ISPyB Collaboration Meeting 2nd July 2018

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Participants

Organisation	Name
Diamond Light Source (DLS)	
	Neil Smith (NS)
	Karl Levik (KL)
European Synchrotron Radiation Facility (ESRF)	
	Stephanie Malbet-Monaco (SM)
	Alex De Maria (AM)
	Olof Svenssson (OS)
Global Phasing	
	Rasmus Fogh (RF)
	Gerard Bricogne (GB)
	Peter Keller (PK)
EMBL Hamburg	
	Ivars Karpics (IK)

Updates from Members

DLS: Work is ongoing to develop ISPyB web services for the SynchLink mobile application. A Swagger/OpenAPI specification was shown – generated from the ISPyB REST annotations. It would be useful to add the updated specification file to the ISPyB software repository to aid documentation. It would particularly help for machine to machine communication (e.g. crystallisation labs automating shipment creation).

ESRF: Investigating serving PDBs, pipelines for auto processing and how better to represent macro molecules and the current modelling of proteins and ligands.

GPhL: Nothing specific to report.

EMBL-Hamburg: Nothing specific to report.

Conceptual modelling, Documentation and Data model

Database tables

KL highlighted the scripts developed to auto-generate documentation from database comments. This is mainly useful for developers to see what the various columns represent. **ACTION:** It was agreed that DLS would open a pull request to add the scripts to the ISPyB repository.

The discussion continued to consider how useful a pure table relationship view would be. While a diagram of tables would also be useful it does not fill the need of the conceptual model. The conceptual models are required as these help bridge the gap between scientists and developers. They should include key information to help scientists understand what is represented in ISPyB.

Database modelling issues, ALL

DLS raised three issues for discussion.

#30 Add AxisStart to EnergyScan / XFESpectrum https://github.com/ispyb/ispyb-database-modeling/issues/30

Longer term these tables can be merged with DataCollection. In short term adding the column to these tables was agreed at the meeting.

#31 Beam calendar – for facilities without access to SMIS. https://github.com/ispyb/ispyb-database-modeling/issues/31

#32 AutoProcProgram refactoring. https://github.com/ispyb/ispyb-database-modeling/issues/32

Agreed that this is a good idea but represents a major change and would affect many clients.

GPhL raised the STARANISO ticket:

#29 https://github.com/ispyb/ispyb-database-modeling/issues/29

Continuing the discussion from last time, the database changes are simple but not currently a priority for ESRF or DLS. As OS pointed out the larger issue is the time required to update user interfaces to show a ranking page. ESRF asked GPhL if they had resource to help update EXI. GPhL suggested there may be multiple views that could be sorted and ranked based on the anisotropic data available. DLS suggested that GPhL might be able to provide mock ups (e.g. wireframe diagrams) of what sample pages might look like. It would then be possible for the facilities to update their user interfaces (EXI, SynchWeb etc.) while providing a consistent approach. **ACTION**: GPhL to prepare design guidelines (e.g. wireframe mock up) of what ranking pages could be useful to users.

Any Other Business

NS asked if anyone in the group had heard about the next face to face meeting at Elettra in Trieste (currently scheduled for 11-13 September). SM suggested that it will probably be up to the ispyb-dev/sci groups to help plan the meeting. NS Agreed to contact Elettra to offer help from the group. **ACTION**: NS contact Elettra to offer help in organising the face to face meeting. **ACTION**: All to consider what papers/talks they want to give at the meeting. The intent is to hold a planning meeting via video conference in the last full week of July where the group can discuss agenda items.

Date of Next Meeting

A date was not set for the next meeting. A planning meeting for the face to face ISPyB/MXCuBE will take place in the last week of July.

Action Summary

Serial	Action	Who	When	Status*
1	Open a pull request to add the scripts to the ISPyB repository.	DLS (KL)	30 July 2018	New
2	Prepare design guidelines (e.g. wireframe mock up) of what ranking pages could be useful to users.	GPhL	2 September 2018	New
3	Contact Elettra to offer help in organising the face to face meeting	DLS (NS)	6 July 2018	New
4	Consider what papers/talks we want to give at the meeting and what agenda items are required	ALL	25 July 2018	New

* Status is one of New, Ongoing, Closed or Completed