The MXCuBE project: Introduction to new developers and partners

Marjolein Thunnissen

Software requirements for MX

Crystal characterisation modes	Cartography, spiral scanning, centering by diffraction...
Crystal diffraction characterization, radiation damage	EDNA, BEST, Stack etc., Multi-crystal approaches, lend etc.
Data collection modes/ protocols	ve, ligand,SAD/MAD, SSX others?
Data analysis and pipelines	DFS, Xia2, Fast_dp, GO,COM, AutoRicksaw, mple, Phenix related ers...
Data transfer and storage	ed at 6.5 GB/sec. aw data?
Sample tracking	e
Remote access	Reliable & s olutions
User friendly, intuitive experiment GUI	

MXCuBE

MX-CuBE history

- 2006 Development started of MXCuBE by ESRF and MRC-UK (in house funding and BIOXHIT)
- Initially deployed at ESRF MX beamlines and the CRG MRC-UK beamline BM14 at the ESRF
- Followed by installations at MAX-lab, HZB-BESSY, EMBL-HH & Soleil
- Installation were not straightforwards and development of MXCuBE2 started —> GUI more independent from both beamline hardware and control software
- MXCuBE2 also allowed for more synergy with ISPyB
- Start of the MX-CuBE consortium, MoM in 2012
- Now 3rd generation development of MXCuBE: Qt4 and v3
- Employed at the majority of MX beamlines in Europe

MXCuBE consortium

Memorandum of Understanding in 2012

Originally a collaboration between 6 European partners.

Grown since with new partners and with an interest from partners from different continents.

Partners are mainly synchrotrons, 1 company involved

Goal of joint use and collaborative development of MXCuBE.

Sharing development, experience, know-how and resources.

Discuss strategies, difficulties and opportunities.

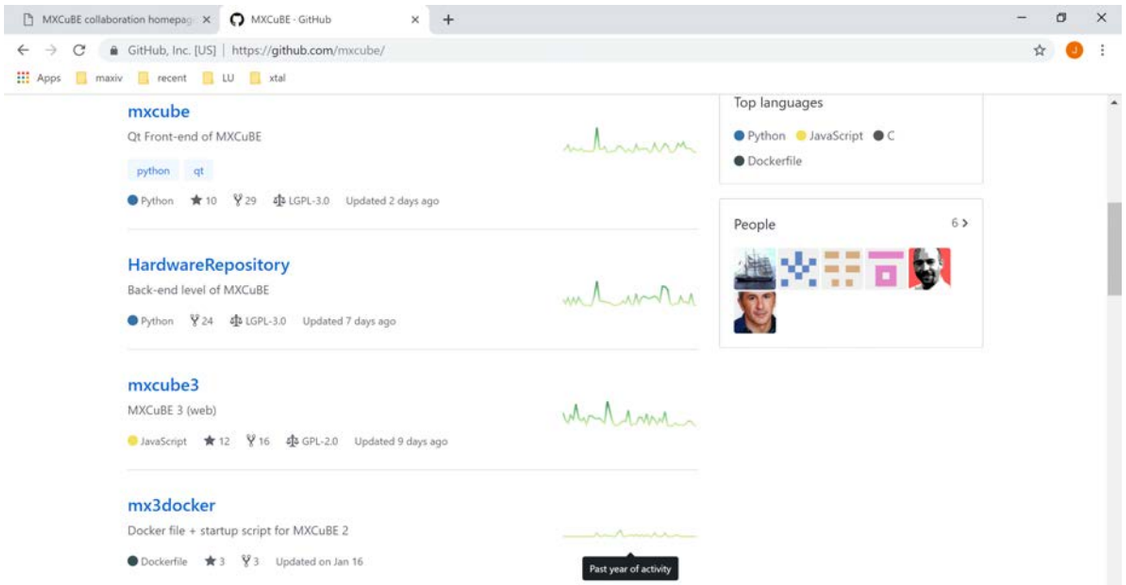
More rapid implementations of new methods for the MX community in Europe.

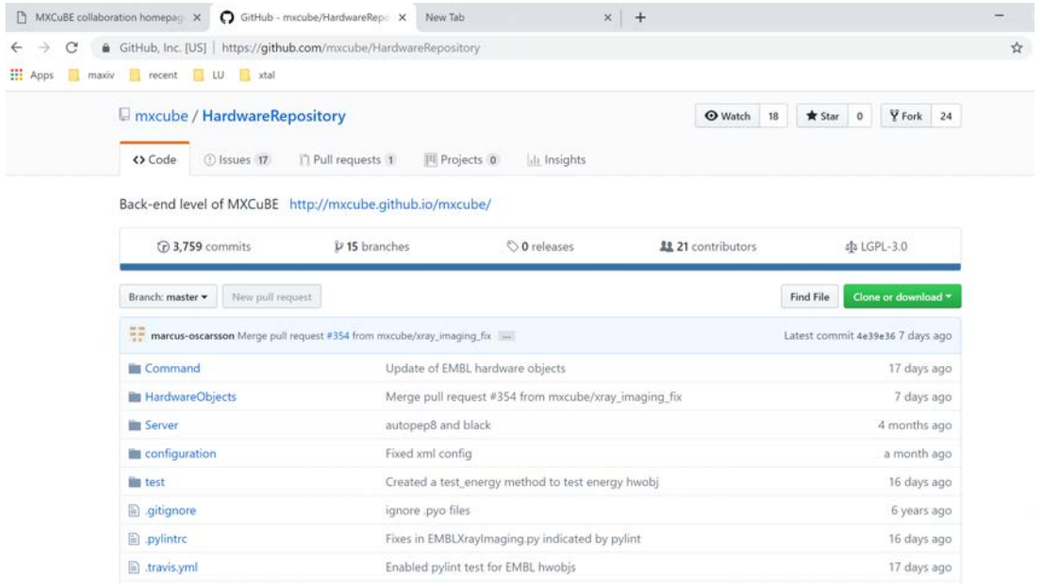
11th MXCuBE meeting, June 2017 at SOLEIL

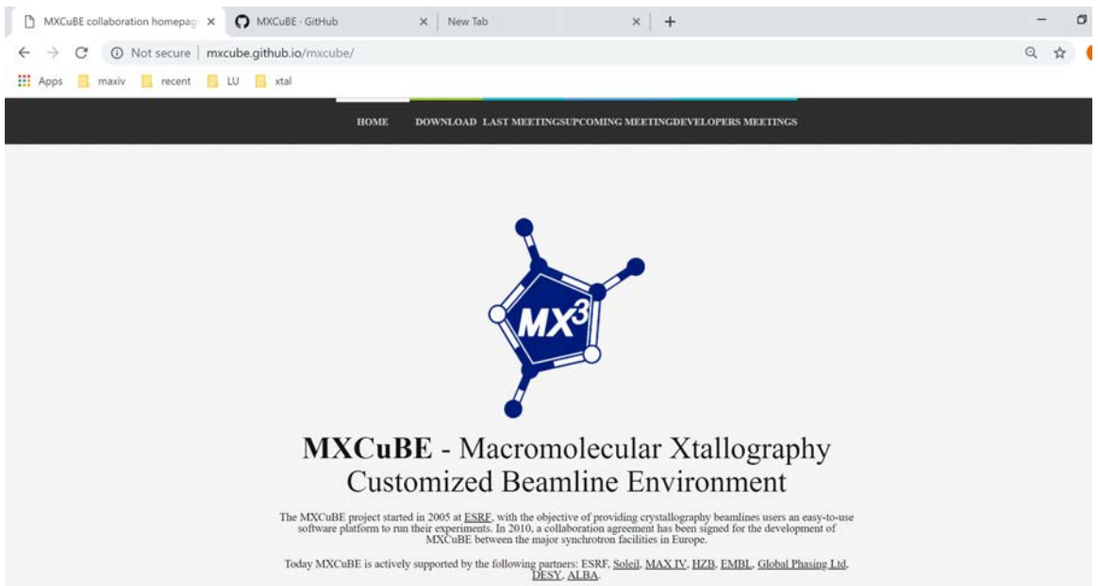
12th MXCuBE meeting, January/ February 2018 at Diamond

Tools to collaborate

- GitHub
- Website
- Videoconferences
- Developers hackatons
- Scrums and agile methods
- MX-CuBE meetings, organise by site to site

