



ESRF HIGHLIGHTS

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(on behalf of the ESRF MXCuBE team)



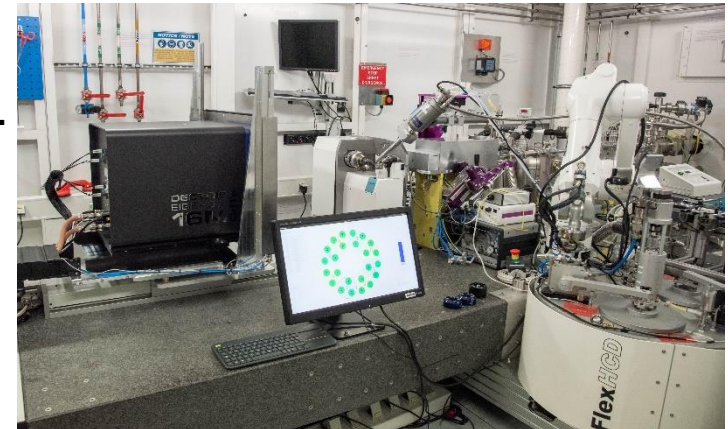
ESRF

- Remote access only. MX beamlines taking full advantage of MXCuBE3 intrinsic remote. Non MXCuBE beamlines use Guacamole.
- From NFS to GPFS for better performance.

Latest news: “...ESRF users for experiments, as well as visitors and contractors, are welcome on-site, as long as they comply with the sanitary and travel regulations applied in France...”

MX Beamlines

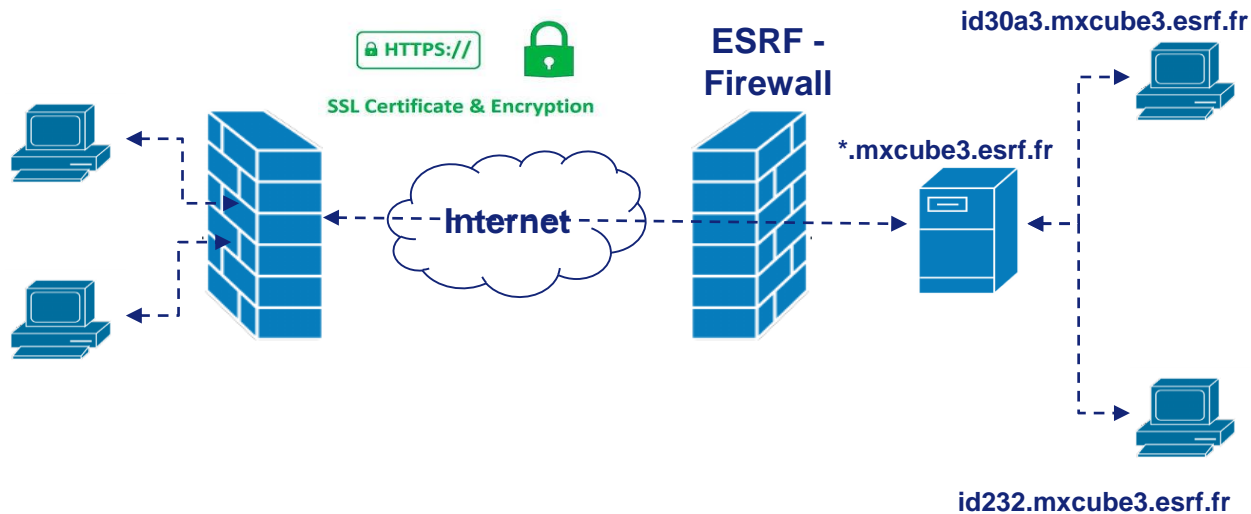
- Refurbishment (2021)
 - MASSIF-1 – MD2 replaced Robodiff, Flex SC
 - ID23-1 – MD2 replaced MiniDiff, Eiger 16M
- New equipment
 - MASSIF-1 – CrystalDirect Harvester 2.
- Construction of SSX Beamline (ID29)
 - See Daniele de Sanctis talk





