

L. Cardonne<sup>1</sup>, S. Delagenière<sup>1</sup>, J. Gabadinho<sup>1</sup>, L. Launer<sup>2</sup>, R. Leal<sup>1</sup>, S. Monaco<sup>1</sup>, D. Spruce<sup>1</sup>, V. Rey<sup>1</sup>, S. Veyrier<sup>1</sup>, M. Walsh<sup>2</sup>

<sup>1</sup> European Synchrotron Radiation Facility, Grenoble, France;  
<sup>2</sup> Medical Research Council, France

## 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 any web browser at <http://ispyb.esrf.fr>

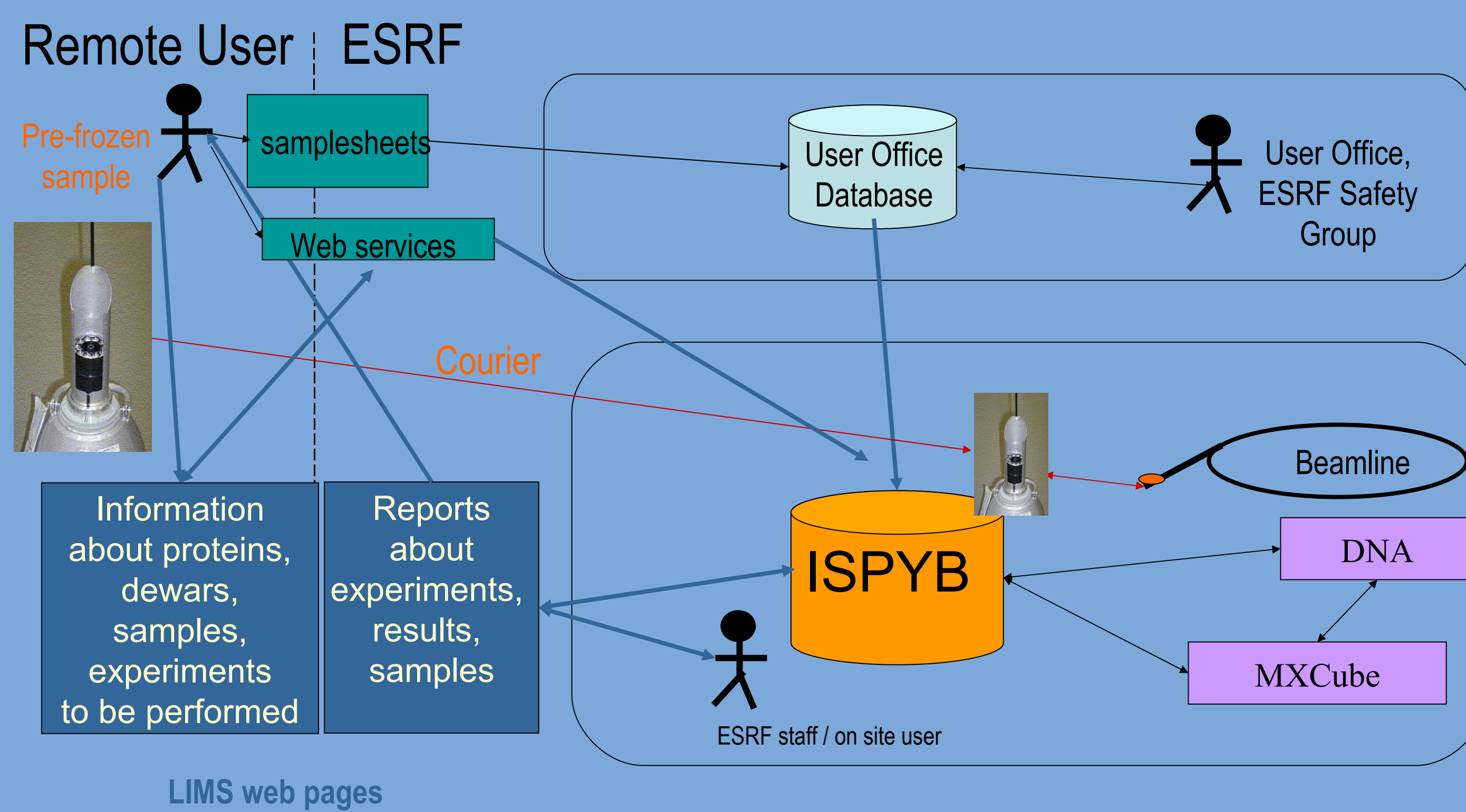
To log-in an ESRF Experiment number and password are required.

