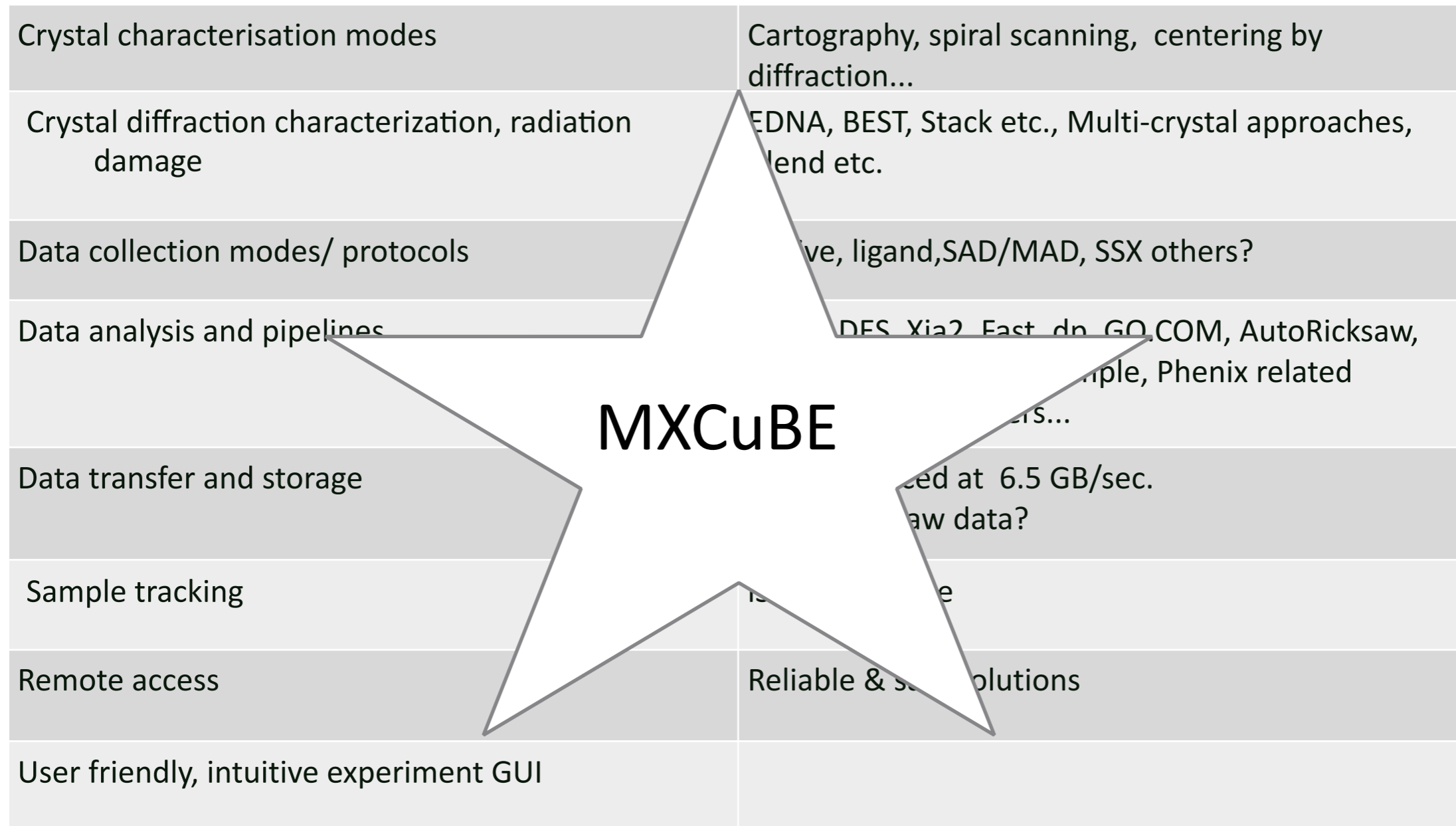




**The MXCuBE project:
Introduction to new developers
and partners**

Marjolein Thunnissen

Software requirements for MX



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 straightforward 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.



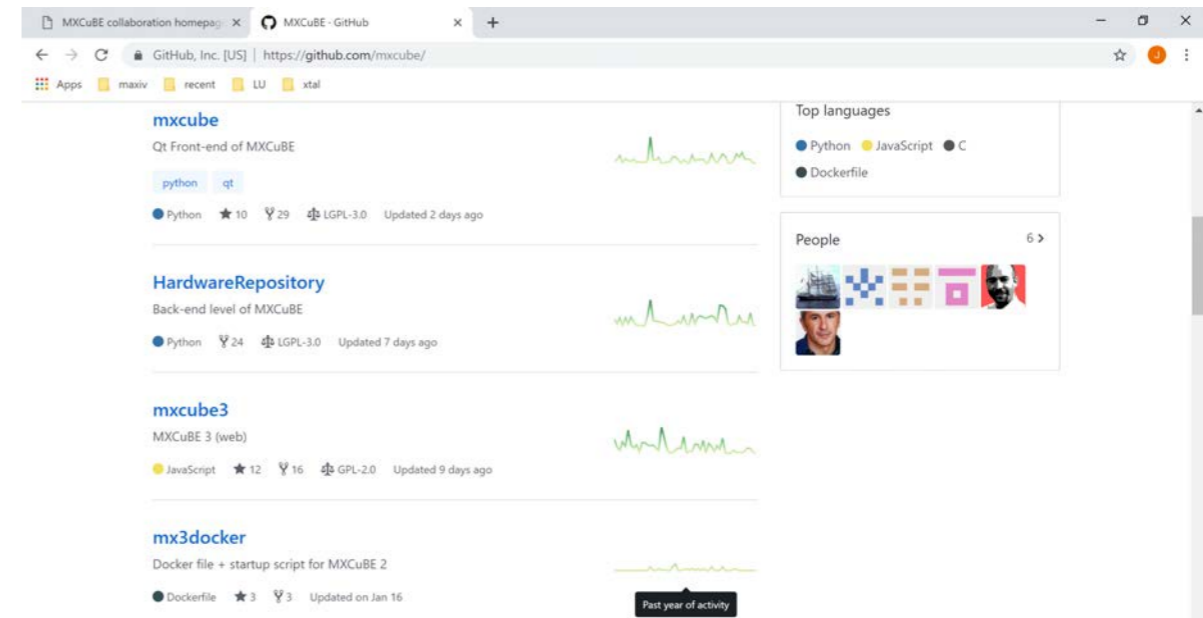
11th MXCuBE meeting, June 2017 at SOLEIL



