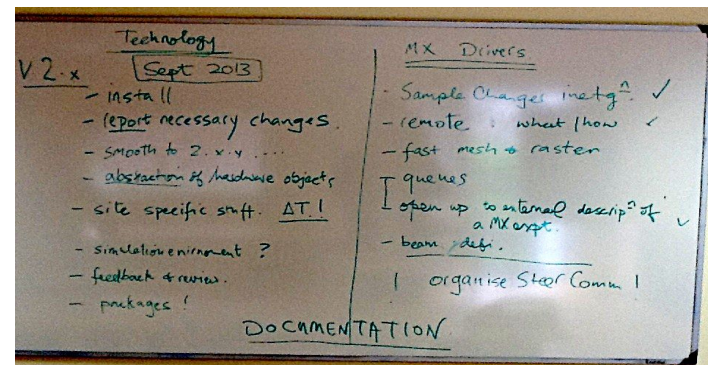
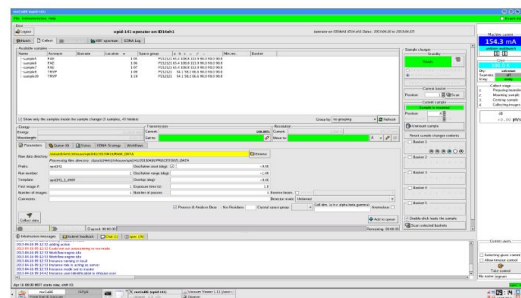
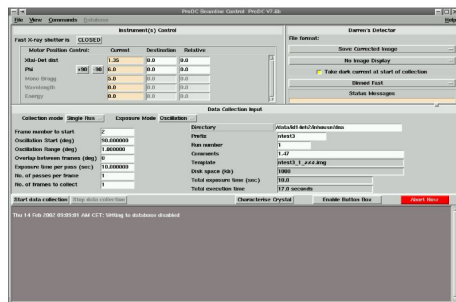


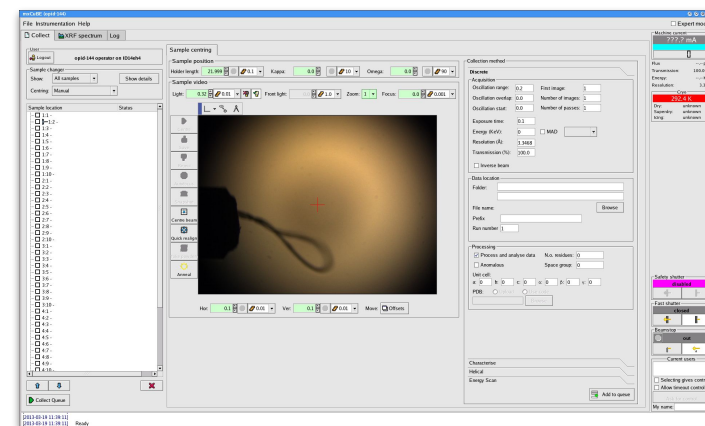
# MXCuBE3 @ ESRF

Daniele de Sanctis  
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# THE ORIGINS



- MXCuBE1 was used for a long time at ESRF
- Eventually installed at Soleil, MAXLab, Bessy, EMBL-HH
- But presented some limitations
  - Capacity of sample changer increased
  - Microbeam capabilities needed to be exploited
  - Complexity of data collection increased
  - Hard to install elsewhere, too many ESRF dependencies (*spec in primis*)
- These common needs paved the way to the design of MXCuBE2 and the begin of the MXCuBE collaboration



# THE MXCUBE COLLABORATION

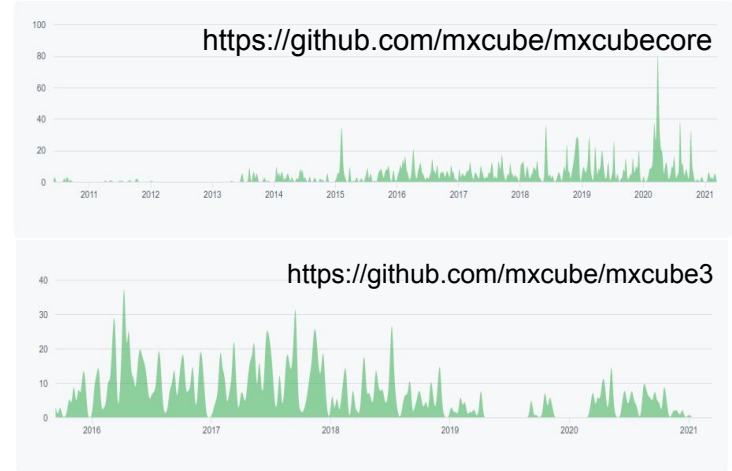


On MXCuBE the sun never sets

Oscarsson et al. 2019. "MXCuBE2: The Dawn of MXCuBE Collaboration." *Journal of Synchrotron Radiation* 26 (Pt 2): 393–405.

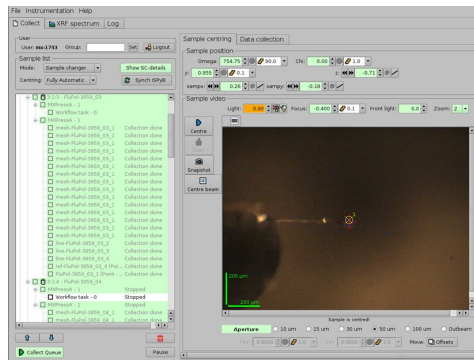
# THE MXCUBE COLLABORATION

Partners meet twice a year in round robin (jointly with ISPyB)  
Collaboration very dynamic both on core and front end





