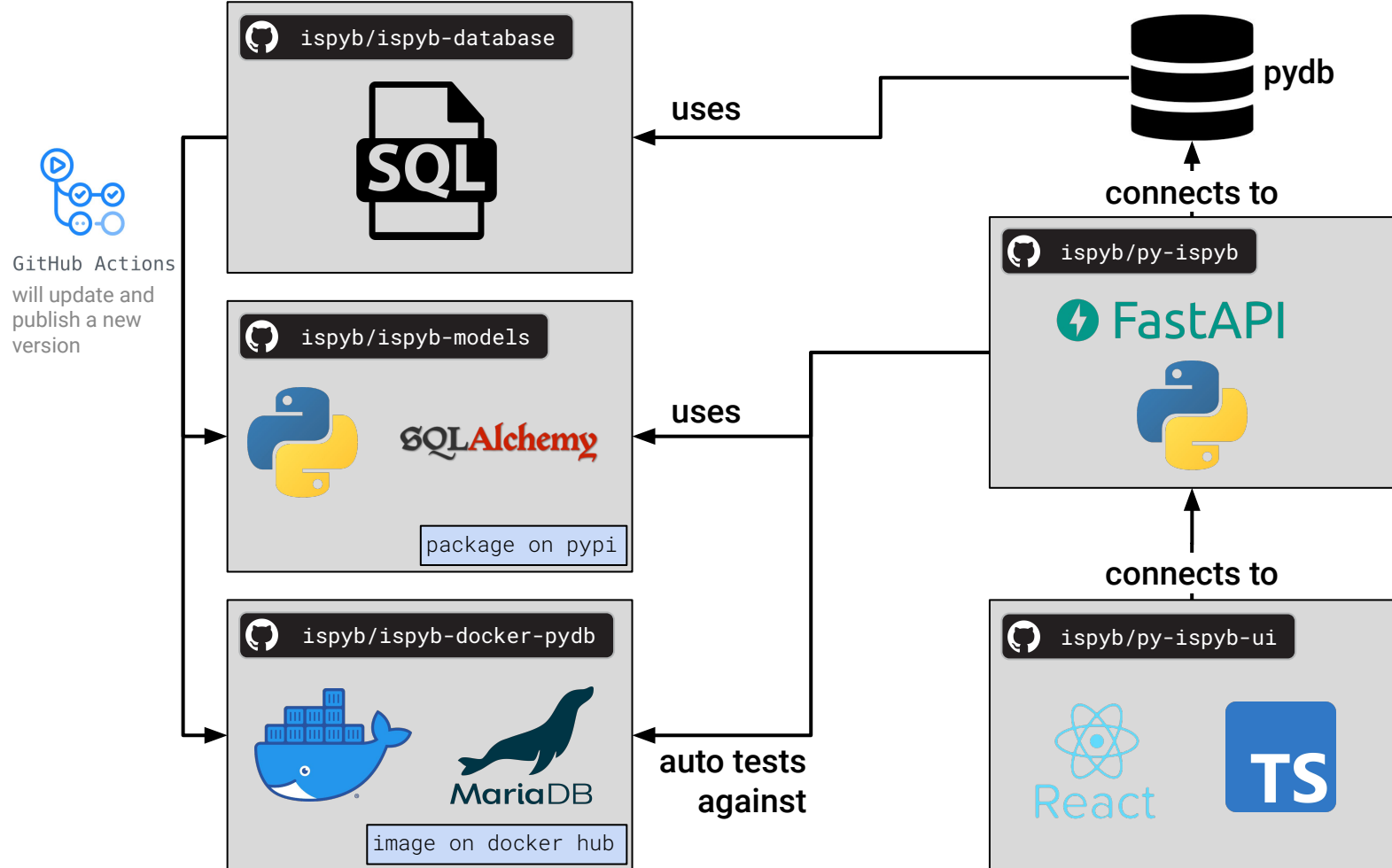
- Latest frontend technologies (React v17)
- Easy to extend
- Included in collaboration
- Backwards compatibility with limited functionalities