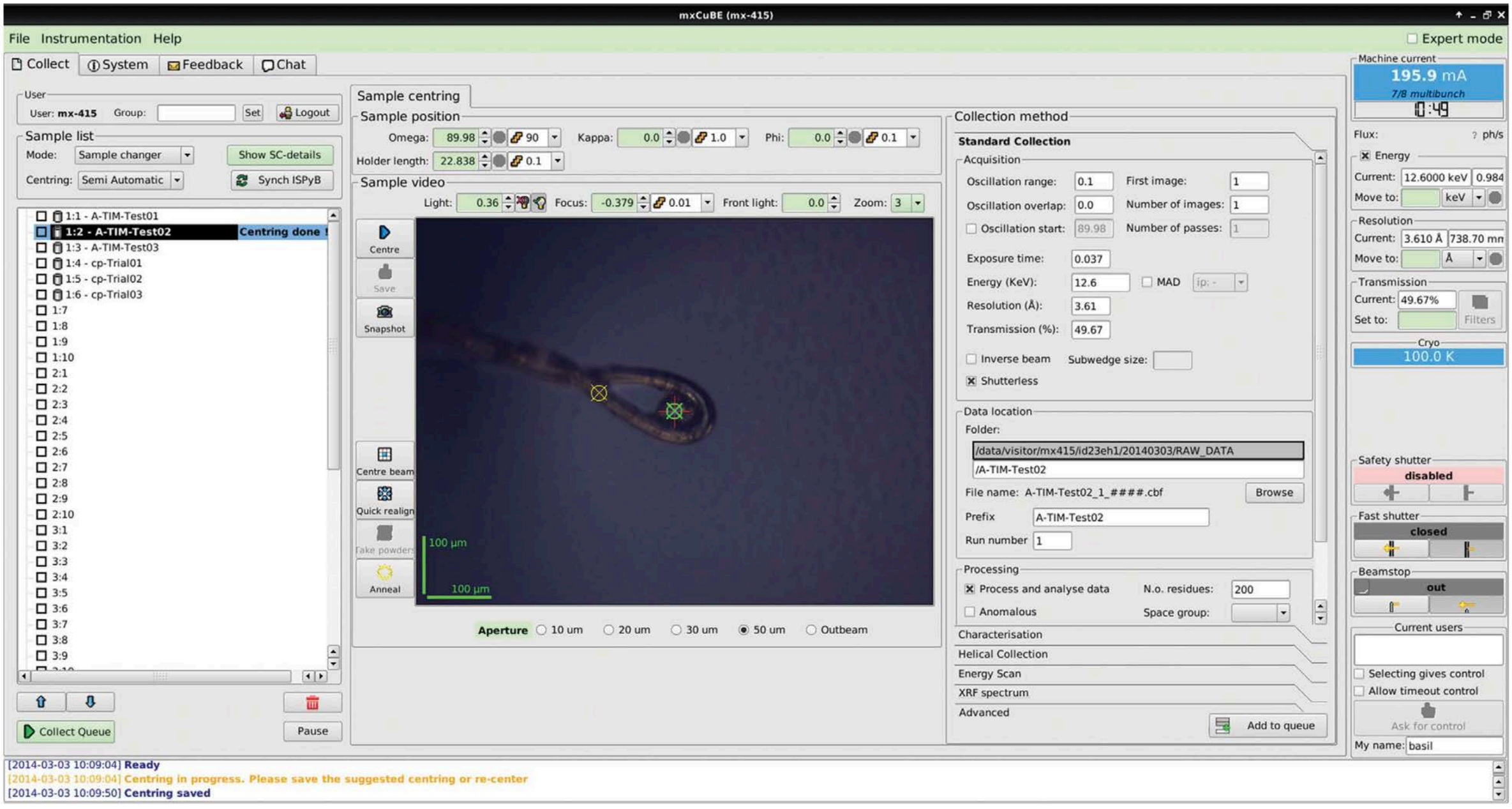






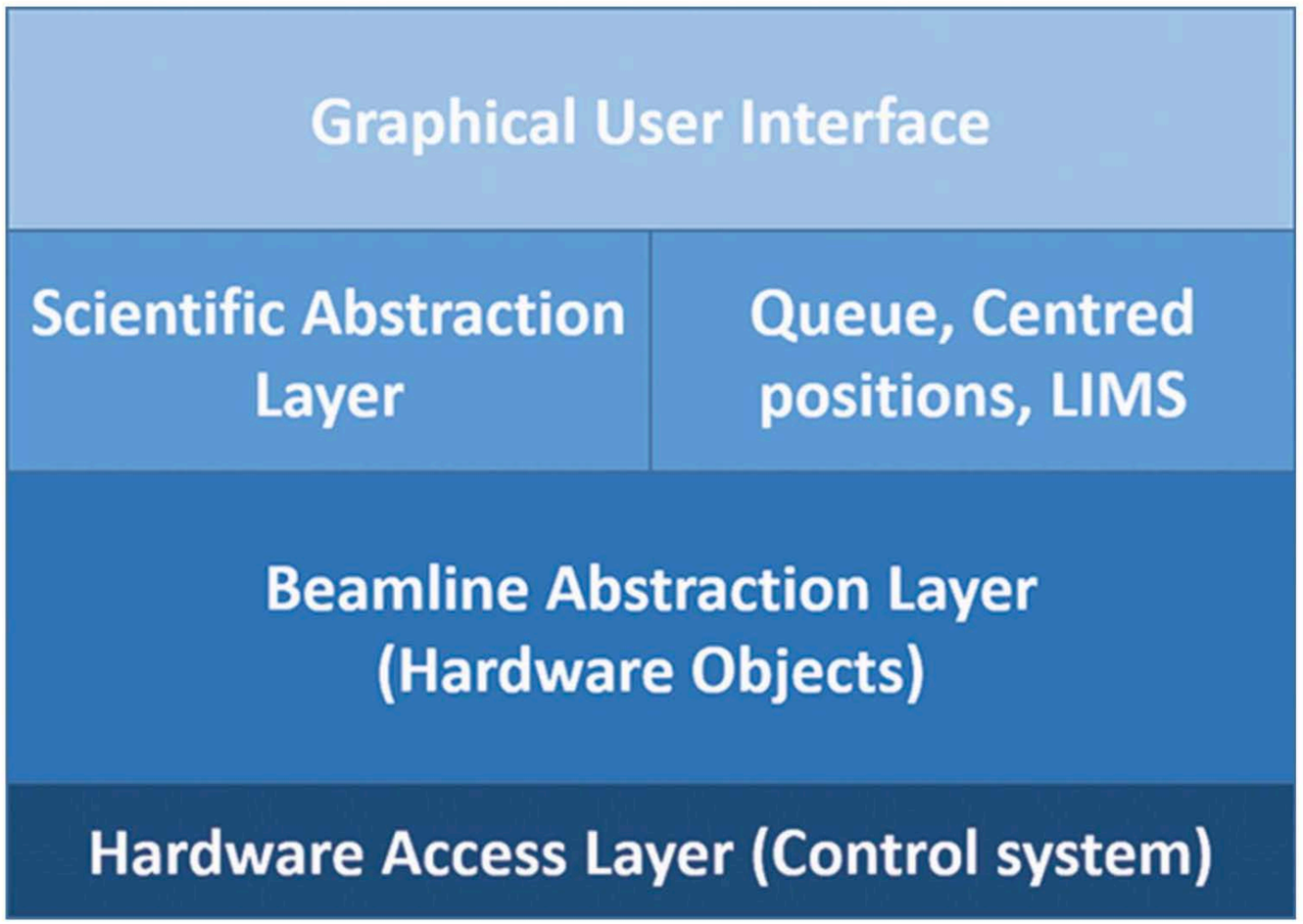
http://mxcube.github.io/mxcube/

MXCuBE2



Oscarsson et al., J. Synch. Rad. (2019) 26, 393-405

Architecture



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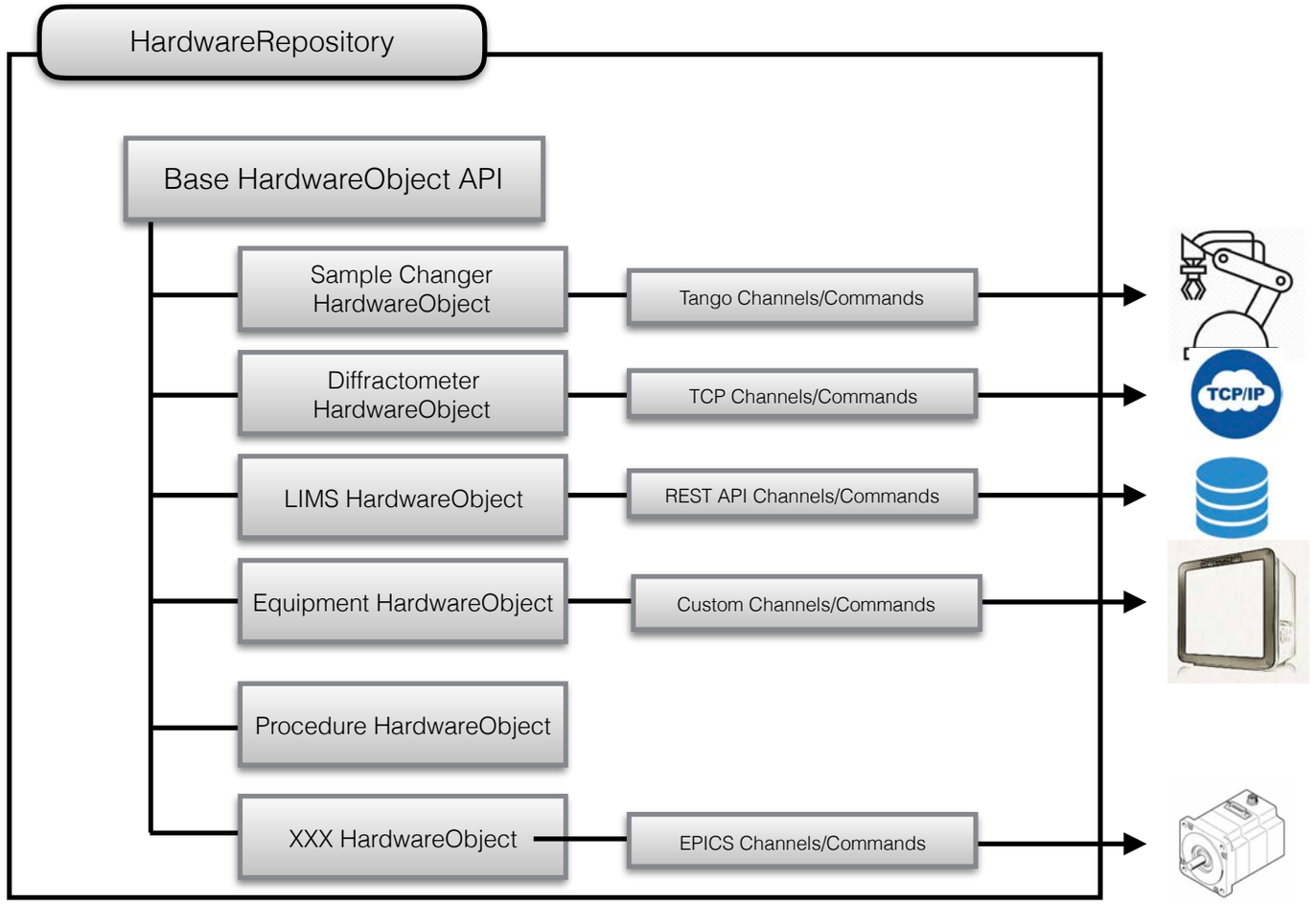
MXCuBE - HardwareRepository

- Hardware Abstraction Layer
- It acts as a container/Pool of single python objects (called Hardware Objects)
  - The information necessary for a hardware object to operate a physical device. Supported protocols: Tango, Spec, Exporter, Sardana, EPICS



MXCuBE - HardwareObjects

- A HO is not only hardware! Procedures/sequences etc
- Link between devices and the graphical interface
  - Through the *HardwareRepository*…
- Configured through xml files
- emitting signals to others HOs, graphical elements

```xml
<device class="MicrodiffMotor">
   <username>Omega</username>
   <exporter_address>130.235.94.124:9001</exporter_address>
   <motor_name>Omega</motor_name>
   <unit>1e-3</unit>
</device>
```

udiff_omega.xml

```python
class MicrodiffMotor(Device):

    def init(self):
        self.position_attr = self.addChannel({"type":"exporter", "name":"position"  }, self.motor_name)

    def getPosition(self):
        return self.position_attr.getValue()

    def move(self, absolutePosition)
        self.position_attr.setValue(absolutePosition)
```

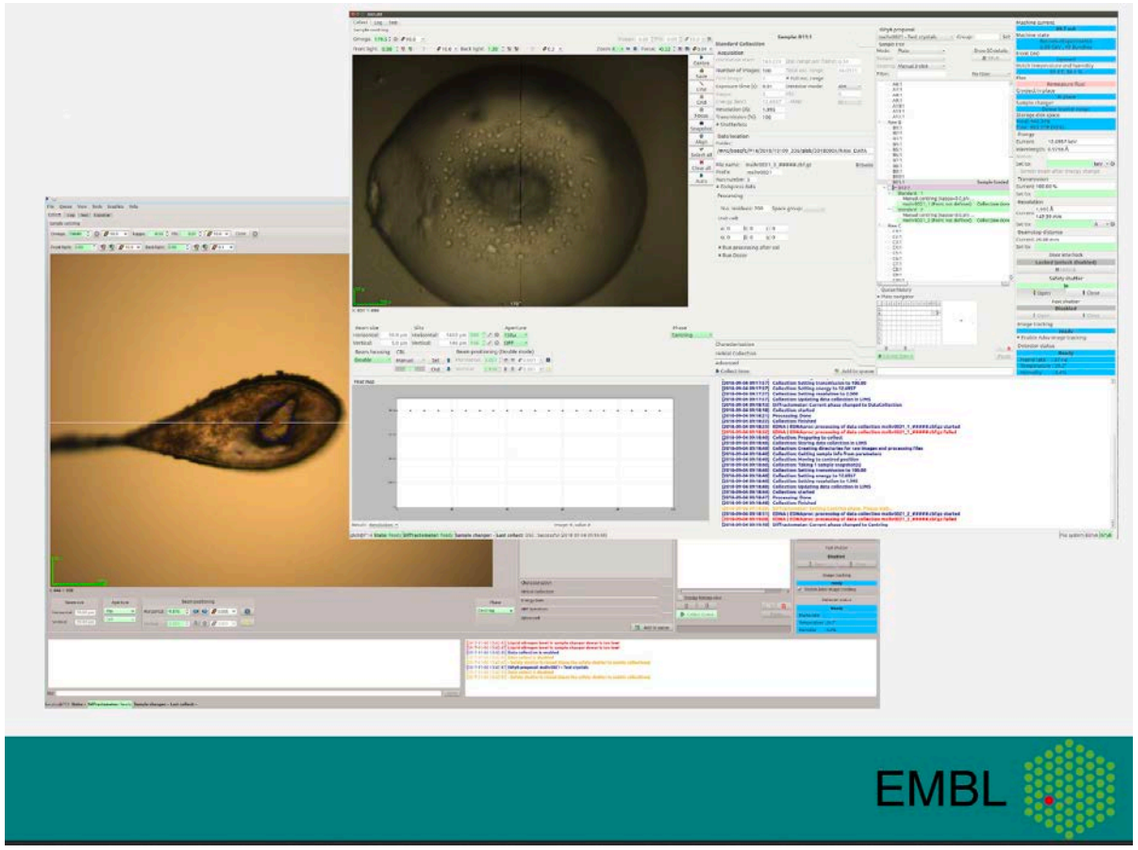
MicrodiffMotor.py

New generation MXCuBE

- More and more need for incorporation of new methods.
- Number of samples within an experiment is increasing fast.
- Better employment of fully automatic data collection methods.
- Better integration of remote data collection protocols.
- There was a vulnerability: MXCuBE2 build on Python and Qt3.
- Better user ergonomics.

Qt4

- Migration of MXCuBE2 from Qt3 to Qt4 spearheaded by EMBL-HH
- Same architecture and feel as MXCuBE2
- Introduction of many new functionalities (EMBL-HH) especially for serial crystallography



From Ivars Karpiĉs, EMBL-HH

MXCuBE v3

- Beamline control and data acquisition as web application
- Modern technologies
- Future easier integration and maintenance
- Remote access in a more *natural* way
- New design for the user interface
- Decoupling logic and interface: any client possible
- Started as a collaboration by MAX IV and ESRF

Feature

MXCuBE targets third phase

Europe boasts several synchrotron X-ray sources offering some 30 experimental stations for macromolecular crystallography. Thanks to the MXCuBE platform, originally developed at the ESRF, users now have a common standard and language to make the most of these facilities.

