

ISPYB :

A web-based laboratory information system
for crystal analysis with X-rays

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SUMMARY

- What is it?
- Main features
- A little tour through some features
- Different levels of usage
- What's next?

What is ISPYB?

- ISPYB is a Laboratory Information Management System (LIMS) linking single **crystal samples** to their corresponding **X-ray data**. It is a web dynamic application using a MySQL database.

- **Access to ISPYB?**

Through a web browser at <http://ispyb.esrf.fr>

To log-in: an ESRF Experiment number and password are required.

- **History:**

2 years old

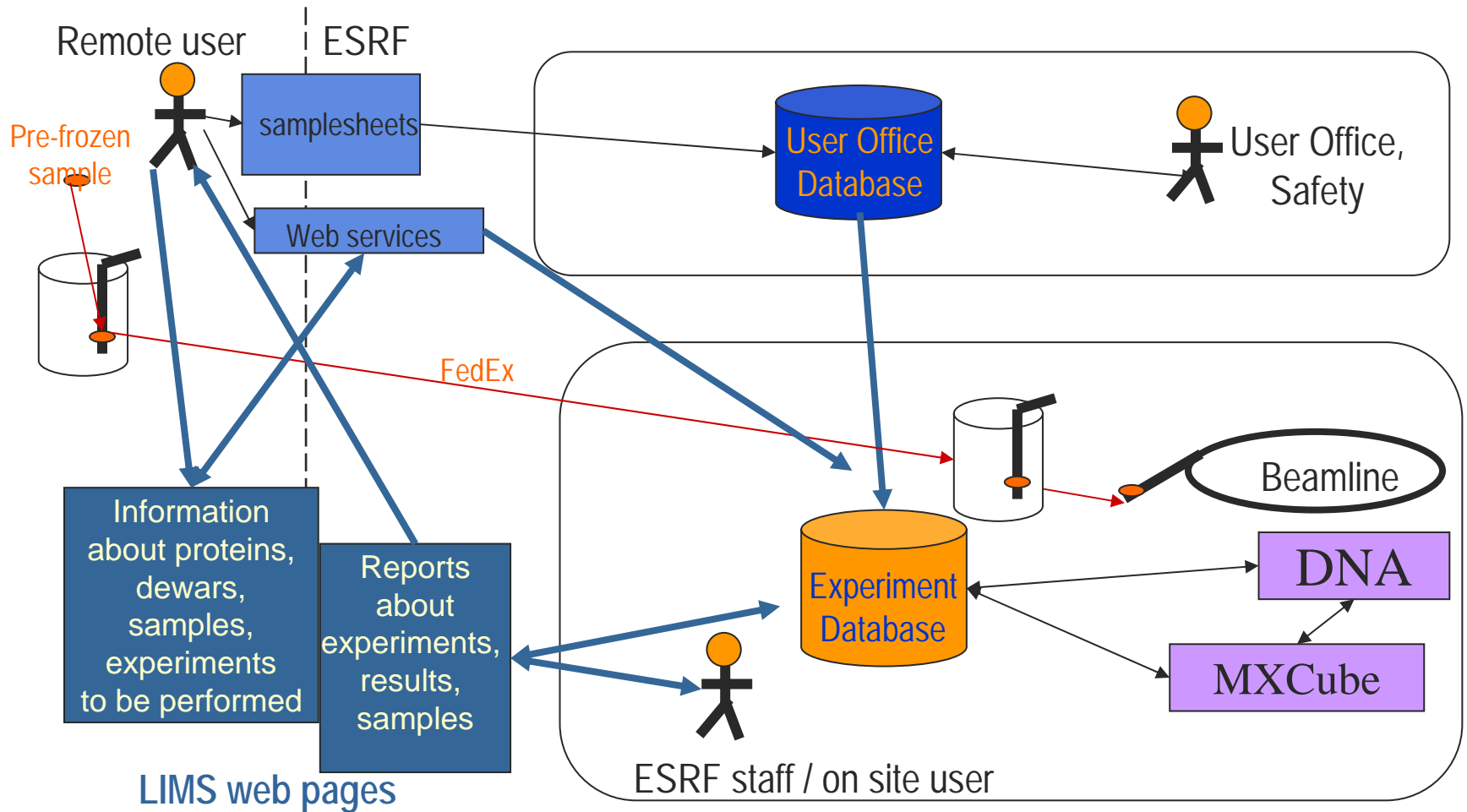
Replaces Pxweb our former LIMS (zope+python/ MySQL database) developed initially thanks to SPINE and BIOXHIT grants