MXCuBE Remote

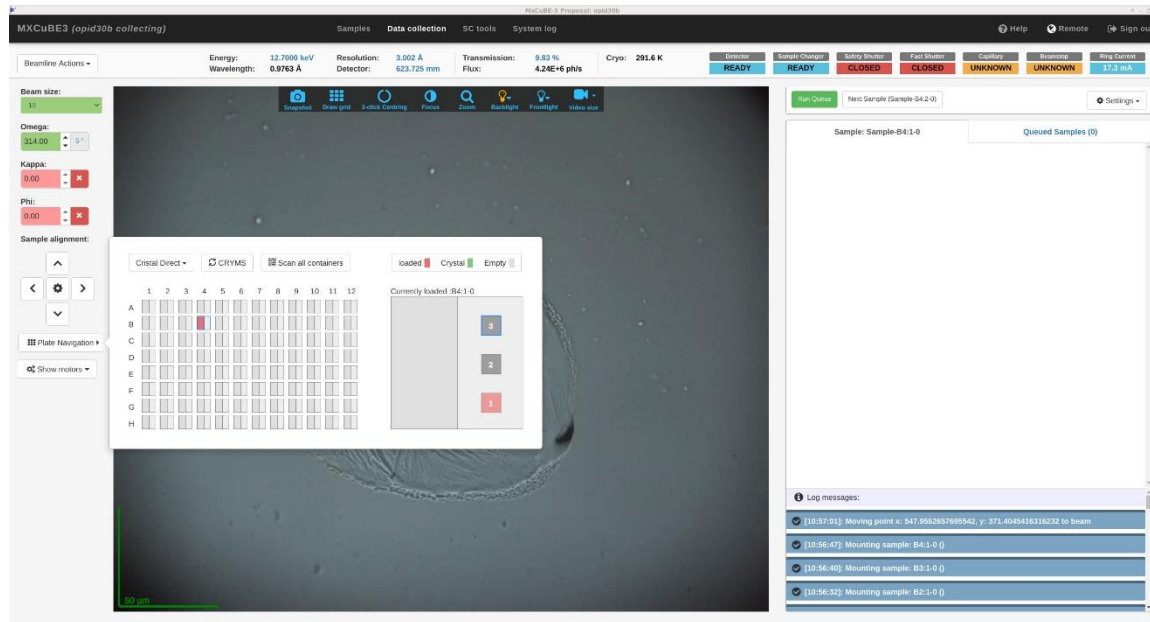
- 2021 statistics:
 - 684 user groups from 12 countries
 - 620 shifts (4960 hours)
- User guide - www.esrf.fr/mx-remote, <https://www.esrf.fr/mxcube3>
- Setup





MXCuBE3

- Using Linux version of the FLEX sample changer software.
- Fully automatic data acquisition (Mxpress*) running on all beamlines.
- Plates (ESRF in collaboration with EMBL Grenoble)





Plates (cont.)

The screenshot displays the MXCuBE3 software interface for data collection. The top status bar shows the following parameters: Energy: 12.700 keV, Wavelength: 0.9793 Å, Resolution: 3.002 Å, Detector: 623.725 mm, Transmission: 9.83 %, Flux: 4.24E+6 ph/s, and Cryo: 291.64 K. The interface includes a central diffraction image of a sample plate with a context menu open over it, listing options such as 'Go To Beam', 'Measure Distance', 'Draw Grid', 'Data Collection (limited OSC)', 'Characterisation (I. Image)', 'MXPressE', 'MXPressI', 'MXPressO', 'MXPressP', 'Trouble shooting', and 'Trouble shooting Dialog'. The left sidebar contains controls for beam size, Omega (314.00), Kappa (0.00), Phi (0.00), and sample alignment. The right sidebar shows a 'Run Queue' with 'Next Sample (Sample-B4-0)' and a 'Log messages' section with entries for delivery, refilling, and mounting.



BSxCuBE3

- BM29 control (beamline open with mail in users).
- New Sample changer implementation.

The screenshot displays the BSxCuBE3 control interface. At the top, there are status indicators for Front End (Wait for permission), Safety shutter (Hutch not searched), Fast shutter (Closed), Energy (12.500 keV), and Transmission (54.47%). The Data path is /data/visitor/mx2276/bm29/. Other indicators include Ring Current (-0.15 mA), CBM20 (Not Controlled), and PDA (Controlled). A Queue button is visible in the top right.

