



# MXCuBE3



# Macromolecular Crystallography Beamline Customized Beamline Environment

- The first version was deployed at the ESRF in 2005
- Soon after followed by installation/adaptation to other soon-to-be partners
- In 2012 the collaboration is established between



- In 2013 the deployment of **MXCuBE2** at ESRF and soon after at the other sites
- In 2014 two new partners join the collaboration

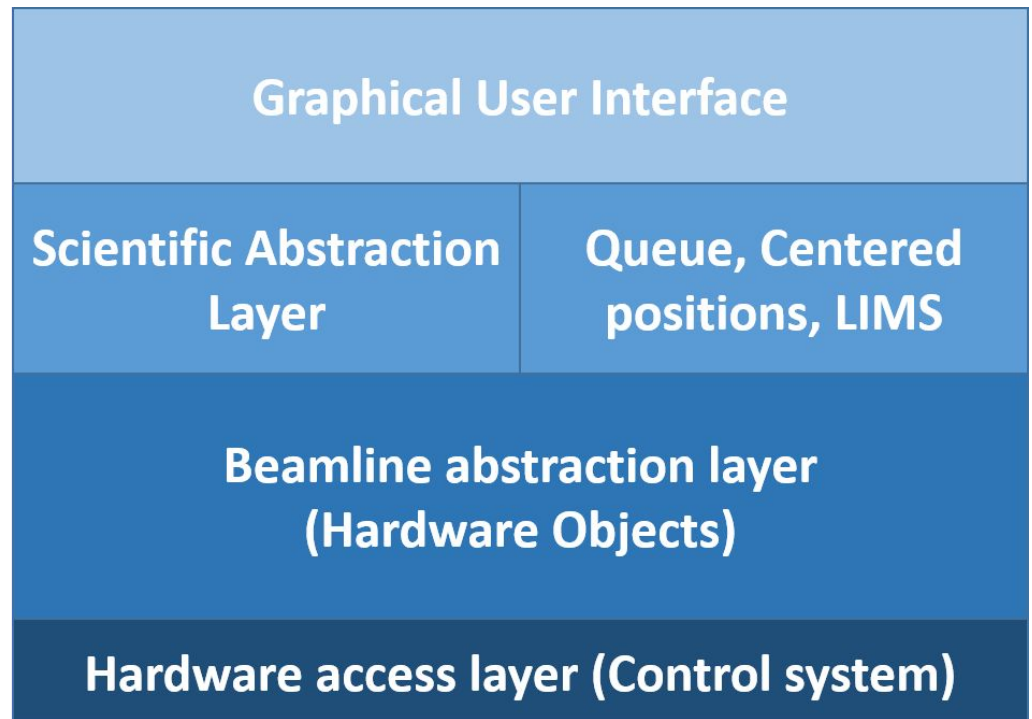


- In 2016 MAXIV and ESRF start working on the new GUI **MXCuBE3**
- In 2018 **MXCuBE3** is being deployed
- Two new partners are in the process of joining the collaboration



- MXCuBE2 introduced a decoupling of interface and an abstraction layer to boost collaboration

- A GUI independent of the control system
  - Data collection methods, on sample tools (points, grid, lines) and a door for external descriptors
  - An abstraction layer to ease compatibility and deployment at any site



MXCuBE2 was explicitly designed for:

- High-throughput data collection
- Hands-off data collection
- Perform more elaborated data collection for complex experiments
  
- Adaptable to any hardware environment
- Scalable with time
  
- But the MXCuBE collaboration eventually became not just MXCuBE
  
- But it stimulates and facilitates collaboration and sharing on EDNA, Workflows, Device servers (CATS), kappa goniometers, automatic centring libraries, autoprocessing pipelines, ...

Sample(s)

Position ( $\kappa$ - $\varphi$ )

Data collection

- MXCuBE2 works by sample:position:data collection
- Any arbitrary combination is possible

Sample(s)

Position-1 ( $\kappa$ - $\varphi$ )

Data collection 1

Data collection 2

Data collection 3

Position-2 ( $\kappa$ - $\varphi$ )

Data collection 4

Position-3 ( $\kappa$ - $\varphi$ )

Data collection 5

Data collection 6

- Sample changers got larger capacity
- Data collection got faster and faster
- And experiment sessions shorter
- More demand for Remote Access
- Synergy with LIMS got stronger
- Novel data collection methods need to be implemented
  
- In other words: MXCuBE2 GUI had to be improved and evolve!

