



MXCuBE 3 web application: on the way to next generation experiment control

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NOBUGS 16

Outline

- MXCuBE project
- MXCuBE v3
 - Technologies in use
 - User interface
 - Demo video
- Next steps & work force



MXCuBE

- Macromolecular Xtallography Customized Beamline Environment
 - Started in 2005 at ESRF
 - Beamline control and data acquisition platform for running MX experiments
- Supported by the following partners: ESRF, Soleil, MAX IV, HZB, EMBL, Global Phasing Ltd, DESY, ALBA.
- Already tested software & builtin experience (many years + many people + many beamlines)



ALBA, Dec. 2015

MXCuBE - Main Features

- Customizable for each beamline/facility
- Reuse of existing code for different beamlines; common solution for users
 - same or similar hardware devices
 - same or similar experimental procedures
- Hardware mockups available, testing and developing without equipment
- Current stable version based on PyQt
- Hide the complexity of the Hardware to the user (and to the developers...) thanks to the usage of the **HardwareObjects**

MXCuBE - HardwareObjects

- Self-contained piece of software linking devices and graphical interface
 - Through the *HardwareRepository*
- Configured through xml files
- A HO is not only hardware! Procedures/sequences etc
- Emitting signals to hardware objects, graphical elements
- Supported protocols: Tango, EPCIS, Sardana...

```
<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>
```

MotorOmega.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

MXCuBE 3



- Beamline control and data acquisition as web application
- Reuse existing HardwareObjects maintaining compatibility with v2
- Modern web technologies for user interface
- Easier integration with LIMS (*laboratory information management system*)
- Maintenance and deployment (decoupling client/server)
- Remote access in a more *natural* way
- Feedback from user community

<https://github.com/mxcube/mxcube3>

MXCuBE 3: Current status

- Under development but first data collection during Biomax commissioning (June 2016, MAX IV)
- Sample imaging and operation
- Basic data collection strategies
 - experiment queue configuration and execution
 - standard dc, characterisation, helical
- Screen mirroring / master-slave operation
- LIMS and sample changer integration very advanced

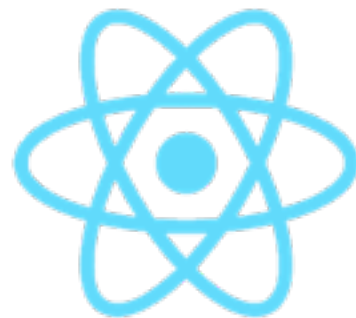


Backend

- Python **Flask** microwebframework:
 - web server made simple
 - extensions (database, login, ...)
 - easily adaptable to your needs while scalable
- http request **API**: rest-like
 - url for each function
 - Simple to add new features without changing existing ones
- Flask **socketio** for sending HO messages
 - server-client bi-directional communication, websocket based
- Reuse the existing Hardware Objects

Frontend REACT

- User interface has been redesigned (compared to MXCuBE v2)
- **Javascript/React** library (Facebook)
- Only for the user interface (the V in MVC)
- UI is described as a collection of components
 - Different components programmed independently
- Reusing existing code when the layout changes



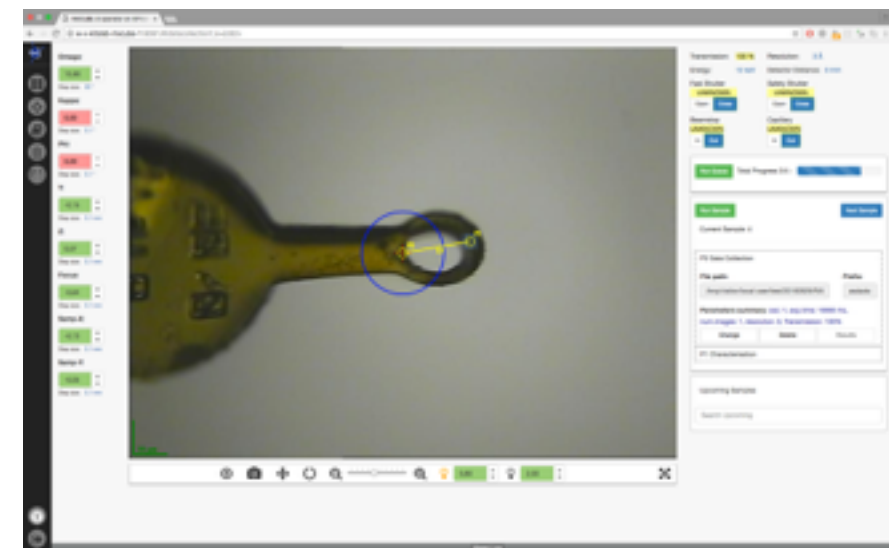
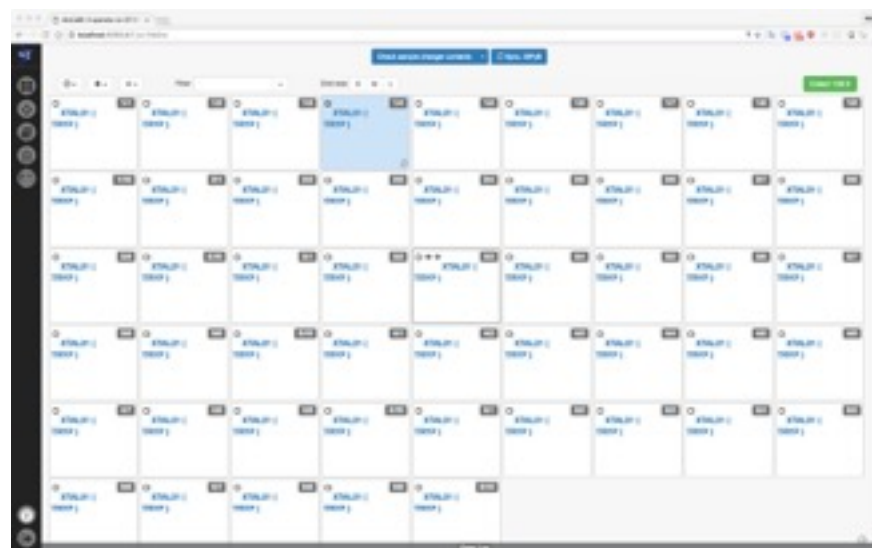
Frontend REDUX