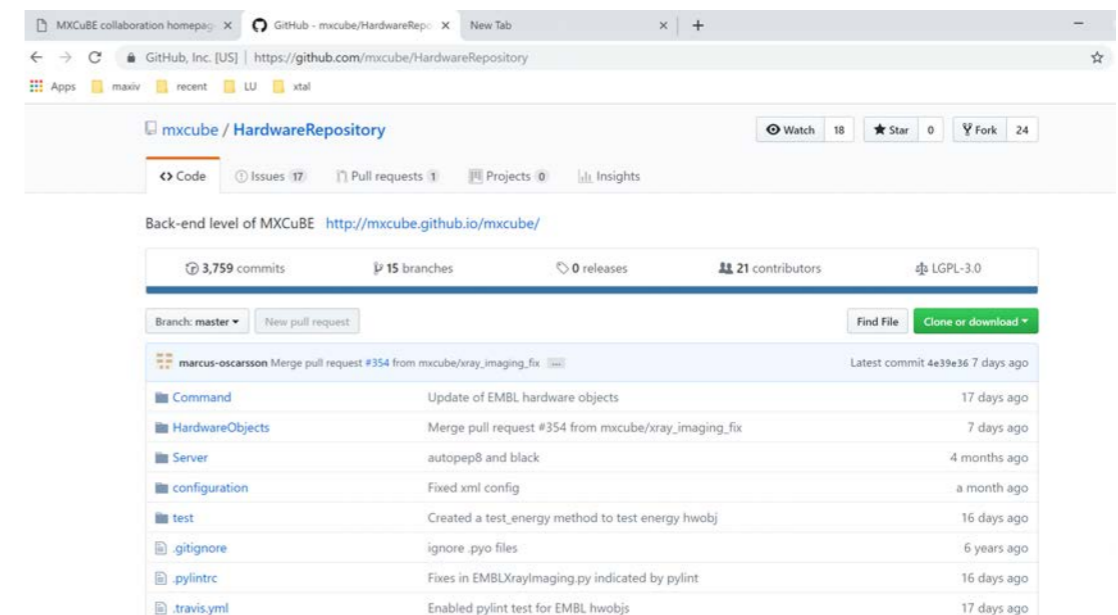
12th MXCuBE meeting, January/
February 2018 at Diamond

Tools to collaborate

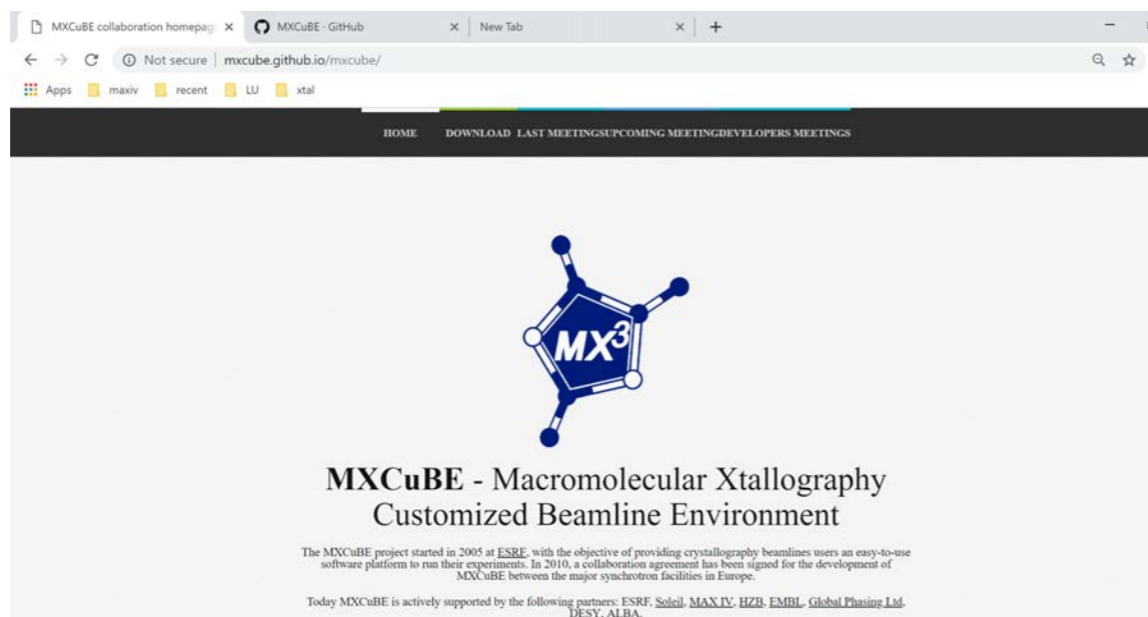
- GitHub
- Website
- Videoconferences
- Developers hackatons
- Scrums and agile methods
- MX-CuBE meetings, organise by site to site



A screenshot of the MXCuBE GitHub repository page. The page shows the repository name 'mxcube' and its description 'Qt Front-end of MXCuBE'. It lists the programming languages used: Python, JavaScript, C, and Dockerfile. The repository is updated 2 days ago. Below this, there are links to other repositories: 'HardwareRepository' (Back-end level of MXCuBE, updated 7 days ago), 'mxcube3' (MXCuBE 3 (web), updated 9 days ago), and 'mx3docker' (Docker file + startup script for MXCuBE 2, updated on Jan 16). The page also features a 'Top languages' section and a 'People' section with 6 contributors.



A screenshot of the MXCuBE HardwareRepository GitHub repository page. The page shows the repository name 'mxcube / HardwareRepository' and its description 'Back-end level of MXCuBE'. It lists the repository statistics: 3,759 commits, 15 branches, 0 releases, and 21 contributors. The repository is updated 7 days ago. The page also features a 'Code' section with a 'Find File' button and a 'Clone or download' button. Below this, there is a list of recent commits and pull requests, including a merge pull request #354 from mxcube/xray_imaging_fix.



A screenshot of the MXCuBE website. The website has a navigation bar with links: HOME, DOWNLOAD, LAST MEETINGS, UPCOMING MEETING, DEVELOPERS MEETINGS. The main content area features the MX³ logo, which is a blue cube with white dots at the corners. Below the logo, the text reads 'MXCuBE - Macromolecular Xtallography Customized Beamline Environment'. A paragraph of text describes the project's history and goals, and a list of supporting partners is provided at the bottom: ESRF, Soleil, MAX IV, HZB, EMBL, Global Phasing Ltd, DESY, ALBA.

<http://mxcube.github.io/mxcube/>

MXCuBE2

The screenshot displays the MXCuBE2 control software interface. The main window is titled "mxCuBE (mx-415)". The interface is divided into several panels:

