

PY-ISPyB

The new Python backend for ISPyB

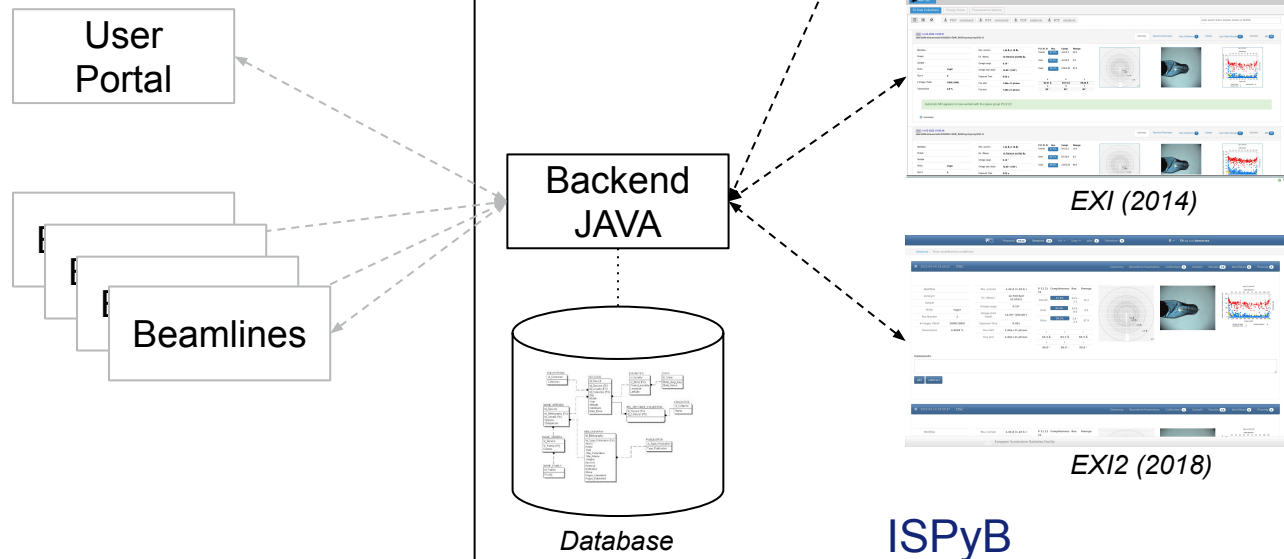
Alex de Maria
Software Engineer
ISPyB Developer

Why this meeting

- Provide feedback about latest developments
- Get your feedback about developments, motivation, participation...
- Reactivate the developers meetings
 - Who
 - When
 - Frequency

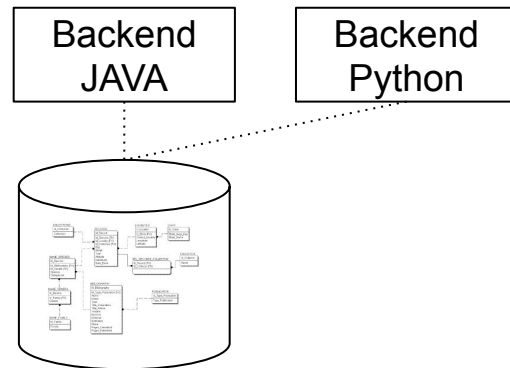
Software overview

- ISPyB full software stack is composed by:
 - Database (MariaDB or MySQL)
 - Backend (JAVA)
 - User interfaces
 - JSP pages embedded (*deprecated*)
 - EXI - Javascript
 - EXI2 - React



