



| The European Synchrotron

AbstractLims

ICAT and SSO integration

Documentation - GitHub and ReadTheDocs

The pull requests and the documentation can be found on GitHub:

[PR # 1079: https://github.com/mxcube/mxcubecore/pull/1079](https://github.com/mxcube/mxcubecore/pull/1079)

[PR # 1492: https://github.com/mxcube/mxcubeweb/pull/1492](https://github.com/mxcube/mxcubeweb/pull/1492)

Documentation on read the docs:

https://mxcubecore--1079.org.readthedocs.build/en/1079/dev/lims_integration.html#ispyb-abstractlims

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And of course the SB and BCU group, *and you guys* !

Current status

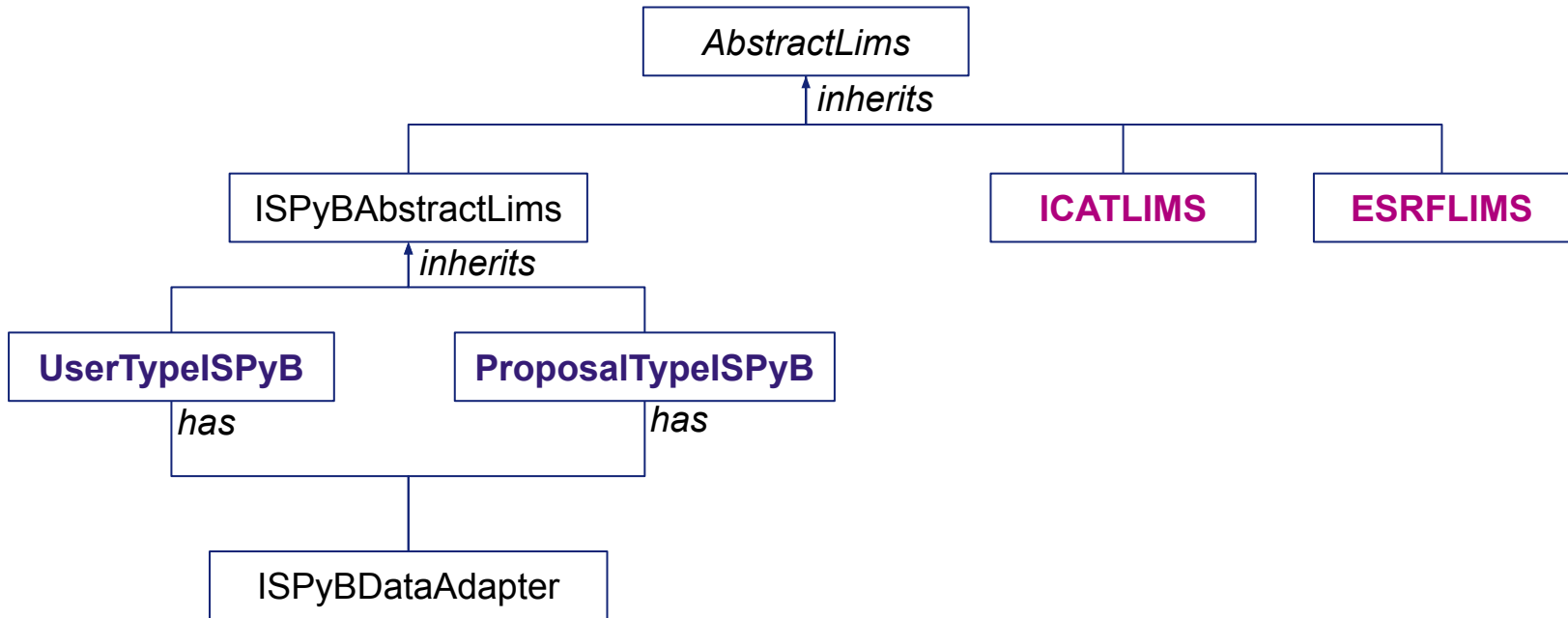
- The work have been tested and validated on the ESRF MX beamlines the last 6-8 months. Most of that work is to make sure that systems (User portal, ICAT, ISPyB, MXCuBE) involved work as expected for synchronization of, users, sessions etc.
- SSO and ICAT tested on MASSIF1 during spring and deployed since August.
- ICAT integration with proposal login deployed on all other MX beamlines since beginning of October. Switch to SSO will be done in January 2025

Background

- ISPyB is no longer the standard LIMS, need for LIMS Abstraction as more sites use other systems
- At ESRF we needed a solution where we could synchronize to and from both **ISPyB** and **ICAT**
- At ESRF, retrieving session information for a user is done via **ICAT** thus a requirement for **SSO**

