ISPyB Collaboration Meeting 3 May 2018

Next meeting Monday June 4th (13:00 UK, 14:00 European Time)

Contents:

- Participants
- Agenda items
    - Updates from members
    - Meta data for plates
    - Conceptual modelling, documentation and data model
    - Database modelling issues
    - Any other business
- Date of Next Meeting

Participants

Organisation	**Name**
Diamond Light Source (DLS)	
	Neil Smith (NS)
	Karl Levik (KL)
	Stu Fisher (SF)
European Synchrotron Radiation Facility (ESRF)	
	Solange Delageniere (SD)
	Stephanie Malbet-Monaco (SM)
	Alex De Maria (AM)
Global Phasing	
	Rasmus Fogh (RF)
	Gerard Bricogne (GB)
	Peter Keller (PK)
EMBL Hamburg	
	Ivars Karpics

Updates from Members

- SD/AdM, ESRF – reported minor changes, enumerations for workflows, Merging of MAXIV branch in progress
- RF/GB/PK, GPhL – nothing specific to report
- IK, EMBL – Set up reprocessing feature some time ago, now expanding to other beamlines and upgrading. User uploads changed XDS input file, which is then run. SF added that Diamond has tables for this.
- NS, Diamond - Work proceeding on adapting ISPyB web services for mobile application. Swagger setup and generating documentation from an endpoint within ISPyB. Challenge now is to integrate with authentication process.

Meta data for plates, DLS

NS circulated a document before the meeting describing the use of plates and associated metadata at Diamond. This expanded on the power point slides developed for the last meeting. SF walked through the document and explained the relationship between the database tables. The information from the document is appended to these meeting notes as Appendix A.

ESRF have a requirement to demonstrate in-situ data collection from plates before their major shutdown in 6 months' time. The document along with SF's description was helpful, however if there are any further questions NS offered to expand the document as appropriate. The tables in use at Diamond have been in place for over 12 months. Most tables should be reusable by ESRF although there are some aspects (e.g. scheduling container inspections) that will not be used/required by ESRF in the short term.

GB expressed his satisfaction at the high degree of collaboration and common planning seen, and hoped to see the results and agreements obtained made public for discussion beyond the immediate parties.

Conceptual modelling, Documentation and Data model, ESRF

AdM reported that a small some work has been done since last meeting; DrawIO still seems like the best candidate for a modelling program. A small part of the model is on GitHub: ISPyB-database-modelling (EM.XML). This is a conceptual model (NOT a database model) and was done by hand, rather than extracted from existing data.

It is agreed to have a substantial part of the model ready modelled by the next meeting, specifically the MX part. Diamond would look at the MX tables, ESRF would look at EM and BioSAXS. (Not quite clear what is and is not included here?)

GB has contacted Jean-Luc Ferrer (JLF) as a possible external expert to contribute to the conceptual modelling, giving his long and varied experience, and the degree of integration already present in his program CRIMS. JLF is willing to contribute time and expertise to review the model, but is not in a position to commit resources to the ISPyB consortium. He would have to be invited as member of and through the FIP beamline rather than as an individual. GB will take the matter up with the steering committee, and will further contact Josan Marquez/EMBL/Arrinax as possible sources of expertise.

There is small discussion on the integration through ISPyB and MXCuBE to allow crystal location data to be tracked from the crystallisation robots through to data collection. FIP apparently is installing MXCuBE2 and looking towards MXCuBE3, but critically short of resources.

Database modelling issues, ALL

Data Collection Limits #12: Group agreed with the proposed changes. ESRF suggested adding aperture sizes. SD agreed to check if Aperture table can be reused.

Goniometer Orientation #16: – Proposed adding a goniometer orientation column to DataCollection table. Discussed if this should be in beamline setup table, but SF noted that some beamlines can switch between goniometers for a collection. Therefore an entry in data collection is preferred by Diamond. No resolution at this point?

