



mxCuBE : software & hardware progress of crystallography beamlines at ESRF

Matías Guijarro

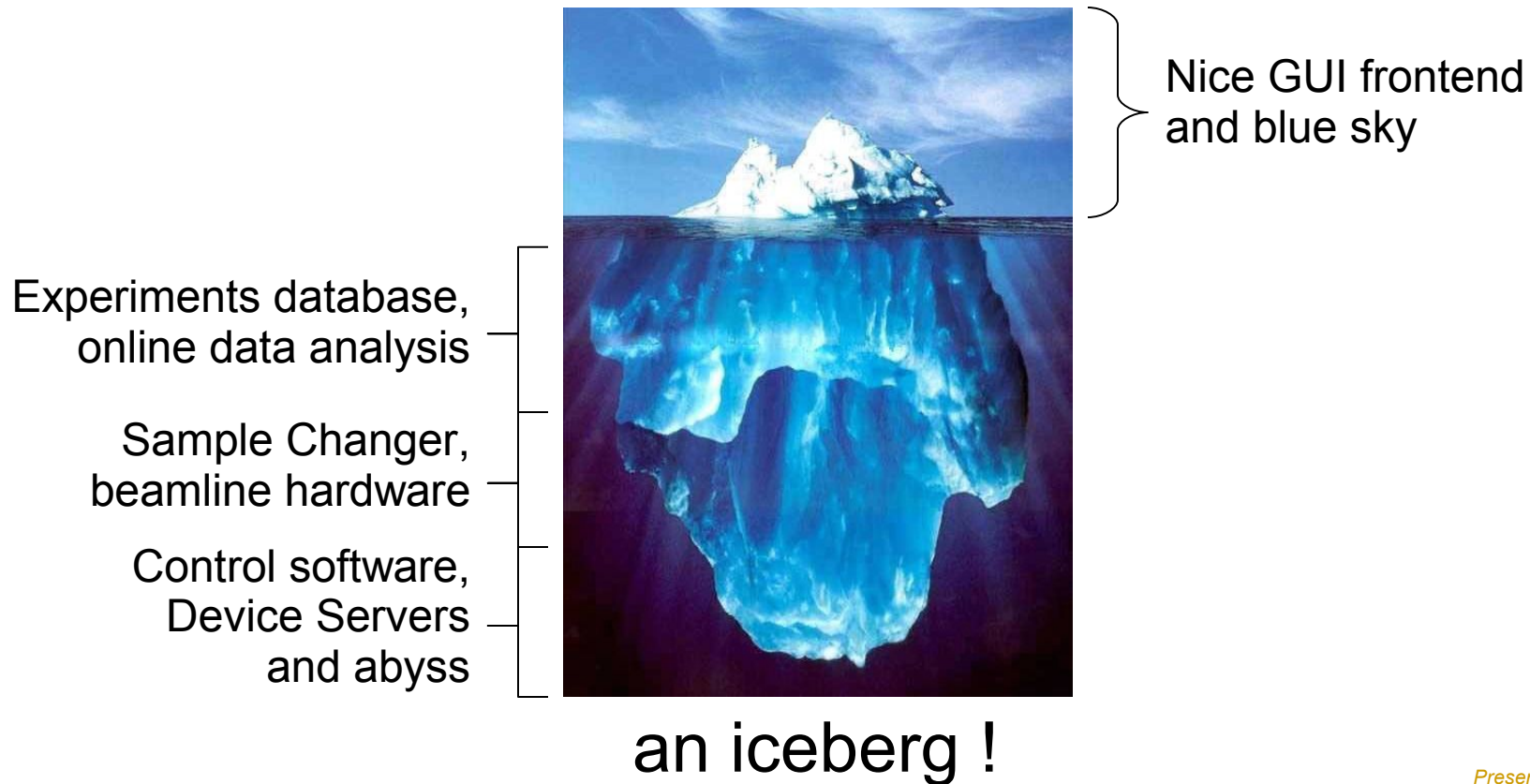


What is mxCuBE ?

- **mxCuBE** stands for
macromolecular xtallography
Customized Beamline Environment
- it is the name of the **graphical frontend application** dedicated to MX beamlines users
- it replaces the former ProDC
- running on **7 MX end-stations since december, 2005**

What is mxCuBE ?

Considering the whole project, it can be seen as...