- ## THE DAWN OF MXCUBE3

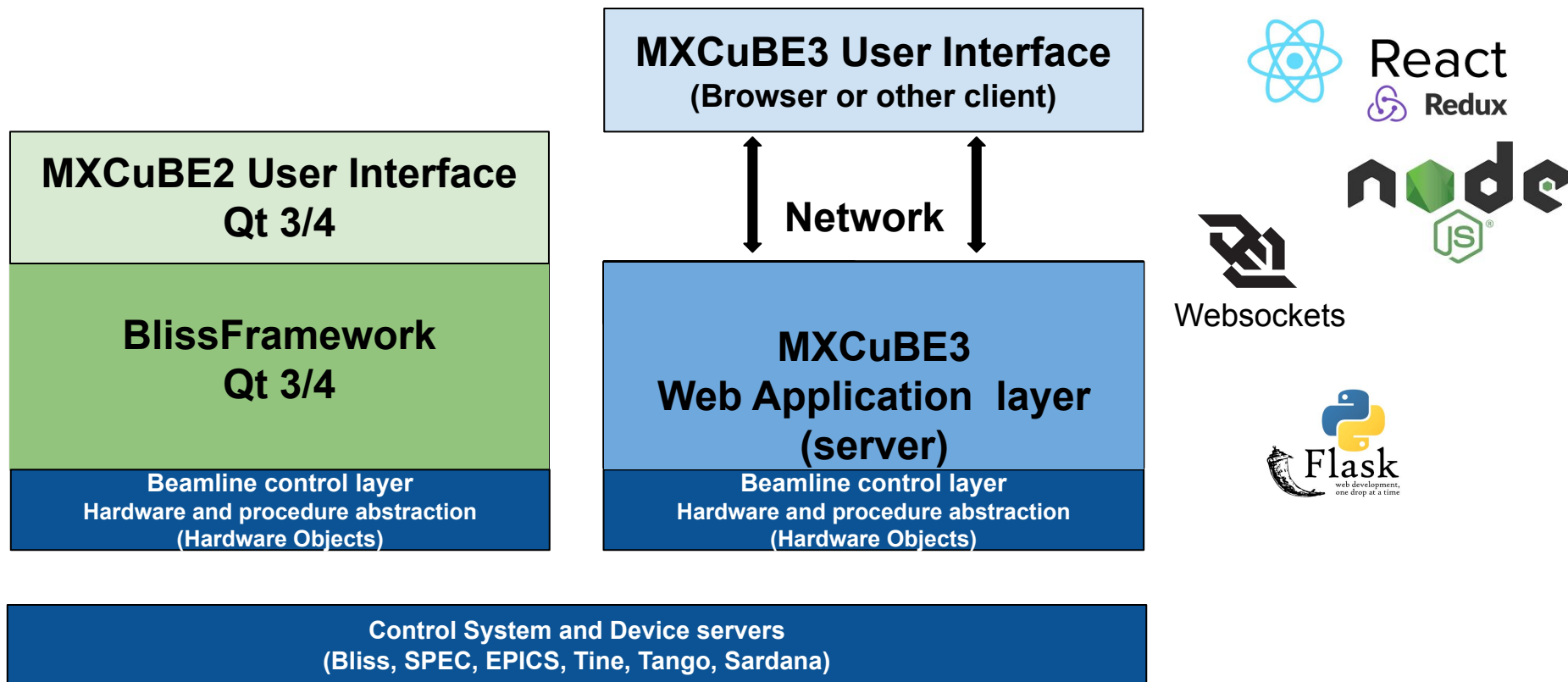


But in the meantime:

- New generation of pixel detectors
- Higher capacity sample changers
- New tools for automated data collection (workflows)
- More demand for Remote access



- Collaboration between ESRF and MAXIV initiated the MXCuBE3 project
- Design a new interface in web technology
- Preserve a common backend with MXCuBE core (Hardware repository)



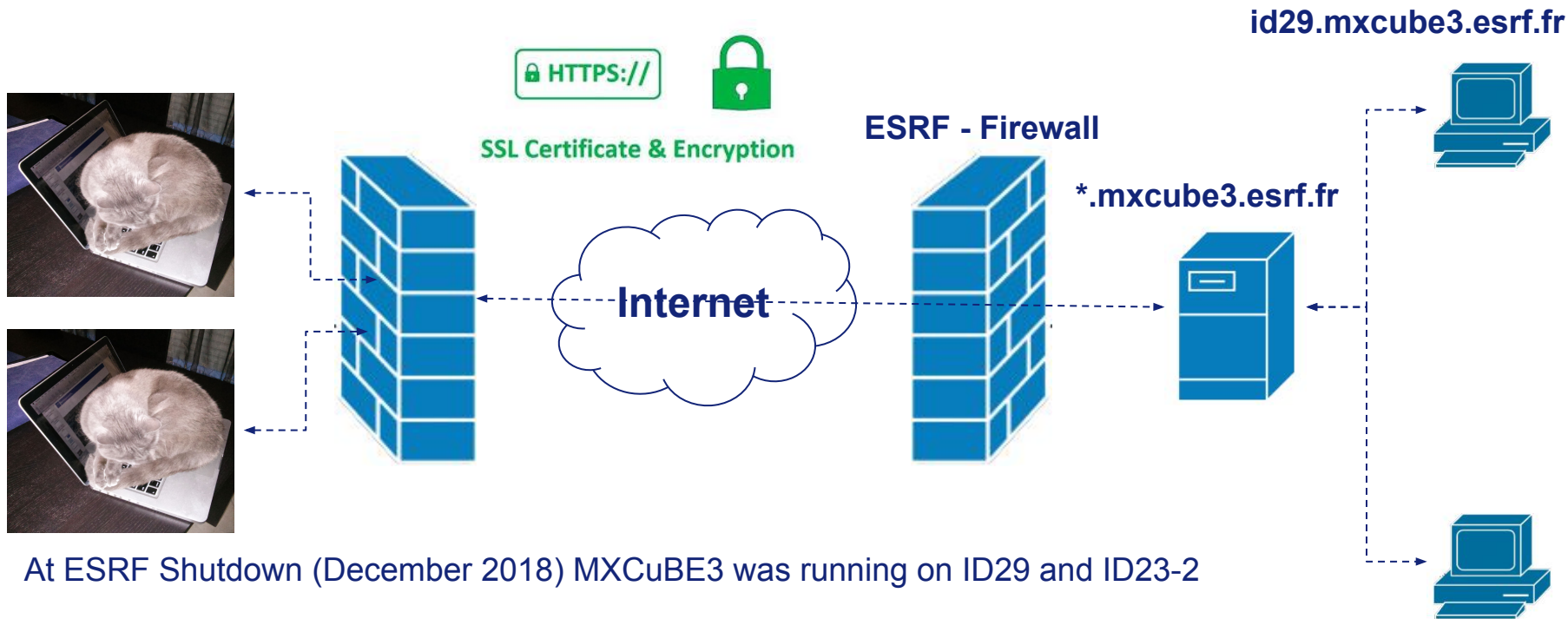
- High-throughput data collection
  - Fully exploit automation
  - Apt to perform more elaborated data collection for complex experiments
- Adaptable to any hardware and control environment
  - Independent from the underlying control system
- Scalable with time
- Interface with external experiment descriptors BES and Global Phasing Workflows