In studying the structure of biological molecules at synchrotron facilities, the macromolecular crystallography (MX) community typically performs complicated and demanding experiments on numerous samples. It is therefore vital that scientists have a user-friendly interface that provides intuitive access to the definition and control of those experiments. MXCuBE (MX Customized Beamline Environement) is a software platform dedicated to beamline control and data acquisition for MX experiments. It was originally developed at the ESRF in 2006 via a combination of in-house funding and support from the FP7 EU project BIOXHIT. The package has since matured into the MXCuBE2 application, which offers better integration with sample changing robots and provides more intuitive workflows for carrying out complex experiments.

MXCuBE is currently deployed on all MX beamlines at the ESRF, and is also used as the general user interface on many MX beamlines at several other European synchrotrons. In 2012 a memorandum of understanding was signed by six partners to establish the MXCuBE Consortium, with the goal of joint use and collaborative development of the platform. The initial partners were: the ESRF, the European Molecular Biology Laboratory; Global Phasing Limited; the HZB-Berlin in Germany; MAX-IV in Sweden; and SOLEIL in France. In 2014 two further light-source laboratories – ALBA in Spain and DESY in Germany – joined the consortium. The MXCuBE consortium thus has an unprecedented seven synchrotron facilities coordinating their efforts and sharing resources to provide an essential tool for MX experiment control and design.

MXCuBE contains mesh tools that allow the diffraction quality in different regions of a sample to be characterised (red indicates weak and yellow indicates strong diffraction quality).

Thanks to the MXCuBE Consortium structural biology researchers now have access to a common software platform, with only certain site-specific customisations, at the majority of European synchrotron sites. This allows users to focus on the experiments they would like to perform with minimal distraction from local beamline idiosyncrasies. For the synchrotron sites themselves, the collaboration has boosted the development of a mature and "battle-tested" system with an enormous amount of built-in scientific experience. For newer synchrotron facilities, or those with limited resources, the project has enabled the rapid implementation of a user interface with high-level functionalities.

