mxCuBE:
software & hardware progress
of crystallography beamlines
at ESRF

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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…

Experiments database, online data analysis
Sample Changer, beamline hardware
Control software, Device Servers and abyss

an iceberg!

Nice GUI frontend and blue sky
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

- **Sample Information**
- **Safety Clearance**
- **Preparation**
  - Beamline configuration, alignment, validation.
- **Sample Screening**
  - Assess crystal quality for required experiment.
- **Collect Diffraction Data**
- **Integrate/Reduce**
- **Phase/Model Build**
- **Mount Samples**
- **Align Samples**
  - Full automatic alignment.
- **Collect 2 images**
  - Indexing (strategy)
- **Xanes Scan**
  - If required for the experiment
- **Plan Experiment(s)**
  - Use results to set-up experiment run

Sample transport
The mxCuBE project responds to the need for MX experiments automation

- Beam delivery
- Diagnostics
- Sample handling
- Data collection
- Data analysis
- Experiment database

Automatic alignment procedures

Hardware records diagnostic data (MUSST)

Sample Changer robot integrated environment (GUI), Pipeline mode

Online data analysis with DNA ISPyB database
General overview of the different pieces

User
- mxCuBE
- DNA
- ISPyB web interface

Services
- SPEC control
- Automated Sequences
- Data analysis
- ISPyB DataBase

Devices
- Device Servers
- Motors
- Diffractometer
- Video

Automation of beam delivery to the sample, including beam alignment, monochromator optimisation and mirror focusing.

Automation of sample alignment, automation of data collection for fixed of multiple wavelength with energy scans of absorption edge when necessary.
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
Sample Changer integration (2/3)

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

Sample Changer “brick” in mxCuBE GUI
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**

- Sample Changer Hardware Object (Python)
- Asks for moving to loading position
- Asks SC to load sample
- Feedback from Sample Changer
- SPEC server
- Moves motors
- Gives software permit
- Wago box
- Wago box checks interlocks, and gives hardware permit to Sample Changer for loading
- Sample Changer
- Tango Device Server (C++)
Automatic Sample Centring

- 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)

SPEC server

Minidiff Hardware Object (Python)

emits “successful” or “error” signal
requests motor moves, get sample snapshots

Data Collection Object (Python)

starts (full automatic)
starts (on demand)

Autocentring procedure

launches

C3D Autocentring program (Matlab, C++)

produces results

reads results

saves snapshots

reads snapshots

emits “successful” or “error” signal
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 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

SPEC server

Data Collection Object (Python)

executes “data collection” macro

Oscillation macro

‘phi’ motor

reads encoder position

GPIB communication

Fast shutter

opens or closes

retrieves recorded data

diagnostic data

SPEC server

executes “data collection” macro

Oscillation macro

‘phi’ motor

reads encoder position

GPIB communication

Fast shutter

opens or closes

retrieves recorded data

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

2. Fast energy scans: continuous motor move

- Energy Scan object (Python)
- SPEC server
- Energy scan macro
- Monochromator motor
- Fluo. detector (MCA)
- GPIB communication
- mxCuBE XANES scan window

Fluo. detector activates and reads counts.
Energy scan macro moves monochromator motor.
Energy Scan object gives feedback.
Monochromator motor reads encoder steps.
SPEC server updates.
GPIB communication.

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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

Remote user → Pre-frozen sample → LIMS web pages

Remote user → Web services → User Office Database

ESRF staff / on site user → DNA

User Office, Safety

Experiment Database

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

Reports about experiments, results, samples
ISPyB web interface
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)
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For more info...

