

# Bringing MX experiments to the web MXCuBE 3



# Outline

- An MX Beamline at glance
- Project background
- Backend, beamline control layer
- Web service layer
- Frontend Development
- Screenshots



## An MX beamline

• Aim is to resolve protein structure



An X-ray beam is focused on a **crystal** 



The crystal is rotated and **diffraction images** are captured



An **electron density map** is calculated from the diffraction images



It's possible to resolve the **molecular structure** from the electron density map





#### **MX-Beamline**

- 2D Detector
- Diffractometer
- Sample changer
- And various other instruments
  - Monochromator
  - Mirrors
  - Filters
  - Aperture
  - o ...

#### MXCuBE is the application used for instrument control and data acquisition



### Project history and background

		₩	0.00
Include (p)//ski/	0000	Ele lettimentiles Mele	Emot not
ne toyustaan nep	C ester nove		- Marbine named
A loss	2013-04-172	L3 Collect BAXRF spectrum Log	???.? mA
	Machine current	User Sample centring	
😭 Hunch 🗋 Collect 🏤 🔛 XRF spectrum EDNA Log	154.3 mA	Legost opid-144 operator on ID14eh4 -Sample position	Colector method
- Available samples	Sample changer unform multibunch	Sample charger Holder length 21,000 B #01 + Kargar 0.0 B #710 + Orregar 0.0 B	Discrete Transmission: 100.87
Name Acronym Шагсобе Location • Space group   a b c α β τ Maxme. Шакен scattering Edd. 106 P272105 64 108 B133 940 901 9300	Standby UU-UU	Show. All samples ¥ Show details Sample video	-Acquisition EnergyK
-sample6 FAE 1.06 P212121 66.4 108.8 113.9 90.0 90.0 90.0	Ready Cryo	Contrior Manual	Oscillation range: 0.2 First image: 1 Resolution: 3.35
	O Surple charger can bad urbad Dry: unknown	Light: 0.32 ∰ 20.01 + 97 57 Front light: 0.6 ∰ 21.0 + Zoont 1 + Focus: 0.6 ∰ 20.01 +	Oscillation overlap: 0.0 Number of images: 1 292.4 K
-sample10 TRYP 1:10 P212121 54.1 58.2 66.6 90.0 90.0 90.0	Mindfimores can maxe     Superdry: of     King     Mindfimores	Sample location Status	Oscillation start: 0.0 Number of passes: 1 Dry: unknown
	Swich to Sample Transfer mode		Eventue time 01
	Carrent basket J. Preparing beamline		
	Position: 1 🖉 🖓 Scan 2. Mounting sample		Energy (Kev): 0 MAD •
	Current sample 4. Collecting images		Istration (v): 1.3468
	Sample is nouried		Transmission (%): 100.0
27 Sharoniy the samely inside the samely channel (Samely, Shidon)	an on this	- 19- Binz	Inverse beam
Fame Commision Besister	Bilmar ante		- Outa location
Energy 12.211 Low Carrent 100.00% Carrent 1.502 Å 141.37 mm		- D 22-	Friday
Wavelength: 0017 A Set to:	Reset sample changer contents	- 27-	
Prameten Gose to Castaus EDNA Searcey Workfows			Ele anno
Manual Annual Control of Control	808808	- 226-	Defe
Raw data directory: Discontine and an an and an	- 🗆 Basket 2	- 27- - 28-	Prov
Processing these stretchy: characterizations are provided as a second stretchy and a sec	3 2 3 4 5 6 7 8 9 10		Kun number 1
Bun survey   Octilation page (det)	- 🗆 Basket 3	- 2:10- Dick reality	- Owners in a
Terrolate solidii 1 aaaa Quedaa (Sea) 40.00	1 2 3 4 5 6 7 8 9 10	- 122-	Process and applying data N.o. myldam: 0
Find image # 1 Exponent time fut	Classed		Anomalous Source group 0
Number of images: 1 Number of passes: 3 Invese bear:	1 2 3 4 5 6 7 8 9 10	- 35- Arrest	Unit celt
Comments: Detector mode: Unbinned +			a 0 b 0 c 0 s 0 p 0 v 0 disabled
Process & Analyse Data : No Besidaes Crystal space assar Cel dim. (a b c alpha beta gamma): Approach	- Basket S	- 38-	PDB: O Ushad O Use cold.
	3 2 3 4 3 6 7 8 9 10	- 39-	Browse Fast shutter
Colocc data	Double click loads the sample	- 41- Hor 0.1 - 20.01 • Move Offices	closed
	Scan selected baskets	- 042-	4 F
		- 44-	Beamstop
Chattering Bester (Chatter Chatter Chatter	Current users	- 045.	O out
2010-04-16 09:1252 adding action 2010-04-16 09:1252 Cadding set autoentring to run mode	<u> </u>	- <u>□</u> <i>ä</i> .	r 😴
2013-04-16 09:12:53 WebBox engine tile	Selecting gives control	- 143-	Characterise Current users
C012-04-10 07.L23 writerow engine ine 2013-04-16 01:23 writerow engine ine 2013-04-16 01:23 writerow engine ine 2016 01-16 01:23 writerow engine ine	Allow timeout control		Helical
2013-04-16 Ort 22-53 Instance role in a carby as server 2013-04-16 Ort 22-53 Instance mode set to moster	<b>6</b>		Energy Scan
2013-04-16 (9:14-42 Instance user Infernitication is Inhouse user	Take control     My party more management	V V X	Allow integet control
	a phone again	Calcot Quese	Ash to compl