Participants of the MXCuBE Consortium meeting held in June at the BESSY-II source in Berlin.

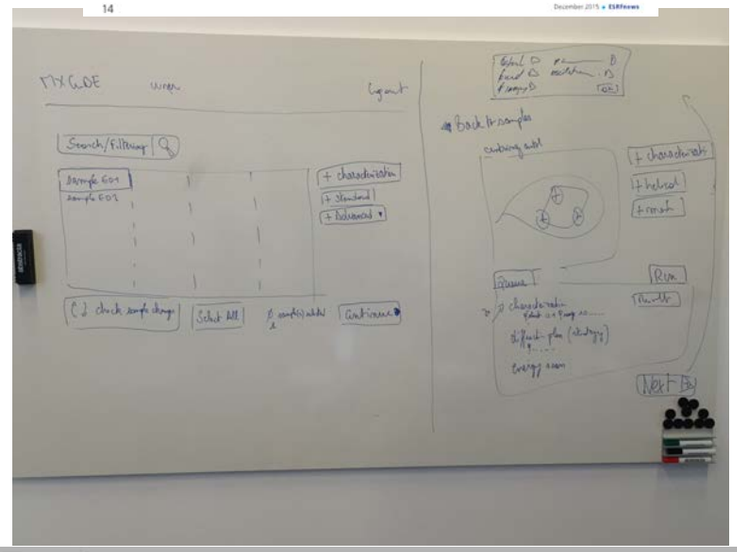
Towards MXCuBE3

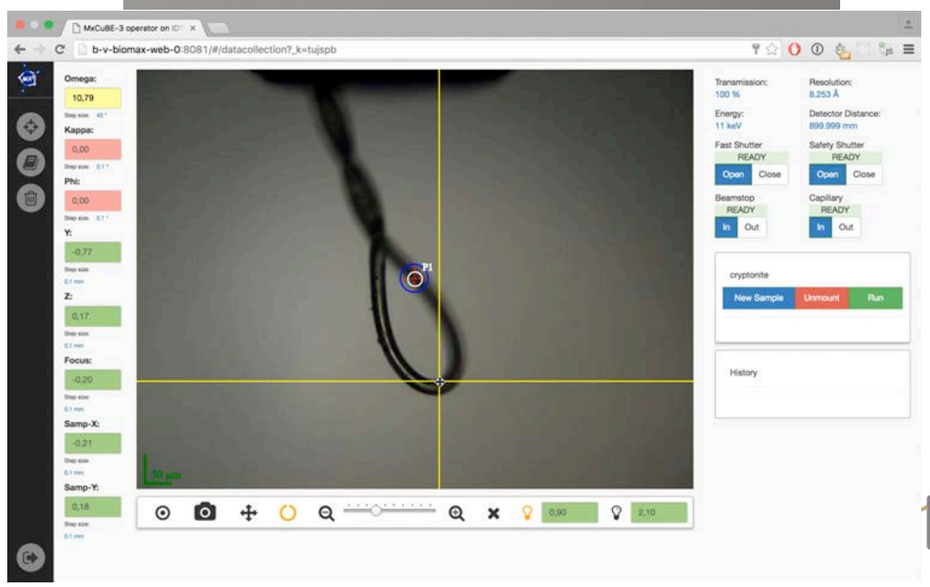
New technologies in synchrotron and beamline instrumentation, as well as detector development, have recently given rise to an explosion of new options for conducting MX experiments including completely automatic data collection and new protocols for synchrotron serial crystallography. A jointly developed version of MXCuBE is the only way for the individual partners to fully exploit these new possibilities in a user-friendly manner.

To ensure the sustainability of MXCuBE the consortium is now collaborating on a common upgrade of the platform towards MXCuBE3 (MX^3), which will incorporate new software engineering paradigms and standards. Here, the goal is to develop a beamline control system that runs as a web application, providing easier integration with future computer platforms and offering a tighter integration with MX experiment database ISPyB and a better remote access experience for both new and experienced users.

This project will be a valuable opportunity to identify the strengths and weaknesses of the current platform and to learn about transitioning mission-critical applications between technologies, enabling MX^3 to offer an even broader portfolio of experimental possibilities to scientists using MX in structural biology and to companies using it as a tool for drug discovery.

MXCuBE Consortium





MXCuBE 3

- Under active development
  - kickoff meeting in September 2015
  - v 3.0.2
- In production in MAX IV, ESRF, Elettra (Roberto?)
- Tests in Soleil?
- Still a few issues to be solved

Latest release

v3.0.2

a0e49fb

MXCuBE 3 (web)