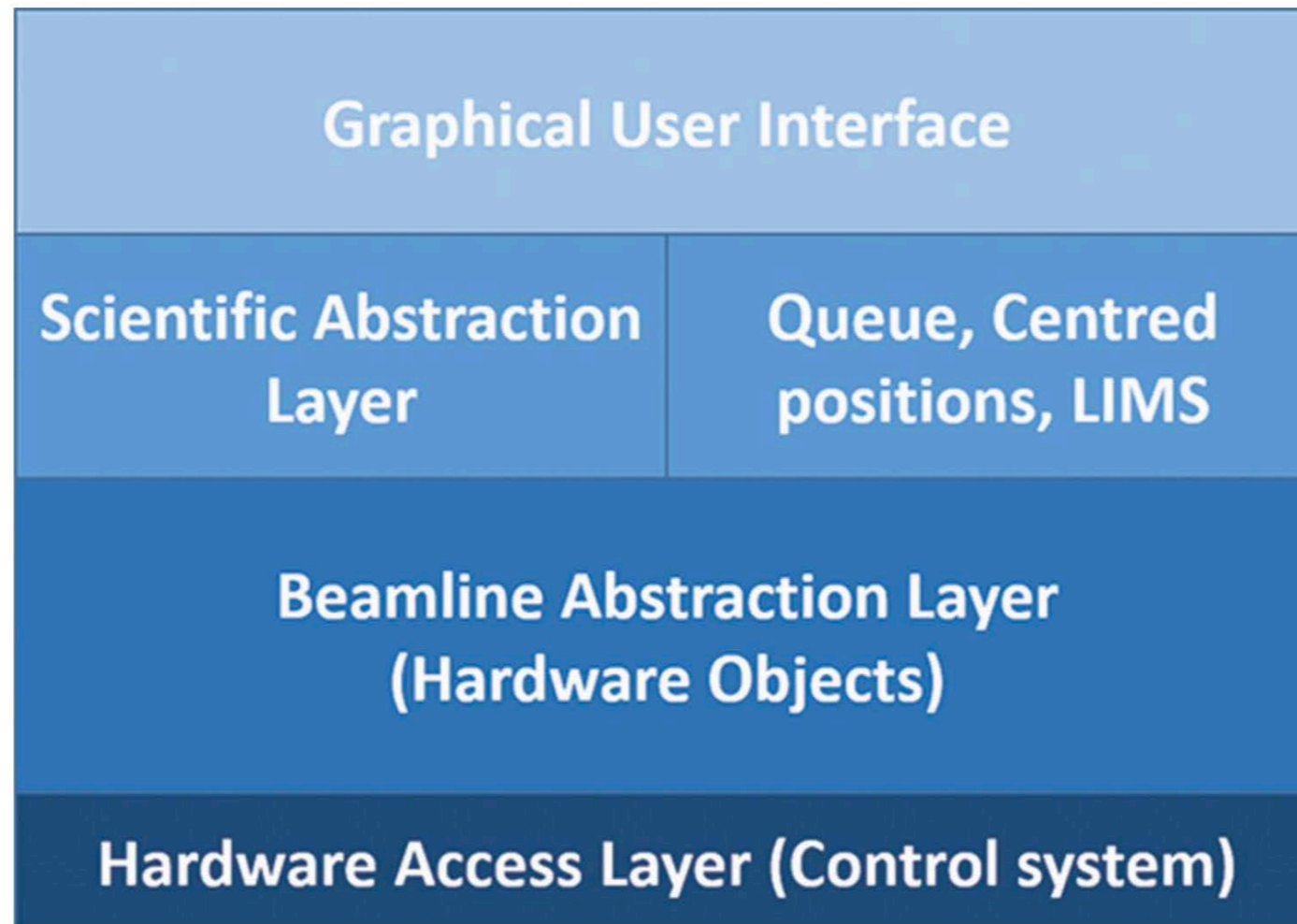
- Sample centring:** Shows sample position parameters: Omega: 89.98, Kappa: 0.0, Phi: 0.0, Holder length: 22.838. Below this is a "Sample video" window showing a live image of the sample with a scale bar of 100 μm . The video controls include Light: 0.36, Focus: -0.379, Front light: 0.0, and Zoom: 3. The aperture is set to 50 μm .
- Collection method:** Shows "Standard Collection" settings: Acquisition (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 (\AA): 3.61, Transmission (%): 49.67. Other options include Inverse beam, Subwedge size, and Shutterless.
- Data location:** Shows the folder path: /data/visitor/mx415/id23eh1/20140303/RAW_DATA and the file name: A-TIM-Test02_1_###.cbf. The prefix is A-TIM-Test02 and the run number is 1.
- Processing:** Shows "Process and analyse data" checked, with N.o. residues: 200. Other options include Anomalous and Space group.
- Characterisation:** Shows Helical Collection, Energy Scan, XRF spectrum, and Advanced options.
- Machine status (right panel):** Shows Machine current: 195.9 mA, Flux: 7/8 multibunch, Energy: 12.6000 keV, Current: 0.984, Resolution: 3.610 \AA , 738.70 nm, Transmission: 49.67%, and Cryo: 100.0 K.
- Safety and Control (right panel):** Shows Safety shutter: disabled, Fast shutter: closed, Beamstop: out, and Current users: basil.

The bottom status bar shows the following messages:

- [2014-03-03 10:09:04] Ready
- [2014-03-03 10:09:04] Centring in progress. Please save the suggested centring or re-center
- [2014-03-03 10:09:50] Centring saved

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

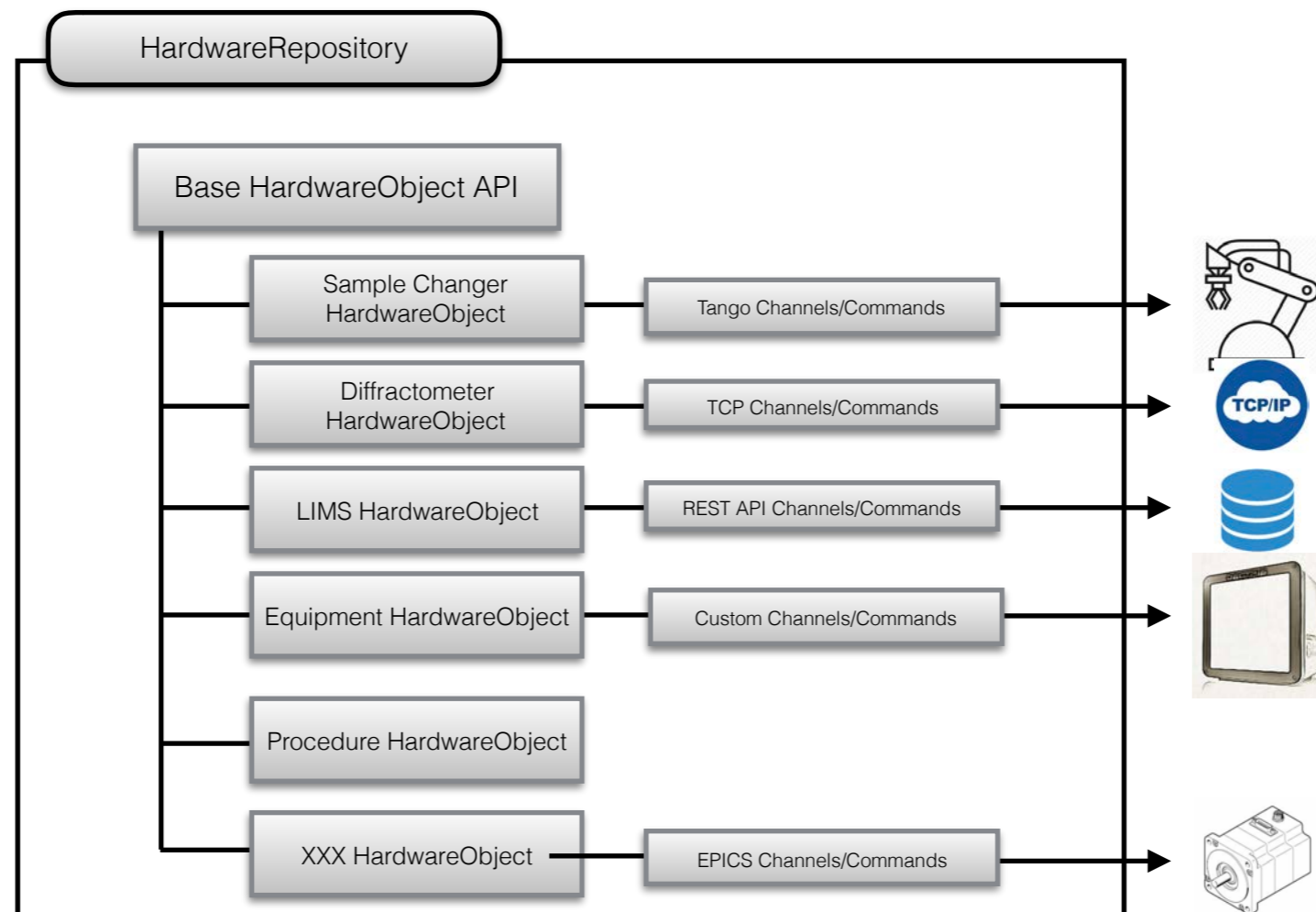
Architecture



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

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

```
<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