- We prepared a survey for the user community to understand (or confirm)
- What users like of MXCuBE2, and what they would improve
- What are their working protocols
- And use the outcome as inspiration for a new GUI

← MXCuBE3 questionnaire

QUESTIONS RESPONSES 171

## MXCuBE3 questionnaire

Form description

⋮

What description better reflects the way you work?

Sample by sample (load,characterize, collect, unload - all manual)

Pipeline (queue data collections to multiple samples - for screening, evaluation, systematic data collection)

Project by project (start from a project, and look for best crystal)

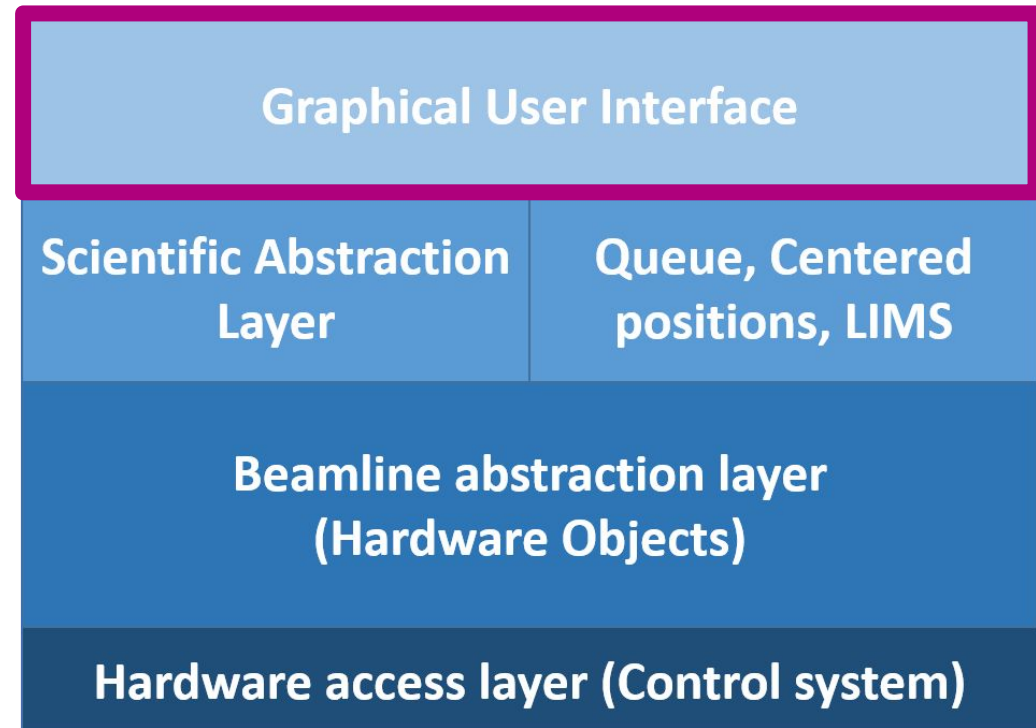
How would you describe your usage of MXCuBE2

Basic (ex. characterize & collect)

ESRF

- In close collaboration with MAXIV we started the MXCuBE3 project
- Design a new GUI, with minimal adaptation to the other parts
- This ensures back-compatibility and facilitates transition to the new interface to every partners

- Qt3 was becoming obsolete
- Design the new interface in web technology: MXCuBE3 as a web app!





- The advantages of a web application:
  - Remote by design
  - No need to install extra software but a recent browser
  - Large developer community
  - Use of modern Library developed and maintained by large IT companies
  - Faster to modify, test, maintain
  - See Marcus' talk for technical details

- An overview on all the projects present in the sample changer robot, with smart filtering and sorting
- Synchronized with ISPyB

The screenshot displays the MXCuBE 3 Sample Overview interface. The window title is "MXCuBE 3" and the main title bar shows "Sample Overview" with sub-tabs for "Data collection", "Sample Changer", and "System log".

At the top, there are controls for "Get samples from SC", "ISPyB", and "Clear sample list". A "Filter:" input field and an "Add to Queue" button are also present. A green button in the top right corner indicates "Collect 14/384".

The main area is a grid of 140 sample project cards, arranged in 14 rows and 10 columns. Each card shows a sample ID (e.g., "Sample-1:1:01") and a timestamp (e.g., "1:1:01"). Some cards have a "DC" button and a checkmark icon. A dashed blue box highlights a group of cards from "Sample-1:1:05" to "Sample-1:1:07".