Written in Java technology in order to be compatible with other synchrotrons and inhouse databases

Co-development between ESRF and BM14 ehtpx



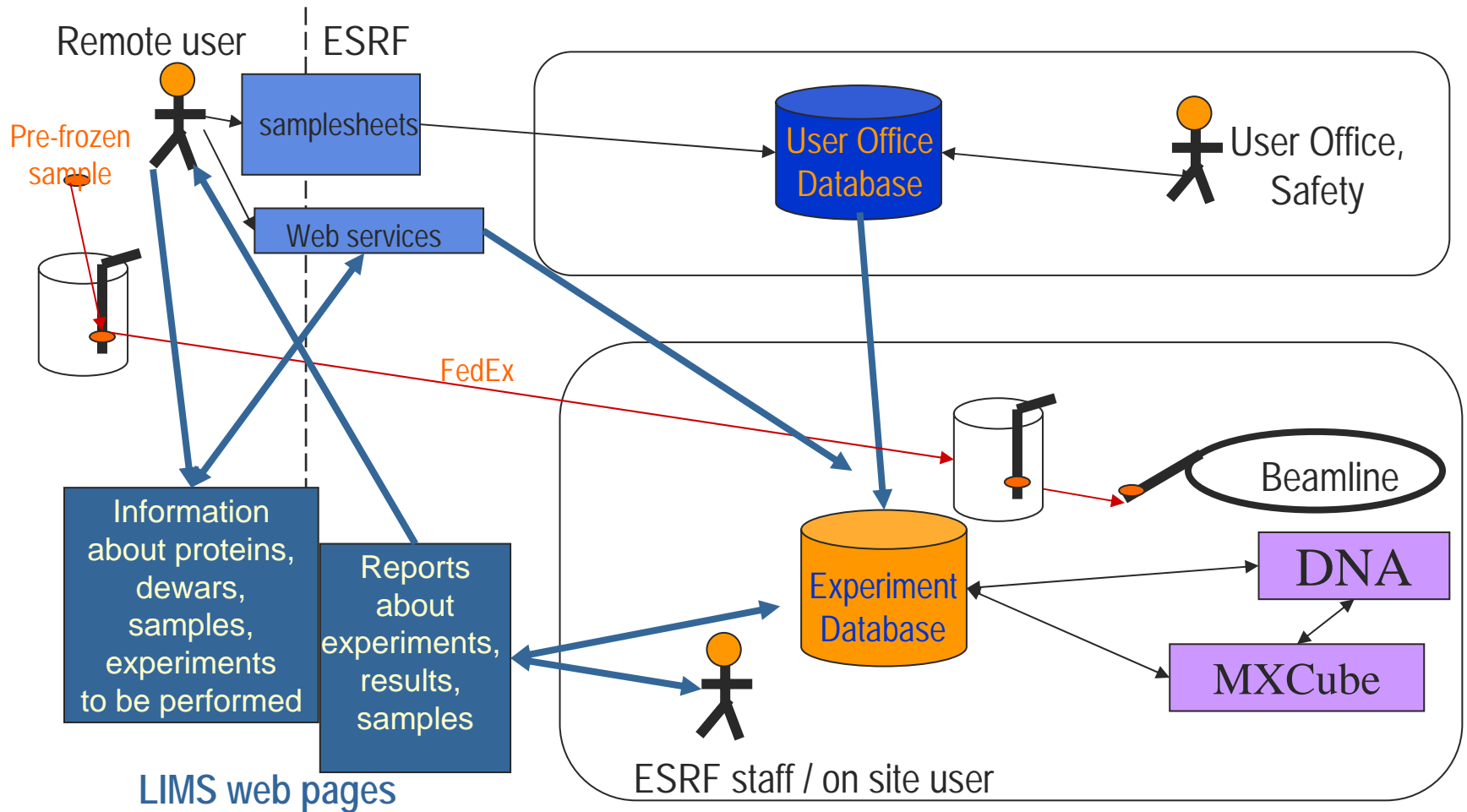
Information flow around an MX experiment



