ESRF Experiment Division Tuesday Events
15/09/2009

From your sample to your data analysis: how to track every step of your experiment in a database.
An example with ISPyB for MX experiments

Patrice Brenchereau ESRF/CS/MIS
Contents

• Tracking, experiments, samples, data analysis…
• What is ISPyB?
• Features
• Architecture
• What’s next?
From your sample to your data analysis: how to track every step of your experiment in a database…
What is ISPyB?

• **ISPyB:** Information System for Protein Crystallography Beamlines
  • Laboratory Information Management System (LIMS) for protein crystallography experiments on synchrotron beamlines
  • Web based interface

• **Access**
  • [http://ispyb.esrf.fr](http://ispyb.esrf.fr)
  • To log-in: ESRF experiment number and password

• **Where is it used at the ESRF?**
  • ID14-1, ID14-2, ID14-4
  • ID14-3 soon (BioSAXS)
  • ID23-1, ID23-2, ID29
  • BM14, BM16
Proposals and Users

• Type of Proposals:
  • IX: Industrial Users who come to the ESRF
  • FX: Industrial Users who don’t come to the ESRF (MXPress Service)
  • MX: Academic Users (mainly BAG / Block Allocation Group)

• ISPyB Users:
  • End user (users on site or remote, Esrf local contact)
  • Local Contacts (dewar tracking)
  • Fx Managers (managing Industrials)
  • Bloms (managing beamlines)
  • Stores (dewar tracking)
History

• 2001-2005: Pxweb
  • Python/Zope, MySql
  • JSBG Project (ESRF/EMBL)
  • Experiment logging for MXPress users (FX users)

• 2005-now: ISPyB
  • Java/Struts/Jboss, Mysql
  • ESRF/Spine/Bioxhit and BM14/MRC/eHTPX collaboration
  • Pxweb features + new features + Dewar Tracking
  • 2009: Collaboration with Diamond (code sharing)
ISPyB Project Management

- Management Structure
  - Steering Committee
  - Executive Committee
  - Scientific and User Committee
  - Project Manager
  - Developers

- Meetings
  - ESRF / DLS once a month (Marratech)
  - Synchrotrons: every 6 months / 1 year (last was April 2009)

- Source Code
  - Shared on SourceForge / SVN
  - Bug & New Feature tracking
  - Site specific statements : is_ESRF(), is_DLS()
ISPyB Features & Modules

- Experiment Management
- Sample Management
- Experiment Recording
- Search and Reporting
Experiment Management

- **Items:**
  - Proposals
  - Sessions (date, beamline, local contact)
  - Lab Contacts (email, address,..)
  - Proteins (approved sample sheets)

- **Features:**
  - Data retrieved from the User Portal (SMIS)
  - Edit Lab Contact Card
### Lab Contacts

#### Select

<table>
<thead>
<tr>
<th>Scientist name</th>
<th>First name</th>
<th>Lab name</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turkenburg</td>
<td>J.R.</td>
<td>YCP Structural Biology Laboratory</td>
<td>Select</td>
</tr>
<tr>
<td>Leonard</td>
<td>Gordon</td>
<td>ESRF</td>
<td>Select</td>
</tr>
<tr>
<td>Monacu</td>
<td>Stephanie</td>
<td>ESRF</td>
<td>Select</td>
</tr>
<tr>
<td>Terradot-Pirot</td>
<td>Laurent</td>
<td>ESRF</td>
<td>Select</td>
</tr>
<tr>
<td>Thibault</td>
<td>Xavier</td>
<td>ESRF</td>
<td>Select</td>
</tr>
<tr>
<td>Pringle</td>
<td>Darren</td>
<td>ESRF</td>
<td>Select</td>
</tr>
<tr>
<td>Guarro</td>
<td>Matteo</td>
<td>ESRF</td>
<td>Select</td>
</tr>
<tr>
<td>Pipeline</td>
<td>Dolo</td>
<td>ESRF</td>
<td>Select</td>
</tr>
<tr>
<td>Cho</td>
<td>Sanghun</td>
<td>Pohang Accelerator Laboratory</td>
<td>Select</td>
</tr>
<tr>
<td>Kim</td>
<td>Inwoon</td>
<td>Department of Chemistry</td>
<td>Select</td>
</tr>
<tr>
<td>Kim</td>
<td>Min-Kyu</td>
<td>Laboratory of Biophysics</td>
<td>Select</td>
</tr>
<tr>
<td>Ahn</td>
<td>Young Iun</td>
<td>Korea Ocean Research &amp; Development Institute</td>
<td>Select</td>
</tr>
<tr>
<td>Seo</td>
<td>Young Hyeon</td>
<td>Department of Chemistry</td>
<td>Select</td>
</tr>
<tr>
<td>Lee</td>
<td>Kim-he</td>
<td>Seoul National University</td>
<td>Select</td>
</tr>
<tr>
<td>Hvidt</td>
<td>Kristian</td>
<td>Department of Biochemistry</td>
<td>Select</td>
</tr>
<tr>
<td>Haapalaenen</td>
<td>Antti</td>
<td>Department of Biochemistry</td>
<td>Select</td>
</tr>
<tr>
<td>Bilaczi</td>
<td>Goran</td>
<td>Institute of Biorganic Chemistry</td>
<td>Select</td>
</tr>
</tbody>
</table>