### Why web?

- Allows for a more graphical experience with direct interaction with the samples
- Lighter interface
- Remote by design
- No need of extra software installation on the client side
- Modern technology
- It scales well on any screen size
- Fast to modify and maintain
- Smooth integration with ISPyB





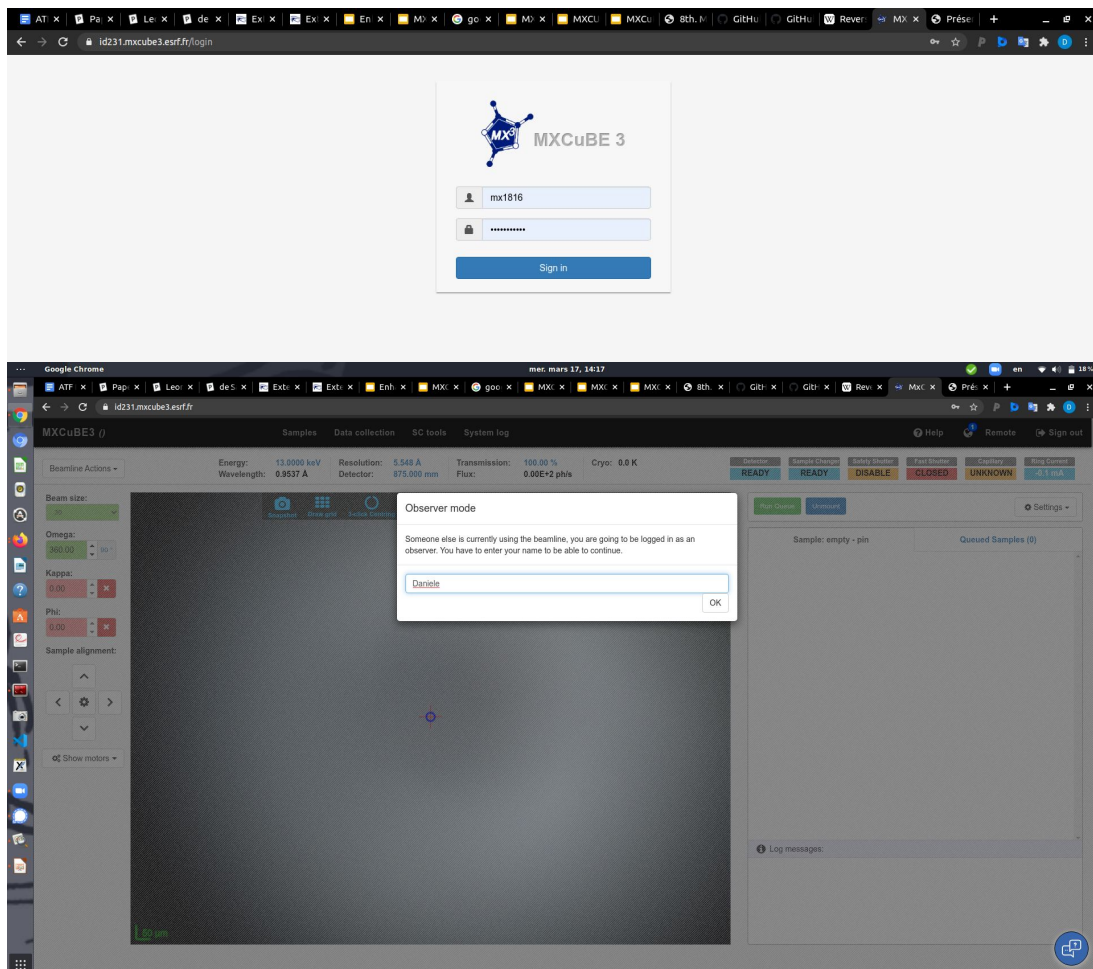
At ESRF Shutdown (December 2018) MXCuBE3 was running on ID29 and ID23-2

ESRF-EBS restarted in complete remote user operation in August 2020

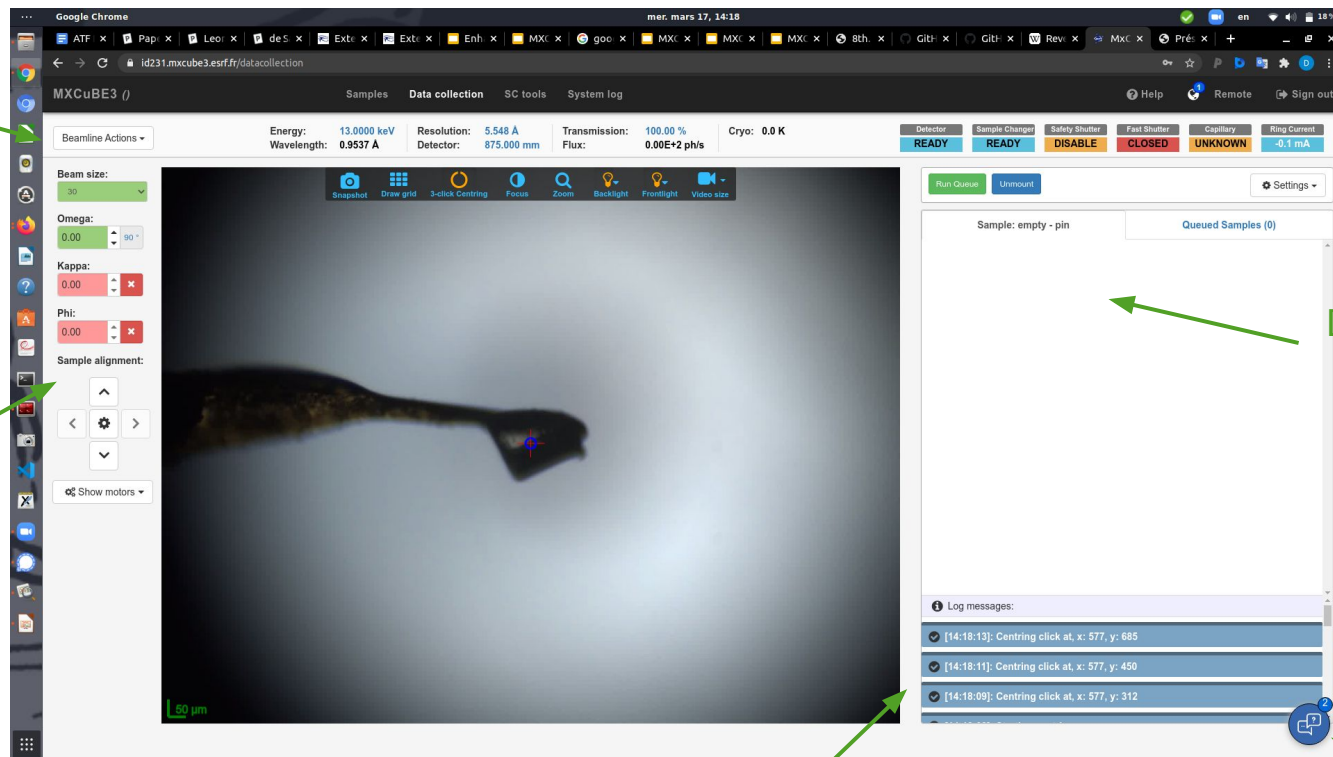
MXCuBE3 used at **ID23-1**, **ID23-2**, **ID30A1**, **ID30A3**, **ID30B**, (soon again on ID29) for 525 user sessions since the restart



