ISPyB Steering Committee Minutes  
30/11/2023 @ ALBA  
DRAFT 3/12/2023

# Agenda

* Future of collaboration
* Other topics

# Attendees

* Andy Götz (chairing) - ESRF
* Martin Walsh – DLS
* Ana Gonzalez – MAXIV
* Gerard Bricogne – GPhL
* Majid Ounsy – SOLEIL
* Judith Juanhuix– ALBA
* Nicolas Demitri (remote) – ELETTRA
* Max Nanao (remote) – ESRF
* Andrew McCarthy (remote) – EMBL Grenoble
* Guillaume Pompidor (remote) - DESY

# Minutes

## Future of the Collaboration

The meeting started with this topic. There was consensus that the comprehensive definition of MX metadata and of how they should be displayed is a topic that interests all partners and that will be at the heart of the continuation of the iCAT-ISPyB Pilot Project presented by ESRF at this meeting.

It was agreed that GPhL would lead this activity in the field of *rotation* MX, on account of (1) GPhL’s long-standing but still unfulfilled requests for extensions of ISPyB that could accommodate multi-orientation datasets and their full processing results, (2) the ongoing (or predictable) accumulation of such datasets as a result of the deployment of the GPhL workflow at several MXCuBE-driven beamlines, and (3) GPhL’s implementation, with the EMBL-HH P14 and Göttingen MPI teams, of a capability to organise all objects produced by the collection and processing of multi-orientation datasets that could provide a useful reference. Crucially, this activity would closely interact with the “Abstract LIMS” project within MXCuBE.

Membership would be spontaneous, i.e. all those interested should participate. The first step would not involve any attempt to connect with mmCIF so as not to get distracted. Majid was interested in defining a second layer related to accessing the underlying metadata store. It was agreed that this step must wait until the first step is done.

**ACTION**: *GPhL to organise and lead the definition of metadata and its embodiment in a Data Model. Results of this activity to be presented at the next ISPyB meeting*.

A discussion was held on which scientific techniques should be included within the scope of the Collaboration, and it was unanimously agreed that it should only cover MX and closely related techniques like BIOSAXS + SSX. Other techniques, that do not have scientists representing them in the Collaboration (e.g. EM, imaging etc.), will not be covered. Andy would like to first see the Collaboration demonstrate its ability to carry out joint activities and to produce results for one technique (MX) before including others.

The topic of SSX was discussed. Max said that the merging of SSX datasets is an important topic for the ESRF. Ana said that she would be interested in discussing how to display SSX results, and that cctbx.xfel gui had some useful displays which could provide guidance or even be copied.

The topic of what is a sample in the SSX case was discussed. This could be a topic for a working group in the future.

**ACTION**: *Create a scientific working group to discuss SSX metadata for samples and displaying processing results. Possible leads – Someone from MAX IV (Ana or, most likely, Oskar Aurelius) / Gleb / Max*

Martin said that shipping could be a separate collaboration as it does not interest all partners.

Gerard brought up the topic of renewing the MoU. Andy said that in view of the current dispersion of the different implementations at the sites (currently at least 4 different solutions with 3 different database schemas are in production) ESRF prefers to wait until we are sharing something again e.g. the ontology. Everyone agreed to wait, the topic will be discussed at the next meeting.

To conclude - the future of the Collaboration will be centred on the scientific use cases and not the software stack.

## Other

The topic of cyber-security was brought up. Everyone is faced with increasing cyber-security challenges. Martin said that DLS had had an audit. Andy said ESRF too. It was agreed it would be useful to share plans for cyber-security put in place for the ISPyB type of applications.

**ACTION**: ALL partners to present plans for cyber-security for ISPyB-type applications at next meeting.

Judith said that they have ICAT installed but not the ingestion. Andy mentioned that ESRF is prepared to help EMBL-HH and ALBA to install the ICAT version of ISPyB (myCAT).

**ACTION**: *ESRF to help EMBL-HH and ALBA to install myCAT in 2024.*

## Next meeting

Ana proposed to organise the next meeting at MAXiV but she needs to confirm. The cost of the meeting was brought up as the meeting was starting to get quite onerous (> 10000 euros). Gerard said GPhL could contribute financially if needed. Andy said we could make the meeting self-financing and ask the participants to pay a registration fee to cover the costs.

**ACTION**: *Ana to confirm if and when MAXIV can organise the next MXCuBe/ISPyB meeting.*

# Appendix – Outcome of Open Discussion on Future of ISPyB

ESRF presented a report on the evaluation of ICAT as a database backend for ISPyB. The results were very positive and ESRF plans to continue with this solution due to the numerous advantages it provides in particular the fact that it unblocks the development for many scientific use cases. In view of this evolution and the fact that the ESRF will stop developing and maintaining the Java and Python based backends the sites were asked to reflect on the future of ISPyB at their site amongst the following options with their implications:

1. stay with the existing solution based on **Java and EXI/EXI2** - but with no new developments or features unless one of the sites decides to implement them, ESRF will provide bug fixes on a best effort basis
2. adopt **py-ispyb** backend - the MX frontend has to be developed from scratch (possibly with a redesign of the data model) and maintained by one or more sites, ESRF can provide help on what they have already developed
3. adopt the ESRF **ICAT**-based solution (**myCAT**) - the MX frontend is ready with new features for reprocessing, more features will be implemented by the ESRF as 3 (at least) permanent staff are allocated to developing and maintaining it, bug fixes and help with installation provided by ESRF + ICAT community
4. adopt **SciCAT** as backend for MX - the MX frontend has to be developed from scratch or an interface to the new ESRF MX frontend developed by one or more of the partners
5. adopt **SynchWeb** - DLS continues to provide support
6. **none** of the above

During the discussion session on the future of the ISPyB collaboration it emerged that the sites plan to do the following in the medium to long term :

**ALBA** – move to ICAT and adopt the ESRF solution (myCAT)

**BESSY** – no input

**DESY** – no input

**DIAMOND** – continue with SynchWeb, a major refactoring is planned as well as a new UI based on React for DIAMOND2.

**ELETTRA** (observer)– continue using SynchWeb but interested in looking at the ICAT solution.

**EMBL** – continue using the Java based version but will test the ICAT based solution.

**ESRF** – move to and continue developing the ICAT based solution (myCAT) for MX, SSX, EM and BIOSAXS. The ISPyB backend will continue to run and metadata ingested for now.

**GPhL –** will continue contributing to the scientific use cases on what needs to be displayed

**MAXIV –** will move to py-ispyb and add support for MX in the backend. ICAT is not an option due to SciCAT already being deployed as generic catalogue.

**PSI** (observer) – continue developing their own solution (HEIDI).

**SOLEIL** – move to py-ispyb for the medium term and in parallel install SciCAT. Eventually replace py-ispyb with SciCAT.