A context menu is open over the "Sample-1:1:06" card, listing the following actions:
 

- Add to Queue
- Collect
- + Add
- Data collection
- Characterisation
- Burn strategy
- Dehydration
- MXPressE
- MXPressI
- MXPressO
- Test RD Express
- Trouble shooting
- Trouble shooting Dialog
- Remove
- Remove tasks

- A Data collection view, with interactive operation on the crystal
- Only pertinent options presented to users (if a mesh only mesh data collection types, if a line helical data collections are proposed, etc)

The screenshot displays the MXCuBE 3 software interface. At the top, the title bar reads "MXCuBE 3" and "MxCuBE-3 Proposal: 291". Below the title bar, there are navigation tabs: "Sample Overview", "Data collection", "Sample Changer", and "System log".

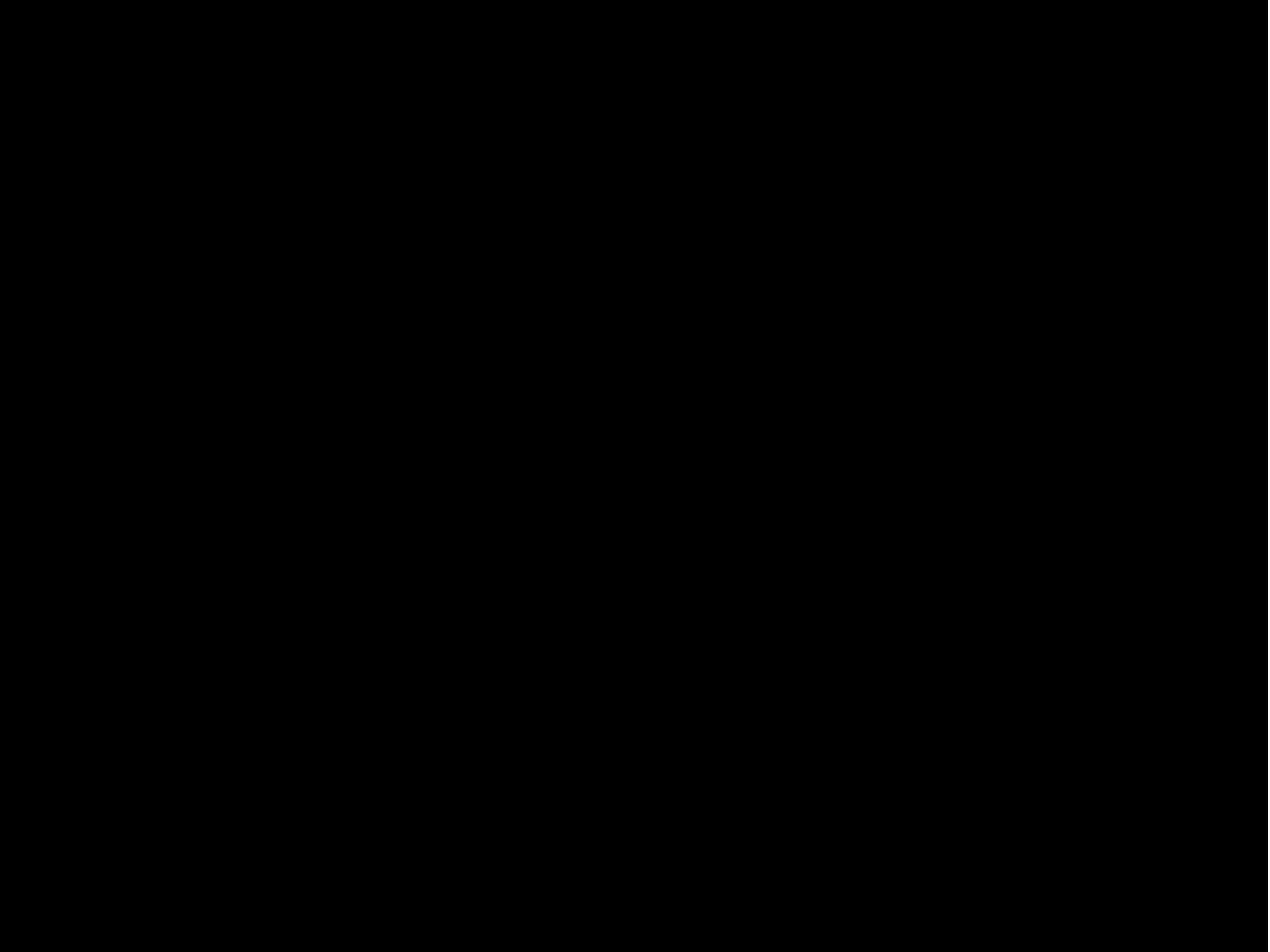
The main interface is divided into several sections:

