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.
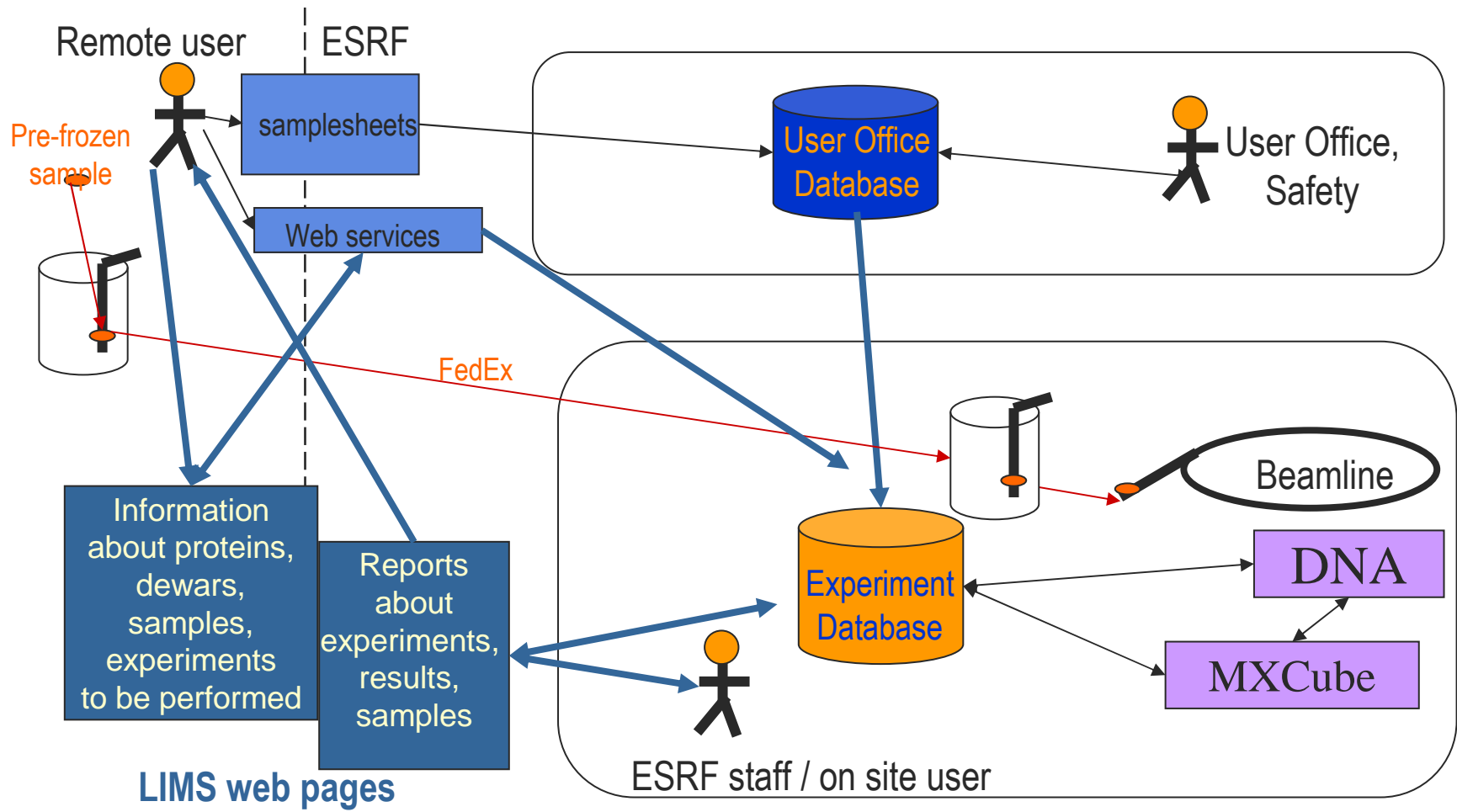
- **History:**

2 years old

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

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

Remote user · ESRF

samplesheets

Pre-frozen sample

Web services

User Office Database

User Office, Safety

FedEx

Information about proteins, dewars, samples, experiments to be performed

Reports about experiments, results, samples

LIMS web pages

Experiment Database

Beamline

DNA

MXCube

ESRF staff / on site user

Available features

- Management of crystal samples and their relative protein information

- Description of samples sent to the synchrotron, including '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 (i.e. for MxPress© clients)