```
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)
```

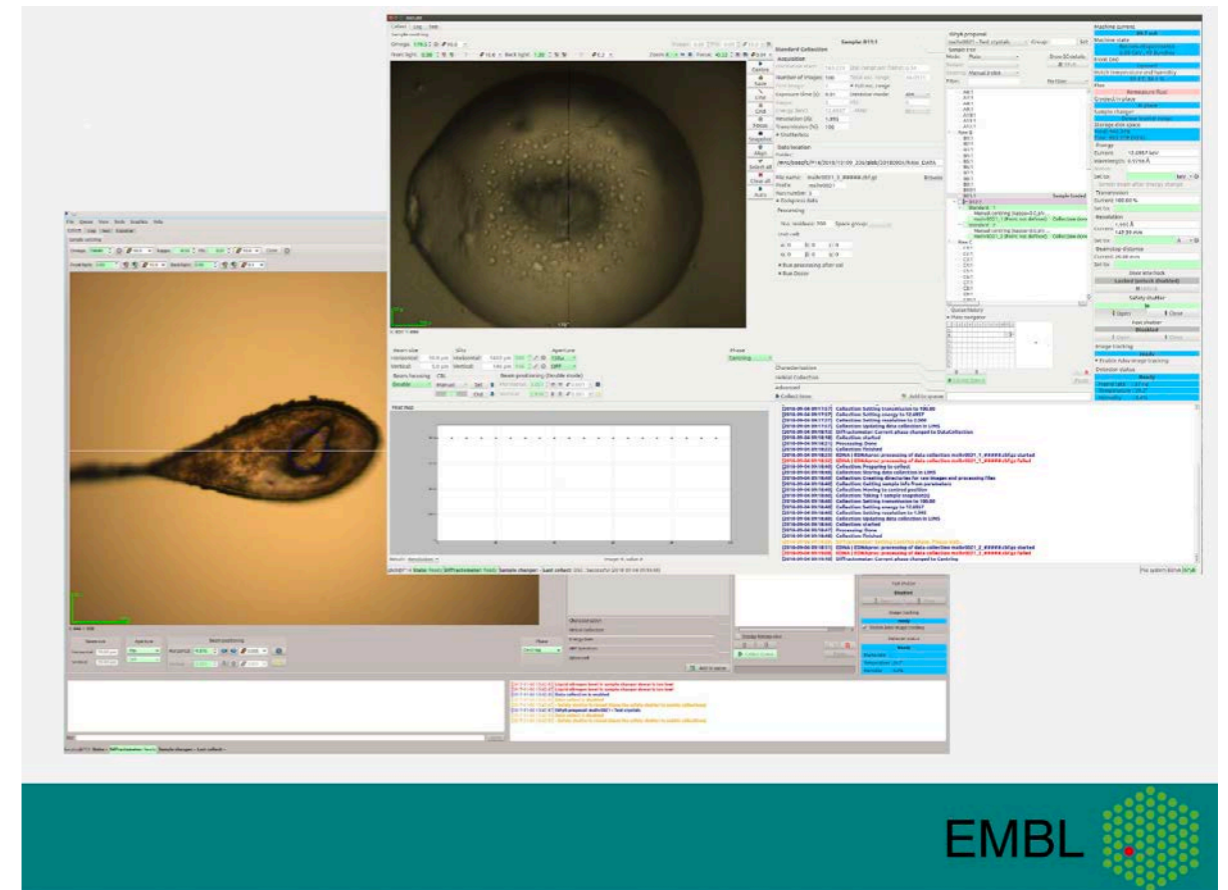
MicrodiffMotor.py

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 Karpīcs, 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

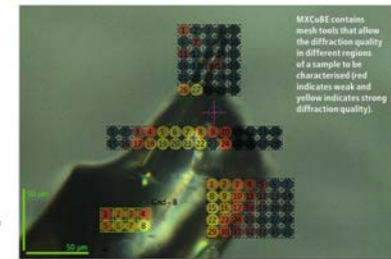
Feature

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 Environment) 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 BIGXHT. 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.



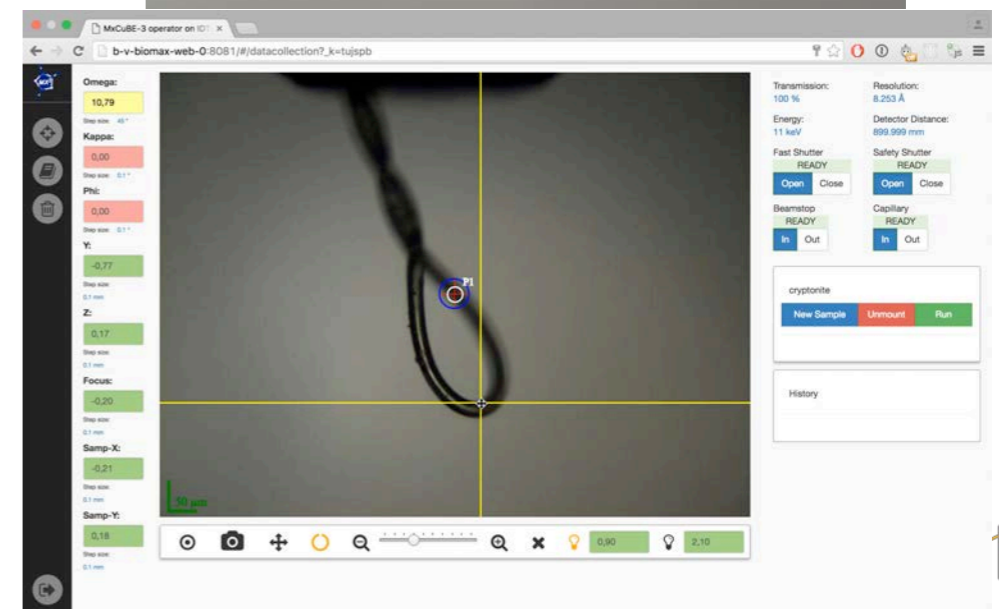
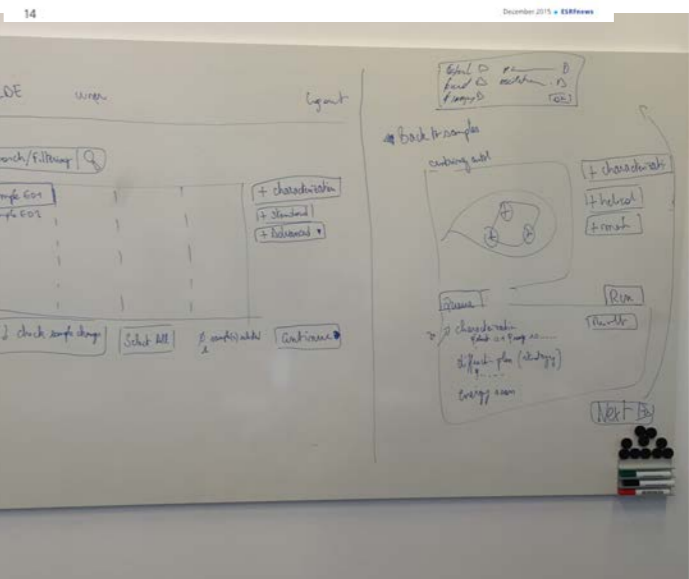
Thanks to the MXCuBE Consortium structural biology researchers now have access to a common software platform, with only certain site-specific customizations, at the majority of European synchrotron sites. This allows users to focus on the experiments they would like to perform with minimal distraction 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.

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 (MX3), 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 (PDB) 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 MX3 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.



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



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

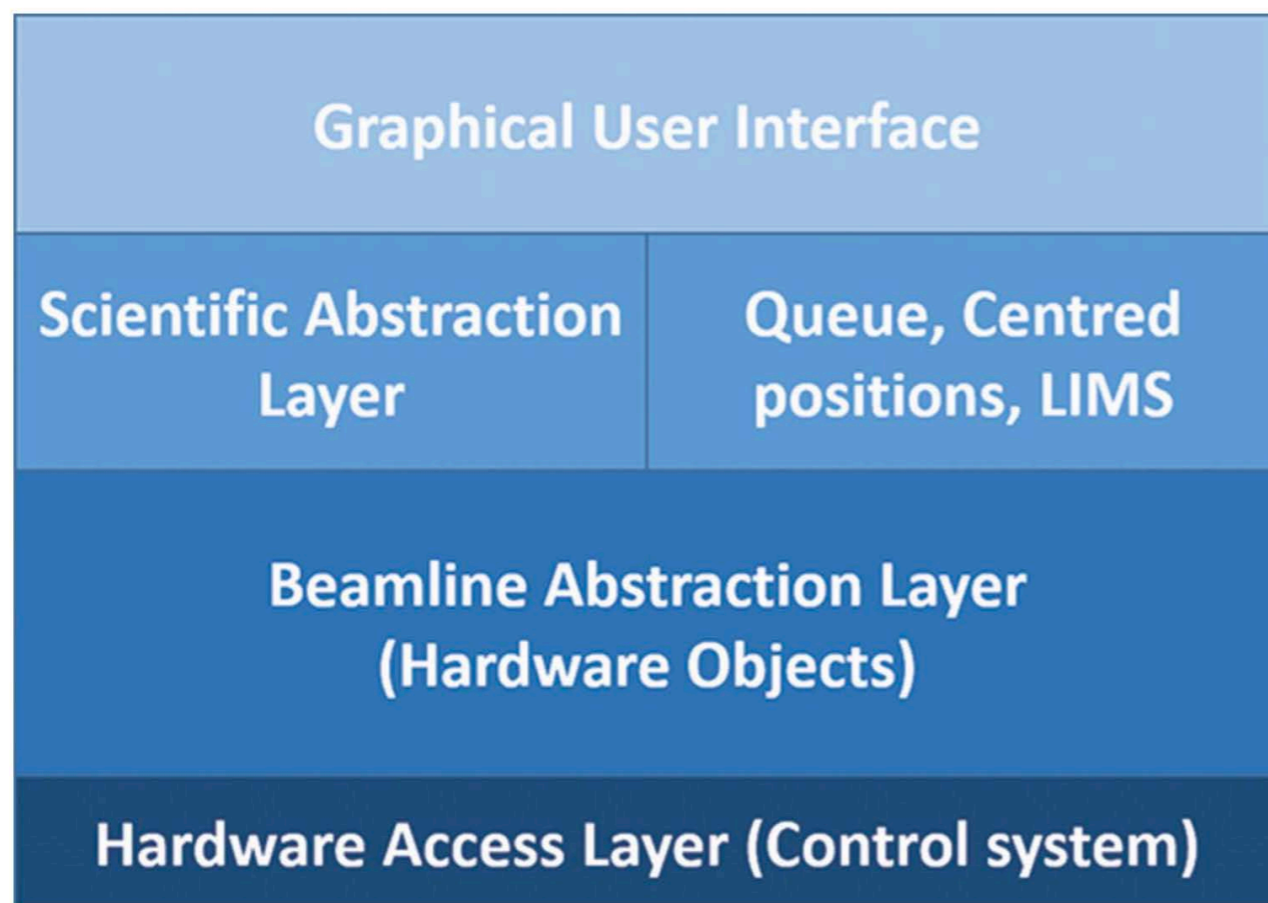
13 branches

7 releases

8 contributors

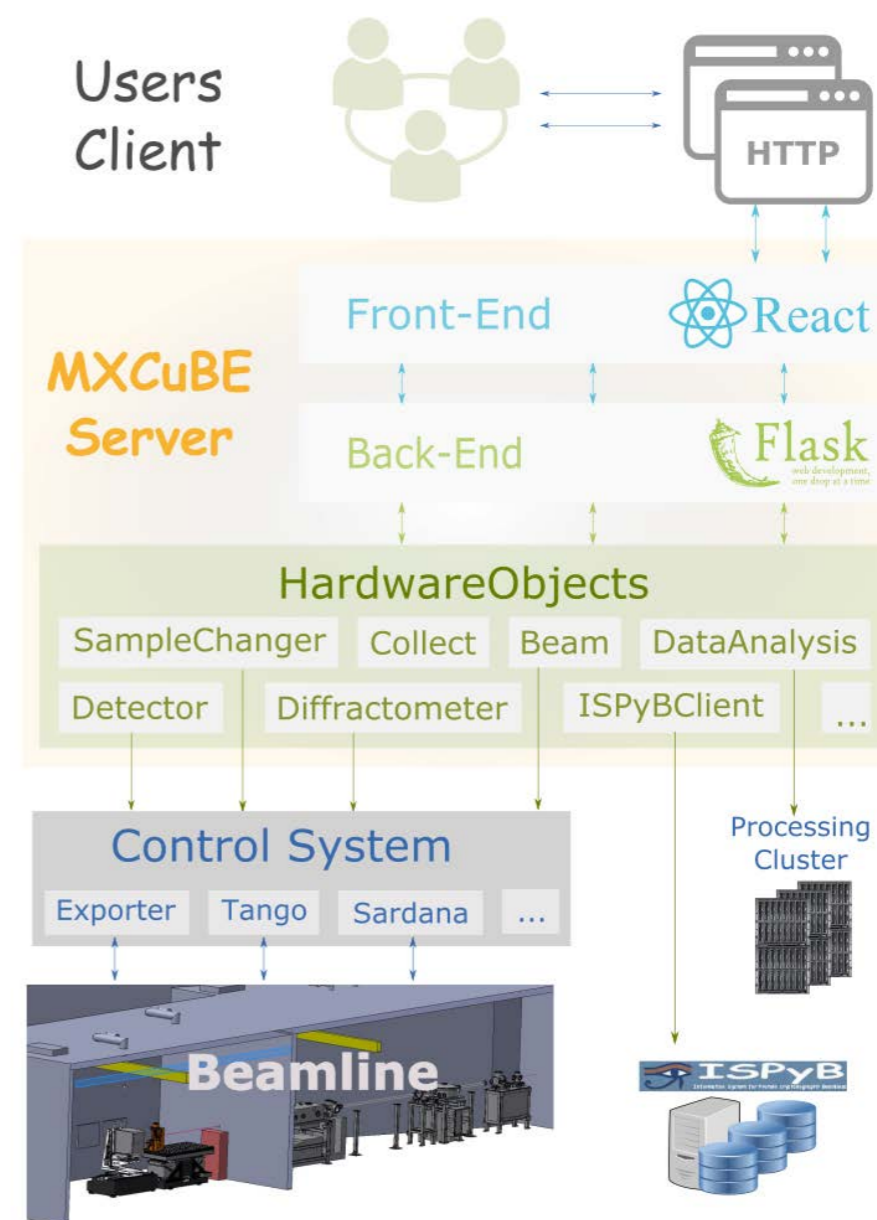
GPL-2.0

Architecture



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

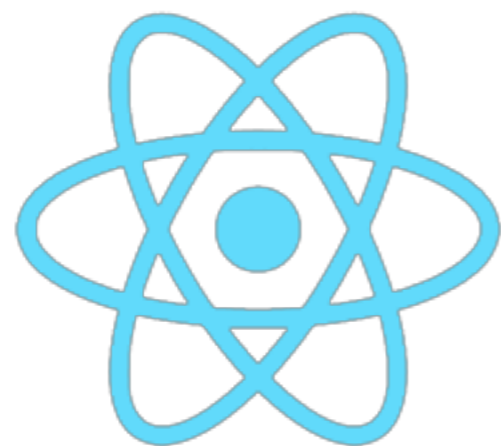
A schematic view of the MXCuBE3 software



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

MXCuBE 3 Sample Overview **Data collection** Sample Changer System log ? Help RA Sign out

Beamline Actions ▾ Energy: **12.0000 keV** Resolution: **3.000 Å** Transmission: **100.000 %** Cryo: **0 K**
 Wavelength: **1.0332 Å** Detector: **277.282 mm** Flux: **0 ph/s**