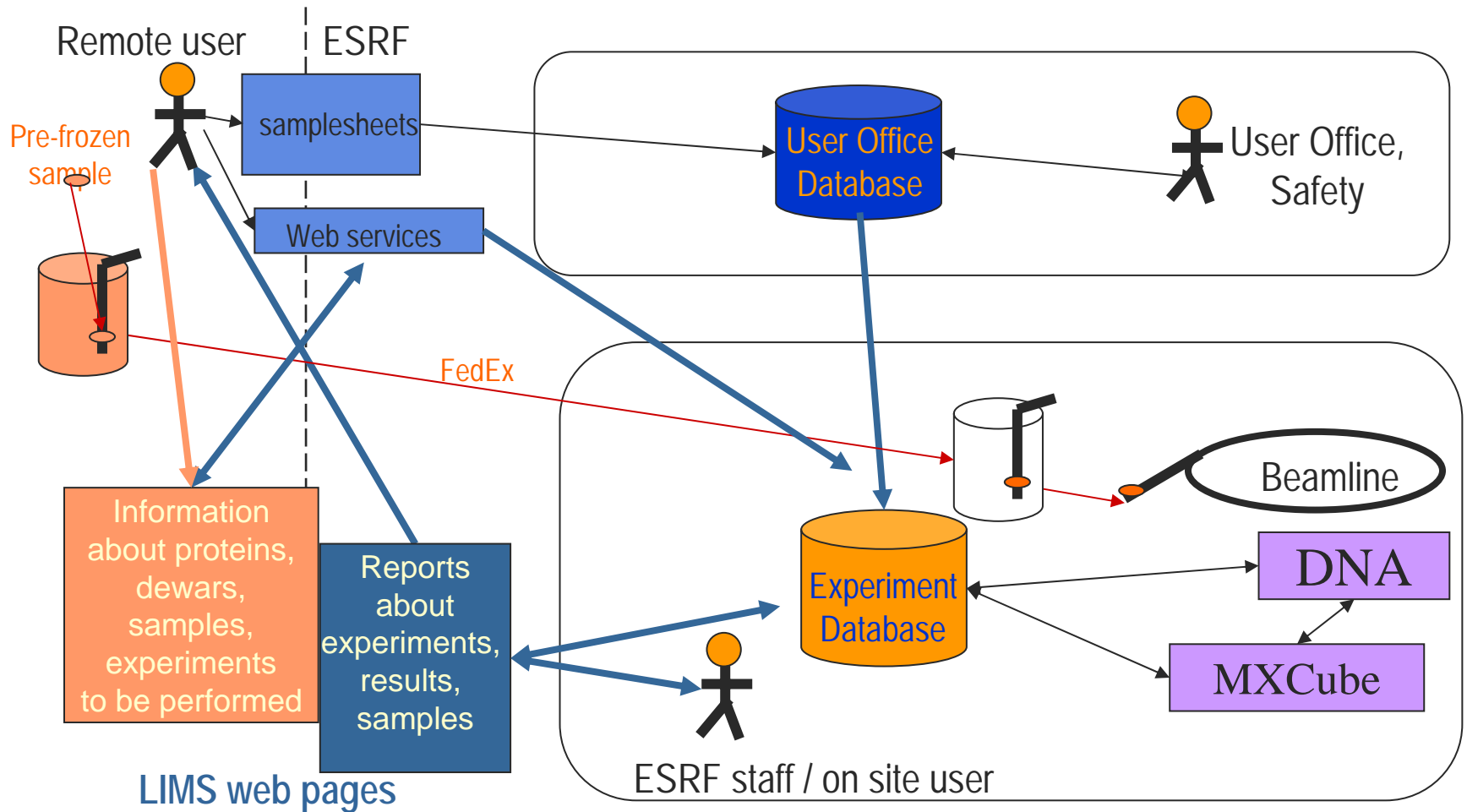
Available features

- Management of crystal samples and their relative protein information
- Description of samples sent to the synchrotron, including their 'diffraction plan'
- Real time monitoring of data collections: diffraction images, crystal snapshots, harvesting of output from data analysis softwares
- Search engines for data mining
- Creation and editing of experiment reports