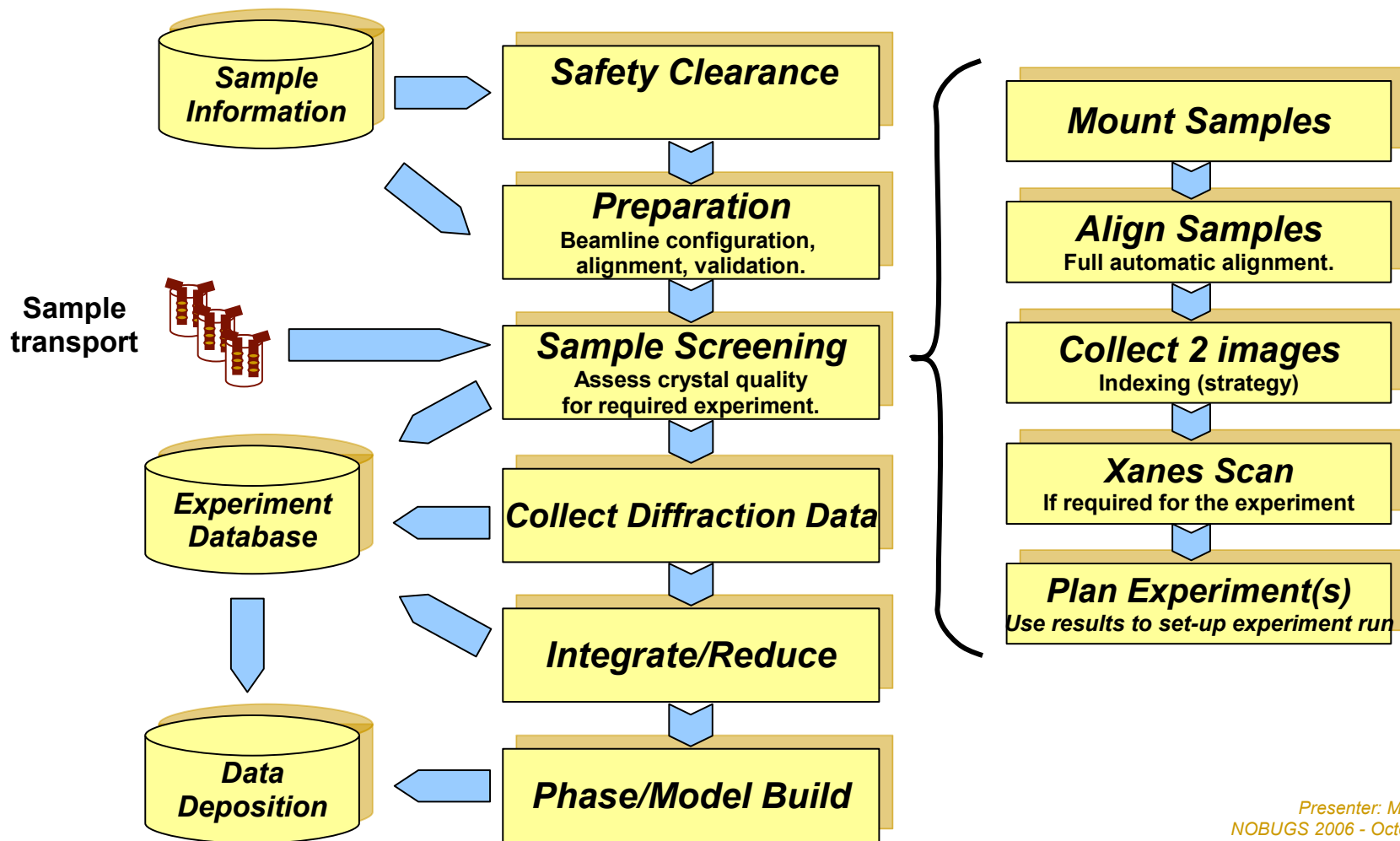


Technical choices

The mxCuBE project follows the Bliss group standards

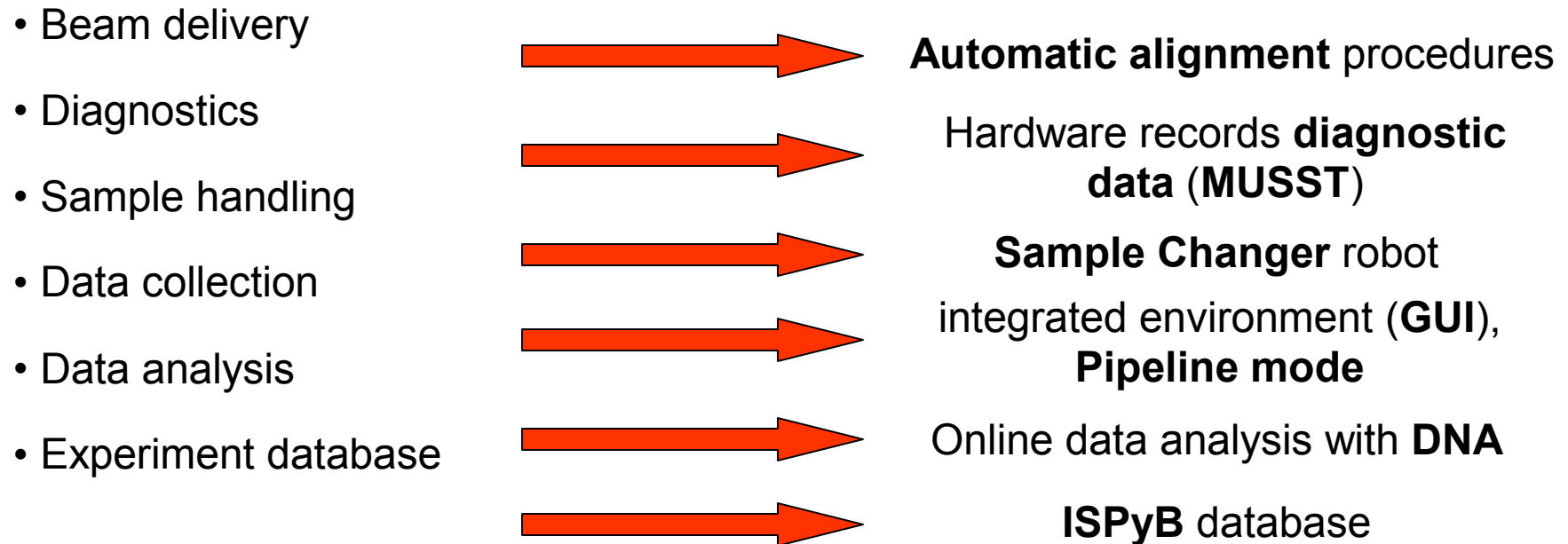
- mxCuBE GUI is built on top of the **Bliss Framework**
(already presented at NOBUGS 2004, PSI, Switzerland)
- **sequences** are mainly run by **Spec** : single data collection, scans, beamline alignment, etc.
- access to hardware is made through **Taco and Tango Device Servers**