MOU status

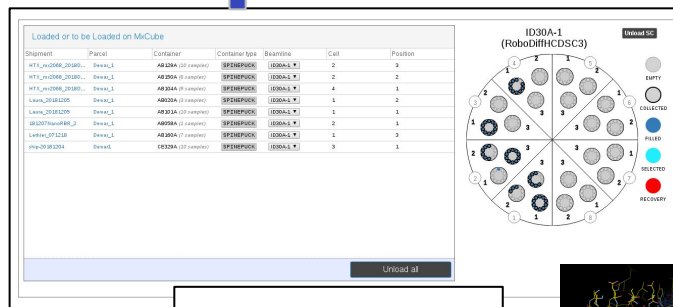
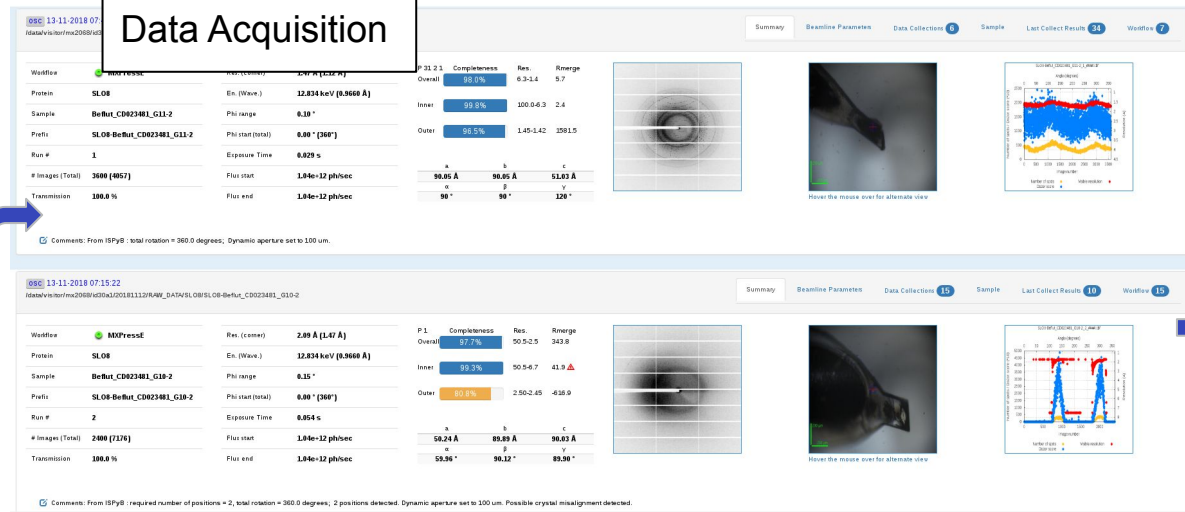
- MOU started on 01 January 2017
 - Collaboration around:
 - Data Model
 - Java Backend
 - Participants: ESRF, DLS, SOLEIL, CELLS, MAXIV, HZB, EMBL, Global Phasing
- February 2020 interim collaboration meeting
 - Implement backend in python -> **py-ispyb**
 - EMBL did a prototype
<https://gitlab.esrf.fr/ispyb/py-ispyb>
 - Develop SSX
- MOU terminated on 31 December 2021



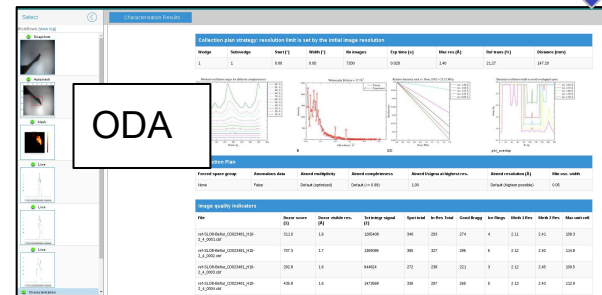
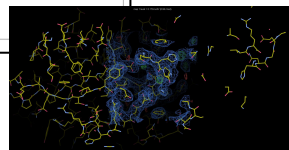
Motivation (MX)

- ISPyB allows:
 - Preparation
 - Monitoring
- Features
 - Real time feedback
 - Display automated DA
 - Friendly web interface
 - Convenient for local and remote access

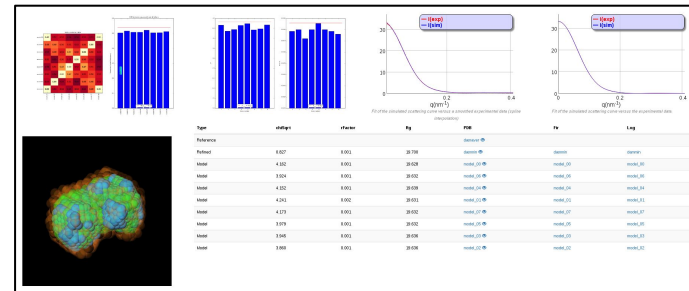
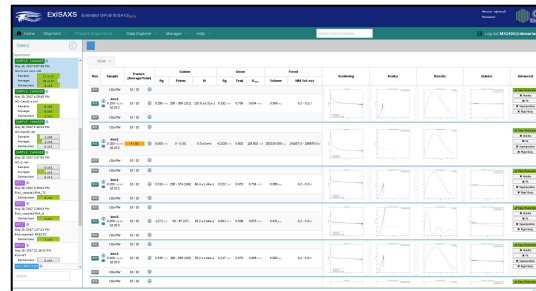
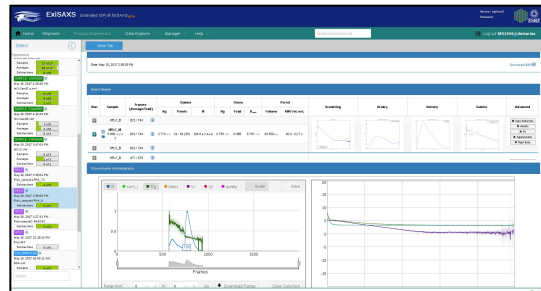
Data Acquisition



