ISPyB Developers

Web meeting

### 2021-01**-21**

**DRAFT**

# Participants:

Ed Daniel, Ivars Karpics, Neil Smith, Rasmus Fogh, Olof Svensson, Alejandro de Maria, Gianluca Santoni,, Daniel Aanchez, Alberto Nardella

Also ’Peter from EMBL’?

# Status

### Olof Svensson

All beamlines are working in remote operation, which is a big change for the non-MX lines.

With people having left, only OS and AdM are working on ISPyB at the moment, and AdM is heavily engaged elsewhere. A replacement for Maxim is expected in march, and a new person to work on EXI and ISPyB should hopefully be in place before Christmas.

There have been improvements in display, with extra information for mesh-and-collect. Work is progressing on a ligand-fit processing pipeline.

The mesh is generated in workf,low. The workflow is now being expanded into a beamline expert system, which is pure Python and open source – Passerelle is used only for design. Move from EDNA to EDNA2. DOZORm is now in production. It is written in FORTRAN and capable of identifying individual crystals. Work is in progress on a new routine for characdterisatoin, based on XDS to replace the rpevious MOSFILM/LABELIT. This is not yet tested, and may be ready in marcxh, at best. New BEST version is to be tested.

### Alberto Nardella

No experiments until April.

### Daniel Sanchez

ALBA plans ot be moving to EXI in 2021. Maybe in April or summer. DS has other projects with higher priority.

### Ed Daniel

Working mainly on Icebear. Will be oding tests with ALBA.

### Rasmus Fogh

GΦL is working quite hard on additions to the mmCIF format to standardise anisotropy and quality parameters and improve deposition. RF himself is mostly working on MXCuBE; it is expected to have the experimental workflows in production beta at EMBL-P14 and ALBA over the coming months.

### Neil Smith

DLS is working on im[proving remote access (for obvious reasons), including interfacing with DHL. Brexit has created additional problems. Beamlines for soft, condensed matter will be added to the system. It is planned to strart expanding EM tables over the coming year. Ther eis a need for a SampleGroup, inn order to allow co-processing and efficient display of data from multiple crystals (plates, ..). At some point also SSX.

IK notes that Hamburg has an SSX data model propopsed, and suggests that DLS should look at this, with a view to agreeing on a model for the end-May virtual meeting organised by EMBL-Hamurg.

OS notes that he would like to move ahead on Cryi-EM issue #64. NS agrees, this should be considered a draft, to be implemented at both sites, in order to gather experience , modify, and agree to a final version.

### Alejandro de Maria

Notes that his perosnal priority is SSX. If the new viewr / PyISPyB goes ahead, that also becomes a priority.

### Peter

Announces development of a production and a development server ‘blue green’ that can eb swapped. There is some consideration on access for users versus robots, these use partially separate access paths, and it is desired to separate them cleanly.

### Ivars Karpics

This year whas been all-remote working. It is the most productive year ever, in terms of PDB depositions, which may suggest more time for users to deposit. IK himself has considerable work on MXCuBE, and has created a Pypi package for PySIPyB.

## Discussion

PyISPyB proposals are on Googledocs, and should be discussed there. Several things still need comments / agreement. The authentication part should ba agreed and preented to the sterring committee well before the next half-yearly meeting in May.

There is a discussion on data policies and embargoes. One argument (DLS) is that actual publishing will be done by a metadata catalog, and ISPyB would mainly need a ‘will be public from’ date. ESRF are aiming more to publish directly from ISPyB, and thinking more in terms of using ISPyB (99d its viewer) for metadata publishing, and so having more detailed description in ISPyB, ways to modify access, possibly support for business rules.

# Next Meeting

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