Edit

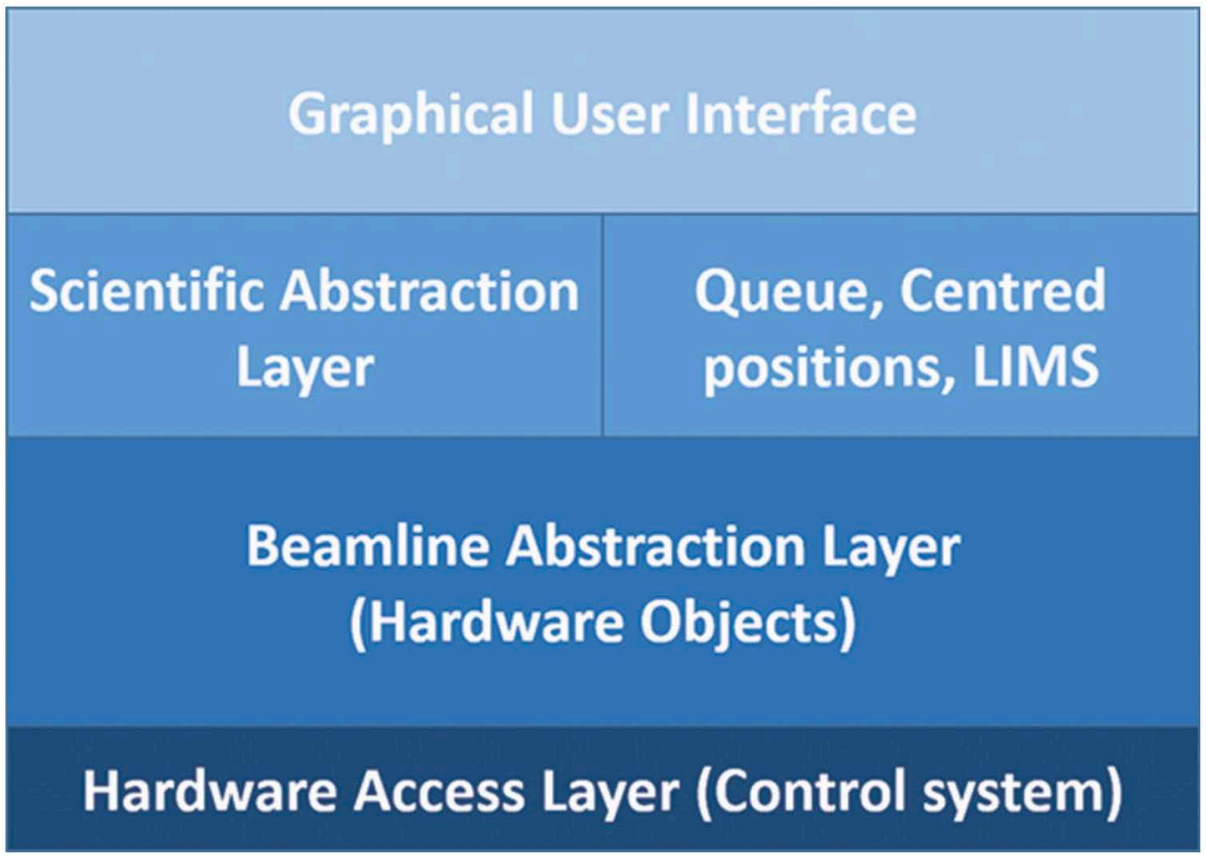
Manage topics

3,328 commits | 13 branches | 7 releases | 8 contributors | GPL-2.0

https://github.com/mxcube/mxcube3

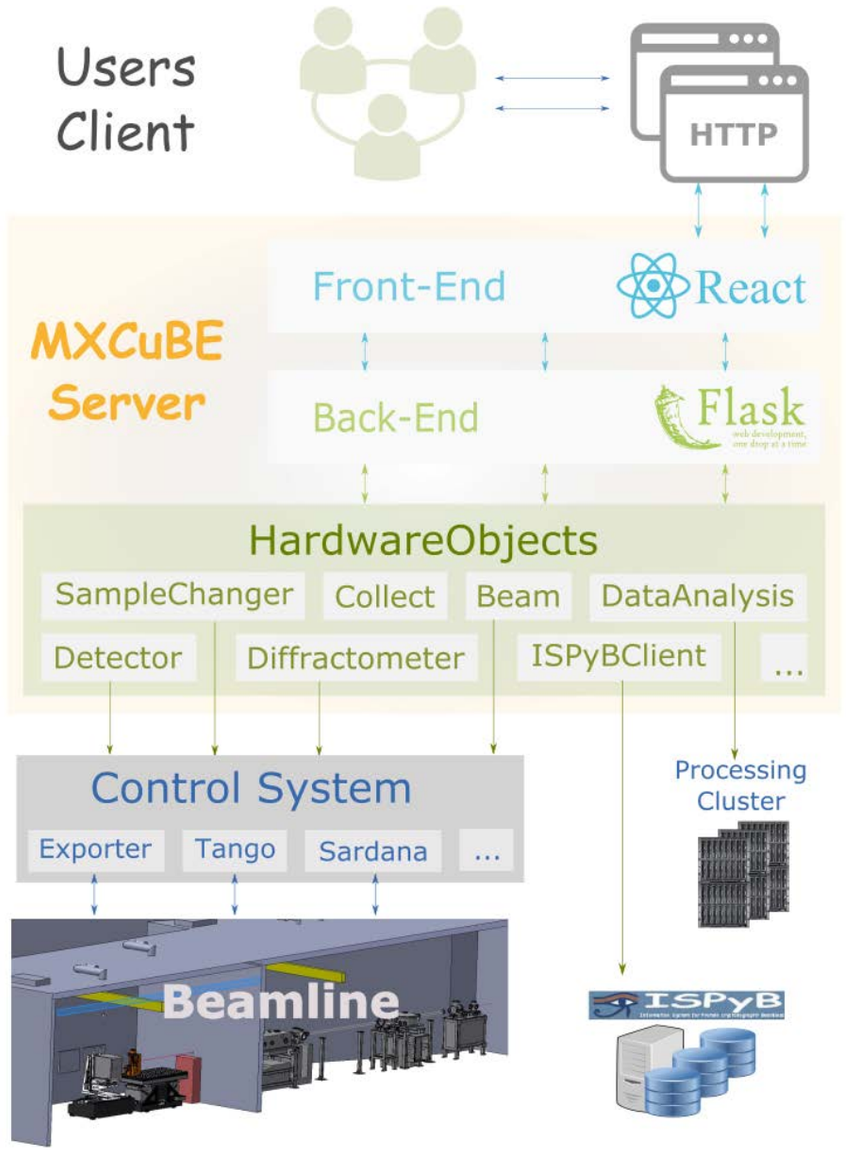
MAX IV

Architecture



Oscarsson et al., J. Synch. Rad. (2019) 26, 393-405

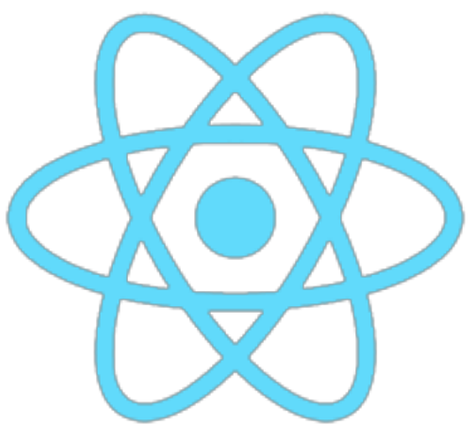
A schematic view of the MXCuBE3 software



Uwe Mueller, et al. (2017) Synchrotron Radiation News, 30:1, 22-27

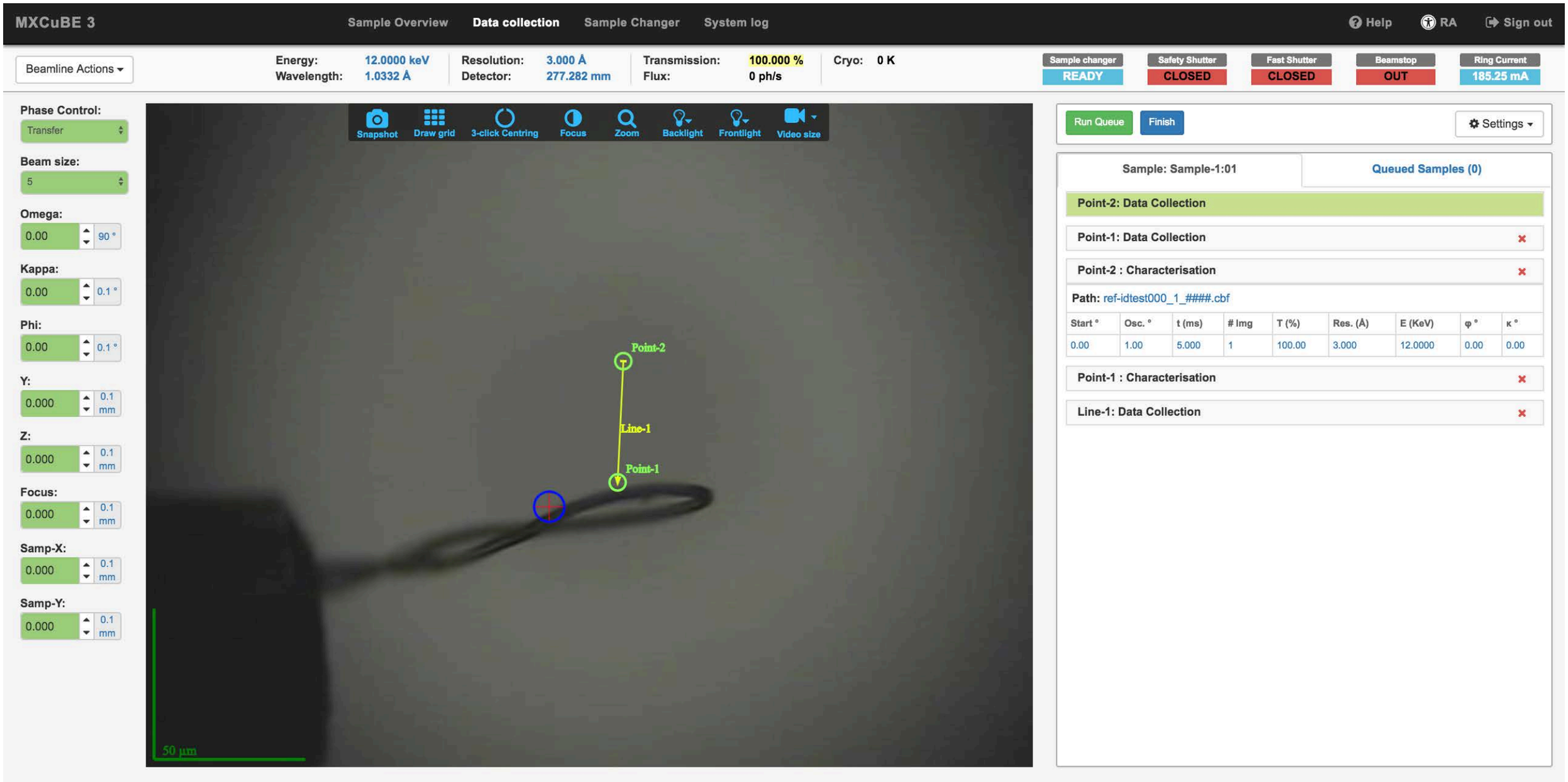
Frontend - REACT

- **Javascript/React** library (Facebook)
- For the user interface (the V in MVC)
- Widgets like in traditional UI development
  - Called **components**
- Reusing existing code when the layout changes
- Express the UI in a markup language called JSX (~html + javascript)