The typical MX experiment

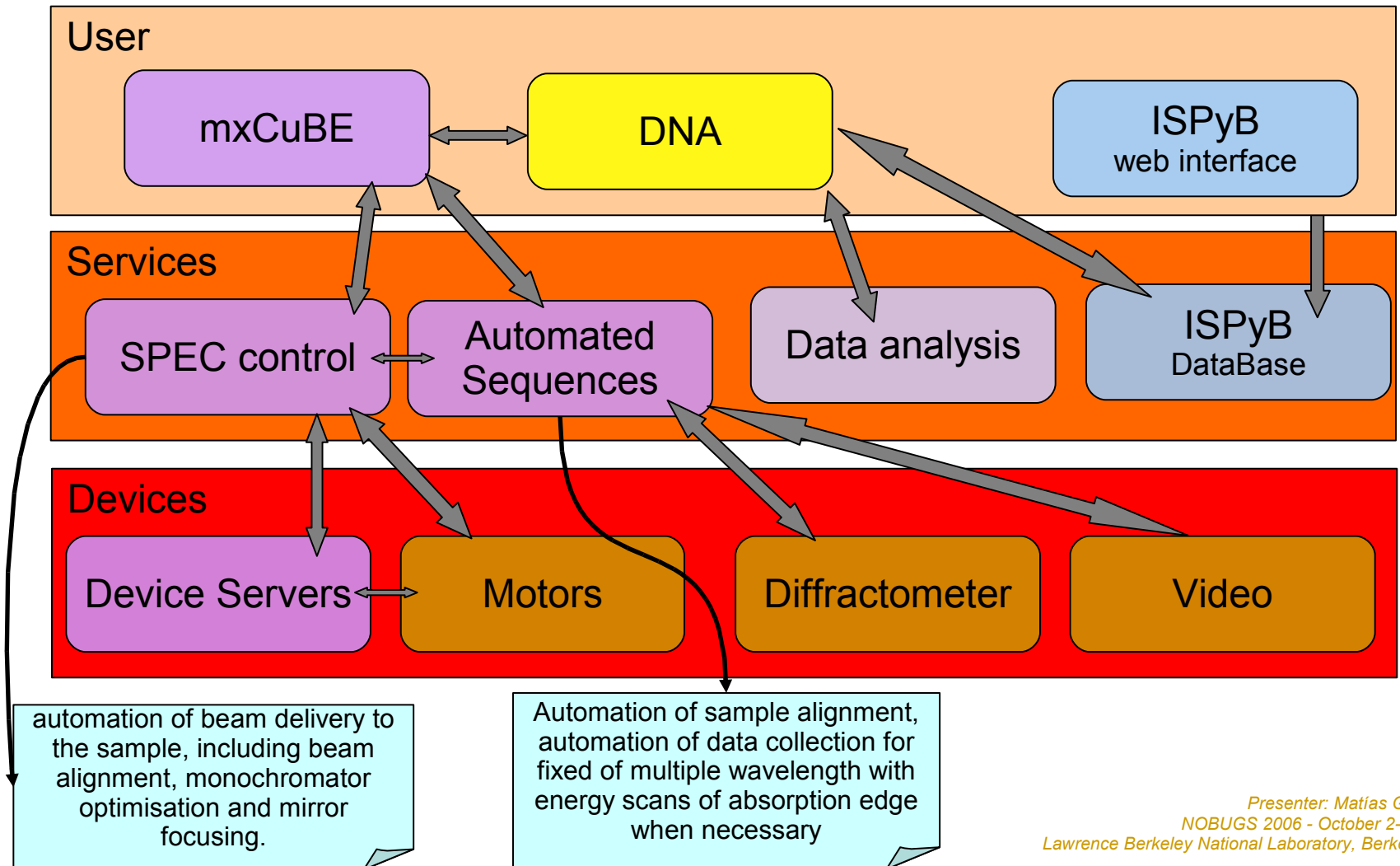


mxCuBE project

The mxCuBE project responds to the need for MX experiments automation



General overview of the different pieces



Presentation highlights

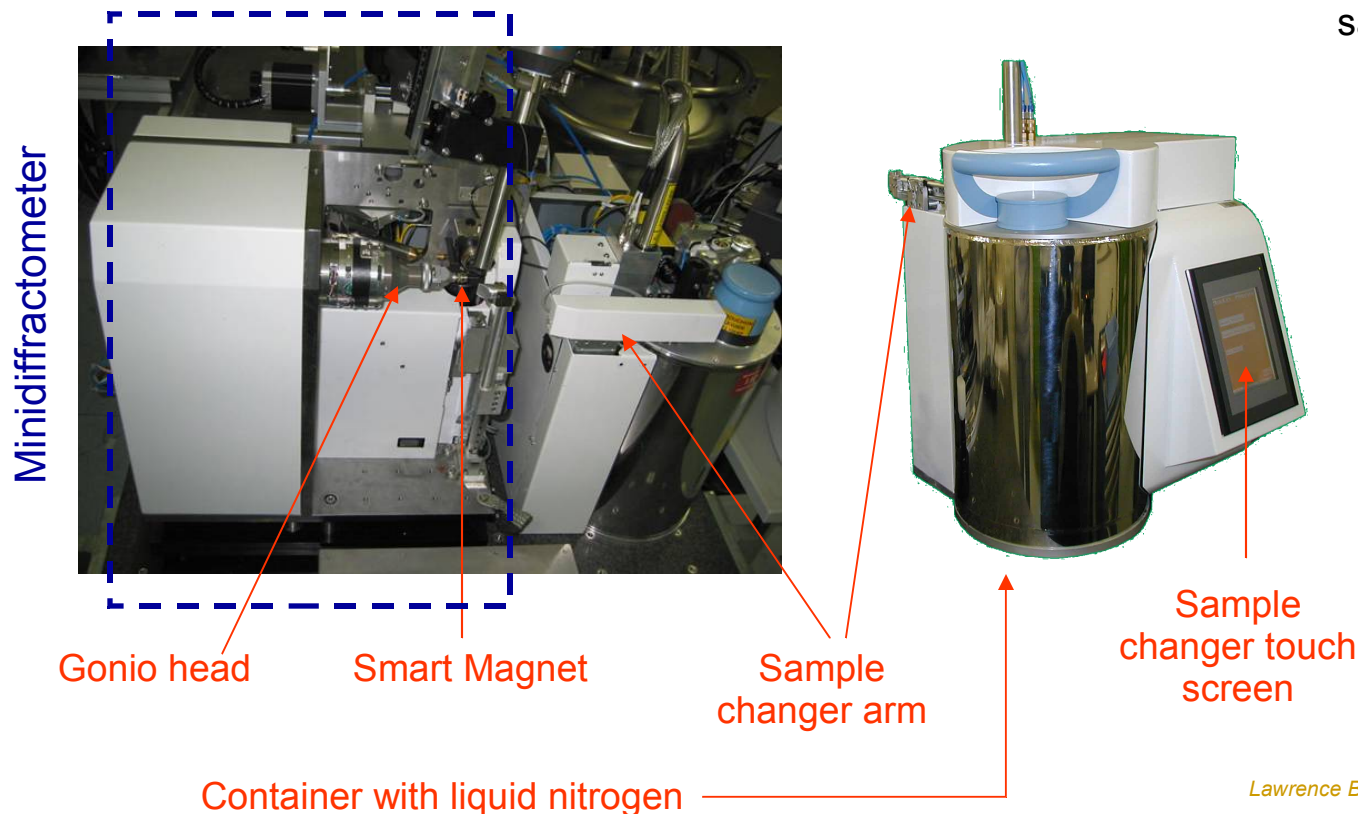
Next slides will focus on

- Sample Changer robot integration within mxCuBE
- automatic centring of samples within mxCuBE
- synchronization, diagnostic and fast energy scans with the MUSST card
- data collection in mxCuBE
- online data analysis with DNA
- integration with ISPyB, our experiments database

Sample Changer integration

SC3 Sample Changer

- can contain 5 baskets of 10 samples each



European SPINE standard
sample holder and vials

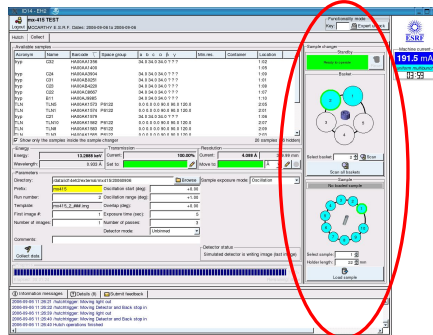
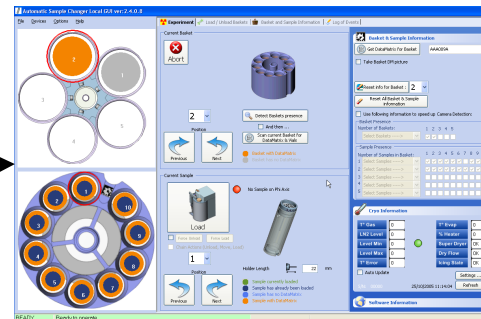


Sample Changer integration (2/3)

The SC3 Sample Changer comes with a Tango Device Server and a Windows control application



PMAC
motor controller



Sample Changer “brick” in mxCuBE GUI

Sample Changer
Hardware Object
(Python)