Sample changer: **READY** Safety Shutter: **CLOSED** Fast Shutter: **CLOSED** Beamstop: **OUT** Ring Current: **185.25 mA**

Phase Control: Transfer ▾

Beam size: 5 ▾

Omega: 0.00 ▾ 90 °

Kappa: 0.00 ▾ 0.1 °

Phi: 0.00 ▾ 0.1 °

Y: 0.000 ▾ 0.1 mm

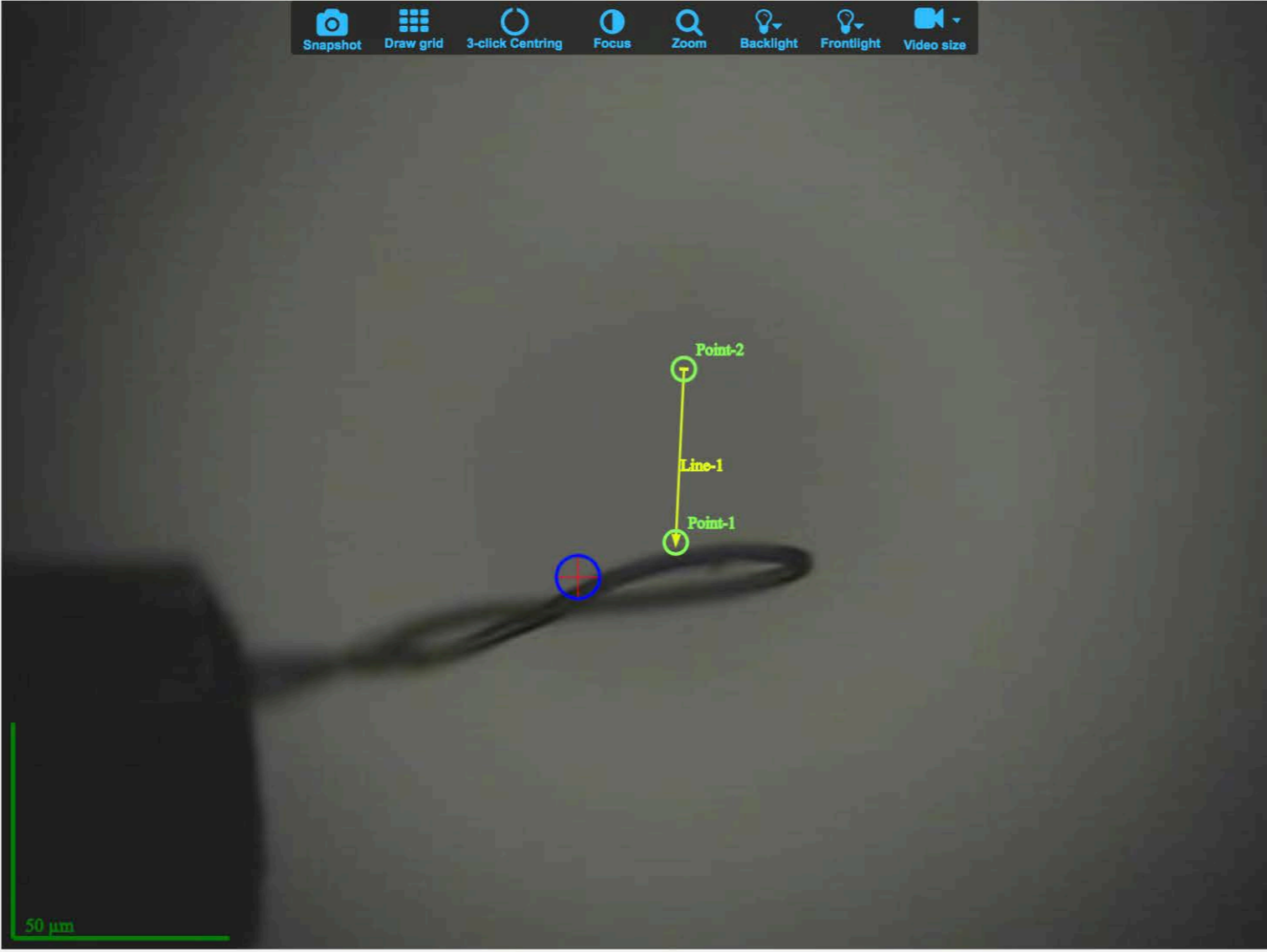
Z: 0.000 ▾ 0.1 mm

Focus: 0.000 ▾ 0.1 mm

Samp-X: 0.000 ▾ 0.1 mm

Samp-Y: 0.000 ▾ 0.1 mm

Snapshot Draw grid 3-click Centring Focus Zoom Backlight Frontlight Video size



Run Queue Finish Settings ▾

Sample: Sample-1:01 Queued Samples (0)

Point-2: Data Collection

Point-1: Data Collection ✖

Point-2 : Characterisation ✖

Path: ref-idtest000_1_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.00	1.00	5.000	1	100.00	3.000	12.0000	0.00	0.00

Point-1 : Characterisation ✖

Line-1: Data Collection ✖

MX-CuBE3 : video as canvas

The screenshot displays the MXCuBE3 web interface. At the top, the browser address bar shows "b-v-biomax-web-0:8081". The interface includes a navigation bar with "Sample Overview", "Data collection", "Sample Changer", and "System log". A status bar shows "Energy: 13.5000 keV", "Wavelength: 0.9184 Å", "Resolution: 1.529 Å", "Detector: 219.996 mm", "Transmission: 0.101 %", "Flux: 0 ph/s", and "Cryo: 0 K". On the right, there are status indicators for "Sample changer" (DISABLED), "Safety Shutter" (OPEN), and "Ring Current" (250.29). The main area is a video feed of the beamline, with a toolbar above it containing icons for "Snapshot", "Draw grid", "3-click Centring", "Focus", "Zoom", "Backlight", "Frontlight", and "Video size". Two points, "Point-2" and "Point-3", are marked on the video. A context menu is open over Point-3, offering options: "Add Datacollections", "Add Characterisations", and "Add Helical Scan". On the left, there are control panels for "Phase Control" (Centring), "Beam