



WHERE WE ARE

The screenshot displays the mxCuBE software interface with three highlighted sections:

- SC - Queue (pink border):** A list of tasks on the left side of the interface, including 'Characterisation - 1', 'Diffraction plan - 1', and 'Centring - 1'. The 'Centring - 1' task is currently active and highlighted in blue.
- Sample - Position (blue border):** A central video window showing a 3D model of a sample (a thin rod) with a yellow crosshair indicating its position. The window includes controls for 'Light', 'Focus', 'Front light', and 'Zoom'. Below the video, the 'Aperture diameter' is set to 30.
- Tasks - Data Collection (green border):** A panel on the right side of the interface containing various parameters for data collection, such as 'Oscillation range', 'Energy (KeV)', 'Resolution (Å)', and 'Transmission (%)'. It also includes a 'Collection method' section with 'Discrete' and 'Shutterless' options, and a 'Data location' section with a file name field.

SC - Queue

Sample - Position

Tasks - Data Collection

- MXCuBE2 has introduced some major features:
 - Abstraction of component and data collections
 - Saved positions
 - Data collection methods
 - xmlRPC “programmable” queue
 - Used by Workflows and other experiment descriptors
 - A better usage of mesh
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- And became the basis of a European collaboration



← MXCuBE3 questionnaire

QUESTIONS RESPONSES 171

MXCuBE3 questionnaire

Form description

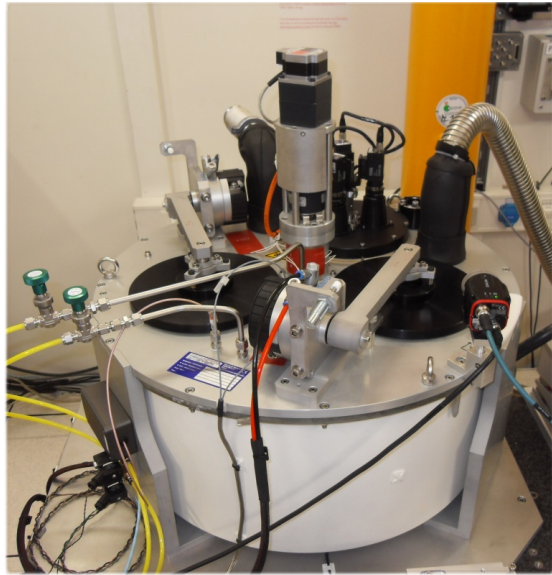
...

What description better reflects the way you work?

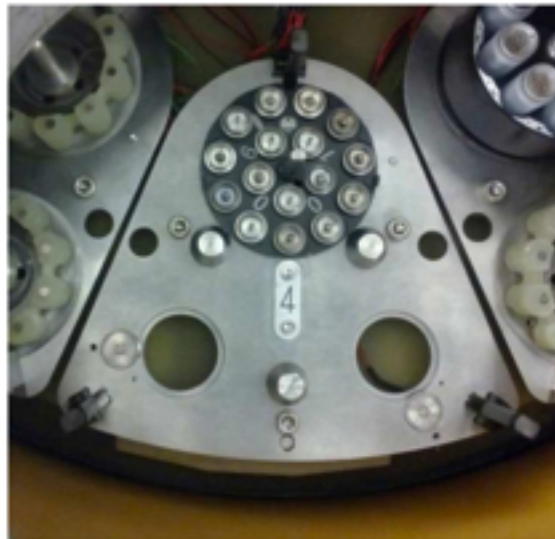
- Sample by sample (load,characterize, collect, unload - all manual)
- Pipeline (queue data collections to multiple samples - for screening, evaluation, systematic data collection)
- Project by project (start from a project, and look for best crystal)

How would you describe your usage of MXCuBE2

- Basic (ex. characterize & collect)



- HCD dewar
 - Spine/Unipuck compatible
 - 12 spine pucks + 11 unipucks + 1 bin
 - 296 Samples
 - 864 MiniSpine samples
- Future sample supports
 - Different support with SBS footprint
 - fluidic chips
 -