ScreeningOutput alignment success #18: Agreed to add alignmentSuccess column (consistent with other Boolean success flags in the table).

Enumeration options for serial crystallography in DataCollectionGroup.experimentType #27: ESRF to discuss the proposal (initial thoughts are it may be too simple) and report back.

Any Other Business

None was raised.

Date of Next Meeting

The next meeting is planned for Monday June 4th at 13h00 UK

Appendix A

Plates and Meta Data at DLS

Description prepared for ISPyB Developer Meeting May 2018

DLS have been conducting in-situ diffraction experiments for some time. ESRF expressed interest in understating what metadata we are capturing. Below is a summary of the data stored and used at Diamond along with a description of the tables. Table names are in bold and key fields described.

In brief terms the additional metadata stored for each plate (over conventional MX experiments) can be described in terms of the crystallization conditions (the screens used) and the inspections taken throughout the process.

The diagram below shows the relationship between plate, drop and well

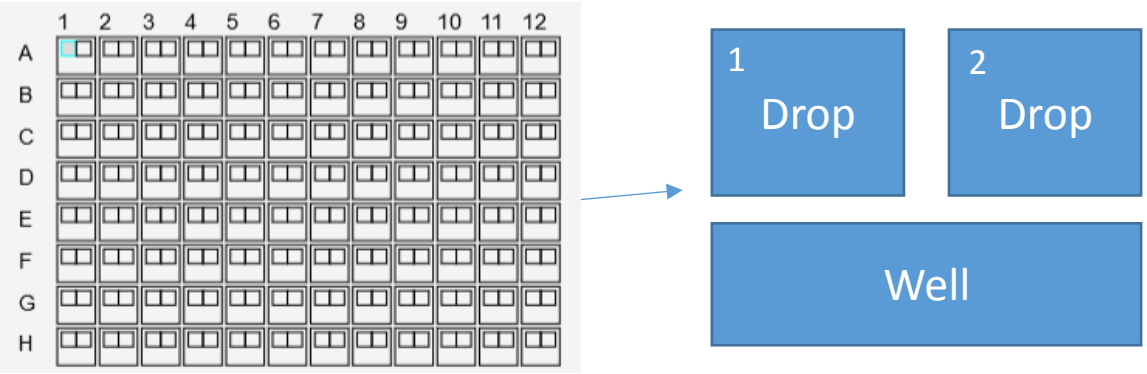

Figure 1- Crystallization Plate. Drop numbering is sequential from left to right, top to bottom. Therefore A1 contains drops 1 and 2, A2 contains drops 3 and 4 etc.

Plate is a Container:

Plates are represented as a **Container** in ISPyB. Each plate consists of a number of wells and drop locations (e.g. 192 drop locations in a CrystalQuickX plate). The plate container is associated with a Screen and a Schedule (for inspections). The Container also defines which imager it is stored in.

1. Crystallization Screens:

The Screen is a combination of chemicals used in the crystallization process. Standard screens are used that define which combination (group) of chemicals are used within each drop location.

Screen

The Screen table is collection of ScreenComponentGroups

ScreenComponentGroup

Describes the chemical composition used in each well/drop. i.e. in one well you may have, PEG400, NaCl, Additive1. The position specifies the well number on the plate

ScreenComponent

One row per component of a group, each component is a link to the Protein (component) table. So NaCl is an entry in the protein table

Protein
Specifies a concentrationtypeid and componenttypeid

ConcentrationType
Some small molecules are recorded as mg/ml, some as %, some as M. This table defines those types.

ComponentType
Defines, protein, rna, dna, small molecule.

2. Scheduling and Inspections:

Each plate is scheduled for regular inspections through software interface to the RockImager machines. At DLS the schedule for a plate is controlled through SynchWeb by creating a Schedule. A Schedule defines a number of ContainerInspections. The ContainerInspection entry records the priority, which imager to be used (20 or 4 degrees) when the inspection was scheduled and when it completed. The imaging itself produces BLSampleImage records. Through SynchWeb we also use a BLSampleImageScore table to identify if the sample has produced good crystals (Hampton Index; clear, precipitate etc).