Working groups

Tasks	Brief description	Responsible(s)	Participant(s)
Framework & architecture	Organize the project structure, choose the libraries and define the best good practices to be adopted (automatic testing and documentation), deployments, etc...	ESRF	ALL
Authentication	Develop the authentication/authorization mechanism(s)	ESRF	SOLEIL, DESY, DLS
User Portal Sync	Development of a fairly generic mechanism to synchronize the data from the user portal. It includes entities like proposals, sessions, proteins and samples, etc...	DESY	ESRF, ALBA, DLS
Shipping	Implementation of the sample tracking system	DESY, ESRF, DLS	SOLEIL, GP
EM	Development of cryo-electron microscopy (cryo-EM) for single particle experiments	ESRF	DLS
MX	Development of MX	GP, SOLEIL	EMBL, DESY, ESRF, MAXIV, ALBA, DLS
SSX	Development of serial synchrotron crystallography (SSX) experiments.	ESRF	EMBL, DESY, DLS, GP
Documentation	Ensure coherent and up to date documentation for Users, Developers and Application Developers	GP	ESRF, SOLEIL

- **Coordination meeting every week**
 - Report decisions and progress from working groups
- **Technical discussions through GitHub issues**
- **Working group meetings when necessary**
 - Take technical decisions

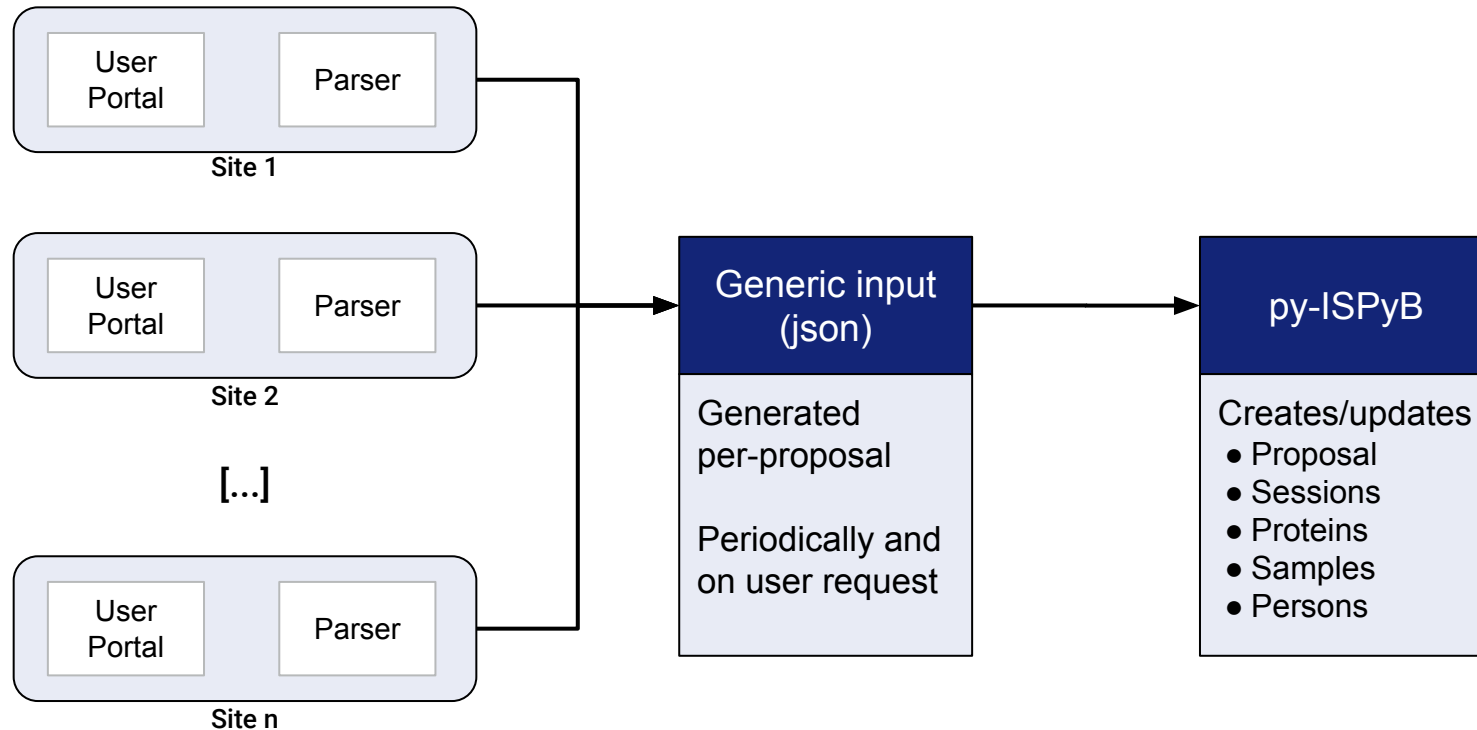
Framework/Architecture Group



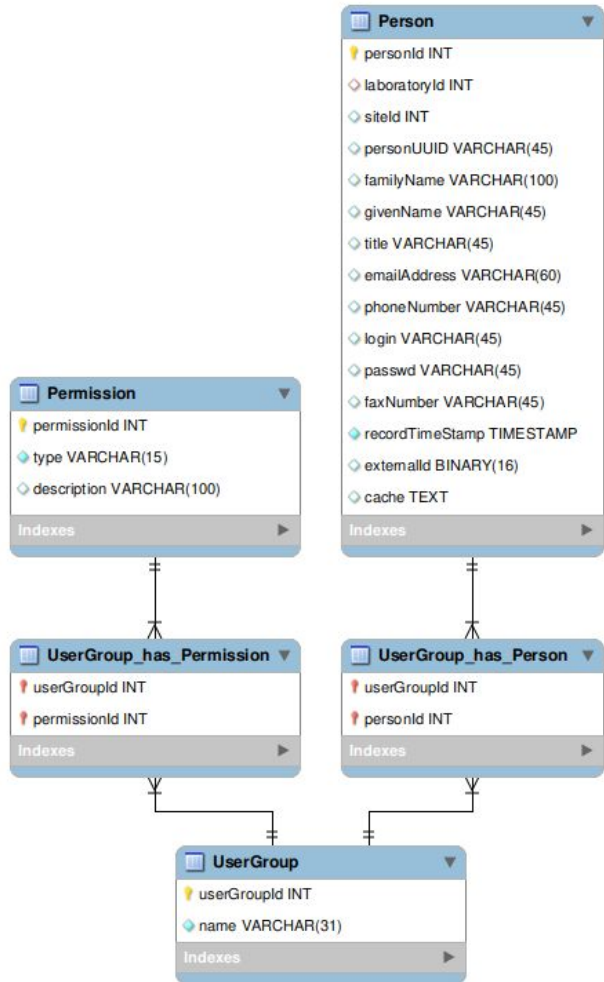
User Portal Sync Group

Goal:

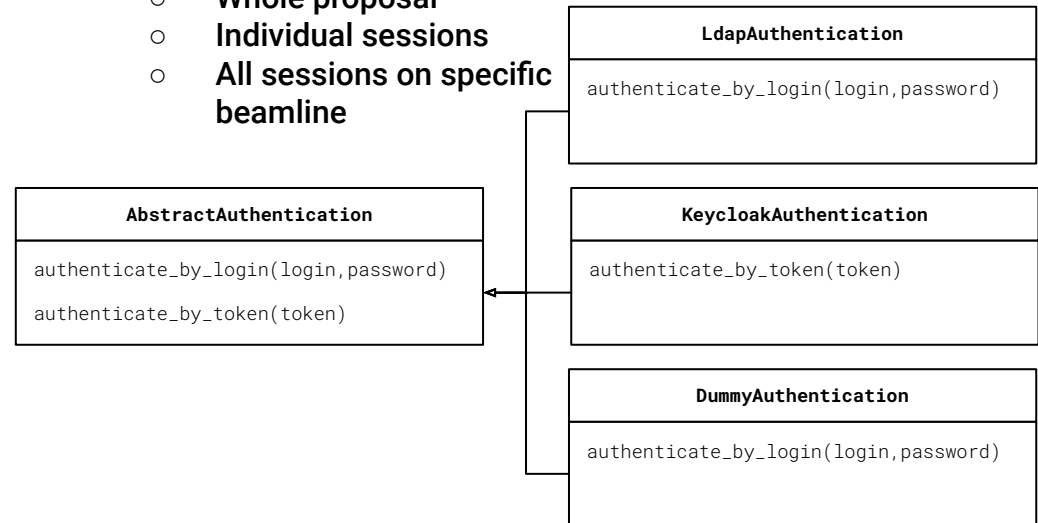
Development of a fairly generic mechanism to synchronize the data from the User Portal. It includes entities like proposals, sessions, proteins and samples, etc...



Authentication/Authorization Group



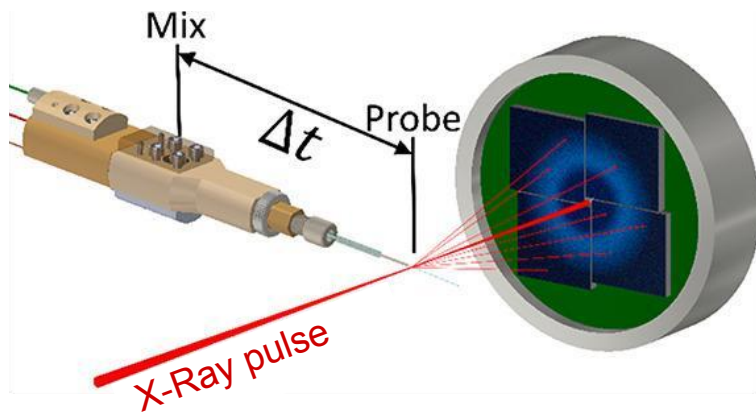
- Groups & permission centralized in DB
- Multiple authentication mechanisms
 - Natively supports:
 - LDAP
 - Keycloak
 - Dummy (For developments)
 - Possibility to add your own auth *via plugin*
- Authorization possible for:
 - Whole proposal
 - Individual sessions
 - All sessions on specific beamline



