MXCuBE goes serial

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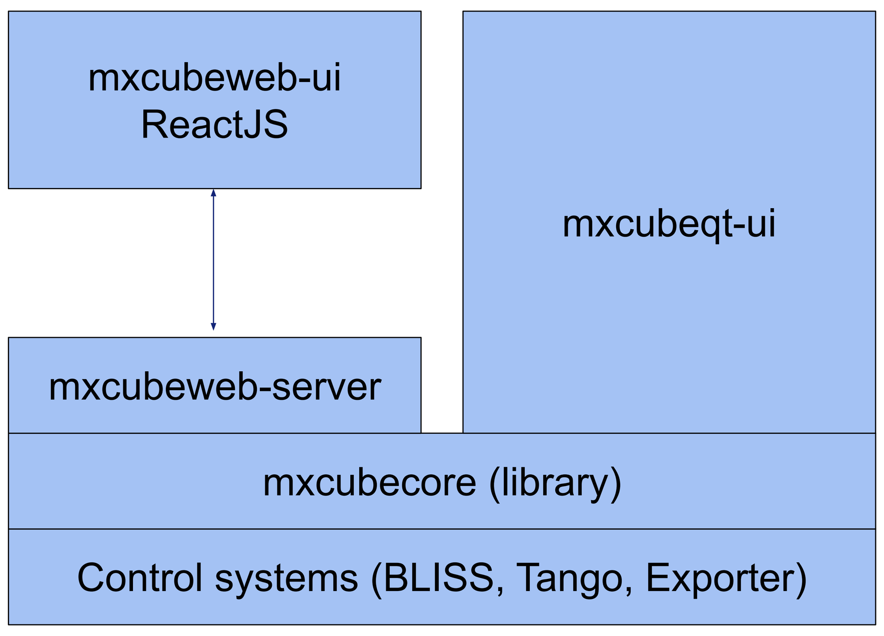
The ESRF Extremely Brilliant Source upgrade programme included the construction of ID29, the first of a kind beamline fully dedicated to room-temperature experiments and time-resolved macromolecular serial crystallography. The beamline presents a flexible sample environment that can accommodate fixed target, viscous injectors, microfluidics or tape drives. The experimental setup is completed with a Jungfrau 4M detector that has been integrated in the ESRF data acquisition pipeline and can be operated at high data acquisition rates.

MXCuBE, the state-of-the-art experiment control software used at all ESRF MX beamlines, for remote, high-throughput attended and unattended data collections, was expanded with new Serial Macromolecular Crystallography features for ID29.

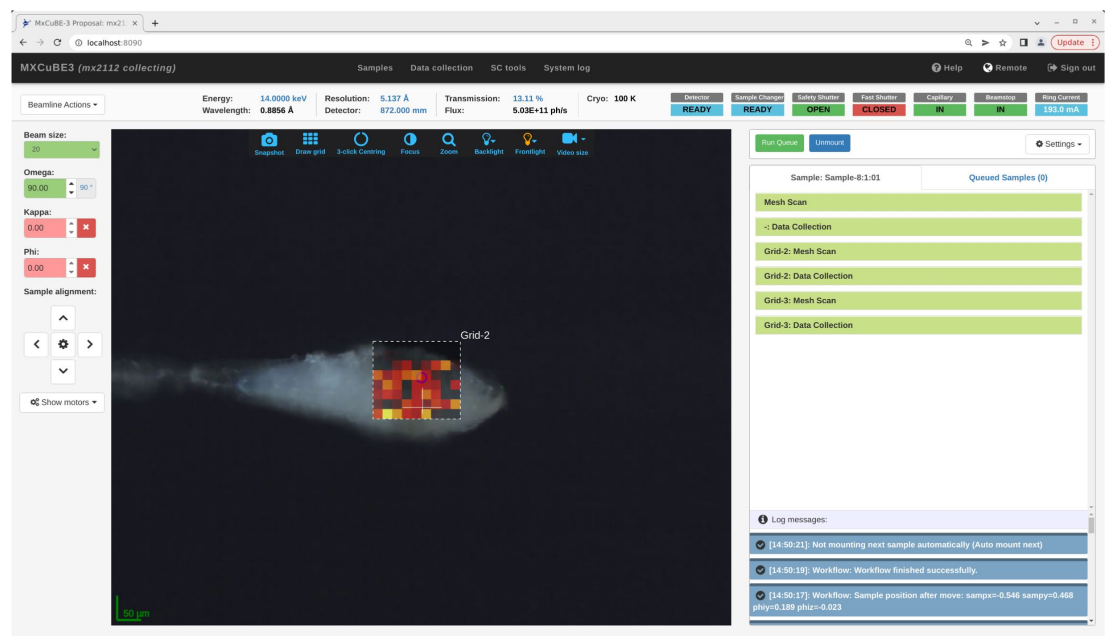
The MXCuBE (Macromolecular Crystallography Customised Beamline Environment) is an application initially developed to control and perform crystallography experiments at synchrotron beamlines. The application is deployed on 7 MX beamlines at the ESRF: ID23-1, ID23-2, ID30A1 (MASSIF1), ID30A3, ID30B, ID29 and BM07. MXCuBE offers a uniform user experience across the different instruments, providing friendly access to the specific features and complexities of each beamline. The application backend is written in Python and consist of two main parts, the mxcubecore[2] library and the MXCuBE-Web[3] user interface.