#### Edit

<table>
<thead>
<tr>
<th>Lab-contact card</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Family name</td>
<td>CHA</td>
</tr>
<tr>
<td>First name</td>
<td>Ehsun</td>
</tr>
<tr>
<td>Telephone</td>
<td>-</td>
</tr>
<tr>
<td>Fax</td>
<td>02-542-276-1556</td>
</tr>
<tr>
<td>Email</td>
<td><a href="mailto:chung@pohang.ac.kr">chung@pohang.ac.kr</a></td>
</tr>
</tbody>
</table>

| Lab name         | Pohang Accelerator Laboratory |
| Lab address [*]  | Download University of Science and Technology 45 Eunpyeong-dong, Yeouido, Seoul, Korea 790-004 |

(*) Address must be in the text box without asterisking.

#### Default info

| Counter company for return (* if ESRF sends a delivery note) | |
| Counter account | |
| Billing reference | |
| Average Custom order value of a deliver (Euro) | 0 |
| Average Transport value of a deliver (Euro) | 0 |

Save card
Sample Management

• Items:
  • Shipments (set of dewars)
  • Dewars (barcode, courier tracking number)
  • Containers (barcode)
  • Samples (barcode, protein acronym, crystal form,…)

• Features:
  • Online shipment description
  • Shipment description upload (Excel file)
  • Dewar Tracking
Creating Shipments

Shipment Creation

Shipment Description (Excel)

Dewar Labels (sending, return)
# Dewar Tracking

## ISPyB Dewar Tracking

<table>
<thead>
<tr>
<th>Laboratory (opened / closed)</th>
<th>Courier (sent to ESRF, sent to user)</th>
<th>ESRF – Stores (Stores-In / Stores-Out)</th>
<th>ESRF – Beamline (Beamline #)</th>
</tr>
</thead>
</table>

- **Create Shipment**
  - Fill shipment or Upload from file
  - Print and stick labels on Dewar
  - Send shipment to the ESRF

- **Shipment transit**
  - Delivered
  - Shipment At Stores

- **Shipments at Stores**
  - Delivered
  - Picked up
  - Track your shipment within ISPyB
  - Receive an email on arrival at the ESRF

- **Shipments at Beamline**
  - Delivered
  - Picked up
  - Track your shipment within ISPyB
  - Receive an email on departure from the ESRF
  - Verify on ISPyB that your shipment is at the beamline
  - Receive an email on departure from the ESRF
  - Track your shipment within ISPyB
  - Picked up
  - Delivered
  - Shipment At Stores

---

**Shipment History:**

<table>
<thead>
<tr>
<th>Label</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dewar1</td>
<td>Dewar1</td>
</tr>
</tbody>
</table>