The Sample Changer section shows the Experiment Name as 'mysc'. It features three plate layouts: Plate 1 (96 Deep Well Plate), Plate 2 (4 x (8 + 3) Block), and Plate 3 (96 well Plate). The Sample and Buffer selection is set to green. The right side of the interface contains a form for well selection (Selected Well: 2B9), Sample Name (water4), Buffer Name (hepes), Concentration (1 mg/ml), Volume (50 µl), SEU Temp. (20 °C), and Storage Temp. (20 °C). An 'Add to Sample Table' button is located at the bottom right of this section.

The Sample Table at the bottom lists the following data:

| Name | Buffer | Plate | Row | Column | C (mg/mL) | Flow | Extra Flow (s) | Volume (µl) | SEU Temp. °C | Storage Temp. °C | Comment |
|------|--------|--------|-----|--------|-----------|------|----------------|-------------|--------------|------------------|-------------------|
| 1 | water | bwater | 2 | D | 11 | 1 | 10 | 50 | 20 | 20 | water calibration |
| 2 | water2 | bwater | 2 | C | 11 | 1 | 5 | 50 | 20 | 20 | |
| 3 | water2 | bwater | 2 | C | 11 | 1 | 5 | 50 | 20 | 20 | |
| 4 | water3 | hepes | 2 | C | 10 | 1 | 5 | 50 | 20 | 20 | |
| 5 | water4 | hepes | 2 | C | 9 | 1 | 5 | 50 | 20 | 20 | |

Additional controls include 'Clear Table', 'Clear Selected Row', 'Optimisation', 'Expand Parameters', and 'Parameters'. At the bottom right, there are buttons for 'Run' and 'Add to Queue', along with 'SC Initial Cleaning' and 'Wait for Beam' checkboxes.



BSxCuBE3 (cont.)

- Ongoing HPLC (High Performance Liquid Chromatography) implementation.

BSxCuBE3 Acquisition result Beamline Setup System log mx1816 Help Signou

Front End Wait for permission Safety shutter Hutch not searched Fast shutter Closed Energy 12.500 keV Transmission 20.05%

Data path : /data/visitor/mx1816/tm29/ Ring Current -0.02 mA CBM20 Controlled PDA Controlled Queue