- Directly accessible from any browser from <https://mxcube3.esrf.fr>
- Remote login with proposal account (soon with personal account)
- When experiment is scheduled and local session allows
- Users from same experiment session can login simultaneously, only one in control
- Users can exchange control without local intervention



# MXCuBE3 LAYOUT



Beamline  
setup

Goniometer  
motors  
control  
Sample  
joystick

Data collection  
queue

User logging

Chat

Shift + dblclick → Move to beam  
R+scroll → Rotate spindle  
Z+scroll → zoom

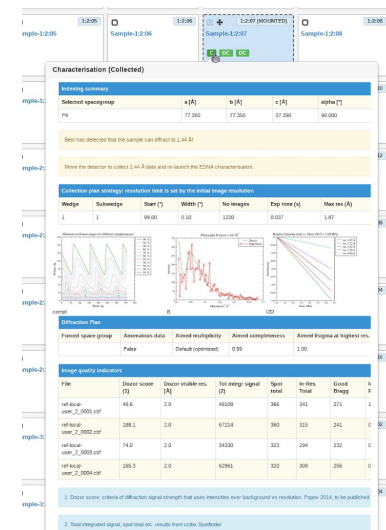
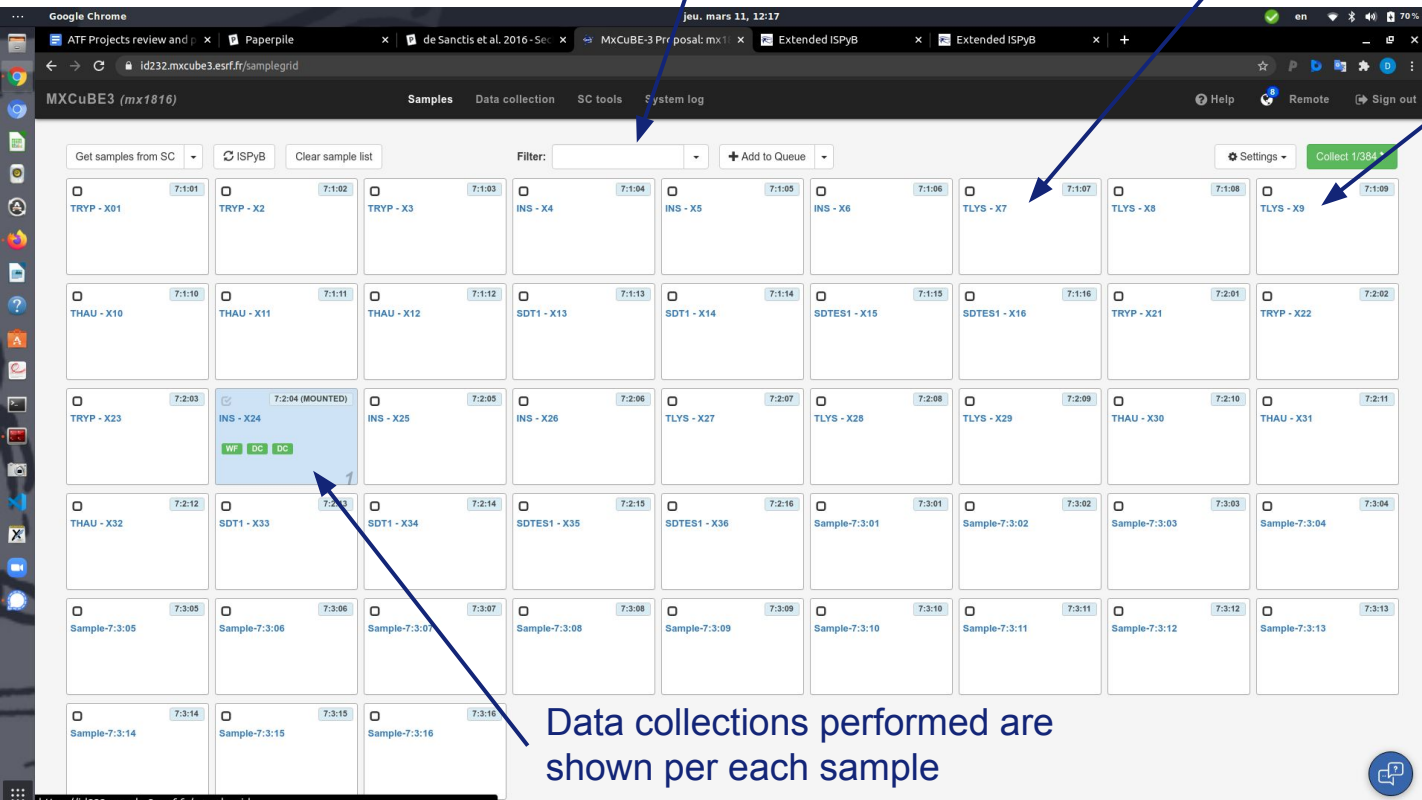
## SAMPLES

Only present pucks are displayed

Smart filtering  
(name, position, ...)