Sample Tracking



Motivation: BioSAXS (2014)



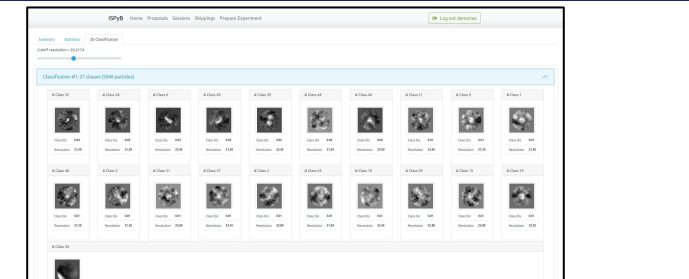
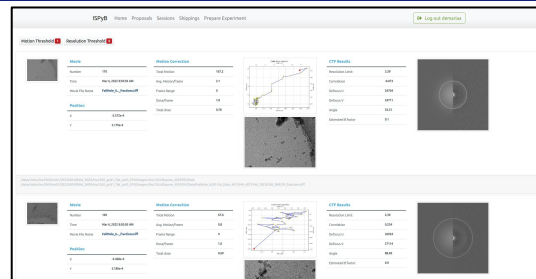
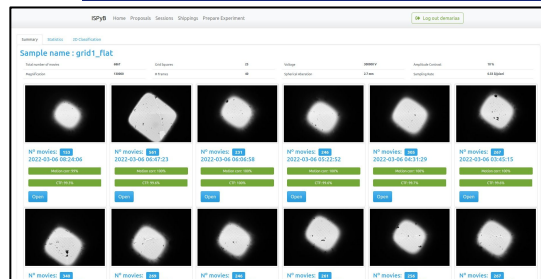
ISPyB for BioSAXS, the gateway to user autonomy in solution scattering experiments

A. De Maria Antolinos, P. Pernot, M. E. Brennich, J. Kleffer, M. W. Bowler, S. Delageniere, S. Ohlsson and A. Round

Upgraded ESRF BM29 beamline for SAXS on macromolecules in solution

P. Pernot, A. Round, R. Barrett, A. De Maria Antolinos, A. Gobbo, E. Gordon, J. Huet, J. Kleffer, Surr, P. Theveneau, L. Zerrad and S. McSweeney

EM (2018)



CM01: a facility for cryo-electron microscopy at the European Synchrotron

E. Kandiah, T. Giraud, A. de Maria Antolinos, F. Dobias, G. Effantin, D. Flot, M. Hons, G. Schoehn, J. Susini, O. Svensson, G. A. Leonard and C. Mueller-Dieckmann

- We evaluated and extended EMBL's work (see Mael's slides)
 - Authentication mechanism
 - Unit Testing
- Implementation of a legacy API
 - Hopefully this will help to adopt py-ispyb sooner
 - That API can be dropped in the future
- Implementation of SSX

Moving forward

- A clear and agreed roadmap that needs to be build within next weeks/months
- Engagement of the partners based on their motivation and resources
- Developments
 - How happy we are with the current proposed software stack/framework
 - Is it viable?
 - Is everybody happy?
 - Can be improved?
 - Compose working groups that can focus in specific area. Example:
 - User portal ingestion: wg that deals with the ingestion of proposals, persons, LC, etc..
 - Authentication/Authorization
 - Shipping
 - SSX
 - MX
 - etc...
 - Each WG needs a coordinator + participants
 - Resume the developers meetings
 - Which frequency?
 - When?
 - Who?



THANKS