**Estimates:**

- Average customs value (Euro): 1000
- Average transport value (Euro): 4000

**Outbound courier:**

- Outbound tracking number: 78964009020

<table>
<thead>
<tr>
<th>Date</th>
<th>Status</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>07-05-2000</td>
<td>In</td>
<td>Stores-In</td>
</tr>
<tr>
<td>17-05-2000</td>
<td>Out</td>
<td>at ESRF</td>
</tr>
<tr>
<td>18-05-2000</td>
<td>At</td>
<td>ESRF Stores-Out</td>
</tr>
<tr>
<td>19-05-2000</td>
<td>Delivered</td>
<td>ESRF Stores-Out</td>
</tr>
<tr>
<td>20-05-2000</td>
<td>Picked up</td>
<td>ESRF Stores-Out</td>
</tr>
<tr>
<td>21-05-2000</td>
<td>Picked up</td>
<td>ESRF Stores-Out</td>
</tr>
<tr>
<td>22-05-2000</td>
<td>Picked up</td>
<td>ESRF Stores-Out</td>
</tr>
</tbody>
</table>

**Inbound courier:**

- Inbound tracking number: 78964009020

---

**Outbound courier:**

- Outbound tracking number: 78964009020

---

**Inbound courier:**

- Inbound tracking number: 78964009020
Experiment Recording

• Items:
  • Session info (date, beamline name, operator,…)
  • Experiment parameters (wavelength, energy, detector distance,…)
  • Beamline parameters (name, beam transmission, beam size,…)
  • Crystal snapshots
  • Images (thumbnails, link to real images)
  • Data Analysis / EDNA results (characterisation & strategy, mosflm.log, pointless.log,…)

Experiment Management
(seessions, lab contacts, proteins, …)

Sample Management
(shaements, devices, containers, sampling)

Experiment Logging
(data collection)

Search and Reporting
(samples, proteins, data collections)
# Data Collections

## Data Collections of a Session

<table>
<thead>
<tr>
<th>Data Collections</th>
<th>Energy Scans</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Image File</strong></td>
<td><strong>Run No.</strong></td>
</tr>
<tr>
<td><strong>Protein Name</strong></td>
<td><strong>Acronym</strong></td>
</tr>
<tr>
<td><strong>Start Time</strong></td>
<td><strong># Images</strong></td>
</tr>
<tr>
<td><strong>Wavelength</strong></td>
<td><strong>Trans.</strong></td>
</tr>
<tr>
<td><strong>Exp. Time</strong></td>
<td><strong>Phi start</strong></td>
</tr>
<tr>
<td><strong>Phi range</strong></td>
<td><strong>Detector</strong></td>
</tr>
<tr>
<td><strong>Resolution</strong></td>
<td><strong>Status</strong></td>
</tr>
<tr>
<td>**Sample **</td>
<td><strong>Rank</strong></td>
</tr>
</tbody>
</table>

**Run 1:**
- Date: 09-07-2009
- Time: 17:15:00
- Images: 14
- Wavelength: 0.976
- Trans.: 100
- Exp. Time: 0.34
- Phi Start: 115.95
- Phi Range: 0.3
- Resolution: 1.54
- Status: **Success**

**Run 2:**
- Date: 09-07-2009
- Time: 17:14:03
- Images: 57
- Wavelength: 0.976
- Trans.: 100
- Exp. Time: 0.1
- Phi Start: 36
- Phi Range: 0.35
- Resolution: 1.54
- Status: **Success**

**Run 3:**
- Date: 09-07-2009
- Time: 17:05:02
- Images: 2
- Wavelength: 0.976
- Trans.: 100
- Exp. Time: 1
- Phi Start: 0
- Phi Range: 1
- Resolution: 1.5
- Status: **Success**

**Run 4:**
- Date: 09-07-2009
- Time: 16:54:21
- Images: 2
- Wavelength: 0.976
- Trans.: 100
- Exp. Time: 1
- Phi Start: 0
- Phi Range: 1
- Resolution: 1.7
- Status: **Success**

**Run 5:**
- Date: 09-07-2009
- Time: 16:42:52
- Images: 21
- Wavelength: 0.976
- Trans.: 100
- Exp. Time: 0.63
- Phi Start: 112.95
- Phi Range: 0.3
- Resolution: 1.7
- Status: **Success**

**Run 6:**
- Date: 09-07-2009
- Time: 16:11:22
- Images: 31
- Wavelength: 0.976
- Trans.: 100
- Exp. Time: 0.4
- Phi Start: 92.8
- Phi Range: 0.45
- Resolution: 1.7
- Status: **Success**