QUEUE NOT SUITABLE

The screenshot displays the MX3 control software interface, which is used for managing X-ray diffraction experiments. The interface is divided into several main sections:

- File Instrumentation Help:** Located at the top left, with sub-tabs for 'Collect', 'XRF spectrum', and 'Log'.
- User:** Shows the current user as 'mx-1743' and includes a 'Logout' button.
- Sample list:** A tree view on the left showing a queue of tasks. The first task, '3:1:3 - FluPol-3959_03', is highlighted in green and contains multiple 'mesh-FluPol-3959_03_1' sub-tasks, all of which are marked as 'Collection done'. Below it, the second task, '3:1:4 - FluPol-3959_04', is marked as 'Stopped'.
- Sample centring / Data collection:** A control panel on the right with tabs for 'Sample centring' and 'Data collection'. It includes sliders and buttons for adjusting 'Omega' (754.75), 'Chi' (0.00), 'y' (0.955), 'z' (-0.71), 'sampx' (0.26), and 'samy' (-0.18).
- Sample video:** A live video feed showing a sample on the beamline. The video has a 'Light' control set to 0.90 and a 'Focus' control set to -0.400. A 'Centre beam' button is visible on the left side of the video frame. A scale bar indicates 200 μm .
- Aperture and Move controls:** At the bottom right, there are controls for the 'Aperture' (set to 50 μm) and 'Move' (set to 'Offsets').

- Moving to MXCuBE to web has the main advantage of a closer layout integration (sample information, Diffraction plan, mesh results, auto-processing results)
- Remote by design
- Modern technology
- No need of extra software installation
- Take advantage of web development
- Fast to modify and maintain
- Smooth integration with ISPyB, sharing components

HARDWARE ABSTRACTION LAYER UNCHANGED

Users
Client



**MXCuBE
Server**

Front-End



Back-End



HardwareObjects

SampleChanger Collect Beam DataAnalysis
Detector Diffractometer ISPyBClient ...

Control System

Exporter Tango Sardana ...

Processing
Cluster



Beamline

ISPyB



SAMPLES VIEW

The screenshot displays the MxCuBE-3 operator interface. At the top, there are browser tabs for 'MxCuBE-3 operator' and 'Getting Started'. The address bar shows 'mxcube3.esrf.fr:8081/#/7_k=ten99m'. The interface includes a control bar with 'Get samples from DC', 'ISPyB', 'Clear sample list', a 'Filter' input field, and a '+ En queue sample' button. A 'Collect 0/50' button is located in the top right corner. The main area is a grid of 60 sample cards, arranged in 6 rows and 10 columns. Each card contains a sample ID (e.g., Sample-101 to Sample-508) and a small green icon with a number. A vertical toolbar on the left side contains various icons for navigation and control. At the bottom center, there is an 'Open Log' button.

DATA COLLECTION VIEW

The screenshot displays the MX3 data collection control interface. At the top, a status bar shows: Fast Shutter: CLOSED, Safety Shutter: CLOSED, Energy: 12 keV, Resolution: 3 Å, Transmission: 100%, Cryo: 0 K, Current: 192.45 mA, and Status: Beam delivered. Below this, a central panel features a large image of a sample with a red crosshair. The interface includes several control panels: Omega (0.00, Step size: 90°), Kappa (0.00, Step size: 0.1°), Phi (0.00, Step size: 0.1°), Y (0.00, Step size: 0.1 mm), Z (0.00, Step size: 0.1 mm), and Focus (0.00, Step size: 0.1 mm). A right-hand panel contains a 'Run Queue' section with a 'Total Progress 0/0' indicator and checkboxes for 'Auto loop centring' and 'Automount next sample'. Below this, there are tabs for 'Current' and 'Upcoming', with 'No Sample Mounted' displayed under the 'Current' tab. The bottom of the interface shows a Windows taskbar with the Start button, taskbar icons, and system tray information including the date and time (14:32 06/02/2017).