size" (20), "Omega" (100.17), "Kappa" (0.00), and "Phi" (0.00). Below these is a "Sample alignment" section with directional arrows and a "Show motors" button. On the right, there is a "Run Queue" section with "Run Queue" and "Unmount" buttons, and a "Queued Samples (0)" list containing "Point-2: Data Collection" and "Point-3: Data Collection". A small video window in the bottom right corner shows a live feed of the synchrotron facility, labeled "BioMAX 2019-03-10 21:30:52".

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

← → ↻ Not secure | b-v-biomax-web-0:8081

Apps maxiv recent LU xtal

MXCuBE 3 Sample Overview Data collection Sample Changer System log Help RA Sign out

Energy: 13.5000 keV Resolution: Wavelength: 0.9184 Å Detector:

Beamline Actions

Phase Control: Centring

Beam size: 20

Omega: 100.17 90°

Kappa: 0.00

Phi: 0.00

Sample alignment: Show motors

Sample changer: DISABLED Safety Shutter: OPEN Ring Current: 249.85

Run Queue Unmount Settings

Sample: cime - cime Queued Samples (0)

Point-2: Data Collection

Point-3: Data Collection

Point-2: Data Collection

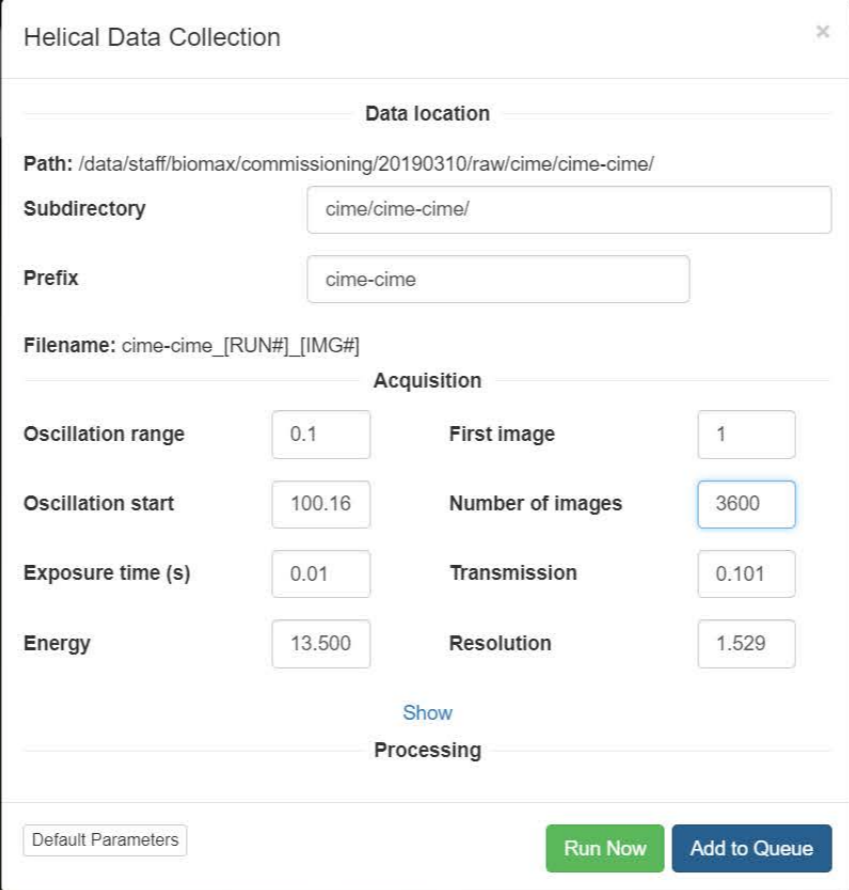
Point-3: Data Collection

Path: cime-cime_4 #####.h5

Start °	Osc. °	t (s)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
100.17	0.10	0.0110	1800	0.10	1.529	13.5000	0.00	0.00

Diffractionmeter

BioMAX 2019-03-10 21:32:11



Helical Data Collection

Data location

Path: /data/staff/biomax/commissioning/20190310/raw/cime/cime-cime/

Subdirectory: cime/cime-cime/

Prefix: cime-cime

Filename: cime-cime_[RUN#]_[IMG#]

Acquisition

Oscillation range: 0.1 First image: 1

Oscillation start: 100.16 Number of images: 3600

Exposure time (s): 0.01 Transmission: 0.101

Energy: 13.500 Resolution: 1.529

Show

Processing

Default Parameters Run Now Add to Queue

Adding a helical scan after adding two collections