AbstractLims

- Cleanup and merging of **ISPyBClient** and **ISPyBRestClient** have resulted in a new **AbstractLims**, very similar to the previous **ISPyBClient** (for now)
- Structures exchanged between **AbstractLims** and the internals of MXCuBE documented, to be modeled in a next iteration



- ISPyBClient have been split into two classes **ProposalTypeISPyB** and **UserTypeISPyB**
- Introduction of adapter to abstract communication technology, such as SOAP and REST
- **ICATLIMS** for ICAT and **ESRFLIMS** for ICAT and ISPyB

Selecting a session

MXCuBE-Web (osc) | Samples | **Data collection** | Equipment | System log | Help | Remote | Proposal (BLC15780) | Sign out (Matthew BOWLER)

Energy: 12.8420 KeV | Resolution: 2.000 Å | Transmission: 100.0 % | Cryo: 100.07 k
Wavelength: 0.97 Å | Detector: 388.6 mm | Flux: 1.35e+10 ph/s

Sample Changer: READY | Detector: UNKNOWN | Capillary: IN | Fast Shutter: CLOSED | **sak@shutter: OPEN** | Ring Current: 187.84 mA

Phase Control
DataCollection: DataCollection
Beam size: A50
Omega: 267.00 | 90
Kappa: -0.0 | 0.1
Kappa Phi: 0.0 | 0.1
Sample alignment: [Controls]

Run Queue | Unmount | Settings

Sample: Sample-1:2:16 | Queued Samples (0)

- MXPressA Global Phasing
- MESH (mesh-Sample-1-2-16_2_2_%05d.h5)
- LINE (line-Sample-1-2-16_2_3_%05d.h5)
- EDNA_REF (ref-fineslice-Sample-1-2-16_2_4_%05d.h5)
- OSC (Sample-1-2-16_2_5_%05d.h5)

Log messages:

- [20:23:54]: Workflow: Workflow finished successfully.
- [20:23:48]: Workflow: Data collection done.
- [20:23:48]: Collection finished
- [20:22:49]: Changing phase to DataCollection, using pmac script

Synchronizing with LIMS - ISPyB or DRAC

The screenshot displays the MXCuBE-Web (osc) interface. At the top, navigation tabs include 'Samples', 'Data collection', 'Equipment', and 'System log'. The main status bar shows: Energy: 12.8420 KeV, Resolution: 2.000 Å, Transmission: 100.0 %, Cryo: 100.07 k, Wavelength: 0.97 Å, Detector: 388.6 mm, Flux: 5.80e+9 ph/s. On the right, status indicators for Sample Changer (READY), Detector (UNKNOWN), Capillary (IN), Fast Shutter (CLOSED), Safety shutter (OPEN), and Ring Current (195.12 mA) are visible.

The central area features a live video feed of a sample with a 50 µm scale bar. To the left of the video are control panels for 'Phase Control' (DataCollection), 'Beam size' (A50), 'Omega' (267.00), 'Kappa' (-0.0), 'Kappa Phi' (0.0), and 'Sample alignment'. Above the video are icons for Snapshot, Draw grid, 3-click centring, Focus, Zoom (LEVELZ), Backlight, Frontlight, and Video size.

On the right side, there is a 'Run Queue' and 'Unmount' button, and a 'Settings' icon. Below this is a 'Sample: Sample-1:2:16' section with a 'Queued Samples (0)' list containing:

- MXPressA Global Phasing
- MESH (mesh-Sample-1-2-16_2_2_%05d.h5)
- LINE (line-Sample-1-2-16_2_3_%05d.h5)
- EDNA_REF (ref-fineslice-Sample-1-2-16_2_4_%05d.h5)
- OSC (Sample-1-2-16_2_5_%05d.h5)

 At the bottom right, a 'Log messages' section shows:

- [20:23:54]: Workflow: Workflow finished successfully.
- [20:23:48]: Workflow: Data collection done.
- [20:23:48]: Collection finished
- [20:22:49]: Changing phase to DataCollection, using pmac script

Future work

- Further refinement of **AbstractLims** and creating models for the data exchanged, internally, between **AbstractLims** and MXCuBE
- mxcubeweb - **UserManager**:
 - Keep the existing **UserManager** as it is (proposal and user based login)
 - Create a new **UserManager** only for user based login
 - Remove proposal login completely ?

Thank you for your attention