Information flow around an MX experiment



Information flow around an MX experiment





The Protein Data Bank: ESD Form

File Edit View Insert Format Tools Data Window Help

Type a question for help

Arial 10

85%

Sample position	Protein Name	Protein Acronym / Description	Image Group	Sample Name	PIN Barcode	Protein(s) / Resolutions	Number of Resolutions	Description Range	Superficial Type	Archaical Feature	Unit Cell	alpha	beta	gamma	Loop Type	Header Length	Comments
1																	
2																	
3																	
4																	
5																	
6																	
7	1								OSC						Nylon	22	
8	2	A-TM - P3							OSC						Nylon	22	
9	3	A-TM - Undefined							OSC						Nylon	22	
10	4	A-TM - P3							OSC						Nylon	22	
11	5	A355 - Undefined							OSC						Nylon	22	
12	6	A355 - Undefined							OSC						Nylon	22	
13	7	hKAJ52 - Undefined							OSC						Nylon	22	
14	8	61 - Undefined							OSC						Nylon	22	
15	9	DNVW - Undefined							OSC						Nylon	22	
16	10								OSC						Nylon	22	

 Required information
 Optional but highly recommended
 Optional

Image Name on the baseline = <Protein Acronym>_<Sample Name>_<Run Number>_<Image Number>

Tip:
 Worksheet name (tab name) is not used during the upload process. Feel free to rename it to anything making sense to you...
 Make sure no drop-down list is selected before saving and submitting the file to ISPyB.