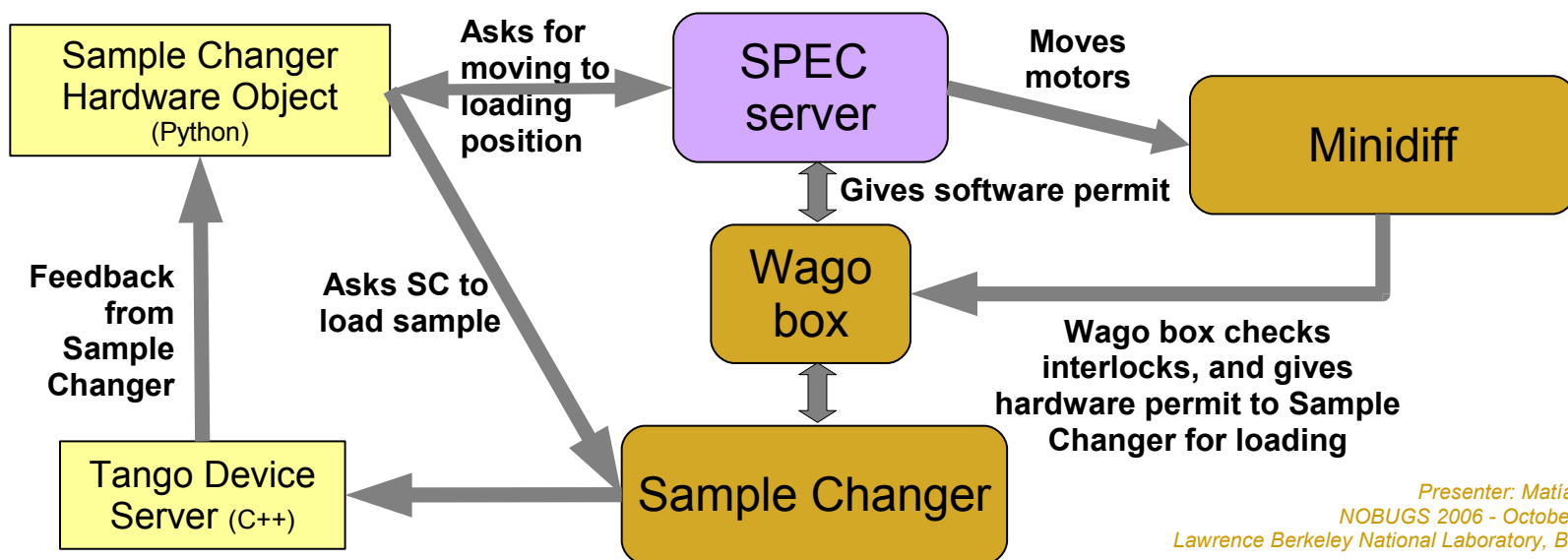
Tango Device
Server (C++)

Sample Changer integration (3/3)

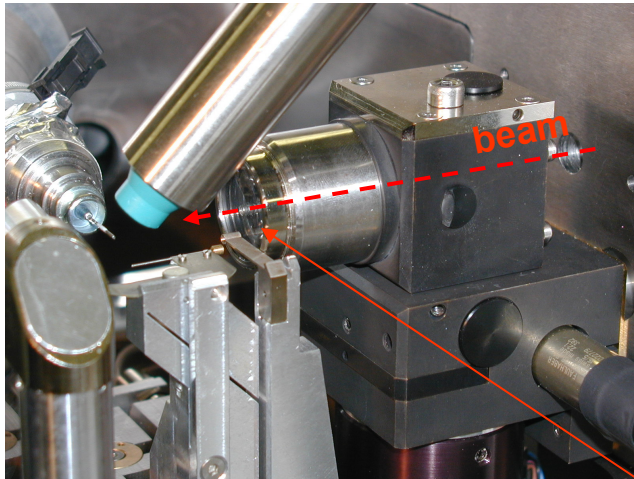
The SC3 Sample Changer is tightly associated with the MD2 Minidiffractometer

- Interlocks have to be managed for safety issues : sample changer cannot load/unload if minidiff is moving, for example
- Checks are done on the Hardware side through a Wago box running a PLC, and software gives or revokes “permits” for Sample Changer and Minidiff