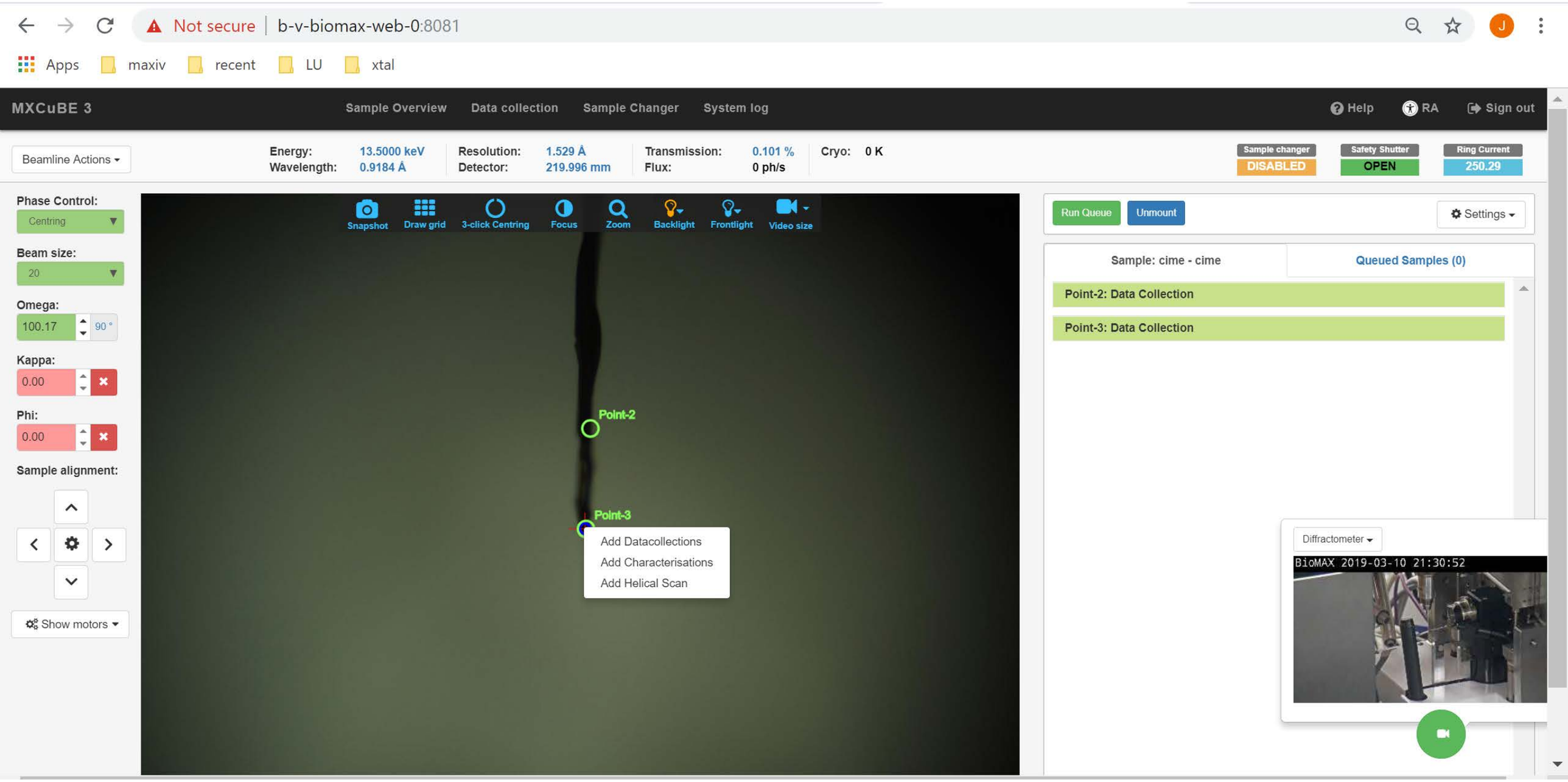


React

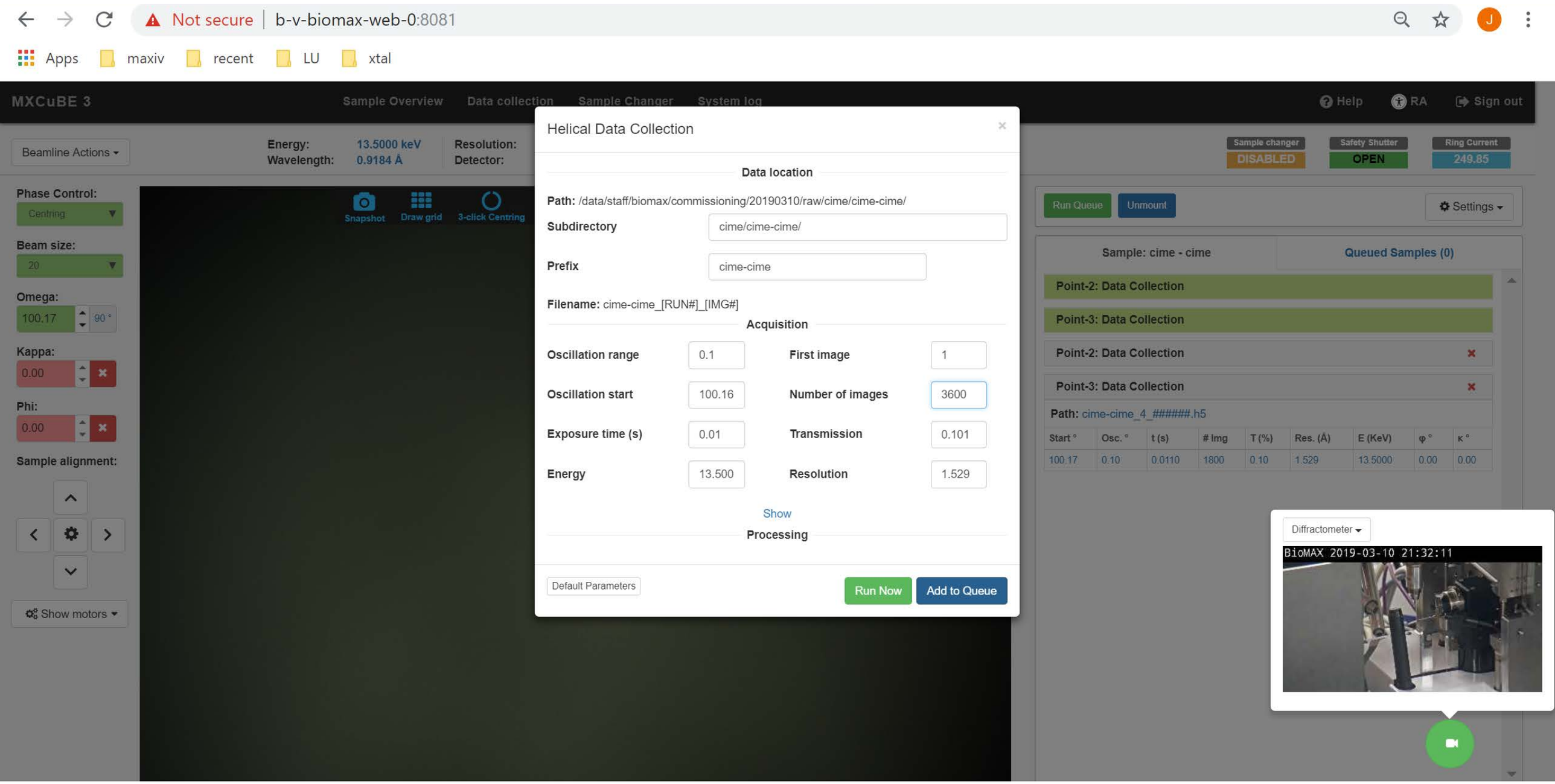
MXCuBE - Today



MX-CuBE3 : video as canvas

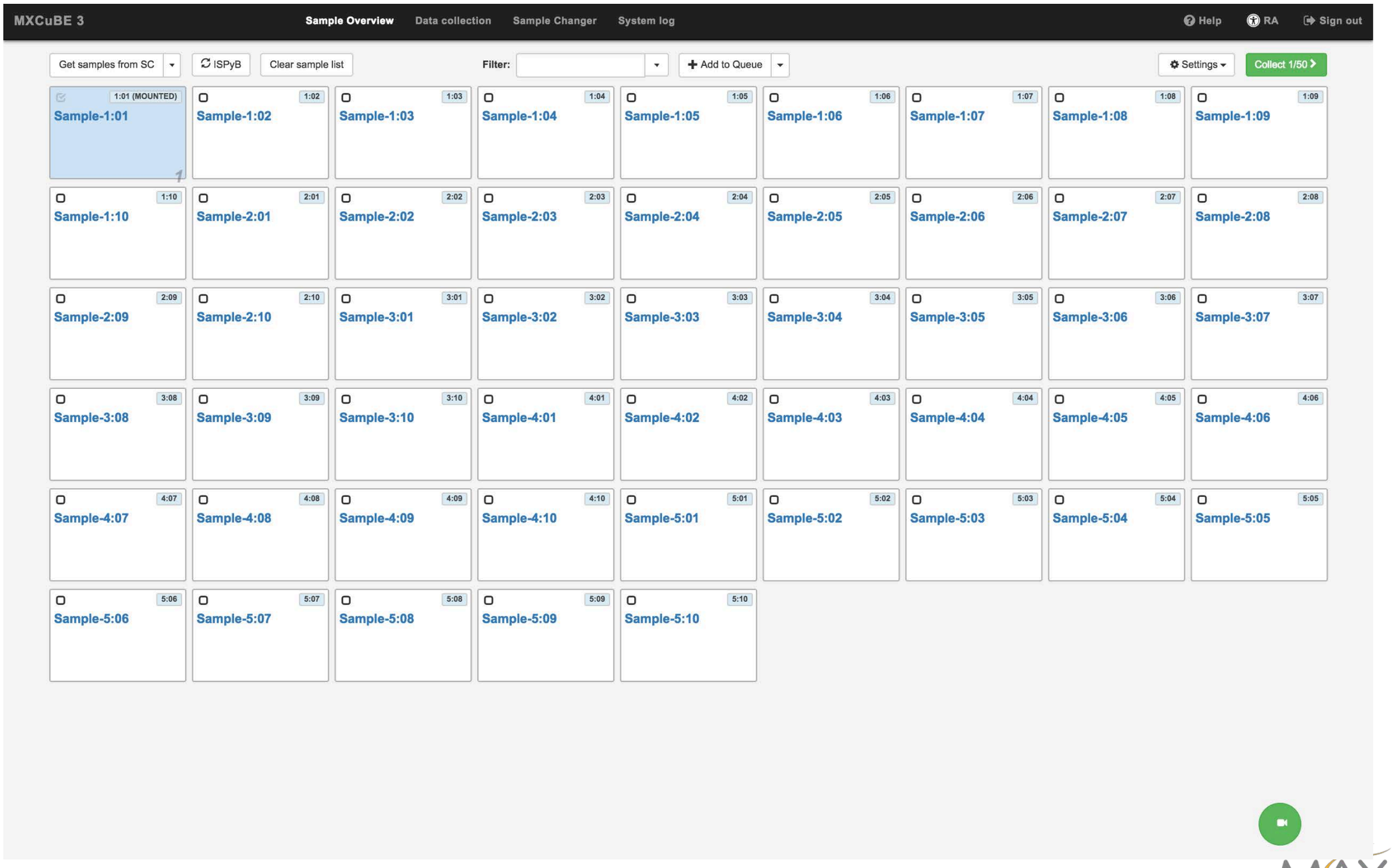


When selecting two points, one can add two collections or characterizations or one helical scan