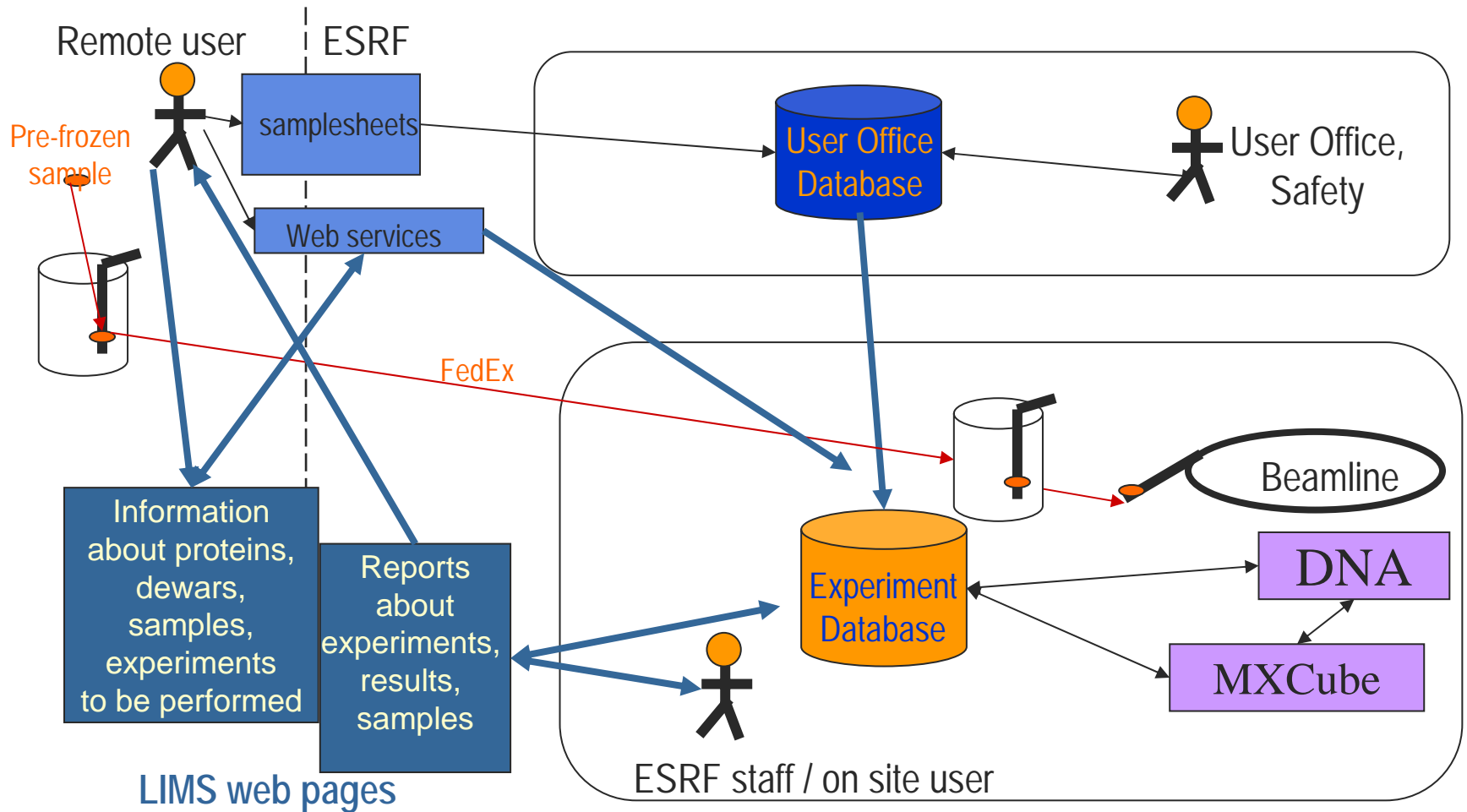
Ready

MM SQL

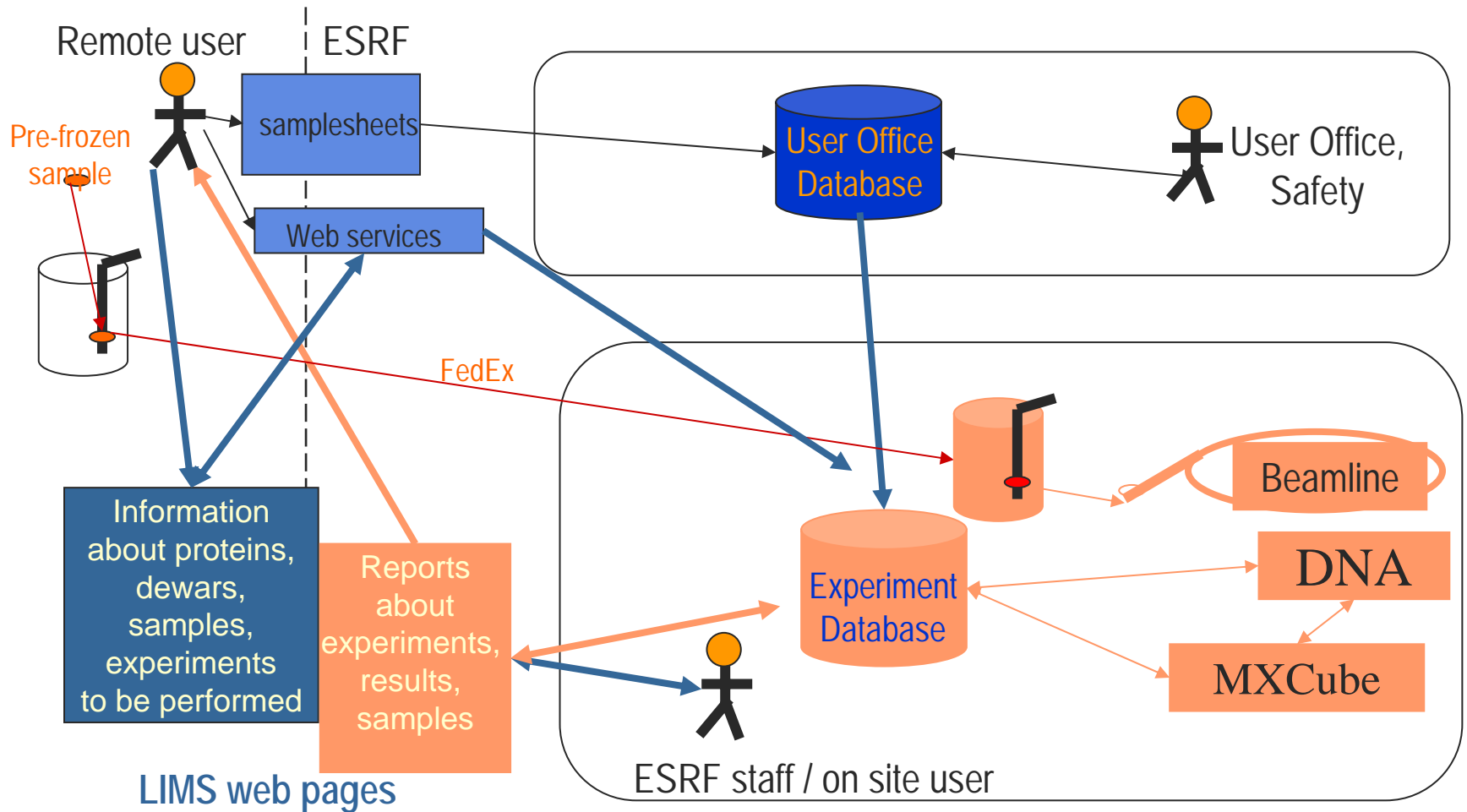
Why describing a shipment?