HPLC Experiment Name : myhplc Load Parameters Save

Equilibrate Sample Collect HPLC Control

Auto Sample : Set OFF Plate : HPLC Well Plate Selected Vial : 91

Auto Sample Temp : (19.9) 20

Sample Parameters

Sample Name * Vial Number * Injection Volume (ul) *

sample_z 91 50

Number of Frame * Column Elution T (min) * Exposure Time (s) *

Recommended Value : 240.0 Recommended Value : 4.0

240 4 1

λ 1 (nm) * λ 2 (nm) * λ 3 (nm) *

260 280 350

λ 4 (nm) * Exposure Temp °C * Flow Rate (mL/min) *

450 20 1

Comment

c

Add to Sample Table

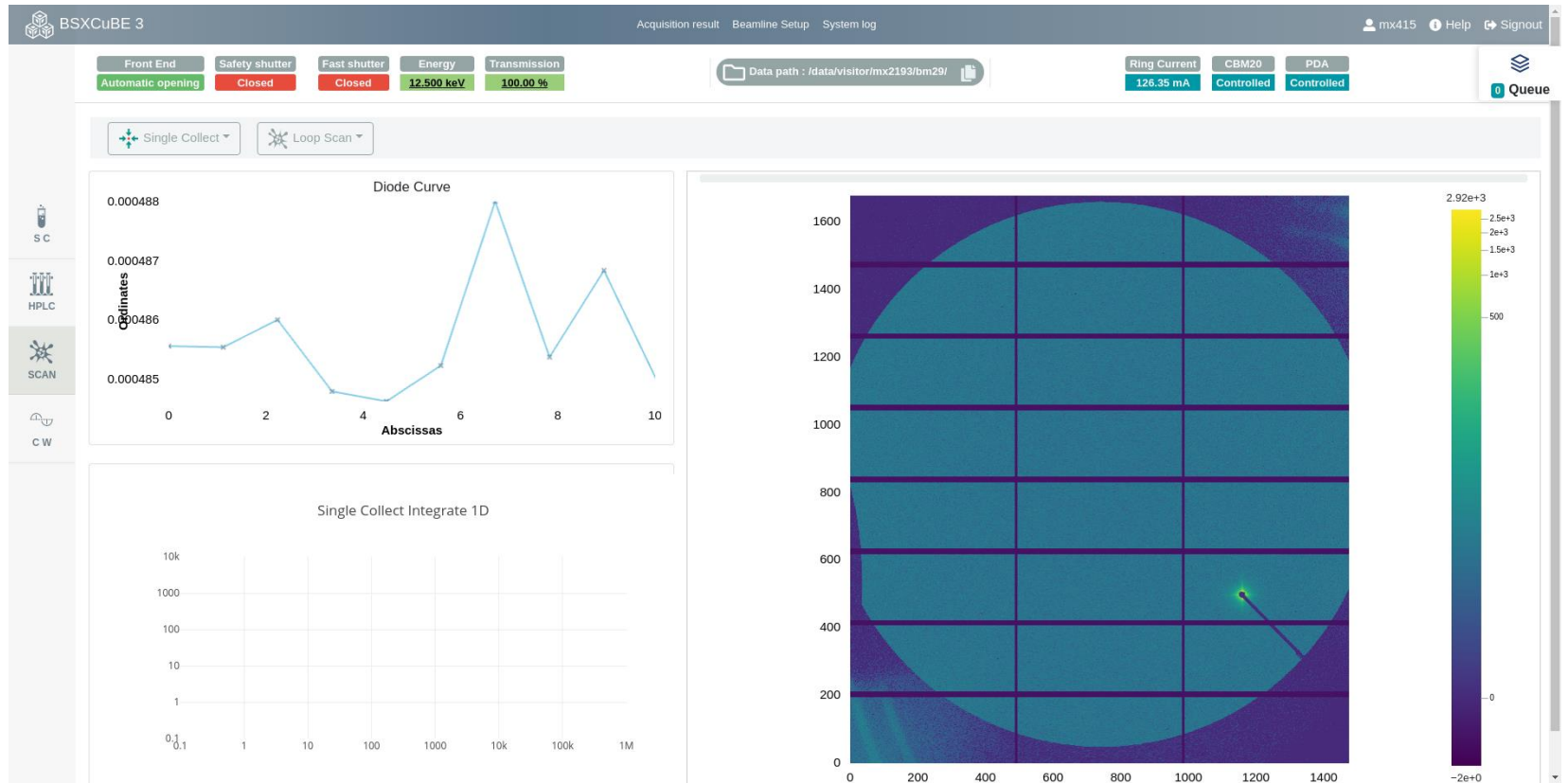
Clear Table Clear Selected Row Optimisation Expand Parameters: Parameters: Number of HPLC Sample's 2

| Sample Name | Inject | Flow R. (mL/min) | Vial Number | Injection Volume (ul) | λ 1 (nm) | λ 2 (nm) | λ 3 (nm) | λ 4 (nm) | Concentration | Exposure Temp °C | Exposure Time (s) | Number of Frames | Column Elution (min) | Comment |
|-------------|-------------------------------------|------------------|-------------|-----------------------|------------------|------------------|------------------|------------------|---------------|------------------|-------------------|------------------|----------------------|---------|
| z | <input type="checkbox"/> | 1 | 91 | 50 | 260 | 280 | 350 | 450 | 1 | 20 | 2 | 10 | 4 | c |
| z | <input checked="" type="checkbox"/> | 1 | 1 | 50 | 260 | 280 | 350 | 450 | 1 | 20 | 1 | 70 | 4 | c |
| sample_z | <input checked="" type="checkbox"/> | 1 | 91 | 50 | 260 | 280 | 350 | 450 | 1 | 20 | 1 | 240 | 4 | c |

SC Initial Cleaning: Wait for Beam: Run Now Add to Queue



BSxCuBE3 (cont.)





Users' corner

“So far we have measured on MASSIF-3, ID23-2 and BM29. The new EBS beam is very nice and we have been getting good data...MXCube3 is an intuitive and easy to use GUI for remote data collection”

“The introduction of the web-based MXCUBE3 was considered a major improvement in beamline remote control.”

“Remote data collection is highly effective and generally works very well... (the) data collection is user friendly and robust.”