The MXCuBE project, initially started at ESRF in the early 2000s, is today a global collaboration among 15 partner institutes and companies, ensuring a large level of compatibility with hardware and control systems.



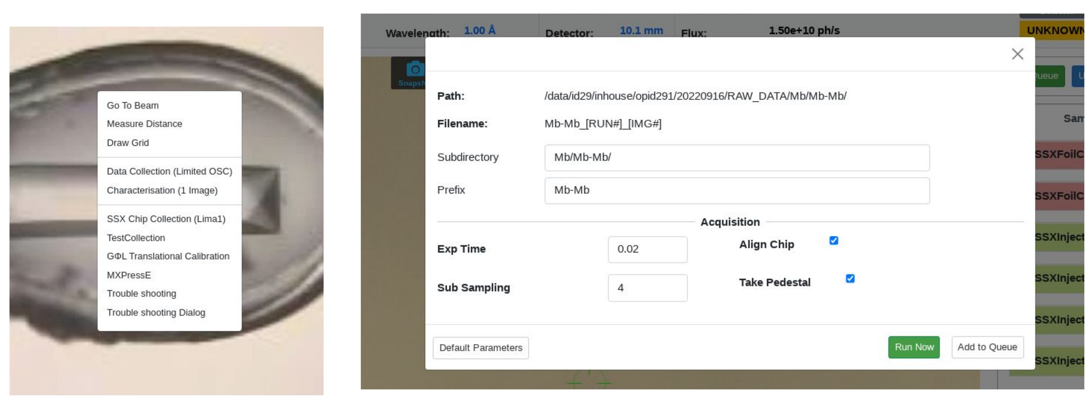
The mxcubecore[2] library provides an abstraction to a number of popular control systems: BLISS, Tango, Tine, Spec, EPICS and EMBL Exporter. It further contains functionality for queue management, integration of third party software and instrumentation control abstractions. Hardware and instrumentation control is implemented by something called HardwareObjects that extends a set of predefined abstract classes.

MXCuBE-Web[3] is a web application and thus supports remote data collection by design. The backend is based on the flask web server and the frontend developed with Javascript using the React library.