Interactions when loading a sample



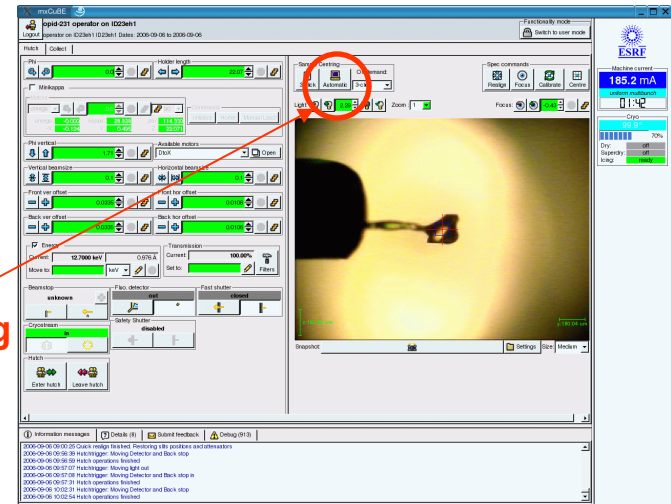
Automatic Sample Centring



Mounted sample on the minidiff

auto-centring
button

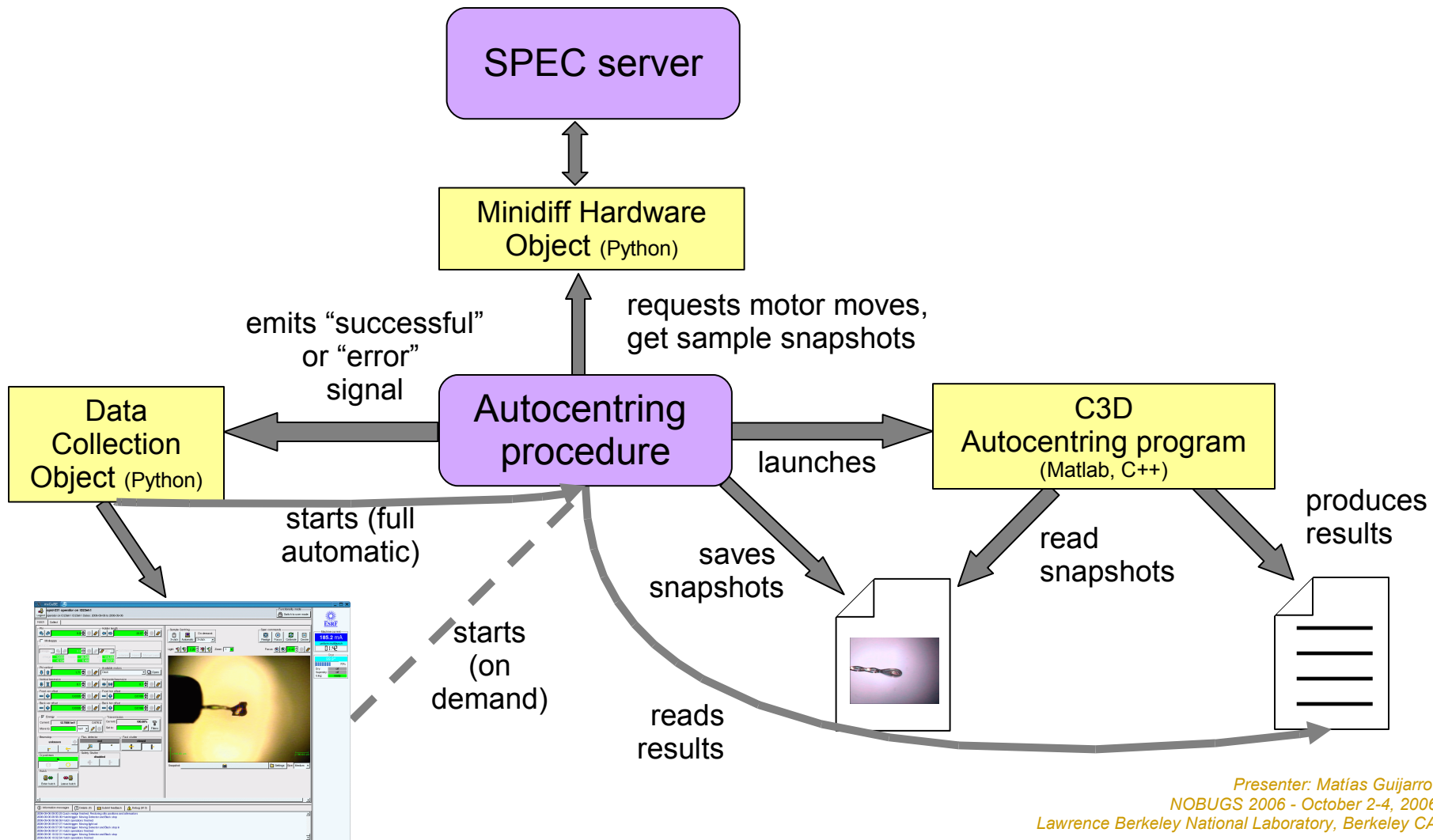
on-axis viewer



Live video in mxCuBE GUI

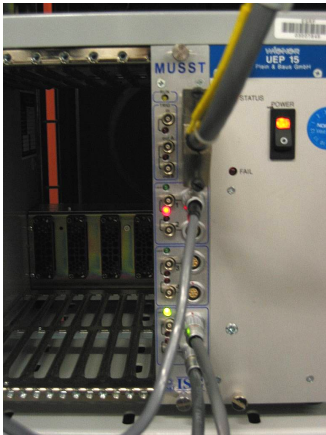
- Automatic Sample Centring is realised by **analysing snapshots** took with the video camera inside the minidiff, through the **on-axis viewer**
- mxCuBE runs **C3D by Bernard Lavault** (EMBL Grenoble) and interprets results to achieve Automatic Sample Centring
- users can decide to do automatic centring with the auto-centring button ; **the full automatic mode (Pipeline) does it by default when a sample is mounted**

Automatic Sample Centring (2/2)



Synchronization, diagnostic and fast scans with the MUSST card

Latest electronics developments at ESRF facilitates hardware and software interaction, and opens new opportunities



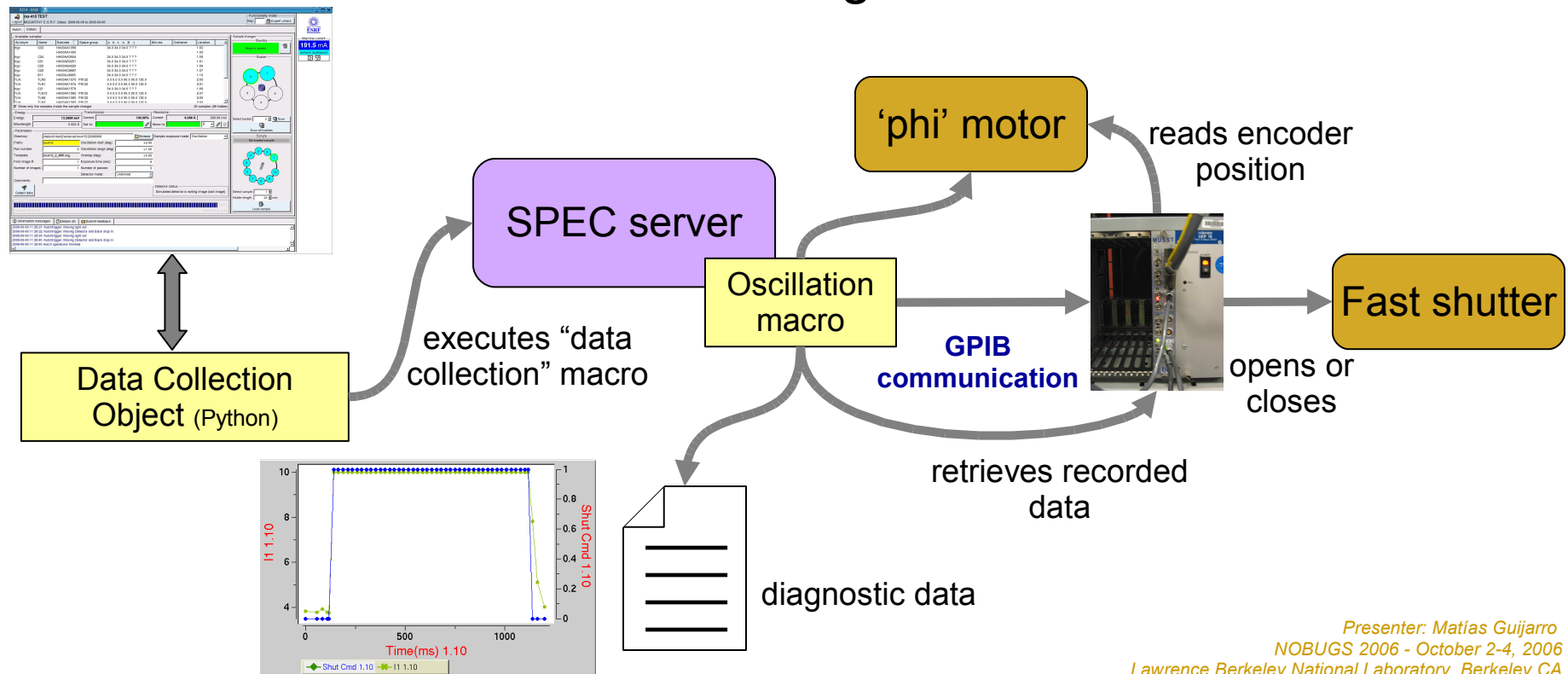
MUSST card in its rack

- MUSST card allows to **synchronize I/O** against **encoder motor positions**
- MUSST card **records I/O data** on different channels at the same time, and **stores it**
- MUSST card **runs programs**, that can be **loaded dynamically**

On MX beamlines, MUSST is used for fast shutter synchro and to do fast energy scans