- Provide information between crystal producers and crystallographers at the beamline
- Provide beamline softwares (DNA, Mxcube) with the exact data directly usable in the experiment (loading a sample using its name instead of loading sample 3 of basket 5- directory path updated)
- Mandatory for automatic screening

Information flow around an MX experiment



Information flow around an MX experiment





ISPYB Tour –II

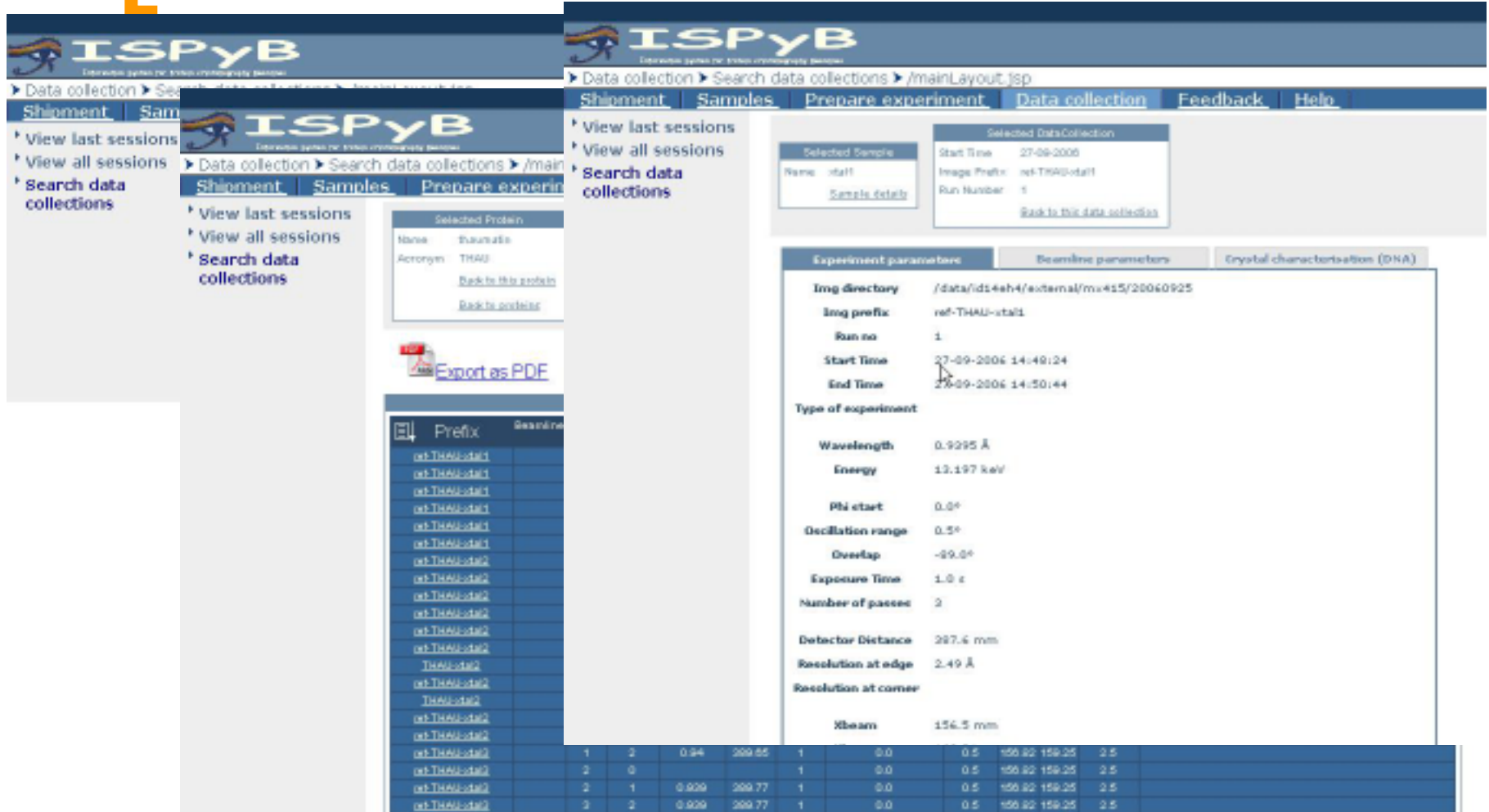
Experimental session viewing

Wink video

Interest of the experimental session viewing

- On the D-day: follow an experiment in real time (facilitate discussion between experimentators and colleagues in their labs)
- Get exact beamline parameters
- Keep track of what crystal shape for what diffraction pattern & analysis
- Crystal ranking results
= Experiment electronic logbook

ISPYB Tour –III search engine



The screenshot displays the ISPYB search engine interface. The top navigation bar includes links for 'Data collection', 'Search data collections', 'Shipment', 'Samples', 'Prepare experiment', 'Data collection', 'Feedback', and 'Help'. The main content area is divided into several sections:

- Selected Protein:**
 - Name: Insulin
 - Acronym: THAU
 - Buttons: [Back to this protein](#), [Back to order](#)
- Export as PDF:** A button with a PDF icon.
- Search Results:** A table with a search bar and a list of results. The results are filtered by 'Prefix' and show a list of 'ref-THAU-stall' entries.
- Selected Data Collection:**
 - Start Time: 27-09-2006
 - Image Prefix: ref-THAU-stall
 - Run Number: 1
 - Button: [Back to this data collection](#)
- Experiment parameters:**
 - Img directory: /data/ids4eh4/external/mx415/20060925
 - Img prefix: ref-THAU-stall
 - Run no: 1
 - Start Time: 27-09-2006 14:49:24
 - End Time: 27-09-2006 14:50:44
 - Type of experiment:
 - Wavelength: 0.9295 Å
 - Energy: 13.197 keV
 - Phi start: 0.0°
 - Oscillation range: 0.5°
 - Overlap: -89.0°
 - Exposure Time: 1.0 s
 - Number of passes: 2