Information flow around an MX experiment
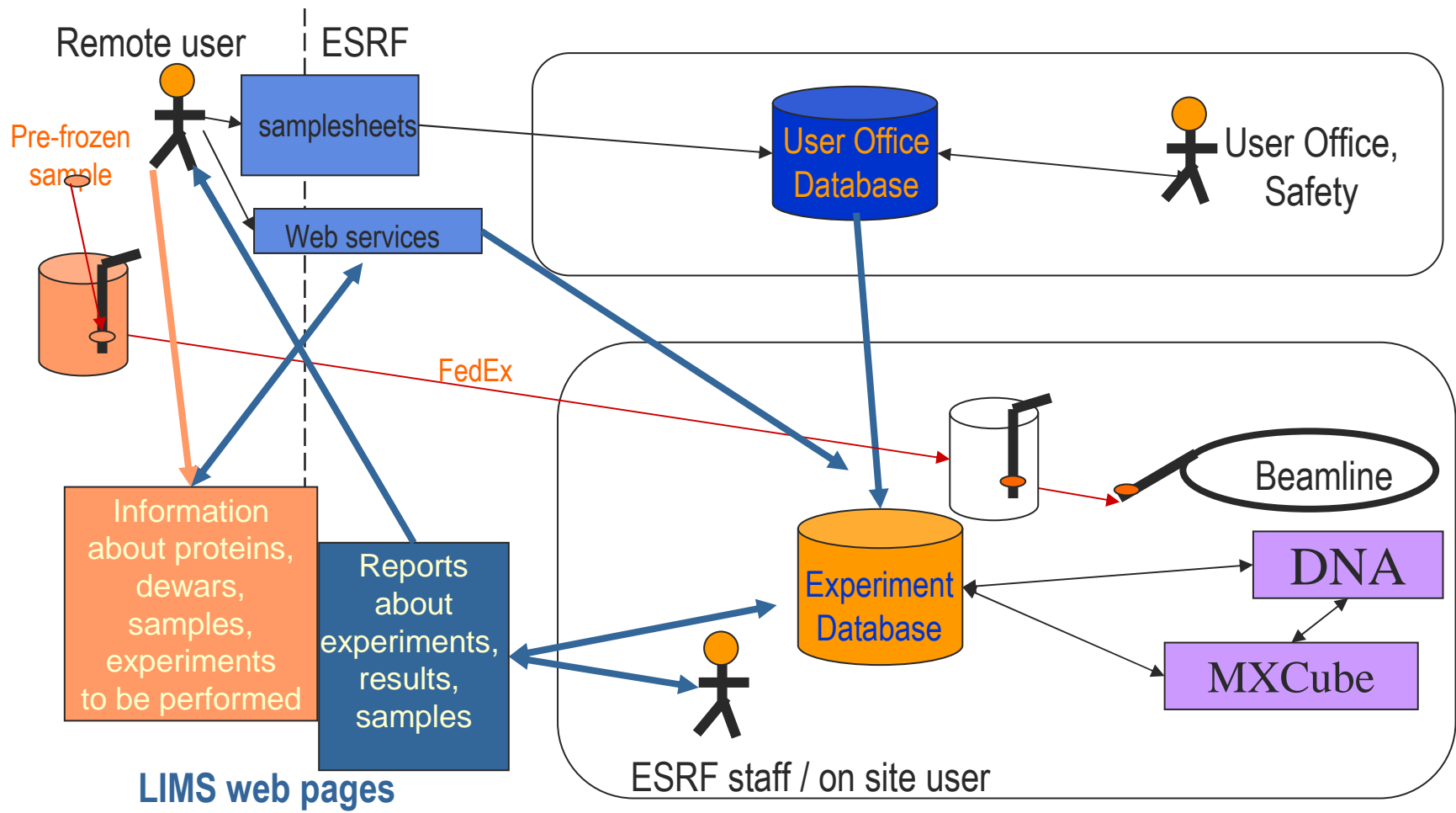
ISPYB Tour – I
shipment description

- Shipment : pool of samples within containers, themselves within dewars & send to the synchrotron.

