

PyISPyB developers' meeting

17 March 2022

Participants:

- Alejandro de Maria, Olof Svensson, Mael Gaonach, Marjolain Bodin, Andy Gotz (ESRF)
- Karl Levik, James Hall (Diamond)
- Rasmus Fogh, Gerard Bricogne, Clemens Vonnrhein (Global Phasing)
- Clemente Borges (DESY)
- Michael Hellmig (HZB)
- Majid Ounsy, Idrissou Chado (SOLEIL)
- David von Stetten (EMBL Hamburg)
- Alexandro Camps Mezquito, Beatrice Lorenzo Gonzalez, Marc Armaito Hierro, Emilio Centenio Ortiz (ALBA)

Minutes: Rasmus Fogh

Alex de Maria introduced the meeting, which has the purpose of sharing information on the current situation and organising a collaboration around implementing a new version of ISPyB, starting from the Py-ISPyB API first prototyped by Ivars Karpics.

Presentations

AdM and MG presented the situation, in general and ESRF. Some highlights:

- The Memorandum of Understanding that organised the ISPyB collaboration expired at the end of 2021. Any rapid advances would have to be organised bottom-up.
- ESRF has three ISPyB front ends, the original ISPyB, EXI and EXI2, all of which are now at least frozen if not deprecated.
- ESRF has evaluated the prototype by Ivars Karpics for real-world robustness. They have added modules for authentication and unit testing, and a legacy API that supports the routes active in the current EXI versions. A minimal code base has been generated and used in porting Cryo-EM front end, and is envisaged to serve for (a start on) SSX.
- ESRF is deciding to proceed with a new front end based on Py-ISPyB, and to use this for SSX. It is a high priority for ESRF that the new collaboration should indeed be a multi-center collaboration with neither all resources nor all decisions centred on the ESRF. At the same time ESRF would wish to have an SSX front end in production by ca. late summer.

- MG presented some new and/or open technical choices:
 - DB access, opting for direct SQL queries where these already exist, but the more maintainable SQLAlchemy joined load for future developments
 - support for multiple authentication mechanisms.
 - The possibility of introducing Python typing and avoiding multiple model definitions, e.g. by changing to the fast-api framework.

Discussion of collaboration activities

AdM proposes to initiate a joint collaboration:

- Joint evaluation of the Py-ISPyB backend proposal and agreement on a framework
- Starting up Working Groups to carry on the workflow
- Regular coordination meetings

GB and KL both support this proposal. James Hall approves the proposal for a joint API and emphasises the need to avoid the introduction of local APIs. AdM points out that given the ESRF deadlines there is a need to fix the frameworks to be used soonest. It is clarified that PyISPyB is not yet ready for production use.

CV raises the point that agreement would hopefully cover not only technical frameworks, but also data content. An API would be exceedingly useful, but it is impossible to use properly unless it is clear what the different data items *mean*. The level of documentation and specification needed is comparable to that used for mmCIF (which is also used for different front ends). Further standardisation on how to present data to users would also be beneficial.

The question is raised whether to have the collaboration include also the front end ('full stack'). Many agree that supporting different front ends is not beneficial, leads to duplication and waste of effort, and has had the effect in the ISPyB collaboration of having all changes happen in the (non-shared) front ends while the (shared) database part became effectively frozen. James Hall notes that 'one-size-fits-all' is not necessarily going to work, that there are specific local requirements to consider, and that there is the question of how to position ISPyB relatively to the developing data catalogues. The discussion is postponed to the relevant meeting at 1500 on the same day.

Site status and resources

- DESY: Clemente Borges has ISPyB as a main area of activity, but is sharing his time with MXCUBE until a new developer arrives in April. DESY wants to keep the Java API for MXCuBE and EXI, and use PyISPyB for new developments. DESY sees a need for a AbstractUserOffice class, and for work on Dewar shipments. There are no specific deadlines, but as always a great hurry.

- SOLEIL Idrissou Chado is in charge of ISPyB work at SOLEIL, while Majid Ounsy (ex experimental control, now data analysis group) is responsible for a number of projects. SOLEIL is limited to development testing for now, though they would like to include the front end in the collaboration. They are looking for a new developer, which would give them resources to invest in ISPyB.
- Diamond cannot commit to anything right now, as they are down a couple of people, have a new department head, and considerable ongoing work.
- ALBA has a group of four people, all new to ISPyB, and all aiming to learn and get involved. They are deploying EXI, and are interested in a full stack collaboration, probably limited to MX.
- HZB do not have ISPyB, but want to start. Alexander Dittmann (not present at the meeting) is being recruited to work on ISPyB. Their situation is similar to ALBAs, needing to get started before they can get into much collaboration, interested in the full stack, and limited to MX.
- Global Phasing does not have a working ISPyB installation (nor a synchrotron), but have a strong interest in ISPyB to transfer parameters and instructions pre-experiment (diffraction plan) and especially to gather and present the results of tailored data processing, particularly for multi-sweep experiments. Their contact person would be RF.
- EMBL-HH David von Stetten is involved as beamline scientist on beamline P14-2 (Trex, SSX beamline), as is Gleb Bourenkov on P14. A replacement for Ivars Karpics is being sought, and there has been no new ISPyB development since he left. Their interest would be in MX and SSX, with no EM and BIOSAXS not involved.
- ESRF: AdM and OS are both working on ISPyB in the internal 'data analysis unit'. ESRF has pressure to start SSX in September – ID29 takes beam for the first time at the start of April. MG is hired for this.

Any Other business

Andy Gotz raises the possibility for synchrotrons to contribute money to pay for outside developer if they cannot contribute manpower. SOLEIL is already subcontracting some ISPyB work on those terms. The meeting reacts favourably to the idea. The areas to cover would depend on who wanted to pay for what, but the work would have to be coordinated.

Next Meeting

There will be a new developers meeting two weeks from this one. AdM to set up a Doodle poll.