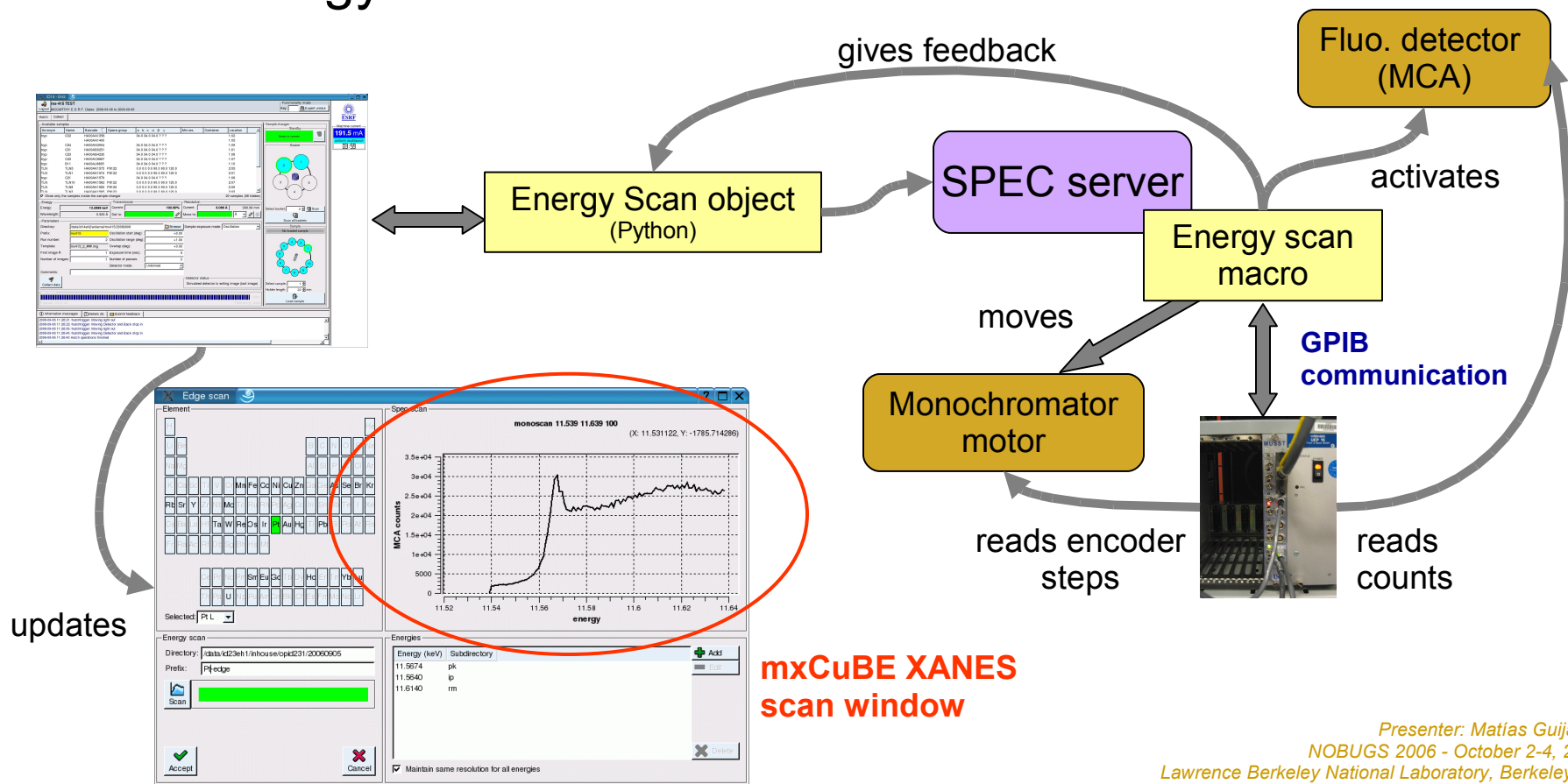
Synchronization, diagnostic and fast scans with the MUSST card (2/3)

1. Synchronization and diagnostic for fast shutter opening and closing



Synchronization, diagnostic and fast scans with the MUSST card (3/3)

2. Fast energy scans : continuous motor move

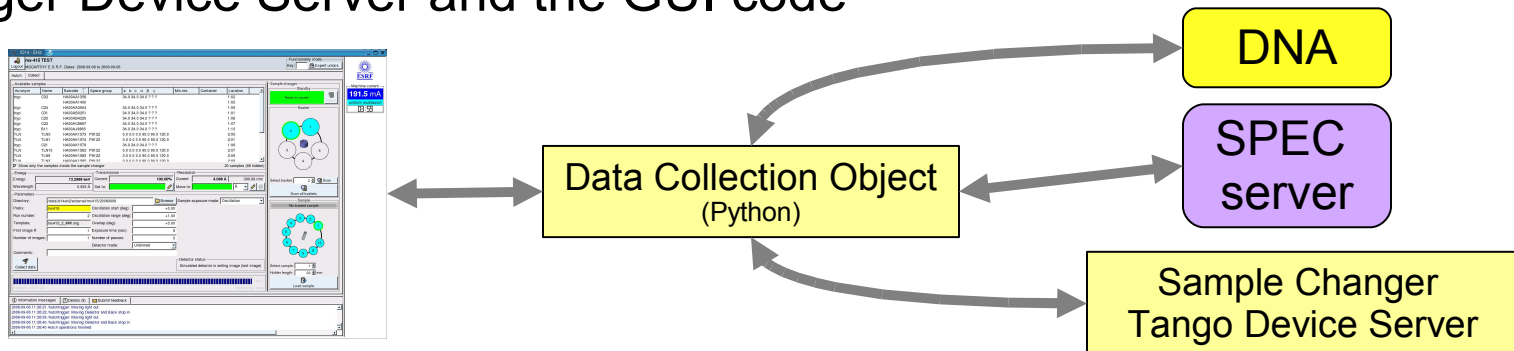


Data collection in mxCuBE

Two ways of collecting data in mxCuBE

- manual mode : users can select a sample to mount, adjust collect parameters and start a Data Collection
- **pipeline mode** : data collection is done automatically ; it loads, centres, screens, collects data, does online data analysis (with DNA) and saves results automatically

The **Data Collection Object** adds a layer between Spec, DNA, the Sample Changer Device Server and the GUI code



What's missing ?