Schedule
A single schedule, eg fibbonaci

ScheduleComponent
Each inspection in the schedule, i.e. one row per 12 hours, specifies an inspectiontypeid

InspectionType
Specifies the type of inspection: visual / uv

ContainerInspection
One scheduled or adhoc inspection per row

BLSampleImage
Each image in a ContainerInspection has a row in here, and can be scored using standard Hampton scoring using a BLSampleImageScoreId from BLSampleImageScore

BLSampleImageScore
Hampton image scorings (clear, precipitate etc.)

3. Data Collection and samples:

Through SynchWeb a user marks the drop with points or regions to ‘shoot’. This produces BLSubSamples.

BLSample
Each drop in a plate is defined as a BLSample

BLSubSample

Each point or region of interest on a single drop is marked as a BLSubSample

DataCollection
Records each datacollection against BLSample AND BLSubSample

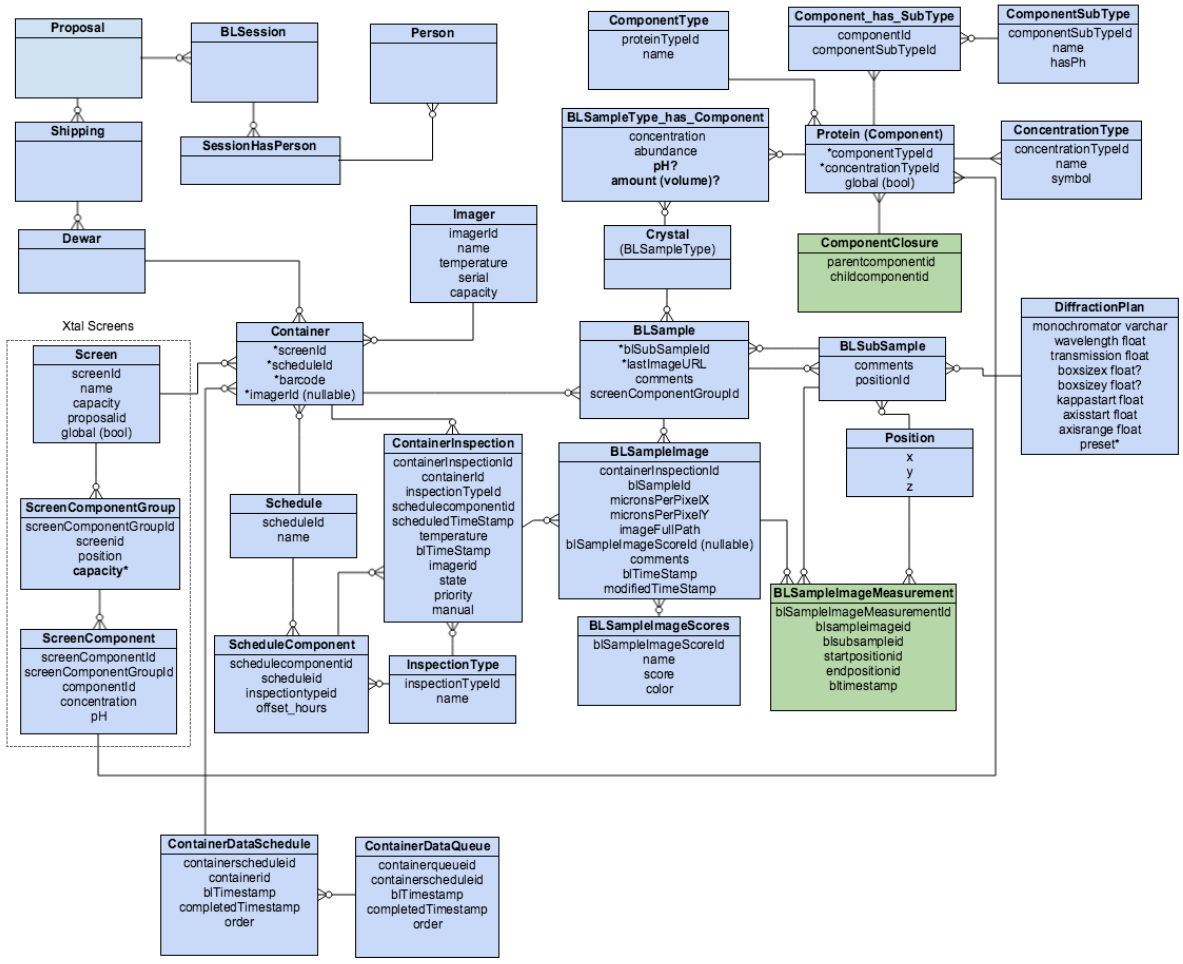

Figure 2 Legacy diagram for discussion showing initial design of ISPyB tables to support VMXi at DLS

ISPyB database table design for VMXi at Diamond. BLSampleImageMeasurement and ComponentClosure were not implemented. An update using the Draw.io package would be helpful to more accurately reflect the implementation. An example work in progress is shown in Figure 3.

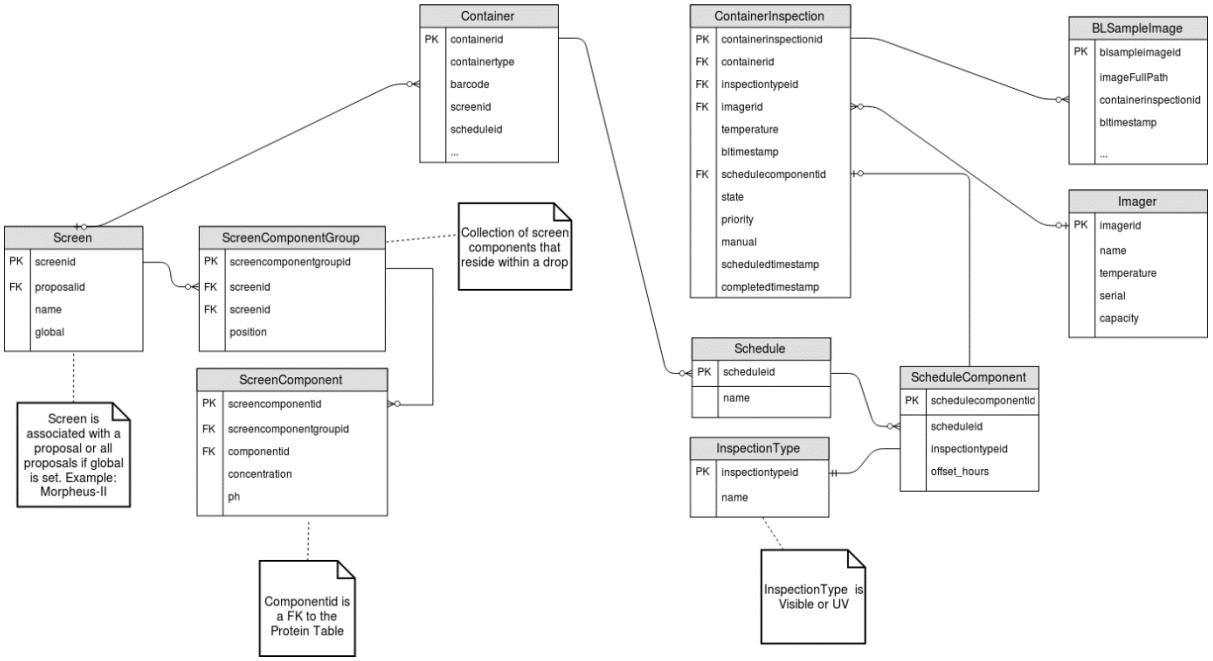

Figure 3 Work in progress to update diagram using Draw.io