- **Redux** application architecture/pattern
 - Predictable state container for JavaScript apps
 - Changes on the internal state in a single place
 - Unidirectional data flow
 - Clear and safe development



User Interface

- Two main operation modes:
 - Automatic:
 - multiple sample selection and configuration
 - Workflows (predefined sequence of automatic operations)
 - Manual:
 - sample by sample
 - manual operation and configuration



Sample Grid

The screenshot displays the MxCube-3 operator interface. At the top, there are two buttons: "Check sample changer contents" and "Sync. ISPyB". Below these, there are controls for "Fiber" and "Grid size" (S, M, L). A "Collect 1/50" button is located in the top right corner. The main area is a 5x10 grid of sample positions. Each cell contains the text "XTAL01 (TRYP)" and a small black box with a white number indicating its coordinates (row:column). The cell at position 1:4 is highlighted in blue. The grid is numbered as follows:

1:1	1:2	1:3	1:4	1:5	1:6	1:7	1:8	1:9	1:10
2:1	2:2	2:3	2:4	2:5	2:6	2:7	2:8	2:9	2:10
3:1	3:2	3:3	3:4	3:5	3:6	3:7	3:8	3:9	3:10
4:1	4:2	4:3	4:4	4:5	4:6	4:7	4:8	4:9	4:10
5:1	5:2	5:3	5:4	5:5	5:6	5:7	5:8	5:9	5:10

At the bottom center, there is an "Open Log" button. The browser address bar shows "localhost:8090/#/?_k=1hk0nz".

Data Collection

MxCuBE-3 operator on IDTES: X

w-v-kitslab-mxcube-1:8081/#/datacollection?k=jz82v

Omega: 10.90
Step size: 90°

Kappa: 0.00
Step size: 0.1°

Phi: 0.00
Step size: 0.1°

Y: -0.15
Step size: 0.1 mm

Z: 0.07
Step size: 0.1 mm

Focus: -0.64
Step size: 0.1 mm

Samp-X: -0.13
Step size: 0.1 mm

Samp-Y: -0.05
Step size: 0.1 mm

Transmission: 100% Resolution: 3 Å

Energy: 12 keV Detector Distance: 0 mm

Fast Shutter UNKNOWN
Open Close

Safety Shutter UNKNOWN
Open Close

Beamstop UNKNOWN
In Out

Capillary UNKNOWN
In Out

Run Queue Total Progress 3/4

Run Sample Next Sample

Current Sample: 4

P2 Data Collection

File path: /tmp/visitor/local-user/test/20160929/TVA/ Prefix: asdads

Parameters summary: osc: 1, exp.time: 10000 ms, num.images: 1, resolution: 3, Transmission: 100%

Change Delete Results

P1 Characterisation

Upcoming Samples

Search Upcoming

50 μm

0.60 2.00

Open Log

Demo video

The screenshot shows a web browser window with the following elements:

- Browser Menu:** Chrome, File, Edit, View, History, Bookmarks, People, Window, Help.
- Address Bar:** localhost:8090/#/login?_k=whxu04
- Page Content:**
 - MX logo (a blue hexagon with 'MX' inside).
 - Text: "Welcome to MX Beamline at MAXIV"
 - Form:
 - Label: "LoginID" above a text input field containing "User".
 - Label: "Password" above a text input field containing "Password".
 - Button: "Sign in" (blue background, white text).

Next steps

- Continue the development
 - Finish LIMS and sample changer interfaces
 - Polish the interface (icons, buttons, minimal layout changes)
 - Debugging
 - Performance improvements
 - Additional views
 - Ready for users

MXCuBE3 People

MAX IV: M. Eguraun, A. Milan-Otero, J. Nan, F. Bolmsten, M. Thunnissen, V. Hardion, D. Spruce

ESRF: M. Guijarro, M. Orkarsson, A. Beteva, D. de Sanctis, G. Leonard, J. Meyer, A. Gotz

Supported by:

MXCuBE collaboration

MAX IV MX and KITS teams

ESRF BCU and SB teams

Thanks for your attention!