 - Detector Distance: 287.6 mm
 - Resolution at edge: 2.49 Å
 - Resolution at corner:
 - Xbeam: 156.5 mm

Interest of the search engine

- Follow the X-ray history of a project (acronym search)
- Follow the the X-ray history of a sample
- Allows to refer to already done experiments on that particular crystal type (help in designing a new X-ray experiment)

ISPYB 'à la carte'

- 1st level: no action by the user.

Log on the beamline control software as proposal number X: all parameters of that session will be stored in ISPYB (snapshots...no data analysis) – updated electronic logbook accessible from anywhere in the world

- 2nd level: use of DNA in parallel to the beamline control software
Same as above plus data analysis from DNA

- 3rd level: use of shipment description without pin barcodes
Same as in level 2. + experiment facilitated on the beamline + link crystal description and X-ray data

- 4th level: use of shipment description with pin barcodes
Same as in level 3. + crystal ranking possible from DNA – storage of results in ISPYB

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What's next for the user interface?

- Improve existing tools: search tool..
- Expand database with other useful parameters (i.e. anomalous spectrum)
- Facilitate data export from ISPYB to user's LIMS
- Expand database to sample analysis: Data integration/scaling in tables...
- Dewar tracking

Not an exhaustive list!...

Thanks to...

- **Joint development (ESRF, eHTPX)**
- **Collaborations**
 - EBI, BioXHit
 - DNA
 - ESRF information system group (MIS) : to be compatible with other dynamic web applications of ESRF
- **Team**
 - D. Spruce (ESRF), J. Gabadinho (ESRF): BLISS
 - R. Leal (ESRF), **L. Launer (Ehtpx)**, **S. Delageniere (ESRF)**, S.Veyrier (ESRF): developers
 - S. Monaco (ESRF), M. Walsh (BM14): Scientific direction and system requirements
- **With the help from Users (feedack at ispyb@esrf.fr), and ESRF MX group**
- **And support from S. Larsen, G. Leonard, S. McSweeney, V. Rey**