ISPyB developers’ virtual meeting

August 4, 2020

# Present:

James Hall, Neil Smith, Karl Levik, Ed Daniels, Ivars Karpics, Rasmus Fogh

# Agenda:

- Status reports

- Feedback from the last ISPyB meeting.

- py-ispyb: latest developments.

- AOB

# Status Reports

**Ivars Karpics** has done a lot of work expending py-ispyb, and will continue to work on this.

**Neil Smith (for DLS):** Work has been done on unattended operation, including work with the user office on the autogeneration of sessions. There has been updates in EM support. A new beamline working on soft, condensed matter is being brought into the ISPyB family, which may need some bespoke data model features.

**Ed Daniels** has been working on integrating Icebear. Integration with DLS is now OK, work is ongoing on a number of other synchrotrons

**Rasmus Fogh (for GphL)**, has mostly been working on MXCuBE. GphL continues to have a particular interest, in topics like diffraction plans, reporting of anisotropy, and multi-sweep acquisition.

# Last ISPyB meeting

The last ISPyB meeting was considered successful, and the message from the developers had come across clearly. Considering the virtual nature of the meeting this was actually a surprise. It is agreed that there is a great need for a physical ISPyB developers’ meeting, which will hopefully become possible soon. The work related to py-ispyb requires a very wide focus and many basic decisions, which will be hard to do in a virtual meeting.

# py-ispyb

The code written by Ivars was ready to download and test. One person (NS) had done this, and reported that it worked, with some points relative to dependencies and not-quite-up-to-date READMEs.

IK has done some refactoring, separating ispyb\_core out from the main app. A new service, for serial crystallography, is being prototyped by IK together with local domain specialists. It was found that the situation was so different that it was a lot easier to write new and separate tables than trying to fit into the existing ones. There were comments from the meeting suggesting the desirability of a discussion on use of common tables, standards, etc. before this work solidifies, to avoid parallel implementations as much as possible

IK gave a demonstration, showing two separate μ-services (ispyb\_core and serial crystallography) running in parallel and communicating.

There was discussion on whether the project actually needed μ-services, which are generally considered a technique to permit parallel running for scalability under very high loads. After some discussion it was clarified that the main goal was not scalability but modularisation, and there was full agreement to continue to work exactly as contemplated until now, but to use henceforth the more precise term ‘services’ (without the ‘μ-’) to avoid confusion.

As part of the discussion it was mentioned that the EM part of ISPyB might be a good candidate for a separate service, given the fairly loose coupling to the non-EM parts of the database, even if the fact that this part of the model was already stable might speak against it.

In spite of the strongly positive reception so far given to the py-ispyb, it was clarified that py-ispyb is still at the stage of proof-of-concept, and especially the performance of the system needs investigation. James Hall strongly recommended a tutorial in modern API techniques available from Apogee, and suggested that we should make sure to build our APIs with the most modern technology.

There was further discussion on the desirability of setting up an API gateway and on setting up a one-shot data entry function, quite likely using JSON input.

The next use case that IK will look at is going to be shipment, and it was proposed to base this on the CVS upload scripts already in place.

# AOB

For the next six months the chairmanship of the developers’ meeting (with the obligation to organise meetings etc. is with IK.

# Next meeting

The next developers’ meeting will be organised for September, as a virtual meeting.