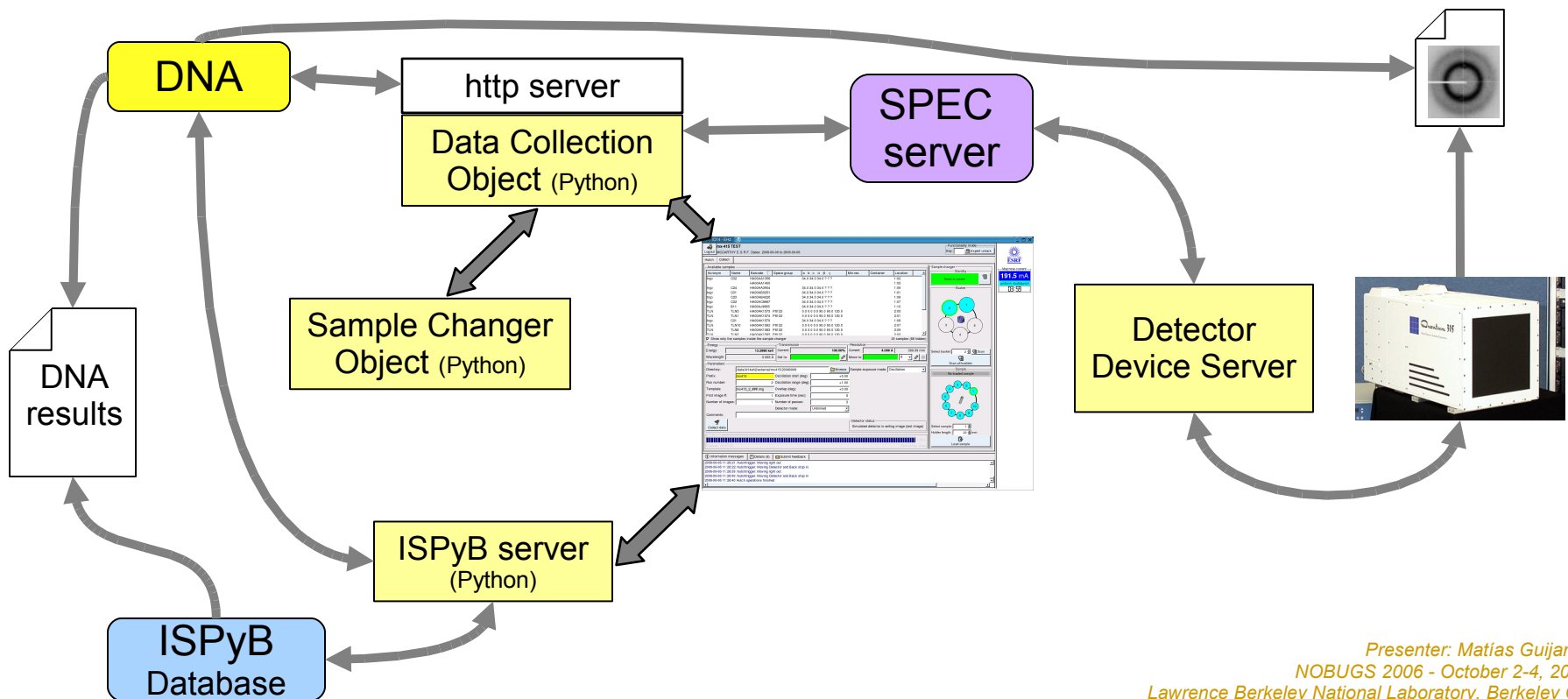
- We should have full-featured **multi-samples, multiple runs** Data Collection available in mxCuBE for christmas



Online data analysis with DNA

DNA asks mxCuBE (BCM) to screen samples and collect data ; it then can produce integration results on the fly (and more...)

- the following scheme shows how everything interacts with DNA



Experiment database : ISPyB

- What is it ?

A Laboratory Information Management System (LIMS)
linking crystals to their corresponding X-ray data