**Run 7:**
- Date: 09-07-2009
- Time: 16:40:39
- Images: 62
- Wavelength: 0.976
- Trans.: 100
- Exp. Time: 0.91
- Phi Start: 62
- Phi Range: 0.9
- Resolution: 1.7
- Status: **Success**

**Notes:**
- This collection has a crystal snapshot.
- Collection was successful.
- No samples for the data collection.
Data Collections

Parameters & Results

<table>
<thead>
<tr>
<th>Experiment parameters</th>
<th>Resolution parameters</th>
<th>Check result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Date directory</td>
<td>2023/09/14/01/01/01/01</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Start date</td>
<td>2023/09/14</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>End date</td>
<td>2023/09/14</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Type of experiment</td>
<td>X-ray</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.979 Å</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Energy</td>
<td>25.89 keV</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Pd start</td>
<td>147.3°</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Oscillation range</td>
<td>0.75°</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Exposure time</td>
<td>0.5 s</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Number of frames</td>
<td>1</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Detector distance</td>
<td>80.7 cm</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Resolution at origin</td>
<td>1.2 Å</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Resolution at corner</td>
<td>1.32 Å</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Mean</td>
<td>1.27 Å</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Volume</td>
<td>126.8 Å³</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Detector 2 theta</td>
<td>5.0</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Step</td>
<td>N/A</td>
<td>(EMBL) data collection</td>
</tr>
<tr>
<td>Step</td>
<td>N/A</td>
<td>(EMBL) data collection</td>
</tr>
</tbody>
</table>

Image thumbnails (image wall)

Crystal Snapshots
Search and Reporting

• Search
  • Data Collection (protein, sample, experiment date, …)
  • Proteins
  • Samples

• Reports
  • Pdf, Word, Csv
<table>
<thead>
<tr>
<th>Sample No</th>
<th>Protein</th>
<th>A@images</th>
<th>Wavelength</th>
<th>Distance (mm)</th>
<th>Phase (pe)</th>
<th>Start Time</th>
<th>Rxn no</th>
<th>Image Prefix</th>
<th>Image no</th>
<th>Wash</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>D01 1</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 2</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 3</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 4</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 5</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 6</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 7</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 8</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 9</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 10</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 11</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 12</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 13</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 14</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
<tr>
<td>D01 15</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.975</td>
<td>0.975</td>
<td>189.14</td>
<td>189.14</td>
<td>0.975</td>
<td>ESRF</td>
</tr>
</tbody>
</table>

Excel / Csv
Sample Ranking

Ranked Samples

<table>
<thead>
<tr>
<th>Sample</th>
<th>Image Factor</th>
<th>Run No.</th>
<th>Start Time</th>
<th>Exposure time</th>
<th>Mobility</th>
<th>Number of spots</th>
<th>Number of time</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>sample1</td>
<td>1</td>
<td>10:15:52</td>
<td>C2221</td>
<td>1200</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>80</td>
</tr>
<tr>
<td>sample2</td>
<td>2</td>
<td>10:30:16</td>
<td>P4</td>
<td>90</td>
<td>3</td>
<td>2</td>
<td>1</td>
<td>70</td>
</tr>
<tr>
<td>sample3</td>
<td>3</td>
<td>11:30:01</td>
<td>P2222</td>
<td>6000</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>50</td>
</tr>
</tbody>
</table>

...
Reporting for Managers Dashboard

Number of logins per week:

Number of dewars per beamline:

Number of dewars per proposal code:
Application Environment and Data Flow
ISPyB Technology

- Pure Web Interface
- Java
- Jboss Application Server (Ejb)
- Struts (MVC Web Application Framework)
- MySql / Oracle Database
- Communication with User Portal (SMIS) via Web Services
- Communication with BCM and EDNA
  - Through the Data Base
  - …soon via Web Services
How does it help?

• Users
  • Prepare Experiment
  • Remote tracking by colleagues at home while the experiment is performed
  • Process experiment results back into the Home LIMS
  • Long term tracking of experiments (stored in the database)

• Communication between Users and ESRF Operations
  • Dewar description (beamline, local contact, user address)
  • Sample description (description, bar-code, location, known unit cell dimensions, space group, diffraction plans, comments)
  • Operator comments on data collections

• Safety (Dewar Tracking)
Next Steps...