Adding a helical scan after adding two collections

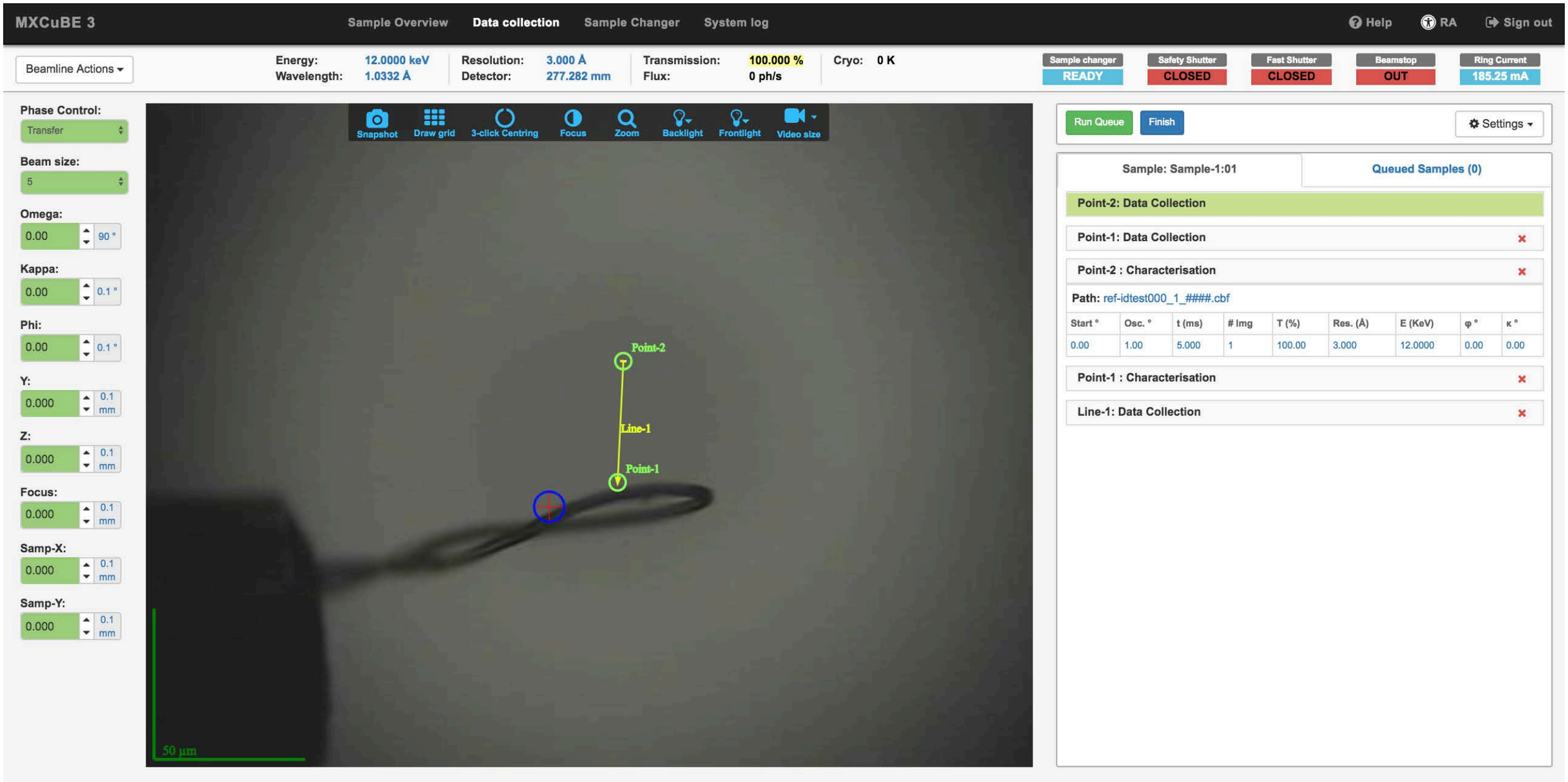
MX-CuBE3 enhanced sample logistics and automatic data collection support



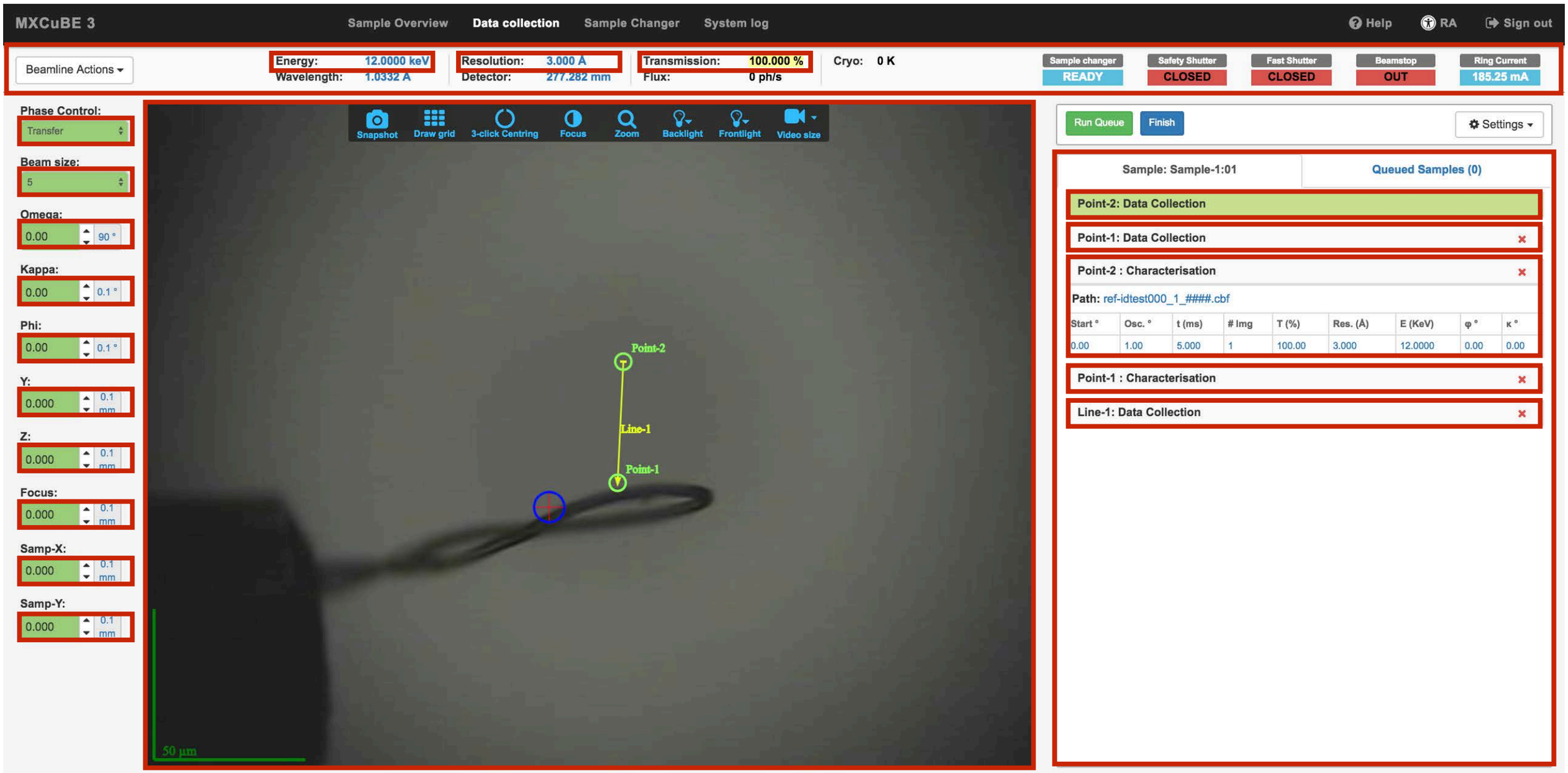
MXCuBE outlook: new methods & beyond MX and Xrays

- Incorporation of new methods, e.g. different serial crystallography methods (fixed target, microfluidics, extruders etc etc).
- Use at other highly standardised beamlines e.g. BioSAXS.
- Use of the front-end technology in other applications.