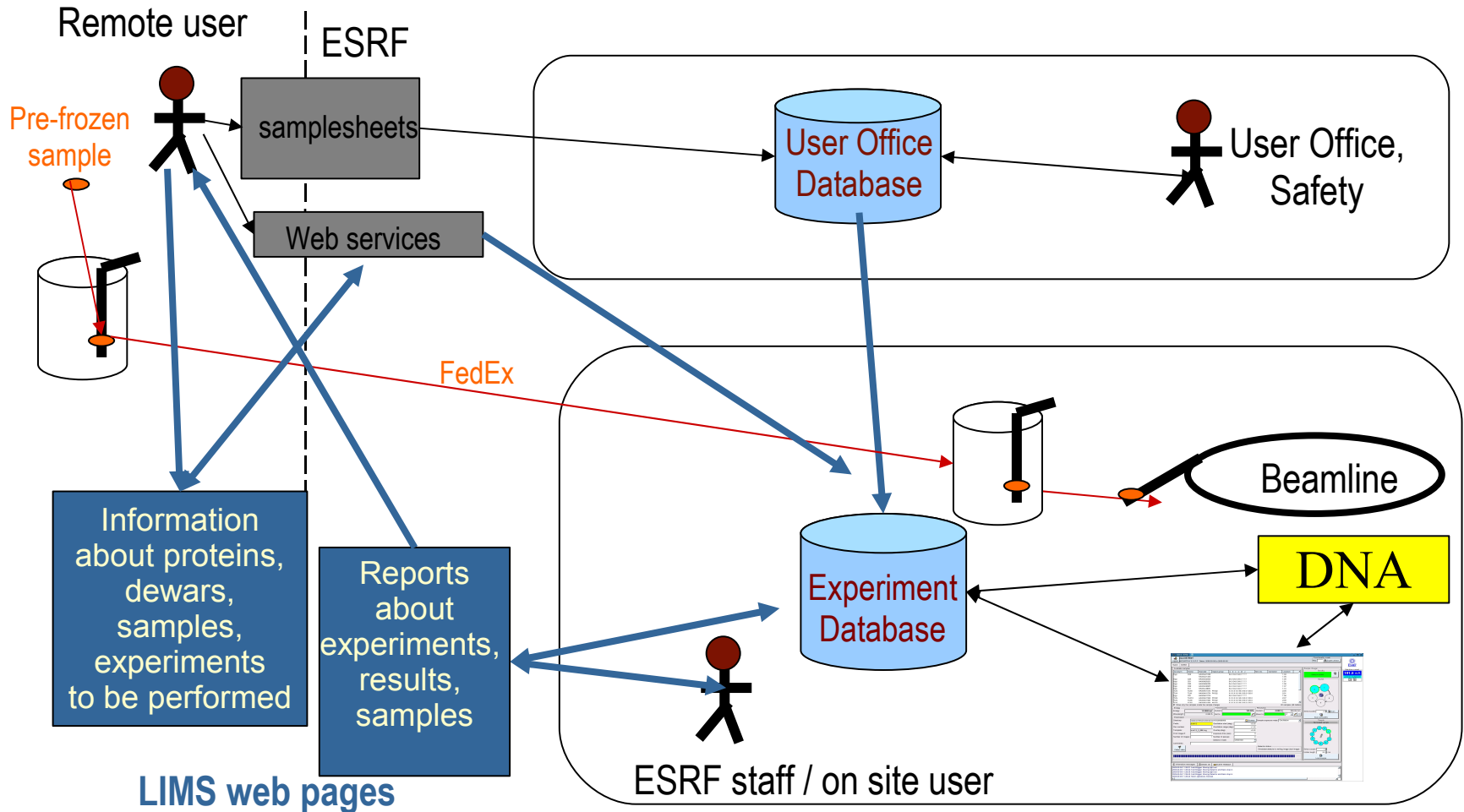


Age: 1 year

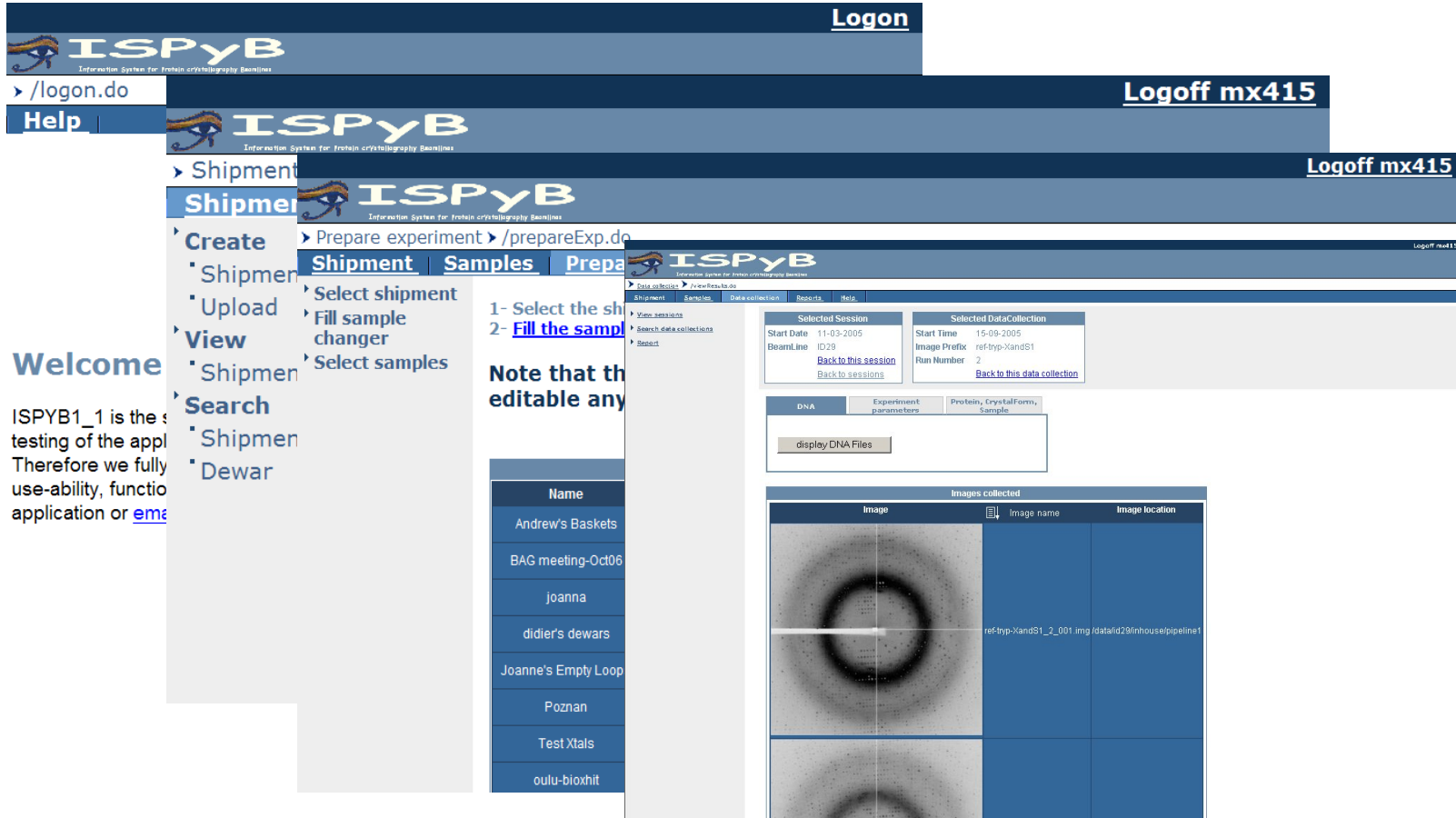
Replaces Pxweb our former LIMS
(zope+python/ MySQL database)

- Written in Java in order to be compatible with other synchrotrons and inhouse databases (SMIS)

ISPyB : information flow



ISPyB web interface



ISPyB
Interaction System for Protein crystallography Beamlines

[Logon](#) [Logoff mx415](#)

[Help](#) [Logoff mx415](#)

[Shipment](#) [Shipmer](#) [Create](#) [Prepare experiment](#) [/prepareExp.do](#)

[Shipment](#) [Samples](#) [Prepa](#)

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Welcome

ISPYB1_1 is the s
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use-ability, functio
application or [eme](#)

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editable any**

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BAG meeting-Oct06
joanna
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Joanne's Empty Loop
Poznan
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Selected Session

Start Date	11-03-2005
BeamLine	ID29
Back to this session	
Back to sessions	

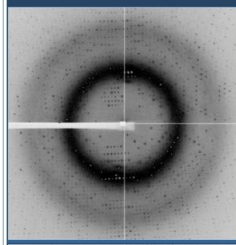
Selected DataCollection

Start Time	15-09-2005
Image Prefix	ref-tyr-xandS1
Run Number	2
Back to this data collection	

DNA **Experiment parameters** **Protein, Crystal Form, Sample**

[display DNA Files](#)

Images collected

Image	Image name	Image location
	ref-tyr-xandS1_2_001_img	IdatId29/inhouse/pipeline1

Conclusion

- mxCuBE is a huge project, the main issue is to deal with all the interactions between "systems"
- The Model-View-Controller pattern enforced by the Bliss Framework helped to have clear "layers of responsibility"
- It is very convenient to have an external Sequencer program, in order to improve robustness and flexibility

Plans for the (near) future :

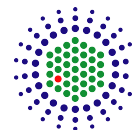
- Remote access facility
- Full featured multi-samples/multi-runs data collections
- Improvements on online data analysis
- Automatic centring with UV light (UV Laser)

Many thanks to...



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Others

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For more info ...

*High-throughput sample handling and data collection at synchrotrons: embedding the ESRF into the high-throughput gene to structure pipeline, **Beteva A. et al.** Acta Crystallographica Section D ((2006) D62 in press)*

*Automation of sample mounting for macromolecular crystallography, **F. Cipriani, F. Felisaz, L. Launer, J.-S. Aksoy, H. Caserotto, S. Cusack, M. Dallery, F.di-Chiaro, M. Guijarro, J. Huet, S. Larsen, Mario Lentini, J. McCarthy, S. McSweeney, R. Ravelli, M. Renier, C. Taffut, A. Thompson, G. A. Leonard and M. A. Walsh**, Acta Crystallographica Section D ((2006) D62 in press)*

*C3D: a program for the automated centring of cryo-cooled crystals, **Andrey, P., Lavault, B., Cipriani, F. & Maurin, Y.** J. Appl. Cryst. 37, 265-269. Acta D (under press)*

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