## Available features:

- Management of sample, crystal and protein information
- Description of samples sent to ESRF, including 'diffraction plan'
- Real time monitoring of data collections: diffraction images, crystal snapshots, harvesting of output from DNA
- Search engines for data mining
- Creation and editing of reports (i.e. for MxPress© clients)

## Information flow

ISPYB interacts with the various beamline components (BCM, DNA...) to provide and store information concerning diffraction experiments.



## Developments foreseen:

- Easier ways of entering of sample information i.e. through file upload
- Dewar tracking
- Improved data mining (i.e. extraction of statistics on beamline use)
- Improvement of data harvesting.
- Better interaction with 'home LIMS'

## Some Details

**Shipment forms:** communication of information concerning individual samples (description, bar-code, location, known unit cell dimensions, space group, 'diffraction plans') from crystallographers in the home lab to those performing the experiments at the ESRF.

Protein	Sample name	Smp code	Dewar	Container	LOC in cont.	Space Group	Cell dim	Cell dim	Cell dim	Crystal	Already	Micro	Sample	comment	Edit sample	Sample status	Data collections
THAU	stab1	HANO/A0501	dewar1	AAV15A	1	P41212	57.3	148.8	90.0	90.0	0	0				TEST_2006-10-02	
TLN	stab0	HANO/A0502	dewar1	AAV15A	10	P6122	92.0	92.0	130.2	90.0	90.0	120.0	0	2.5			
THAU	stab2	HANO/A0511	dewar1	AAV15A	2	P41212	57.3	148.8	90.0	90.0	0	0					
THAU	stab3	HANO/A0521	dewar1	AAV15A	3	P41212	57.3	148.8	90.0	90.0	0	0					
THAU	stab4	HANO/A0526	dewar1	AAV15A	4	P41212	57.3	148.8	90.0	90.0	0	0					
Prot_K	stab5	HANO/A0529	dewar1	AAV15A	5	P4212	68.2	68.2	108.3	90.0	90.0	90.0	0	0			
Prot_K	stab6	HANO/A0531	dewar1	AAV15A	6	P4212	68.2	68.2	108.3	90.0	90.0	90.0	0	0			
Prot_K	stab7	HANO/A0524	dewar1	AAV15A	7	P4212	68.2	68.2	108.3	90.0	90.0	90.0	0	0			
TLN	stab8	HANO/A0517	dewar1	AAV15A	8	P6122	92.0	92.0	130.2	90.0	90.0	120.0	0	2.5			

**Storage of experimental parameters:** Data collection is automatically recorded & reported. These can then be tracked via the web interface.

The screenshot shows the 'Data collection' tab in ISPYB. It displays a table of data collections with columns for Image Prefix, Run No., Start Time, #Images, Wavelength, Exposure Time, Phi, start Phi, range, deflection, Run Status, Step, and Comments. A red circle highlights a row, with an arrow pointing to a 'Click for more details' label. Below the table, a detailed view of an experiment is shown, including 'Experiment parameters' (Image prefix, Run no, Start Time, End Time, Wavelength, Detector Distance, Exposure Time, Phi start, Phi range, Xbeam, Ybeam, Detector Resolution) and 'Crystal snapshots' (Image collected, image name, image location). A red circle highlights the 'DNA files' link in the 'Experiment parameters' section, with an arrow pointing to a 'Results from DNA screening in this tab' label.

Experimental details & results for each experiment

The 'data collection' tab allows tracking of experiments

Results from DNA screening in this tab