SAMPLE DETAILS

matr2_1

Characterisation 2:1

matr2_2

Characterisation 2:2

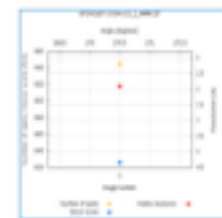
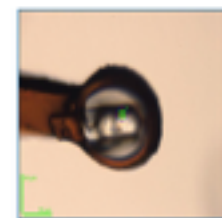
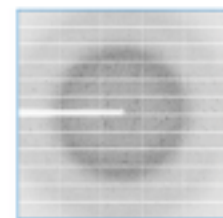
matr2_3

Characterisation 2:3

Run #1: CHARACT[1]18C186 Nov 29, 2016 5:33:44 PM
 /data/125/inhouse/matr1/20161129/RAW_DATA/datasets/b4Gat7/b4Gat7-cn094-x10

Summary | Beamline Parameters | Data Collections 1 | Sample | Results | Workflow

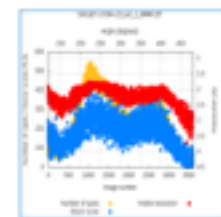
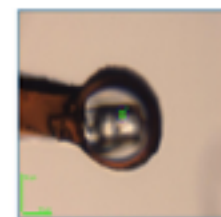
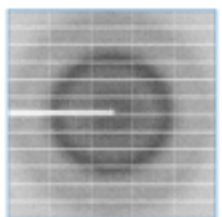
Workflow	Characterisation	Type	Characterisation	Index	Mosicity	0.30
Protein	b4Gat7	Res. (corner)	2.11 Å (1.57 Å)	Strategy	Space Group	P4
Sample	cn094-x10	Wavelength	0.977 Å	Dark Res.	Exp. Time	0.037 s
Prefix	ref-b4Gat7-cn094-x10	Phi range	1°	Images	Total rotation	0.1°
Images	2	Phi start (total)	400° (180°)	Transmission	26.76%	
Transmission	100.00%	Exposure Time	0.037 s	cell A	cell B	cell C
Flux start	6.77e+11 ph/beam	Flux end	6.76e+11 ph/beam	123.79	123.79	87.01
				Alpha	Beta	Gamma
				90.00	90.00	90.00



Run #1: 096 Nov 29, 2016 5:34:45 PM
 /data/125/inhouse/matr1/20161129/RAW_DATA/datasets/b4Gat7/b4Gat7-cn094-x10

Summary | Beamline Parameters | Data Collections 1 | Sample | Results 2 | Workflow

Workflow	096	1 1 2 2	Completeness	Res.	0.5	7.6
Protein	b4Gat7	Inner	100%	2.0	173.4	
Sample	cn094-x10	Outer	100%	2.0	29.9	
Prefix	b4Gat7-cn094-x10_w1	Overall	100%	2.0	29.9	
Images	3600	cell A	cell B	cell C		
Transmission	26.76%	123.94	123.94	87.00		
Flux start	2.01e+11 ph/beam	Alpha	Beta	Gamma		
		90	90	90		



