

ISPyB Meeting

Wednesday 20180131 - minutes

Scientific and Steering Committees

(Presented together to reduce duplication)

Cryo-EM

DLS and ESRF have very similar data models for this area, and both use (different versions of) SCIPION. It is believed that harmonising the two should be relatively simple; the main problem seems to be knowing for sure the meaning of what goes into some of the columns. It is decided that the two sites should agree on a single database model for both to use, and that they should bring into the discussion some scientific domain specialists from among their leading edge users to settle uncertainties and improve the model.

SAXS

The ongoing work on modelling and integration for SAXS is approved, including framework, development plan, and data model extension, as proposed by Dmitry Molodenskiy.

Consortium membership

- ISPyB membership of Elettra is approved, based on a letter of intent stating willingness to abide by the ISPyB Memorandum of Understanding, and installing and using ISPyB locally
- LNLS Brasil is asked to provide a letter of intent
- Consortium members to consult internally on the question of streamlining the joining of new members, for which a template based on a text used by the ESRF in other collaborations was circulated by Gordon Leonard to the members of the Steering Committee

Data model changes

- Addition of JSON columns to accommodate provisional or program/site-specific information, as discussed by the Developers Committee, is approved throughout ISPyB, subject to technical feasibility. This should hopefully reduce the pressure for crowbarring new data into tables and columns that were designed for a different use.
- Extension/ modification of the ISPyB structure to accommodate multipins and other composite sample structures is considered essential. Developers are tasked with a detailed analysis of all relevant use cases, to lead to a proposed solution. Once in place, MXCuBE must use the new ISPyB capabilities in preference for local ad-hoc solutions.

- Further model reorganisation and clean-up should be considered. This would be important for the long-term sustainability of ISPyB. It is, however, difficult, and might not be possible without the commitment of additional resources, e.g. through communal hiring of an additional developer. For the moment it is decided to task a small working group with exploring the issue and prototyping possible solutions.
 - Specifically Olof Svensson raised the problem of tracking and processing combinations of parts of data sets from different crystals, different samples, and different runs. Because of differences in crystal form etc. there will be a requirement to combine these data sets after acquisition and track their provenance and the sample content they relate to, requiring a many-to-many relationship between images, samples, and processing runs. A solution to this problem might potentially require wide-ranging model changes.
 - More generally there is the long-standing problem of overloading the ISPyB tables with multiple inconsistent uses, especially the main data collection table (currently at 96 columns and counting).

Organisation

- The standard procedure for changes should be to open an issue on github and send an email to ispyb-dev
- It was agreed that model changes need to be simpler to carry out, and at the same time to be better disseminated and discussed. For small changes it should be enough to post the issue on github and presume consent after 3-4 weeks if no one comments. For bigger issues or in the case of disagreement one might select an issue manager to oversee the discussion and hold separate video conferences to find a solution. It was not agreed how to distinguish between small/big issues or what the precise procedures should be.
- The ISPyB developers shall start a series of regular Webex conferences to discuss and coordinate issues. Meetings will be on the last Monday of every month as 1500 GMT, and Neil Smith (was) volunteered to call and steer them. It is expected that these meetings will keep track of open and upcoming model change issues. Meetings must be minuted, and minutes circulated to the Scientific Committee. The Scientific Committee will be overseeing the Developers Committee meetings and actions, and SC members are encouraged to take part in DC meetings. The Scientific Committee will in turn inform the Steering Committee as necessary.
- A working group will be formed to explore and prototype ways to reorganise the overall ISPyB model, with a view to split and rationalise tables, and to reduce overload of individual table items by multiple uses and techniques. The groups should invite interested parties, including e.g. ESRF (Solange, Olof), GPhL, Diamond, and EMBL-Hamburg