Proposed layout and agenda for the first 2018 ISPyB-MXCuBE meeting

This document outlines significant proposed changes in the format and focus of the forthcoming ISPyB-MXCuBE meeting (30th January to 2nd February) compared to previous ones, for reasons and with aims that are hopefully made clear.

Rationale

The main and ubiquitous challenge in developing software at synchrotrons is to bridge the divide between the science and the software engineering components of the work, both in terms of *Weltanschauung* and in terms of resource allocation.

The overall guiding principle behind the layout and agenda proposed below is to promote a greater degree of discussion and coordination aimed at bridging this divide, not only between the members of each collaboration but also across the two collaborations, and to place the scientific goals of current and future MX at the helm in defining and prioritising collaborative actions.

Coordination between ISPyB and MXCuBE

Evolving experiments and pattern of usage at synchrotrons are giving rise to requirements for ever closer and better designed integration between MXCuBE and ISPyB.

Auto-processing and re-processing capabilities are in increasing demand, and a certain amount of indecision prevails in this respect – e.g. some ISPyB or EXI based proposals have been mooted, and some prototyping may have been carried out, but further assessment is required.

This situation makes it crucial to have some overlap between the two meetings to allow significant contact and discussion between both sets of participants, while avoiding the chronological overlap of mutually exclusive sessions that generates frustration in those wanting to attend both and leaves no room for organised discussion.

It is proposed here that this dilemma be addressed by a joint discussion session after the Wednesday 31st dinner, taking advantage of the fact that DLS logistics enable dinner to be served in the Atrium of Diamond House, right next to the meeting room.

ISPyB participants are therefore urged to extend their stay beyond the strict minimum, and leave on Thursday morning rather than Wednesday afternoon. MXCuBE participants should similarly plan to arrive in the afternoon or early evening on Wednesday.

Coordination within ISPyB and MXCuBE themselves

It was pointed out at the last MXCuBE Steering Committee (StC) meeting that the Scientific Committee (ScC) had never actually met as such, even though both Collaboration Agreements put their respective ScC in charge of defining the scientific goals that the other two Committees are to help achieve. Somehow, this goal-defining role of the ScC was thought to be "subsumed" under the influence exerted by those of its members who are also members of the StC.

Now that the initial setup phase of the MXCuBE collaboration has produced a strong shared development and communication infrastructure that has been exercised to a very significant extent by the MXCuBE partners, with the ramping up of the ISPyB collaboration expected to follow a similar path, it seems appropriate and desirable to put scientific goals in the driving seat in an explicit rather than an implicit manner, and thus reach the mode of operation envisioned in both Collaboration Agreements.

A major practical hindrance to operating in this way has been that the absence of meetings of the ScC *per se* was compounded by the fact that the meetings of the StC and of the Developers' Committee (DvC) took place in parallel, with little time allowed to take stock of both viewpoints and/or meeting outcomes in defining sufficiently detailed coordinated actions among the Members to overcome the centrifugal forces that tended to lead to divergent and/or duplicate implementations.

The two agendas detailed below propose that the meetings be structured as follows:

- first, the traditional brief status reports (~10mn each) from all the Members;
- then, three distinct sessions, Session 1 being developer-oriented, Session 2 science-oriented and Session 3 collaboration-oriented, with an extra discussion session on all previous topics in the MXCuBE meeting;
- finally, a succession of meetings of the three committees, starting with the ScC in plenary format (i.e. with no other committee meeting taking place in parallel) in an after-dinner slot in the case of MXCuBE, followed a pattern of presentation of recommendations leading to decisions and resolutions in which everyone (and every viewpoint from those with dual membership of some committees) will have had its say.

Orientation of the three sessions

This is illustrated for MXCuBE, which is the more advanced of the two collaborations, but the transfer of the guiding principles to ISPyB should be quite straightforward.

Note that all three types of orientation are relevant to everyone. This introduction of a degree of pre-formatting into three categories for the invited contributions departs from previous modes of operation, where the program was structured around whatever submissions were received.

Session 1: MXCuBE development highlights (developer-oriented).

This will consist of detailed technical presentations of substantial advances in developing and/or deploying MXCuBE, e.g. interfaces to new devices, including new GUIs.

Session 2: Evolving scientific capabilities (science-oriented)

This session will include presentations with an emphasis on the science motivating some recent, ongoing future developments, referring to technical requirements but not on implementation as such. Viewpoints and contents would include e.g.