MX-CuBE3 enhanced sample logistics and automatic data collection support

The screenshot displays the MXCuBE 3 Sample Overview interface. At the top, there is a navigation bar with the title 'MXCuBE 3' and tabs for 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. On the right side of the navigation bar are links for 'Help', 'RA', and 'Sign out'. Below the navigation bar, there is a control area with a dropdown menu 'Get samples from SC', a 'Clear sample list' button, a 'Filter:' input field, an 'Add to Queue' button, a 'Settings' dropdown, and a 'Collect 1/50' button. The main area is a grid of 50 sample slots, arranged in 5 rows and 10 columns. Each slot contains a sample ID (e.g., 'Sample-1:01') and a small icon in the top right corner. The first slot, 'Sample-1:01', is highlighted in blue and has a '1:01 (MOUNTED)' label in its top right corner. A small number '1' is visible in the bottom right corner of this slot. The other slots are white with a small square icon in the top left corner. The grid ends with 'Sample-5:10' in the bottom right corner.

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

MXCuBE 3

[Sample Overview](#)
[Data collection](#)
[Sample Changer](#)
[System log](#)
? Help
RA
Sign out

Beamline Actions ▾

Energy: **12.0000 keV**
 Wavelength: **1.0332 Å**

Resolution: **3.000 Å**
 Detector: **277.282 mm**

Transmission: **100.000 %**
 Flux: **0 ph/s**

Cryo: **0 K**

Sample changer
READY

Safety Shutter
CLOSED

Fast Shutter
CLOSED

Beamstop
OUT

Ring Current
185.25 mA

Phase Control:

Transfer ▾

Beam size:

5 ▾

Omega:

0.00 ▾ 90 °

Kappa:

0.00 ▾ 0.1 °

Phi:

0.00 ▾ 0.1 °

Y:

0.000 ▾ 0.1 mm

Z:

0.000 ▾ 0.1 mm

Focus:

0.000 ▾ 0.1 mm

Samp-X:

0.000 ▾ 0.1 mm

Samp-Y:

0.000 ▾ 0.1 mm

Run Queue
Finish
Settings ▾

Sample: Sample-1:01

Queued Samples (0)

