

ISPyB developers' front end meeting

17 March 2022

Participants:

- Alejandro de Maria, Olof Svensson, Mael Gaonach, Marjolain Bodin (ESRF)
- Karl Levik, James Hall (Diamond)
- Rasmus Fogh, Gerard Bricogne, Clemens Vonnrhein (Global Phasing)
- Clemente Borges (DESY)
- Alberto Nardella (MaxIV)
- Majid Ounsy, Idrissou Chado, Tatiana Isabet (SOLEIL)
- Gleb Bourenkov, David von Stetten (EMBL Hamburg)
- Alexandro Camps Mezquito, Beatrice Lorenzo Gonzalez, Marc Armaito Hierro, (ALBA)

Minutes: Rasmus Fogh

The purpose of the meeting is to discuss the way forward for ISPyB front ends using, considering the new PyISPyB backend work.

Discussion

The meeting consisted of a wide-ranging discussion that did not coalesce into clear decisions; the minutes try to do justice to the points made.

Soleil has been doing a fair amount of work on EXI2 over the past year, implementing support for SSO and the sample tracking. ESRF has refactored the code in a fork of the code. Key words were single-sign-on, Typescript, React 17.0 interface, Storybook, CRA 5.0.0. EM has been ported, MX is in development. Backwards compatibility of the Python backend is seen as important. Main missing parts are shipping and experiment preparation. Soleil is interested in collaboration for a new UI, introduction of tests (Storybook?) .

ESRF (AdM) had the SSX data model from EMBL, but no implementation. Ivars Karpics did a backend prototype but no work on SSX front end. ESRF will have SSX users on ID29 in summer 2022 (?) and need a working interface by September at the latest. That makes it necessary to agree rapidly on the back end, and then move fast. ESRF agrees on the need to collaborate also on the front end, UI.

Majid Ounsy (SOLEIL) Reminds of all the work that went into ISPyB, memorandum of understanding etc. - is this now obsolete? Supporting multiple front ends was emphatically not a success, and a restart this time should collaborate on the full stack. Not everybody has

skills for every part, and for now SOLEILs skills are for the front end, not back end, given that SOLEIL uses the same software stack (react Typescript, ...) for other programs. Future contributions and skills would depend on management-level decisions.

There is some discussion whether a decision can be taken now, and where that would leave Diamond. MO proposes a decision by majority vote. AdM points out that it will be necessary to operate without any formal MOU for the next two years, while MO emphasises the need for a solid organisation for the next 1-2 years, with management buy-in to guarantee the required resources. AdM emphasises the lack of time, the existing agreement on the back end, and the need to move together now.

Gleb Bourenkov opines that it is too early for setting precise terms. There is currently one database, two backends, four front ends, and the first need is to formulate shared goals, with Diamond included in the discussion. If there is agreement on the back end already, the front end can be settled in a similar way. But: It needs a name; what is the precise objective; Is this just a technology change for EXI, or what is the scope? AdM opines that ESRF does not want to do this alone. EXI2 was stopped in part for technical reasons, in part to get out of the long-running competition with Synchweb.

KL (Diamond) is really happy with the proposal to make workgroups and would like to participate. Diamond is special in that it has a number of beamlines with particular requirements, which need extra database tables. How could Diamond support these under a collaboration? A one-size-fits-all front-end development would be very hard for Diamond to fit into. AdM points out that ISPyB was created for MX and expanded from there. Many techniques have mostly orthogonal needs. KL points out that many tables are common, but AdM notes that many other techniques use metadata catalogues, which have not been done for MX. KL does not see any contradiction between using ISPyB and data catalogues.

MO makes a strong case for relying increasingly on data catalogues, and points out that a shared software stack will be an important step in the right direction. The EU-level 'European Commission in Data Viewers (??)' and other high-level projects are in progress and will eventually force a convergence on accessing data via data catalogues, as part of the move to open science and open data. KL does not see this as a good reason to make major changes to ISPyB now, and wonders if the two could not coexist. Gleb Bourenkov sees little scope for harmonisation as ISPyB and the data catalogues have little in common beyond being based on databases and web viewers, and the data catalogues have not yet produced major successful applications in this field. RF points out that the high degree of success of the MXCuBE collaboration – in spite of multiple front ends and splittist tendencies of their own – has depended on a shared concrete focus on running synchrotrons, and warns against making goals too wide-ranging.

Tentative conclusions

A final round of discussion covers the current status of the discussion and who would come to a continuation meeting next week. ESRF, DESY, SOLEIL, and MaxIV all want to participate and to include front-end development in the collaboration. Gleb Bourenkov (EMBL-HH) would like to be involved as much as resources allow. He emphasises the need for up-front agreement on requirements and goals ('what a user must be able to do with it'), and would like to see the newest version in action. EMBL-HH has at least one technique to add – full field X-ray imaging. AdM can deliver a working installation for testing, provided EMBL can use https for access instead of http. He hopes that it should be possible to make a modular architecture so that one technique does not clash with others. Global phasing want to participate in the discussions, and would provide time and manpower rather than financial contributions. James Hall, from Diamond would like to be involved in further discussions, and is interested in a modular architecture, but is not in a position to make commitments on behalf of Diamond.