Developers' meeting – discussion summary

ISPyB project meeting, Trieste, September 2018

- Monthly meetings are judged successful and will continue, using appear.in. The responsibility for organising them now passes to ESRF (Alex de Maria) for the next six months.
- Elettra has found it very hard to get started using ISPyB. One question was: What does the term 'ISPyB' cover in conversation? Databases, servers, GUI, EXI, Synchweb? Answer: 'All of the above'. Many things need doing just to get set up, e.g. what must be set in the LDAP server to make the initial ISPyB installation work? What are the roles and their definition for the access control? Milan will write down that they have found out, and what the questions are, but essentially there is a need for a complete step-by-step guide for a fresh install, which likely none of the established participants really know how to do. Alexandra Kastner will write this up, but needs input. It is agreed to use the Github Wiki, although this may need moving later as this system does not scale that well.
  It was proposed that at some point there should be a gathering of developers at Trieste to see (and go through) how a de novo installation is done.
- The ranking of results for both different samples and different processing runs was discussed. (see also summary of MXCuBE/ISPyB session on the subject). It was agreed that a scientific discussion on metrics was required. Following a previous conversation with Gerard Bricogne, Olof Svensson proposed (to silent agreement) that a face-to-face workshop was necessary. The problem is mostly scientific but also has important technical aspects, in order to find a way to display the ever increasing amount of information in a way that makes sense to the user.
- The subject of the protein/monomer table was raised. Some information is technically mandatory but not actually filled in (space group,. Unit cell, …). There is a need for compound type information, and for describing multi-molecule assemblies.
- Karl Levik raises the issue of adding a BeamCalendar table with beam state fields, to use for storing beam calendars even though some sites are handling the problems already outside ISPyB. There were no objections.
- The meeting consensus seems to be for NOT introducing soft deletes (with isDeleted fields) but instead making hard deletes and taking care of avoiding cascading deletes.
- The EM data model was mentioned, but the discussion was referred to the discussion in the relevant Github issue.

- The high level data structure diagrams that were agreed in the 2018 Diamond meeting have not progressed significantly. Alex de Maria did a test for the Cryo-EM model, but it was realised that the high level model would not be usable without a mapping to the low level model, which would mean three different levels that had to be maintained. Also the idea of bringing in outside scientific experts for model development has not progressed, possibly for lack of volunteer experts. It is decided that the main need at the moment is for up-to-date lower-level documentation, and for documentation of installation and set-up. Meanwhile the high level documentation has been down-prioritised pending an urgent use case.