Each card a sample

Sample name  
retrieved from ISPyB



# THE CONCEPT

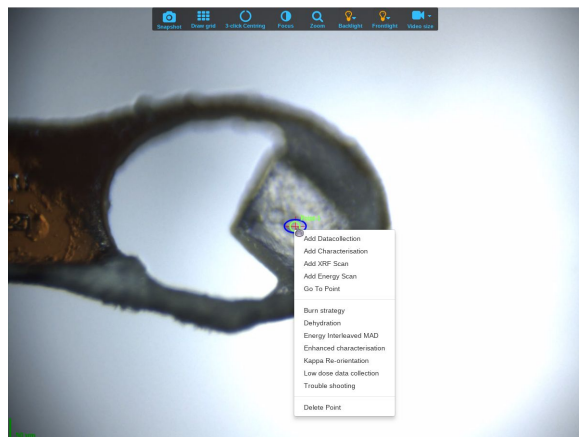
Sample(s)

Position, line, grid

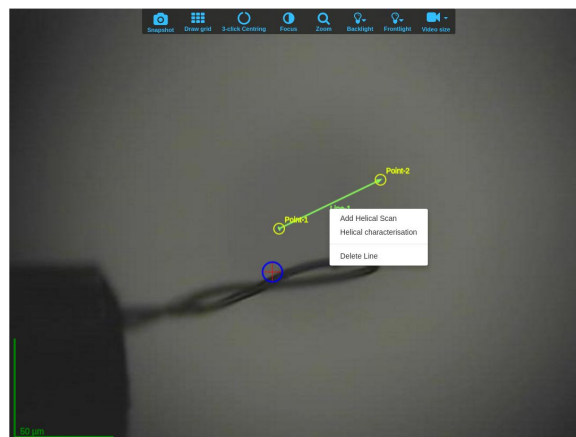
Data collection method

This is the basis to build any complex data collection sequence (automatically when combined with workflows)

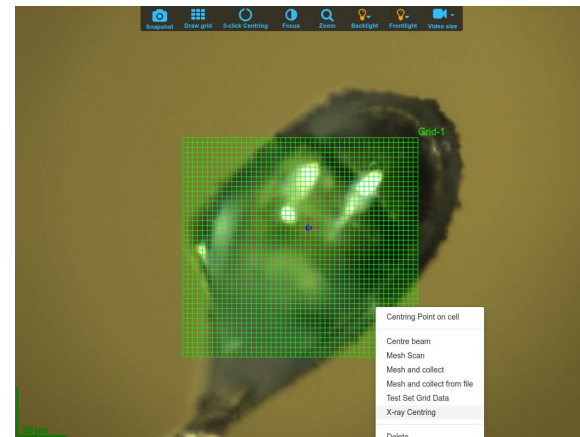
Point (3D or 2D)



Line



Grid





Google Chrome mer. mars 17, 14:18

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: UNKNOWN Ring Current: -0.1 mA

Beam size: 30  
Omega: 0.00  
Kappa: 0.00  
Phi: 0.00  
Sample alignment:   
Show motors

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

Point-4

- Add Datacollection
- Add Characterisation
- Add XRF Scan
- Add Energy Scan
- Burn strategy
- Dehydration
- Energy Interleaved MAD
- Enhanced characterisation
- Kappa Re-orientation
- Low dose data collection
- TestCenterOfRotationAxis
- TestInversedLineScans
- Save Point
- Delete Point

Run Queue Unmount Settings

Sample: empty - pin Queued Samples (0)

Log messages:

- [14:18:35]: Centring click at, x: 670, y: 482
- [14:18:33]: Centring click at, x: 665, y: 487
- [14:18:31]: Centring click at, x: 665, y: 515

50 µm

# DATA COLLECTION

Google Chrome mer. mars 17, 14:18

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: UNKNOWN Ring Current: -0.1 mA

Run Queue Unmount Settings

Sample: empty - pin Queued Samples (0)

Log messages:

Standard Data Collection

Path: /data/visitor/mx1816/id23eh1/20210317/RAW\_DATA/empty/empty-pin/  
Filename: pin-empty\_[RUN#]\_[IMG#]

Subdirectory: empty/empty-pin/  
Prefix: pin-empty

Acquisition

Oscillation range	0.1	First image	1
Oscillation start	0.0000	Number of images	100
Exposure time (s)	0.0083	Transmission	100.00
Energy	13.0000	Resolution	5.548

Show Processing Show

Default Parameters Run Now Add to Queue

50 µm

ESRF

# CHARACTERISATION

Google Chrome mer. mars 17, 14:19

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 ()

Samples Data collection SC tools System log

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.00 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: UNKNOWN Ring Current: -0.1 mA

Run Queue Unmount Settings

Sample: empty - pin Queued Samples (0)

Beam size: 30

Omega: 0.00

Kappa: 0.00

Phi: 0.00

Sample alignment:

Show motors

Characterisation

Path: /data/visitor/mx1816/id23eh1/20210317/RAW\_DATA/empty/empty-pin/  
Filename: pin-empty\_[RUN#]\_[IMG#]

Subdirectory: empty/empty-pin/  
Prefix: pin-empty

Reference acquisition

Number of images: 4 Transmission: 100.00  
Exposure time (s): 0.05 Resolution (Å): 5.548  
Oscillation range: 1 Energy: 13.0000  
Oscillation start: 0.0000

Show

Characterisation

Account for radiation damage: ☒ Optimised SAD: ☐  
Strategy complexity: SINGLE

Crystal

Show

Radiation damage model

Show

Optimization parameters

Show

Routine DC

Log messages:

50 µm

ESRF

ENERGY SCAN

European Synchrotron | ESRF



Google Chrome | je. mars 11, 12:19

id232.mxcube3.esrf.fr/datacollection

MXCuBE3 (mx1816)

Samples Data collection SC tools System log

Help Remote Sign out

Beamline Actions

Energy: 14.2000 keV Resolution: 2.497 Å Transmission: 20.61 % Cryo: 99.18 K

Wavelength: 0.8731 Å Detector: 337.565 nm Flux: 2.50E+11 ph/s

Detector: READY Sample Changer: READY Safety Shutter: OPEN Fast Shutter: CLOSED Capillary: IN Beamstop: IN Ring Current: 32.9 mA

Beam size: 5x5 µm

Omega: 91.00

Kappa: 0.00

Phi: 360.00

Sample alignment:

Show motors

Helical Data Collection

Data location

Path: /data/visitor/mx1816/id232eh2/20210311/RAW\_DATA/INS/INS-X24/

Subdirectory: INS/INS-X24/

Prefix: INS-X24

Filename: INS-X24\_[RUN#]\_[IMG#]

Acquisition

Oscillation range: 0.0502 First image: 1

Oscillation start: 91.000 Number of images: 2000

Exposure time (s): 0.006 Transmission: 5

Energy: 14.200 Resolution: 2

Show Processing

Default Parameters Run Now Add to Queue

Sample: INS - X24 Queued Samples (0)

X-ray Centring

-> Data Collection

-> Data Collection

Log messages:

ESRF

# INTERLEAVED

Google Chrome | jeu. mars 11, 12:23

id232.mxcube3.esrf.fr/datacollection

MXCuBE3 (mx1816)

Energy: 14.2000 keV | Resolution: 2.000 Å | Transmission: 4.75 % | Cryo: 99.18 K

Wavelength: 0.8731 Å | Detector: 262.865 nm | Flux: 2.50E+11 ph/s

Detector: READY | Sample Changer: READY | Safety Shutter: OPEN | Fast Shutter: CLOSED | Capillary: IN | Beamstop: IN | Ring Current: 32.6 mA

Beam size: 5x5 µm | Omega: 191.50 | Kappa: 0.00 | Phi: 360.00

Sample alignment: < [Settings] >

Interleaved data collection

Data location

Wedge	Path
1	/data/visitor/mx1816/id232h2/20210311/RAW_DATA/INS/INS-X24/INS-X24_2_###.cbf
2	/data/visitor/mx1816/id232h2/20210311/RAW_DATA/INS/INS-X24/INS-X24_3_###.cbf

Interleaved parameters

Wedge size: 216 ° | No of images per wedge: 2160

Sub wedge size: 200 (images) | Sub wedge size: 20 °

Subwedge	Start °	Osc. °	# img	t (ms)	T (%)	Res. (Å)	E (KeV)	φ °	κ °
1:1	191.5	0.1	200	0.006	4.745176	2	14.2	360	0
2:1	191.5	0.1	200	0.006	4.745176	2	14.2	360	0
1:2	211.5	0.1	200	0.006	4.745176	2	14.2	360	0
2:2	211.5	0.1	200	0.006	4.745176	2	14.2	360	0
1:3	231.5	0.1	200	0.006	4.745176	2	14.2	360	0
2:3	231.5	0.1	200	0.006	4.745176	2	14.2	360	0
1:4	251.5	0.1	200	0.006	4.745176	2	14.2	360	0
2:4	251.5	0.1	200	0.006	4.745176	2	14.2	360	0
1:5	271.5	0.1	200	0.006	4.745176	2	14.2	360	0
2:5	271.5	0.1	200	0.006	4.745176	2	14.2	360	0
1:6	291.5	0.1	200	0.006	4.745176	2	14.2	360	0
2:6	291.5	0.1	200	0.006	4.745176	2	14.2	360	0
1:7	311.5	0.1	200	0.006	4.745176	2	14.2	360	0
2:7	311.5	0.1	200	0.006	4.745176	2	14.2	360	0

Run Now | Add to Queue

Sample: INS - X24 | Queued Samples (0)

X-ray Centring

~> Data Collection

~> Data Collection

~> Data Collection

Point-2: Data Collection

Point-2: Data Collection

Path: INS-X24\_3\_###

Start ° | Osc. ° | t (ms) | T (%) | Res. (Å) | E (KeV) | φ ° | κ °

191.50 | 0.10 | 0.006 | 4.745176 | 2 | 14.2 | 360 | 0

Log messages:

- [12:20:14]: Queue execution finished
- [12:20:09]: Not mounting next sample automatically (Auto mount next)
- [12:20:09]: Collection finished

Interleave multiple data collection

Energy  
Angle (inverse beam)  
Kappa

European Synchrotron | ESRF

Google Chrome | jeu. mars 11, 12:10

id232.mxcube3.esrf.fr/datacollection

MXCuBE3 (mx1816) | Samples | Data collection | SC tools | System log | Help | Remote | Sign out

Energy: 14.2000 keV | Resolution: 2.497 Å | Transmission: 20.61 % | Cryo: 99.2 K

Wavelength: 0.8731 Å | Detector: 337.565 mm | Flux: 2.87E+11 ph/s

Detector: READY | Sample Changer: READY | Safety Shutter: OPEN | Fast Shutter: CLOSED | Capillary: IN | Beamstop: UNKNOWN | Ring Current: 33.4 mA

Beamline Actions

Beam size: 5x5 µm

Omega: 91.00°

Kappa: 0.00°

Phi: 360.00°

Sample alignment:

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

Grid-1

50 µm

Centring Point on cell

Centre beam

Mesh Scan

Mesh and collect

Mesh and collect from file

Test Set Grid Data

X-ray Centring

Delete

Run Queue | Next Sample (INS - X25) | Settings

Sample: INS - X24 | Queued Samples (0)

Log messages:

- [12:10:45]: Centring Failed
- [12:10:45]: User canceled centring
- [12:10:26]: Centring click at, x: 699, y: 623

Mesh data collections methods

Mesh&collect  
Mesh  
X-ray centring



# X-RAY CENTRING

Google Chrome | je. mars 11, 12:17

id232.mxcube3.esrf.fr/datacollection

MXCuBE3 (mx1816) | Samples | Data collection | SC tools | System log | Help | Remote | Sign out