MXCuBE - Today

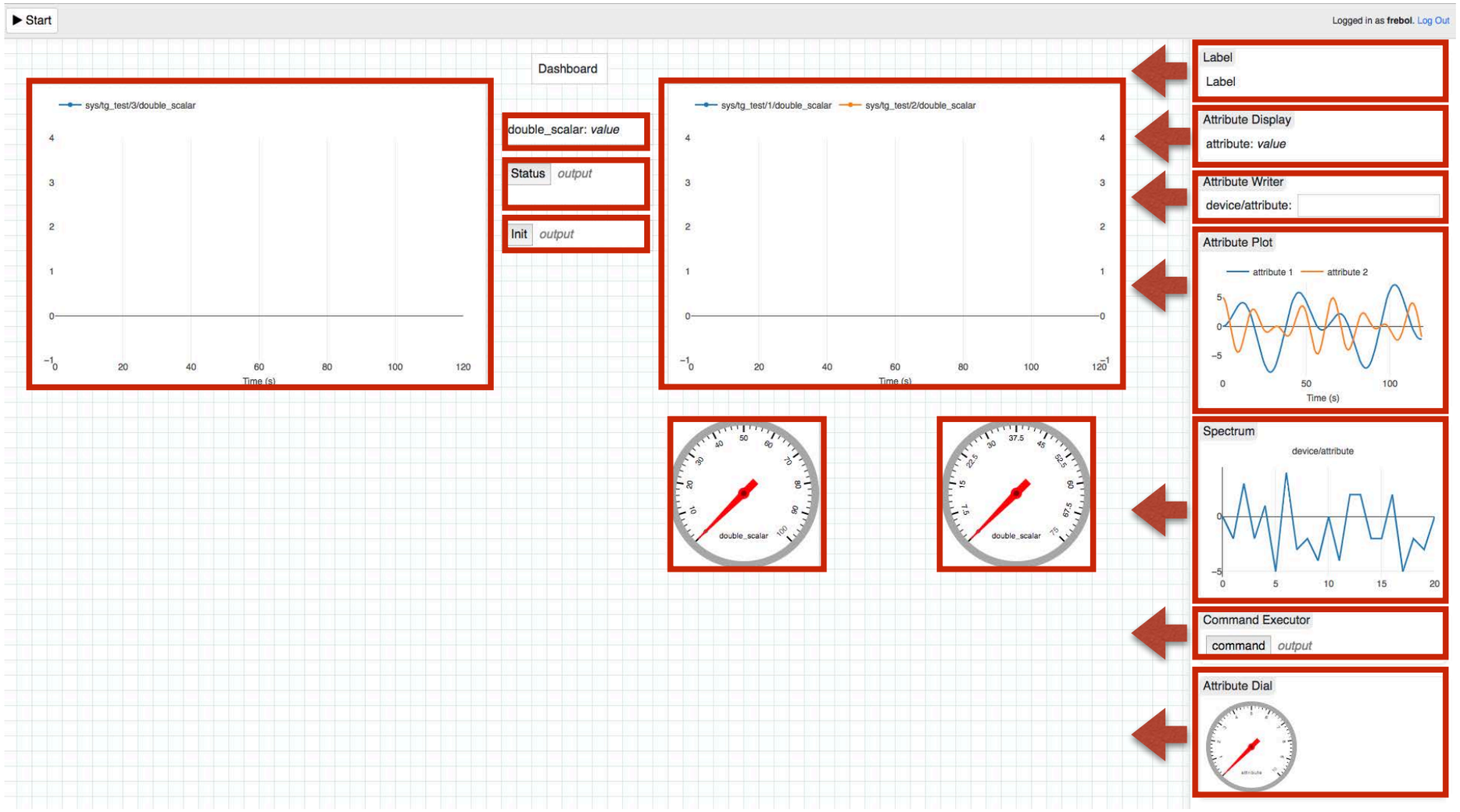


Layout - Fixed component based



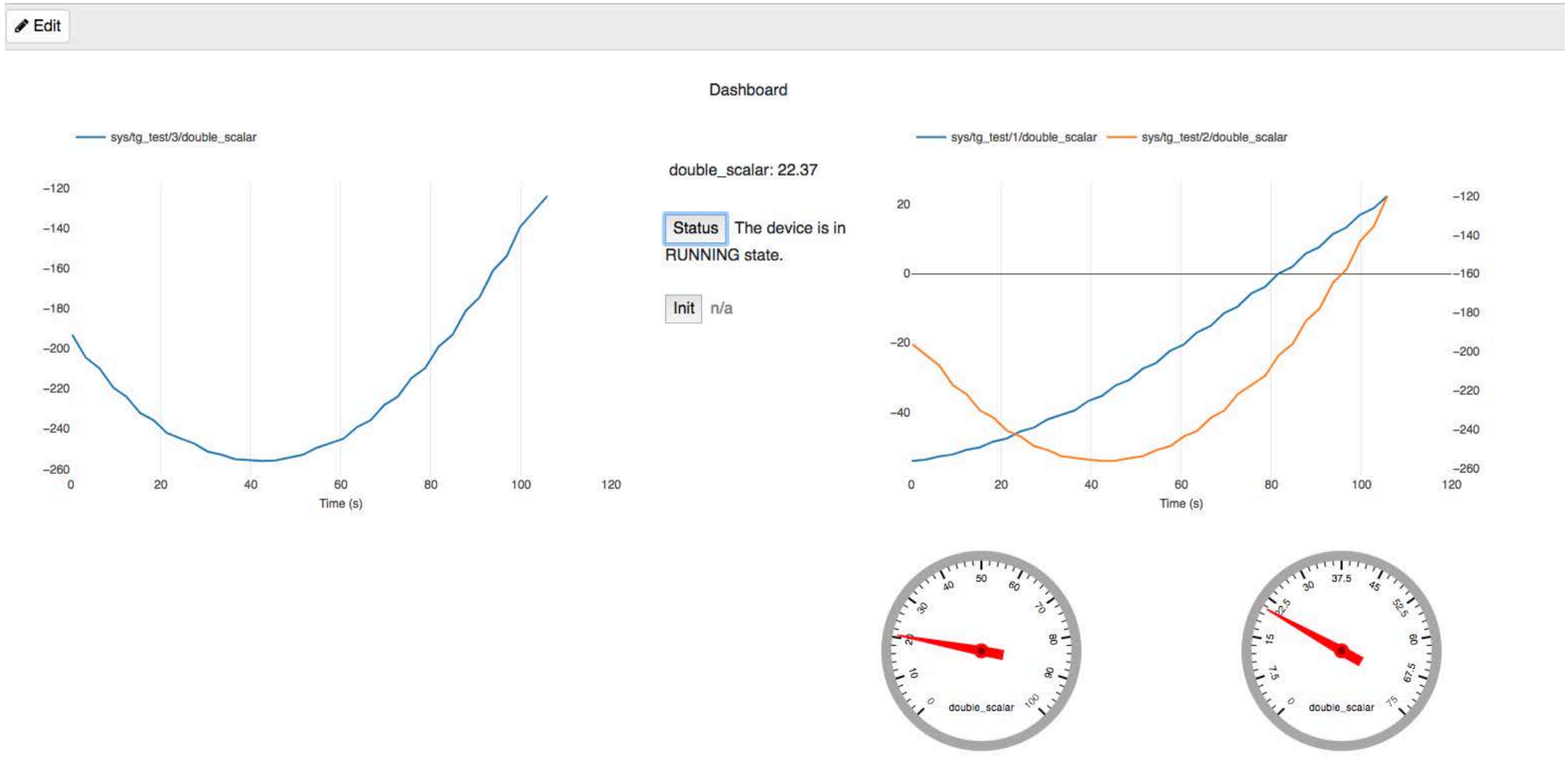
Future - Flexibel Component based

MAXIV - Mar. 2019



- GUI creator
  - Drag and Drop
  - Extendable
  - Shareable
- Generic
  - Available to all beamlines
  - User driven development

WebJive


Edit
Dashboard
sys/tg_test/3/double_scalar
−120
−140
−160
−180
−200
−220
−240
−260
0
20
40
60
80
100
120
Time (s)
double_scalar: 22.37
Status
The device is in RUNNING state.
Init
n/a
sys/tg_test/1/double_scalar
sys/tg_test/2/double_scalar
20
0
−20
−40
Time (s)
double_scalar
double_scalar

Thanks to

- Many people at the ESRF, in particular Matias Guijarro, Marcus Oscarsson & Daniele de Sanctis
- EMBL-HH, in particular Ivar Karpiĉs
- MAX IV in particular Mikel Eguiraun, Fredrik Bolmsten & Jie Nan
- All involved with the MXCuBE consortium