MXCuBE 1 in 2005

MXCuBE 2 released in May 2012



Collaboration website: http://mxcube.github.io/mxcube/

- MXCuBE is now an international collaboration, with 8 partner institutes
- Same familiar interface on all sites
- Partners can easily adapt to existing solutions



New requirements on software as new instruments are introduced

UI gets less user friendly as new functionality is added

At the same time software industry also evolves New software needed, decision made to implement MXCuBE as a Web Application

- Better remote access performance
- Keeping up with new instrument capabilities
- Improved user experience
- Easing the maintenance and client install



## MXCuBE 3 - Roadmap

- MXCuBE 3 Development started by ESRF and MAXIV in September 2015
- MXCuBE 3.0 to be released in **early November 2017** 
  - Pre release already in use at MAXIV since June 2016
  - Preliminary user feedback is very positive (Poster presentation by Mikel Eguiraun TUMPL08 this afternoon)
- Version 3.1 scheduled for second quarter 2018





- Built on top of the same beamline control layer as MXCuBE 2 (Hardware Objects)
- Instruments and procedures are implemented as what is called Hardware Objects
- The beamline control layer is control system agnostic and supports for instance SPEC, EPICS, Sardana, BLISS and TANGO, (BLISS Talk by Matias Guijarro, WEBPL05)
- Base classes define a common API for a particular instrument or procedure, which facilitates cross site adaption





- Defines an API for clients to access the HardwareObjects, and relays events between Hardware Objects and clients (not necessarily a browsers)
- Thin utility layer for providing new **functionality exclusive to MXCuBE 3** and ease access to Hardware Objects
- Websockets, via SocketIO, used to relay events from backend
- Implemented on top of a Flask web server, WSGI container



#### Frontend development - Babel and Webpack

- Application written in HTML 5, Javascript 6 (JS6) and CSS
- JS6 gives us the possibility to use reusable components and modules
- Problem, no browser have full JS6 support

Babel and webpack allows us to use reusable modules and classes (https://babeljs.io/) and (https://webpack.github.io/)



ES6 Code is "transpiled" with babel to ES5 which have good support in most browsers

Webpack is used to bundle the various assets, JS, CSS, LESS, Fonts and images to a set of static files that can be loaded by the browser.

![](_page_10_Picture_8.jpeg)

![](_page_11_Picture_1.jpeg)

#### React <u>https://facebook.github.io/react/</u>

- React is a library for creating user interfaces
- React makes it possible to use widgets like in traditional UI development
- Provides a way to express the UI in a markup language called JSX
- Can be used with state management library, in order to avoid per widget state

![](_page_11_Figure_7.jpeg)

import React from "react" class Example extends React.Component { constructor(props) { super(props) console.log("Hello world") render() { return (<div> This is an example JSX embedded code </div>)

## Redux http://redux.js.org/

- Application wide state, only source of data for components.
- The redux store is an immutable data structure and can only be updated (replaced) by a pure function, a reducer
- The reducer function is called by dispatching an action for instance when user interacts with UI
- Provides unidirectional data flow, easy to debug
   Marcus Oskarsson (marcus.oscarsson@esrf.fr)
   The European Synchrotron | ESRF

#### **Screenshots - Data Collection**

![](_page_12_Picture_1.jpeg)

Data collection view, for interactive data collection and sample alignment

![](_page_12_Picture_3.jpeg)

### **Screenshots - Sample overview**

![](_page_13_Figure_1.jpeg)

Sample overview, samples represented as cards. Gives the possibility to apply data collections over a set of samples and run them in a **automatic sequence** 

![](_page_13_Picture_3.jpeg)

# **Questions ?**

![](_page_14_Picture_1.jpeg)

Thanks to everybody involved in the project, especially staff from MAX IV and ESRF (Picture from last MXCuBE ISPyB meeting at Soleil)

![](_page_14_Picture_3.jpeg)