Beamline Actions

Energy: 14.2000 keV | Resolution: 2.49 | Wavelength: 0.8731 Å | Detector: 337.4

Heat map: | Crystal map: | Capillary: IN | Beamstop: IN | Ring Current: 33.0 mA

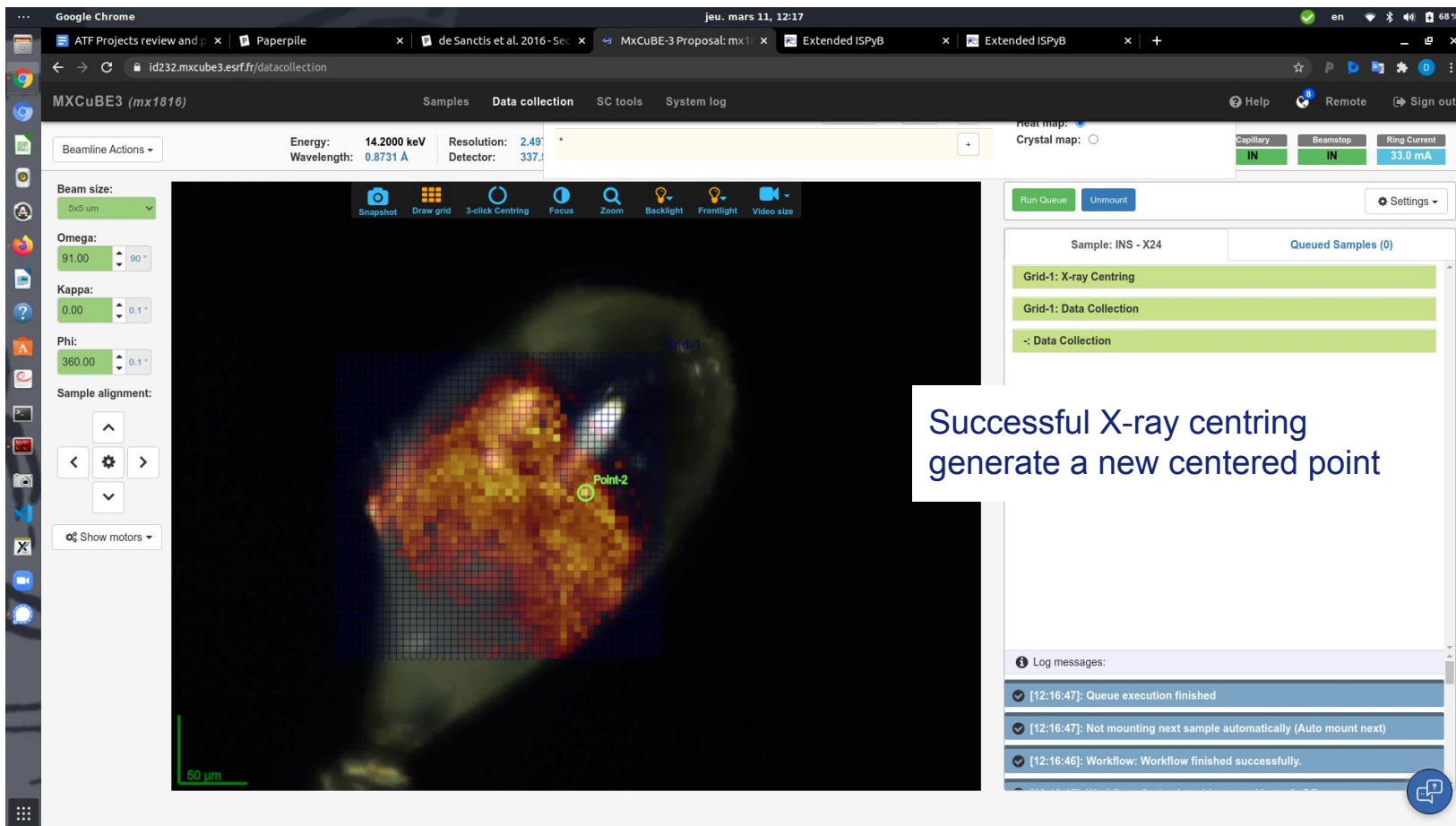
Run Queue | Unmount | Settings

Sample: INS - X24 | Queued Samples (0)

Grid-1: X-ray Centring  
Grid-1: Data Collection  
-: Data Collection

Log messages:  
✓ [12:16:47]: Queue execution finished  
✓ [12:16:47]: Not mounting next sample automatically (Auto mount next)  
✓ [12:16:46]: Workflow: Workflow finished successfully.

Successful X-ray centring generate a new centered point





Google Chrome mer. mars 17, 21:52

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 (mx1816) Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: IN Ring Current: -0.1 mA

Beam size: 30

Omega: 118.88 90°

Kappa: 0.00

Phi: 0.00

Sample alignment:

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

50 µm

Go To Beam  
Measure Distance  
Draw Grid  
Data Collection (Limited OSC)  
Characterisation (1 Image)  
MXPressE  
MXPressI  
MXPressO  
MXPressP  
Trouble shooting  
Trouble shooting Dialog

Run Queue Unmount Settings

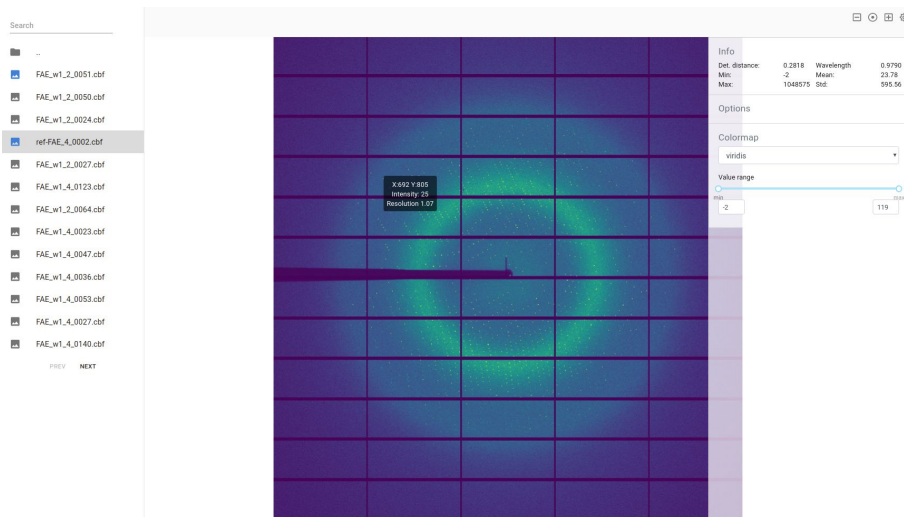
Sample: empty - pin Queued Samples (0)

:- Data Collection  
:- Data Collection

No point  
Shoot here, no rotation  
Do everything automatic  
Same methods are available from Samples for pipeline mode

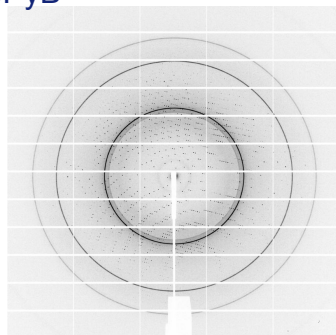
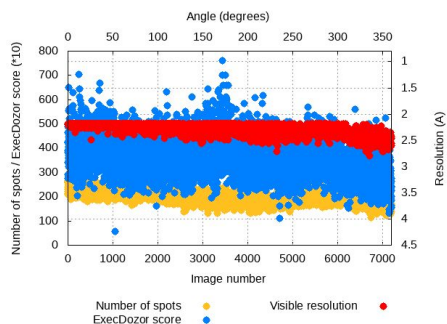
Log messages:  
[14:24:46]: Queue execution finished  
[14:24:46]: Not mounting next sample automatically (Auto mount next)  
[14:24:46]: Collection finished