Point-2: Data Collection

Point-1: Data Collection ✖

Point-2 : Characterisation ✖

Path: ref-idtest000_1_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.00	1.00	5.000	1	100.00	3.000	12.0000	0.00	0.00

Point-1 : Characterisation ✖

Line-1: Data Collection ✖

Layout - Fixed component based

MXCuBE 3 Sample Overview **Data collection** Sample Changer System log Help RA Sign out

Beamline Actions ▾ **Energy: 12.0000 keV** **Resolution: 3.000 Å** **Transmission: 100.000 %** Cryo: 0 K

Wavelength: 1.0332 Å Detector: 277.282 mm Flux: 0 ph/s

Sample changer: **READY** Safety Shutter: **CLOSED** Fast Shutter: **CLOSED** Beamstop: **OUT** Ring Current: **185.25 mA**

Phase Control: Transfer ▾

Beam size: 5 ▾

Omega: 0.00 ▾ 90 °

Kappa: 0.00 ▾ 0.1 °

Phi: 0.00 ▾ 0.1 °

Y: 0.000 ▾ 0.1 mm

Z: 0.000 ▾ 0.1 mm

Focus: 0.000 ▾ 0.1 mm

Samp-X: 0.000 ▾ 0.1 mm

Samp-Y: 0.000 ▾ 0.1 mm

Snapshot Draw grid 3-click Centring Focus Zoom Backlight Frontlight Video size

Point-2
Line-1
Point-1

50 µm

Run Queue Finish Settings ▾

Sample: Sample-1:01 Queued Samples (0)

Point-2: Data Collection

Point-1: Data Collection ✕

Point-2 : Characterisation ✕

Path: ref-idtest000_1_####.cbf

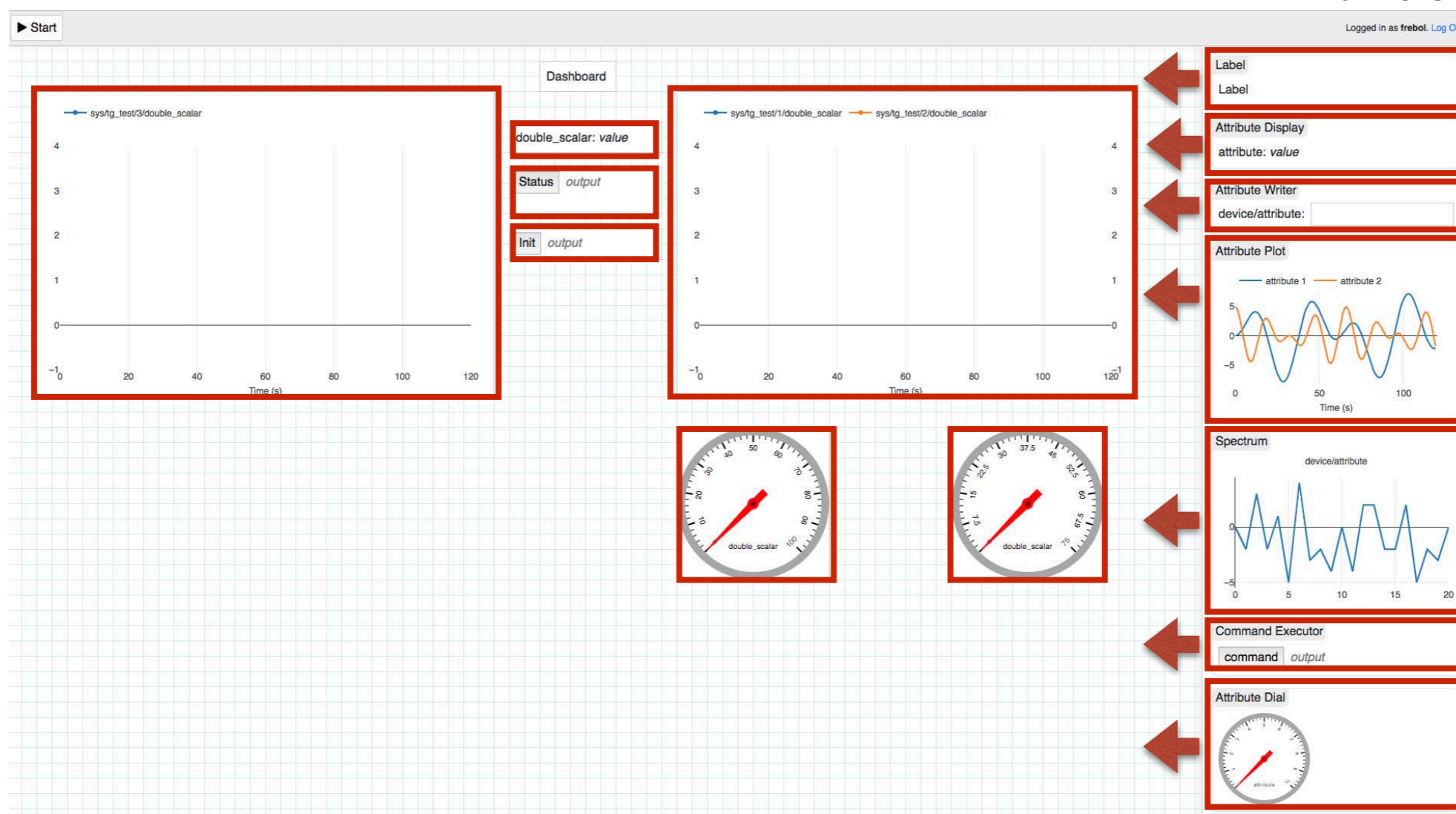
Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.00	1.00	5.000	1	100.00	3.000	12.0000	0.00	0.00

Point-1 : Characterisation ✕

Line-1: Data Collection ✕

Future - Flexibel Component based

MAXIV - Mar. 2019



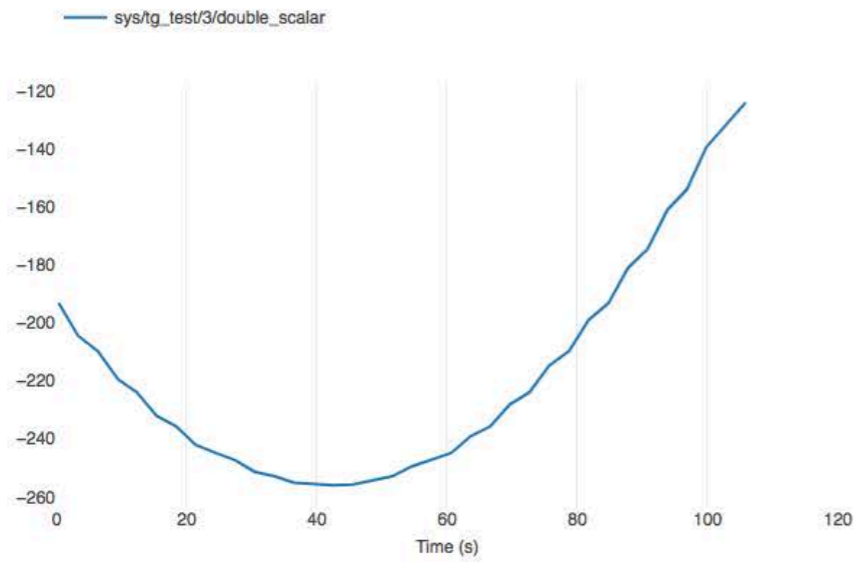
- GUI creator
 - Drag and Drop
 - Extendable
 - Shareable

- Generic
 - Available to all beamlines
 - User driven development

WebJive

Edit

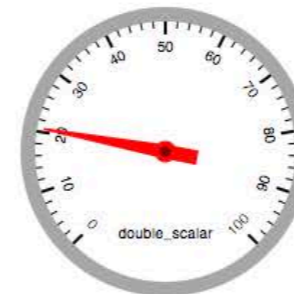
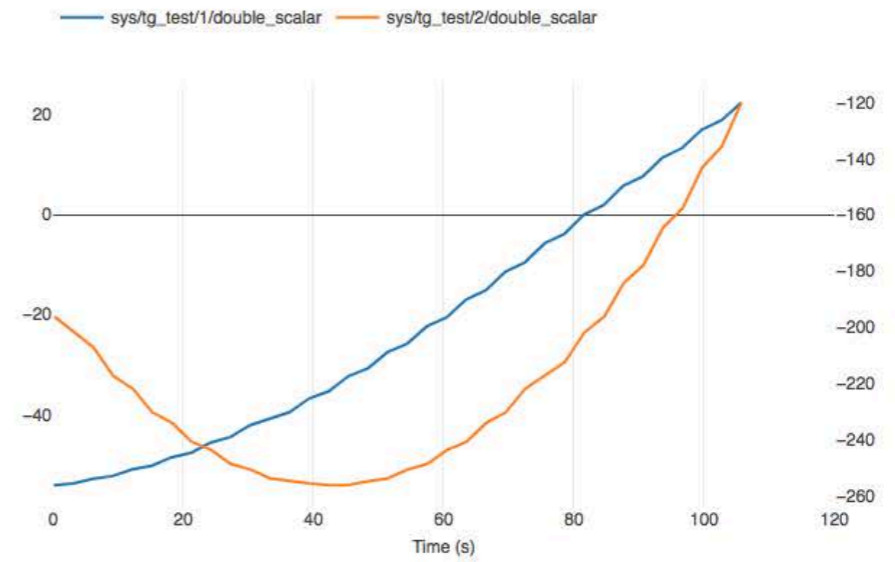
Dashboard



double_scalar: 22.37

Status The device is in RUNNING state.

Init n/a



Thanks to

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