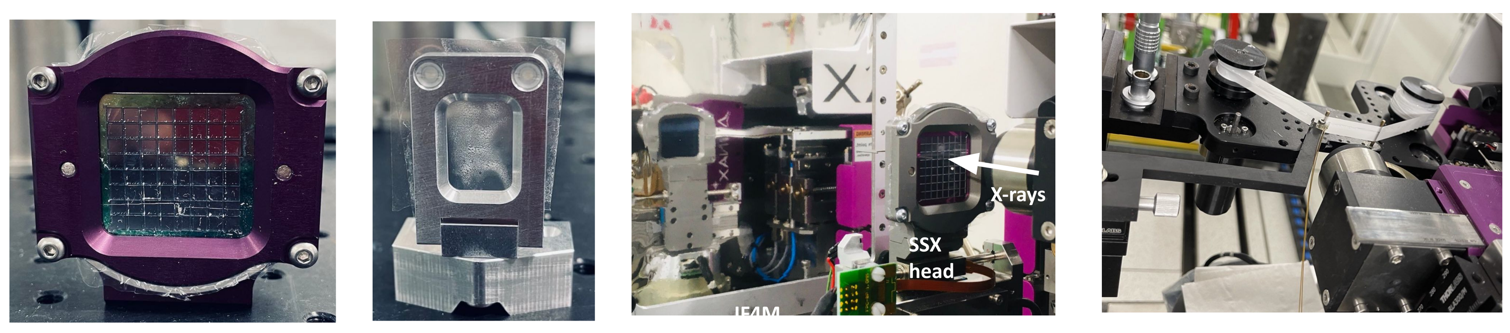


MXCuBE can be further extended with functionality in three different ways. Collection protocols can be added by implementing a **task**. Procedures that are performed routinely, that are not a collection protool, such as alignment can be implemented as something called **beamline actions**. Devices and instrumentation control is added by implementing a **HardwareObject**. The collection protocols, the **tasks**, can further be enqueued to achieve automation.

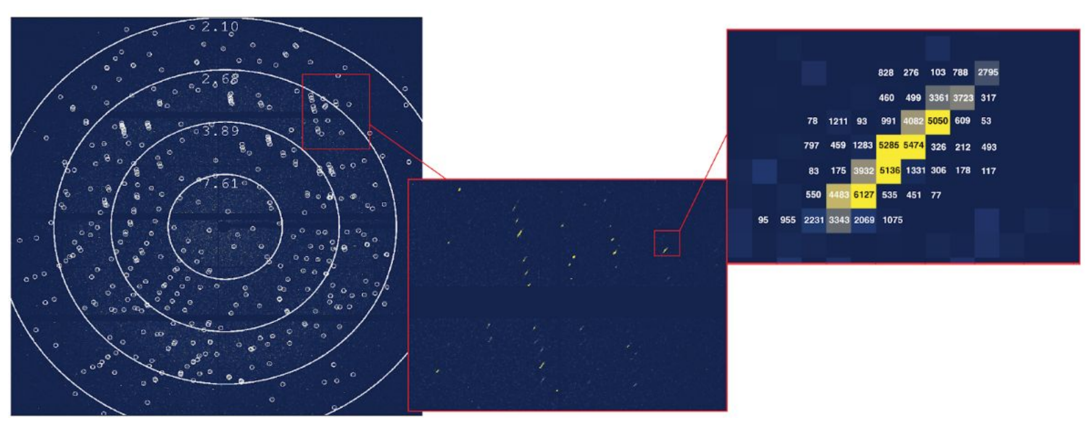
The application can generate parts of the user interface automatically based on the data models defined and specified in the method type hints. This flexibility is essential to quickly adapt to novel emerging methods and fields as in the case of **Serial Crystallography**.



MXCuBE was extended with new data collections protocols for the new ID29 beamline. Three sample delivery methods are routinely available: Fixed target, High Viscosity Extruders and Tape drive.



These methods are implemented in MXCuBE-Web4 [3] with a light interface that eases data collection also for non expert users. Fixed target acquisition is either performed on foils or Silicon chips by continuous scanning along an S-shape trajectory. Silicon chips are automatically aligned prior the data acquisition.



Diffraction data is recorded with the Jungfrau 4M detector, which is controlled by MXCuBE via a new version of LImA2 [5], which is integrating automatic hit detection and can discard empty frames on-the-fly.

[1]Collaboration website: **https://github.com/mxcube**, [2] mxcubecore: **https://github.com/mxcube/mxcubecore.** [3]mxcubeweb: **https://github.com/mxcube/mxcubeweb**
[4]Oskarsson et al. 2019. "MXCuBE2: The Dawn of MXCuBE Collaboration." *Journal of Synchrotron Radiation* 26 (Pt 2): 393–4
[5] https://gitlab.esrf.fr/limagroup/lima2

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