2:1

matr2_1

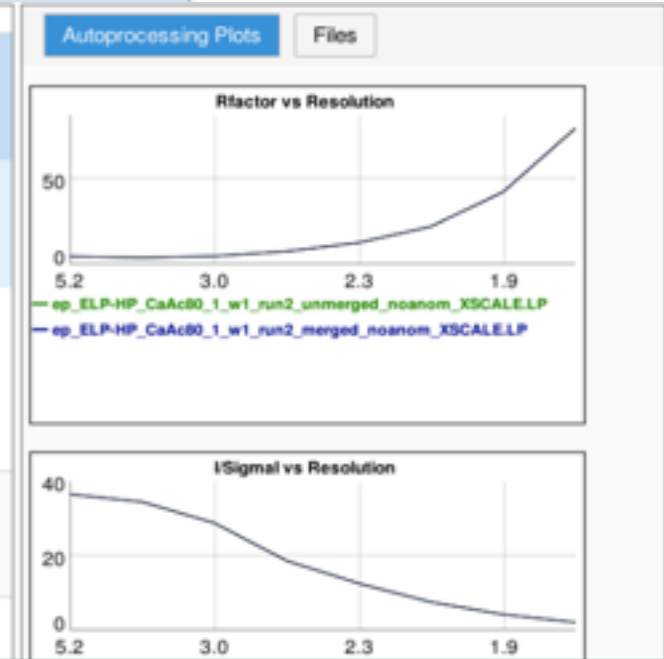
2:2

matr2_2

2:3

matr2_3

Autoprocess...	Unit cell			Statistics				Phasing	
EDNA_proc P 41	a	b	c	Data Range	Resolution	Multiplicity	Completeness	I/σ	
	164.1	164.1	84.0	innerShell	47.4 - 7.2	5.6	99.5	39	
	α	β	γ	outerShell	1.9 - 1.9	5.6	99.0	1.1	
	90.0	90.0	120.0	overall	47.4 - 1.9	6.0	99.6	13	
EDNA_proc P 41	a	b	c	Data Range	Resolution	Multiplicity	Completeness	I/σ	
	164.1	164.1	84.0	innerShell	47.4 - 7.2	5.6	99.5	40	
	α	β	γ	outerShell	1.9 - 1.9	5.6	99.0	1.1	
	90.0	90.0	120.0	overall	47.4 - 1.9	5.9	99.6	14	
grenades_f_ P 4	a	b	c	Data Range	Resolution	Multiplicity	Completeness	I/σ	Space Group
	164.0	164.0	83.9	overall	100.0 - 1.8	5.9	99.5	12	P6
	α	β	γ	innerShell	100.0 - 3.9	5.8	99.8	34	P61
	90.0	90.0	120.0	outerShell	1.9 - 1.8	5.8	99.1	1.1	P62 P63
Open Phasing									
grenades_f_ P 4	a	b	c	Data Range	Resolution	Multiplicity	Completeness	I/σ	
	164.0	164.0	83.9	overall	100.0 - 1.8	5.9	99.5	12	
	α	β	γ	innerShell	100.0 - 3.9	5.8	99.8	34	
	90.0	90.0	120.0	outerShell	1.9 - 1.8	5.8	99.1	1.1	
grenades_ P 321	a	b	c	Data Range	Resolution	Multiplicity	Completeness	I/σ	
	164.0	164.0	83.9	overall	100.0 - 2.1	5.9	99.6	3.1	



SELECT SAMPLES FOR DATA COLLECTION



SELECTED SAMPLES

MX3 operator interface showing a grid of sample cards. The interface includes a top navigation bar with 'Get samples from SC', 'ISPyB', 'Clear sample list', 'Filter', and '+ En-queue sample'. A 'Collect 8/50' button is in the top right. The grid contains cards for samples 101 through 508. The selected cards are Sample 102, 103, 104, 105, 310, 402, and 410. Each selected card has a blue background, a magnifying glass icon, and a 'DC' button. The grid also shows sample numbers 1 through 7 in the bottom right corner of the selected cards.

SMART SORTING/FILTERING

The screenshot displays the MeCuBE-3 operator interface. At the top, there is a browser window with the URL `mxcube3.esrf.fr:3081/#/?_k=ben99m`. Below the browser, a navigation bar includes a "Click to go back, hold to see history" button, an "iSPyB" button, a "Clear sample list" button, a "Filter: 30" input field, and an "En-queue sample" button. A "Collect D/50" button is located in the top right corner. The main area contains a grid of sample cards. The first row consists of eight cards labeled "Sample-301" through "Sample-308", each with a green status indicator in the top right corner. The second row contains a single card labeled "Sample-309" with a green status indicator. A vertical toolbar on the left side of the interface contains several icons for navigation and control. At the bottom center, there is an "Open Log" button.