- ISPyB new features (new EDNA data, AutoProcessing,…)
- Object Tracking
- ISPyB for BioSAXS (ID14-3)
- ISPyB for other beamlines
- ISPyB for other MX facilities
- ISPyB and UPBL10/MASSIF
Gas Tracking

- Why Tracking bottles of gas?
  - Gas available at storage -> Users
  - Location of old bottles -> Safety, Finance
  - Location of ‘dangerous’ bottles -> Safety
- Uses Dewar Tracking architecture and technology
ISPyB For BioSAXS (ID14-3)

- BioSAXS needs
  - Sample Tracking
  - Experiment Management (sample preparation, …)
  - Experiment Recording (images, data files, beamline parameters, …)
  - Search and statistics on past experiments
  - Web interface (remote access)
  - Link with MX experiments and SANS experiments…

![BioSAXS Experiment Workflow](image)
ISPyB For BioSAXS (ID14-3)

• Architecture

• Developments
  • Experiment Management: as it is in ISPyB
  • Sample Management: little customization (dewar/box, container/plate)
  • Experiment Management:
    • Data model extensions for BioSAXS data
    • GUI for BioSAXS data
  • Search and Report: customization for BioSAXS data
  • BCM/BsxCuBE evolutions

• An opportunity to see how we can use the ISPyB 'framework' and data model on other beamlines
ISPyB for Other Beamlines

• Features
  • Sample Tracking
  • Experiment Logging

• Developments
  • Experiment Management: as it is in ISPyB (link with User Portal/SMIS)
  • Sample Management: beamline sample description (generic ?)
  • Experiment Recording
    • Experiment data model (one per experiment type … or generic data model)
    • Gui to browse & view data collections
  • Search and Reports: depends on experiment data model
  • BCM (Beamline Control Management)
    • MX: MxCuBE
    • BioSAXS: BsxCuBE
    • …
ISPŷB Light for Other MX Facilities

- Facilities interested in using ISPŷB
  - Max-Lab, Bessy, Soleil, APS,… (ISPŷB meeting, April 2009)
- Features
  - Sample Management: as it is in ISPŷB
  - Experiment Recording: as it is in ISPŷB
  - Search and Report: as it is in ISPŷB
  - Experiment Management: link with Proposal Submission System
    - Proposals, Sessions, Lab Contacts, Sample sheets,…
    - Current ISPŷB: data filled in by User Portal / SMIS
    - ISPŷB Light: API or Gui to fill in / manage this information
UPBL10 / MASSIF

- Many more samples…
  - Instead of a few samples, hundreds will be evaluated to select the best ones for data collection
  - An order of magnitude increase in samples and data
- …and new Architecture / Workflow
  - Automated end stations for sample screening
  - End station for data collection
- Needs
  - As automation increased – more reliant on information from user (crystal mounting, size, composition, …)
  - Automated links with Home Lab Systems
  - Tracking by individual Samples
  - Sample Ranking (over hundreds of samples)
  - New data arrangement: not by session, by project?
  - Sample Management: sorting facility associated with beamlines
Thanks to...

Elspeth Gordon  ESRF
Stéphanie Monaco  ESRF
Gordon Leonard  ESRF
Gianluca Cioci  ESRF
Pernot Petra  ESRF
Adam Round  EMBL
Matthew Bowler  ESRF
Martine Moroni  ESRF
Serges Ronseaux  ESRF
Thierry Caruana  ESRF
Eric Fertin  ESRF
Olof Svensson  ESRF
Darren Spruce  ESRF
Matias Guijarro  ESRF
Bernard Lavault  EMBL

Alun Ashton  DLS
Martin Walsh  DLS
Karl Levik  DLS
Graeme Winter  DLS
Solange Delagenière  ESRF
Ludovic Launer  MRC/BM14
Emmanuel Eyer  ESRF
Christian Rolland  ESRF
Samuel Jones  ESRF
CS/MIS Group  ESRF
Oleg Konovalov  ESRF

... people I don't know but who have contributed to ISPyB
... people I forgot to mention (sorry)
... and all users for their constructive feedbacks

Questions...