- Beamline Actions:** A dropdown menu on the left.
- Parameters:** Energy: 11.5627 keV, Wavelength: 1.0723 Å, Resolution: 4.000 Å, Detector: 754.569 mm, Transmission: 50.104 %, Flux: 0, Cryo: 0.
- Aperture Control:** A dropdown menu set to "30".
- Omega:** 164.34 (range 10°).
- Kappa:** 0.00 (range 0.1°).
- Phi:** 0.00 (range 0.1°).
- Y:** -0.486 (range 0.1 mm).
- Z:** -0.145 (range 0.1 mm).
- Focus:** -0.000 (range 0.05 mm).
- Samp-X:** 0.453 (range 0.1 mm).
- Samp-Y:** 0.287 (range 0.1 mm).

The central area shows a live video feed of a dark, elongated crystal sample with a circular hole at one end. A blue crosshair is centered on the hole. A 50 µm scale bar is visible in the bottom left corner. Above the video feed is a toolbar with icons for Snapshot, Draw grid, 3-click Centring, Zoom, Backlight, Frontlight, and Video size.

On the right side, there are status indicators for "Beamstop" (OUT), "Fast Shutter" (CLOSED), "Safety Shutter" (---), and "Ring Current". Below these is a "Run Queue" section with a "Settings" dropdown and a "Queued Samples (0)" indicator.









# Miscellanea

The screenshot displays a software interface for a microscope system. The main window is titled "Microscope" and contains a large dark field image with a bright spot in the center. The interface is divided into several sections:

- Top Panel:** Contains status information such as "Range: 1.000 um", "Resolution: 0.000 um", "Temperature: 0.000 °C", and "Speed: 0.000 um/s".
- Left Panel:** A vertical sidebar with various control buttons and indicators, including "Range", "Focus", "Z", "Y", "X", "Home", "Stop", and "Start".
- Right Panel:** A control panel with buttons for "Stop", "Home", "Start", and "Pause". It also displays "Range: 0.000 um" and "Speed: 0.000 um/s".
- Bottom Panel:** A horizontal bar with a green arrow pointing right.



Source Status: ON

Energy: 22.700 keV  
Wavelength: 0.00054

Resolution: 0.002 Å  
Detector: 001001 (mm)

Transmission: 100.000 %  
Pile: 0.00e+00

Exp: 0

Start Stop Pause Clear

- Aperture Control ⊞
- Energy ⊞
- Slits ⊞
- PS ⊞
- W ⊞
- Y ⊞
- Z ⊞
- Power ⊞
- Step 1 ⊞
- Step 2 ⊞

⊞
⊞
⊞
⊞

Characterization: Energy: Reflector being estimated, time to reach Henderson limit: 24.8 s

Characterization: Energy: Slits: used completeness = 2.6, aimed resolution = 0.002 Å, complexity = none

Characterization: Energy: Collector pair 1: Resolution limit is set by the crystal detector max distance limit

Characterization: Energy: Slitting resolution: 0.002 Å

Characterization: Energy: wedge 1: resolution 0.002 Å, roll wedge 1: start 0.00, image 0.0, width 0.00, time 0.00 (s), transmission: 1.00

Characterization: Energy: Wedge no (image 0.0, Wedge exposure time: 7.0 (s)

Characterization: Energy: calculated successful

Characterization: Energy: Reflector being estimated, time to reach Henderson limit: 24.8 s

Characterization: Energy: Slits: used completeness = 2.6, aimed resolution = 0.002 Å, complexity = none

Characterization: Energy: Collector pair 1: Resolution limit is set by the crystal detector max distance limit

Characterization: Energy: Slitting resolution: 0.002 Å

Characterization: Energy: wedge 1: resolution 0.002 Å, roll wedge 1: start 0.00, image 0.0, width 0.00, time 0.00 (s), transmission: 1.00

⊞ Settings

Sample: 000 - 01
Current Samples: (0)

**PS Characterization**

- A docker image is available here  
[https://hub.docker.com/r/oscarosso/mxcube3\\_debian9/](https://hub.docker.com/r/oscarosso/mxcube3_debian9/)
- Install and start docker
- follow the instruction in the page above
- I have tested successfully in windows (where command should be given in powershell), Linux, and others on MacOS

- ID29 now
- ID23-2 and MASSIF-1
- ID30B and MASSIF-3
- ID23-1

- The MXCuBE Collaboration
- The ESRF Structural Biology Group
- The ESRF Beamline Control Unit (M. Oscarsson, M. Guijarro, A. Beteva)
- MAXIV Biomax team