- 'Manual description' : create and describe each crystal sample individually in ISPYB

- 'Semi-automatic description': prepare an excel sheet (pre-filled with the projects) and upload it to ISPYB.
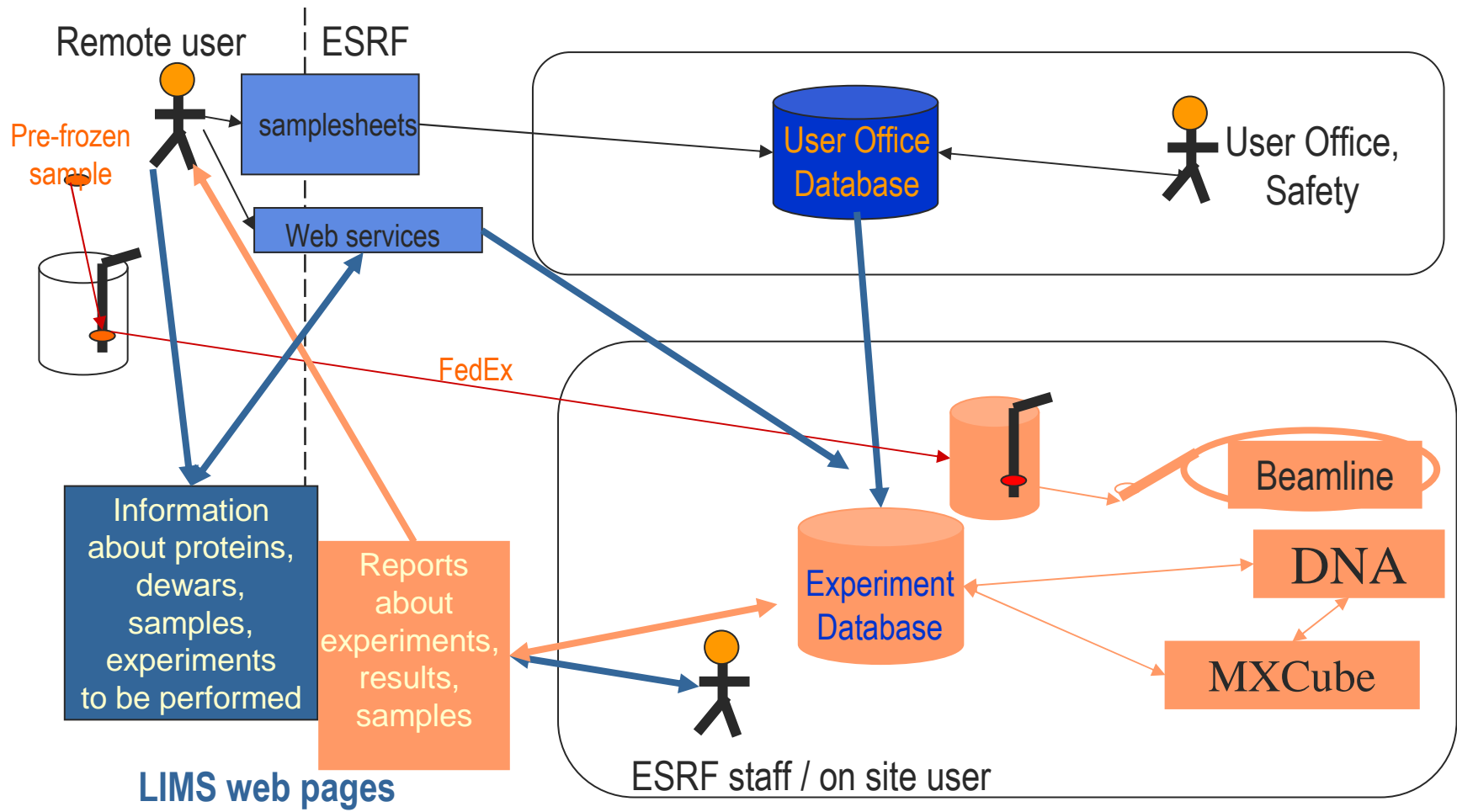
ISPYB Tour – I

Interest of describing my shipment in ISPYB?

- Provide information between crystal producers and crystallographers at the beamline

- Provide beamline softwares with exact data directly usable in the experiment (loading sample X instead of loading sample 3 of basket 5, directory path updated)

- Mandatory for automatic screening

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LIMS web pages

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 bewtween 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

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

What's next for the user interface?

- Improve existing tools: search tool..

- Expand database with other useful parameters: anomalous spectrum – Flux at sample position…

- 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**