- What kinds of new experiments has MXCuBE become capable of supporting?
- In what directions does it need to be moving?
- Who has what plans, over what time scales? E.g.
    - Lattice upgrades
    - New beamlines
    - Serial experiments – with what mode of sample delivery?
    - Detector upgrades
    - Goniometer upgrades
    - New protocols - with what built-in processing requirements?

Session 3: The collaboration in action (collaboration-oriented)

- How good are we at sharing new developments across sites (and user interfaces)?
- How good are we at avoiding duplication and reinventions of the wheel?
- How could the collaboration be made closer and more efficient, encouraging convergence and discouraging divergence?
- Is manpower adequate, and adequately coordinated?

Apologies are offered, and amendments keenly invited, if this attempt to introduce such a deliberate formatting into these meetings is seen as overly prescriptive or even presumptuous: this proposal has been written from the standpoint that the status of GPhL as the only non-synchrotron member of two strongly synchrotron-oriented collaborations might provide an opportunity to introduce some potentially useful variation from the format of previous meetings.

Proposed agenda for the ISPyB meeting

Tuesday 30th January	
14:00 – 14:30	**Registration of early participants**
14:30 – 16:00	Visit of eBIC cryo-EM facility
16:00 – 17:30	Optional session on cryo-EM in ISPyB
19:30 – 22:00	**Dinner (unformatted – arrangements TBD)**

Wednesday 31st January	
08:30 – 09:00	**Registration**
09:00 – 09:15	Welcome and admin
09:15: – 10:30	Updates and Status Reports from Members
10:30 – 11:00	**Coffee**
11:00 – 12:30	**Session 1**: ISPyB development highlights
12:30 – 13:30	**Lunch at Diamond House**
13:30 – 15:00	**Session 2**: Evolving scientific capabilities, logistical requirements and user expectations
15:00 – 16:30	**Session 3**: The ISPyB collaboration in action
16:30 – 17:00	**Coffee**
17:00 – 18:45	Committee meetings // Developers' contact time The detailed schedule will be agreed at the time, but will follow a similar "layered" pattern to that of MXCuBE, ensuring that the Scientific Committee meeting happens first, with no other committee meeting taking place at the same time, and that each meeting will present its recommendations and/or decisions to all participants
19:00 – 20:30	**Joint dinner in Diamond House Atrium with MXCuBE participants**
20:30 – 21:30	Joint discussion session with MXCuBE participants Topics to include: "Where ISPyB will (and won't) meet MXCuBE"

Proposed agenda for the MXCuBE meeting

Wednesday 31st January	
16:30 – 17:00	**Coffee / Registration of early participants** **Sign-up for visit of Diamond MX beamlines on Friday afternoon**
19:00 – 20:30	**Joint dinner in Diamond House Atrium with ISPyB participants**
20:30 – 21:30	Joint discussion session with ISPyB participants Topics to include: "Where ISPyB will (and won't) meet MXCuBE"

Thursday 1st February	
08:30 – 09:00	**Registration** **Sign-up for visit of Diamond MX beamlines on Friday afternoon**
09:00 – 09:15	Welcome and admin
09:15: – 10:30	Updates and Status Reports from Members
10:30 – 11:00	**Coffee**
11:00 – 12:30	**Session 1**: MXCuBE development highlights
12:30 – 13:30	**Lunch at Diamond House**
13:30 – 15:00	**Session 2**: Evolving scientific capabilities at beamlines and in MXCuBE
15:00 – 16:30	**Session 3**: The MXCuBE collaboration in action
16:30 – 17:00	**Coffee**
17:00 – 18:30	Chaired general discussion
18:30 – 20:00	**Dinner in Diamond House Atrium**
20:00 – 21:30	Scientific Committee meeting // Developers' contact time

Friday 2nd February	
09:00 – 09:30	Presentation of Scientific Committee recommendations
09:30: – 10:30	Parallel meetings of Steering and Developers' committees
10:30 – 11:00	**Coffee**
11:00 – 11:15	Presentation of Steering Committee's meeting outcome
11:15 – 11:30	Presentation of Developers' Committee's meeting outcome
11:30 – 12:30	Formulation of plans for the next 6 months and of resolutions for the medium-term future
12:30 – 14:00	**Lunch at the Diamond canteen**
14:00 – 15:30	Guided visit of Diamond MX beamlines (for those who signed up)
14:00 – 17:00	Free-format contact and activity time.