The screenshot displays the MXCuBE-3 operator interface. At the top, the browser address bar shows the URL `mxcube3.esrf.fr:8081/#/?_k=w01vmg`. The interface includes a control bar with buttons for "Get samples from SC", "ESPyB", "Clear sample list", a "Filter" input set to "10", and "+ En-queue sample". A "Collect 7150" button is located in the top right corner.

The main area contains a grid of sample cards, each representing a different sample. Each card displays a sample ID (e.g., Sample-101 to Sample-110) and a status indicator in a green box (e.g., 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 1.10, 2.10, 3.10, 4.10, 5.10). Some cards also feature a blue button with a white icon (e.g., "DC" or "C").

At the bottom center, there is an "Open Log" button. The left sidebar contains several circular icons for navigation and control.

THE IDEA

The screenshot displays a control interface for a synchrotron beamline. On the left, a list of experiments is shown, with '1:2 - A-TIM-Test02' selected and a blue circle containing the number '1' next to it. The status 'Centring done!' is visible next to the selected experiment. The central area shows a dark image of a sample with a yellow crosshair and a red crosshair, both marked with a blue circle containing the number '1'. A green scale bar indicates 100 μm. Below the image, the 'Aperture' is set to 10 μm. On the right, a 'Standard Collection' dialog box is open, showing acquisition parameters: Oscillation range: 0.1, First image: 1, Oscillation overlap: 0.0, Number of images: 1, Oscillation start: 89.98, Number of passes: 1, Exposure time: 0.037, Energy (KeV): 12.6, Resolution (Å): 3.61, Transmission (%): 49.67. The dialog also shows data location information: Folder: /data/visitor/mx415/d23eh1/20140303/RAW_DATA, File name: A-TIM-Test02_1_###.cbf, Prefix: A-TIM-Test02, Run number: 1.

Omega: 50.80
Step size: 0.1°

Kappa: 0.00
Step size: 0.1°

Phi: 0.00
Step size: 0.1°

Y: 0.50
Step size: 0.1 mm

Z: 0.22
Step size: 0.1 mm

Focus: -0.27
Step size: 0.1 mm

Samp-X: 0.00
Step size: 0.1 mm

Samp-Y: 0.47
Step size: 0.1 mm

Fast Shutter: Open Close
Safety Shutter: Open Close
Beamstop: In Out
Capillary: In Out

Energy: 12.67 keV
Resolution: 1.797 Å

Transmission: 100 %
Detector Distance: 250 mm

Current: -1

Run Queue: Total Progress 56 %

Current: Run Sample
Upcoming: Next Sample

Sample: 3

Open Log

MXCuBE-3 operator on IDTES1b1 - idtest - Chromium

mxcube3.esrf.fr:8081/#jsonDataCollection?k=rgi60z

Omega: 0.00 Step size: 90°

Kappa: 0.00 Step size: 0.1°

Phi: 0.00 Step size: 0.1°

Y: 0.00 Step size: 0.1 mm

Z: 0.00 Step size: 0.1 mm

Focus: 0.00 Step size: 0.1 mm

Samp-X: 0.00 Step size: 0.1 mm

Samp-Y: 0.00 Step size: 0.1 mm

Fast Shutter: Open Close

Safety Shutter: Open Close

Beamstop: In Out

Capillary: In Out

Energy: 12 keV Resolution: 3 Å

Transmission: 100% Detector Distance: 0 mm

Current: 187.47 mA ATTENTION: ktop in 49 secs

Run Queue Total Progress 1/9

Auto loop centring

Autamount next sample

Current Upcoming

Search Upcoming Create new sample

1:03	Mount
1:04	Mount
1:05	Mount
3:10	Mount
4:02	Mount
4:10	Mount

50 μm

Open Log



- Marcus Oscarsson
- Matias Guijarro
- Antonia Beteva



- Mikel Eguiraun
- Jie Nan
- Fredrik Bolmsten
- Marjolein Thunnisen
- Antonio Milan Otero