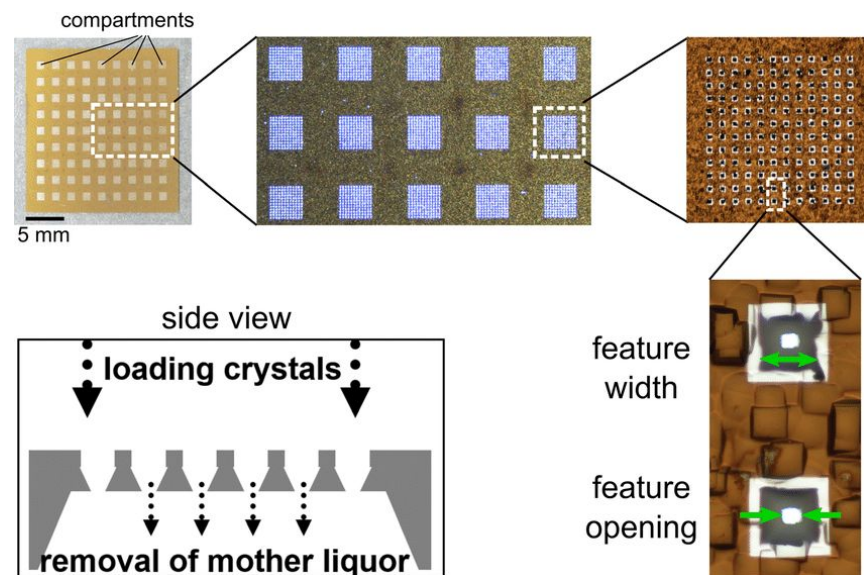
First use case: Serial synchrotron crystallography

MX	SSX
1 crystal	Many crystals
Many images	1 image per crystal
Rotation	Static
Frozen loop	Various support

Jet experiments



Chip experiments



Improved : sample definition

ISPyB My proposals My sessions

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Proposal SSX1 [Sessions](#) Prepare experiment

SSX1 on ID29 - Session from 20/09/2022 12:00:00 to 25/09/2022 12:00:00

20/09/2022 18:21:38 **SSXChip** 17 collections

Sample

Processing

Monitor
experiment

Sample name	rphvi
Protein	zklua
Avg crystal size (X, Y, Z)	5828.9541298867, 9102.611898082, 1033.4600075552
Crystal concentration	1352.11
Support	TODO

Sample components

	Name	Concentration	Composition
Buffer	bytuh	191.183	mgujd
Jet material	cztem	2777.93	uguig
Ligand	uzjdx	5324.89	nkdkp

20/09/2022 18:28:33 **SSXInjector** 17 collections

Sample

Processing

Monitor
experiment

Sample name	mkurr
Protein	jbkrm
Avg crystal size (X, Y, Z)	8925.4676631456, 7601.5418174401, 5146.9575426521
Crystal concentration	7186.21
Support	TODO

Sample components

	Name	Concentration	Composition
Buffer	elrgu	7914.23	ncpbx
Jet material	ircjb	2287.51	etteo
Ligand	kuare	9313.34	xffmt

20/09/2022 18:29:18 **SSXChip** 12 collections

Sample

Processing

Monitor
experiment

Sample name	ronyn
Protein	xfbiv
Avg crystal size (X, Y, Z)	4951.9001006718, 3492.7597611604, 1944.8108790331
Crystal concentration	6054.19
Support	TODO

Sample components

	Name	Concentration	Composition
Buffer	rvajs	5476.41	itnmd
Jet material	kbqqq	9859.93	tydpe
Ligand	ujevv	4515.86	edxri

New feature : SSX Data collection summary

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Proposal SSX1 Sessions Prepare experiment

SSX1 on ID29 - Session from 20/09/2022 12:00:00 to 25/09/2022 12:00:00

Details for experiment:

20/09/2022 18:29:18 SSXChip 12 collections

Sample name	robyn
Protein	xfbr
Avg crystal size (X, Y, Z)	4951.900/1066718, 3492.7597611604, 1944.8108790331
Crystal concentration	6054.19
Support	TODD

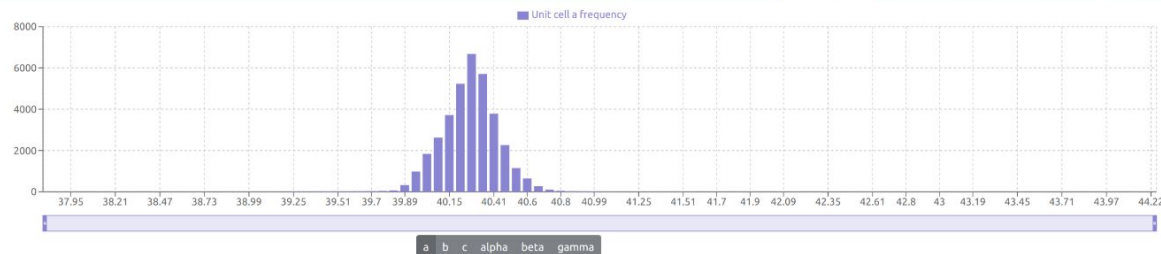
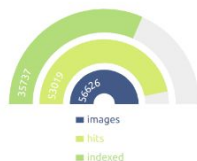
Sample components

	Name	Concentration	Composition
Buffer	rvqs	5476.41	itnmd
Jet material	kbqq	9859.93	tydpe
Ligand	ujev	4515.86	edxi

Back to experiments

20/09/2022 18:29:31

Sample name	robyn
Experiment type	SSXChip
Support	TODD
Exposure time	1808.95 s
Repetition rate	9640.75
Wavelength	7908.55
Flux	9133.7146645084
Transmission	585.778 %
Detector distance	1831.79 mm



20/09/2022 18:29:30

Sample name	robyn
Experiment type	SSXChip
Support	TODD
Exposure time	3725.04 s
Repetition rate	8673.49



New feature : SSX Data collection

20/09/2022 18:29:31									
								Summary	Parameters
Workflow	TODD	Res. (corner)	8151.04 Å (4073.28 Å)	Beamline Name	ID29	Synchrotron name	Focusing optics		Detector Type
Protein	xfblv	En. (Wave.)	0.002 KeV (7908.5500)	Detector Distance	1831.79 mm	Synchrotron filling mode	Monochromator type		Photon counting
Sample	royn	Exposure Time	1808.95 s	X Beam	4578.84 mm	Synchrotron Current	Beam size at Sample Hor (Vert)	4952130(6925910) µm	Detector Model
Prefix	ajcpf	Flux start	9.13e+3 ph/sec	Y Beam	7183.19 mm	Undulator types	Beam divergence Hor (Vert)	null(null) µrad	Manufacturer
Run	8332	Flux end	8.89e+3 ph/sec			Undulator gaps	Polarisation		In-house
# Images	56626	Temperature	2516.54						Pixel Size Hor (Vert)
Transmission	585.778 %								(t) µm

20/09/2022 18:29:31

Summary

Parameters


Sample

Sequence

Sample name	royn
Protein	xfblv
Avg crystal size (X, Y, Z)	4951.9001006718, 3492.7597611604, 1944.8108790331
Crystal concentration	6054.19
Support	TODD

Sample components

	Name	Concentration	Composition
Buffer	rvqjs	5476.41	ltmnd
Jet material	kbqqq	9859.93	tydpe
Ligand	ujevv	4515.86	edxri





20/09/2022 18:29:30

Summary

Parameters

Sample

Sequence

Detections

3 events

time	type	duration	period	repetition
20/09/2022 18:24:34.375	Laser excitation	8.88958	7.23178	4374
20/09/2022 18:21:23.950	Xray detection	4.41098	4.79728	183
20/09/2022 18:36:22.362	Xray detection	0.0356328	4.81722	6063

Sample preparation

1 events

time	type	name
20/09/2022 18:25:53.996	Reaction trigger	mixed vrubq

Roadmap

- **Serial synchrotron crystallography**
 - Improve UI with experiment feedback
 - Develop experiment processing results
- **Switch all techniques to py-ISPyB UI**
 - Re-implement (with improvements) missing features from EXI
 - MX data collection visualization
 - Shipments management
- **Switch all techniques to py-ISPyB**
 - Re-implement (with improvements) missing features from Java
 - backend for techniques: MX, EM
 - backend for shipments
 - backend for experiment preparation

Thank you!

Any question?