

ISPyB Developers

Web meeting

2020-01-20

Participants:

ALBA: Daniel Sanchez, **Diamond:** Karl Levik, Neil Smith, James Hall, **ELETTRA:** Alberto Nardella, **EMBL Hamburg:** Ivars Karpics, **ESRF:** Olof Svensson, Gianluca Santoni, GPhL: Rasmus Fogh, **Oulu** Ed Daniel, **SOLEIL:** Majid Ounsy (?)

Status reports:

- **ALBA** Setting up PyISPyB on a test server
- **DLS** SynchWeb development has occasioned some database schema changes. EM-related shcma schema changes are being discussed – virtual meeting for interested developers on Friday.
- **EMBL Hamburg** Has been working on PyISPyB, to be discussed below.
- **ESRF** (OS) Minor changes to EXI.
Q: When will EXI2 be made publicly available on github?
A: EXI2 is used internally for EM, but MX and SAXS are not quite ready yet. The code is on an internal gitlab server for now.
- **MAX-IV** Work on backend fixes and sample management.
- **Oulu** Nothing new; working on MaxIV shipments.
- **GPhL** Nothing new to report.

PyISPyB

IK reports on discussions with Peter Murphy, from the CRIMS group, who has experience on moving from a single monolithic database to a set of microservices. They are happy with the move, but in their case it took two years to complete. We plan to keep existing ISPyB as a single service (for now?) to avoid the considerable work of splitting. CRIMS will send an example configuration file – they are **not** using

many of the available features of the Kong framework. They have promised to provide a few slides describing technical issues, and/or give a presentation.

IK is using a set-up with two services, one for core ISPyB, one for SSX. They communicate on separate ports, but Kong combines everything together. This includes having a single central location for all logs. Currently requests must pass in the server name, to protect from potential name clashes in the two services. NS comments that this is not ideal, and a different system using prefixes to disambiguate might be better. Kong is not the only framework possible, but both IK and CRIMS apparently went for the top Google hit.

CRIMS has a separate service for authentication. This might be a good idea, as authentication is both crucial and different at different sites. James Hall notes that certain operations may be prohibited even if the gateway passes them in the first instance. JH suggests EngineXplus (a commercial program) as a possible framework.

IK has made a `get_db_item` request for generic querying. Agreement is needed on the form of the response. He has also started to implement the interface for shipments – only to find that he also needed to add LocalContact and Laboratory for this to work.

NS has tried to run the PyISPyB framework. He could get to the point where he got data back from the current database, which is a **good** result. He notes that

- Configuration is complex
- It would be preferable if configuration did not involve code changes, but only a configuration file
- PyISPyB uses headers rather than the more standard POST.

Pull requests

KL had several proposed database changes

(PR numbers refer to <https://github.com/ispyb/ISPyB>):

- #487 Add name column to BLSampleGroup table (that until now had only the one key column). The table serves to group samples, through a many-to-many link. *Accepted*.
- #488 Add DiffractionPlan.userPath. For better user control of result location, particularly useful in remote operation. It is noted that DiffractionPlan is getting

quite complex (it 'sort of mirrors' the DataCollection table), but this attribute would fit in. *Accepted.*

- #489 Add DewarRegistry table for storing the physical dewars and their facility code, with DewarRegistry_has_proposal table to allow many-to-many links from dewars to proposals. These are new tables and will not cause problems for any existing code. *Accepted.*
- New columns for safety information in Protein table – description, hazardGroup, and containmentLevel. ContainmentLevel and hazardGroup are of type tinyint, since different countries use different string enums but all match basic numeric levels (1,2,3,...). *Accepted.*
- KL has been working on attributes for automatic scoring of drops and images, but does not intend to make a PR since this work is only done at DLS.

Next Meeting:

Tentatively planned for first two weeks of October. IK will make a Doodle poll.