# FUTURE PLANS



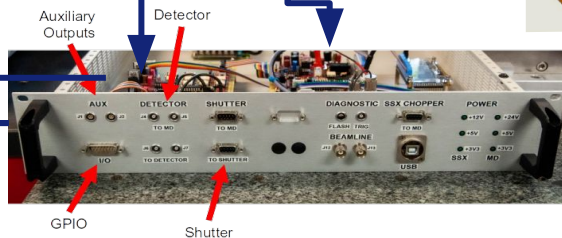
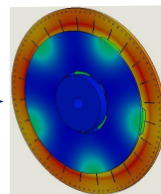
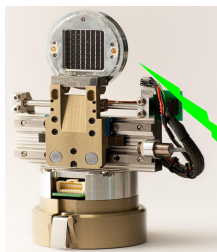
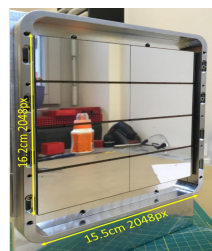
<https://github.com/marcus-oscarsson/braggy>

Dozor score and png available in ISPyB



- Integrate a new Web based diffraction image viewer
- Continue the improvement in the ergonomics
- Improve Samples list visualisation and results
- Complete implementation of DozorM and MeshBest combined with mesh results
- Port GP workflows to MXCuBE3
- Finalise integration of crystallisation plate screening
- Implement novel SSX data collection methods
- Controller for “liquid” based delivery systems, pumping, mixing
- Fixed targets, new type of mesh on periodic supports

RF



Develop a graphical interface for timing mode:

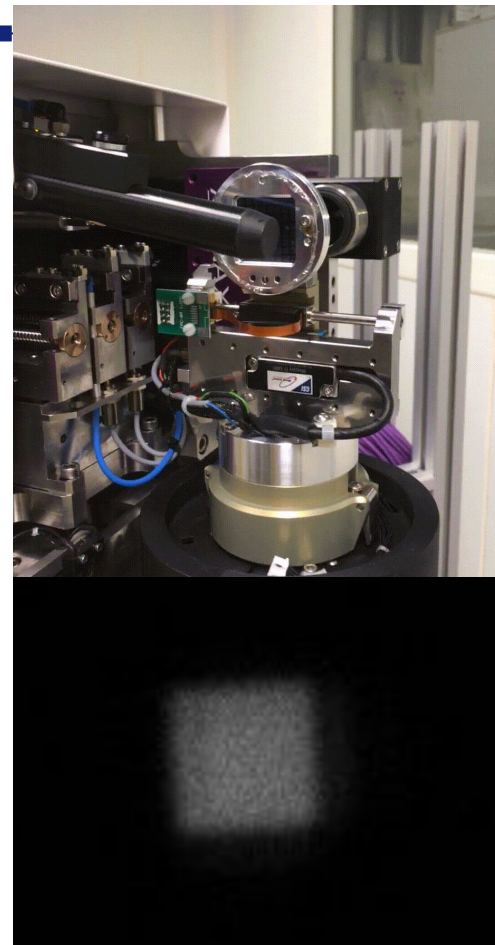
- Defines trigger, offsets and delays
- Be able to retrieve the signals (oscilloscope mode) to monitor the events



X-ray  
Trigger 1  
Trigger 2

ESRF Electronic Unit  
EMBL Instrumentation Team

Opening for PostDoc for ID29  
<https://www.esrf.eu/Jobs>



- MXCuBE is part of a large collaboration
  - on a common control layer and user interface
  - That makes a great effort in sharing generic components that are commonly used (ex. Detectors, Diffractometers)
  - “Standardisation” is part of a iterative process, continue refactoring
- MXCuBE3 is the web front end
  - Specifically optimised for remote access
  - Facilitate all kind of MX related experiments by hiding the complexity (not removing it)
  - From user perspective it has a flat learning curve
- The home of MXCuBE is <https://github.com/mxcube>
- The MXCuBE meeting are usually opened to observers, feel free to contact if interested





# ACKNOWLEDGEMENTS

ESRF - EMBL Joint Structural Biology Group  
**The MXCuBE collaboration**  
<http://mxcube.github.io/mxcube/>

ESRF - Marcus Oscarsson, Antonia Beteva  
MAXIV  
EMBL  
Global Phasing  
SOLEIL  
BESSY HZB  
ALBA  
DESY  
ELETTRA  
LNLS  
NSRRC



EXTRA SLIDES



Google Chrome | je. mars 11, 12:19

id232.mxcube3.esrf.fr/datacollection

MXCuBE3 (mx1816) | Samples | Data collection | SC tools | System log

Beamline Actions

Energy: 14.2000 keV | Resolution: 2.497 Å | Transmission: 20.61 % | Cryo: 99.18 K  
Wavelength: 0.8731 Å | Detector: 337.565 nm | Flux: 2.50E+11 ph/s

Detector: READY | Sample Changer: READY | Safety Shutter: OPEN | Fast Shutter: CLOSED | Capillary: OUT | Beamstop: OUT | Ring Current: 32.8 mA

Beam size: 5x5 µm | Omega: 96.02 | Kappa: 0.00 | Phi: 360.00

Sample alignment:

Show motors

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

Stop | Pause | Settings

Sample: INS - X24 | Queued Samples (0)

X-ray Centring

-: Data Collection

-: Data Collection

Line-1: Data Collection

Path: INS-X24\_1\_####.cbf

Start °	Osc. °	t (s)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
91.00	0.05	0.006	2000	5.00	2.000	14.2000	360.00	0.00

Log messages:

- ✓ [12:19:26]: Taking 4 sample snapshot(s)
- ✓ [12:19:21]: Detector Cover done.
- ✓ [12:19:15]: Moving Diffractometer to CentringPhase

Google Chrome mer. mars 17, 14:24

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector RUNNING Sample Changer READY Safety Shutter DISABLE Fast Shutter CLOSED Capillary IN Ring Current -0.1 mA

Beam size: 30

Omega: 116.43

Kappa: 0.00

Phi: 0.00

Sample alignment:

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

Point-4

50 µm

Stop Pause Settings

Sample: empty - pin Queued Samples (0)

Point-4: Data Collection

Path: pin-empty\_1\_####.h5

Start °	Osc. °	t (s)	# img	T (%)	Res. (Å)	E (KeV)	$\varphi$ °	$\kappa$ °
360.00	0.10	0.008	100	100.00	5.548	13.0000	0.00	0.00

View Results

Point-4: Data Collection 90.0 %

Path: pin-empty\_2\_####.h5

Start °	Osc. °	t (s)	# img	T (%)	Res. (Å)	E (KeV)	$\varphi$ °	$\kappa$ °
14.44	0.10	0.008	1000	100.00	5.548	13.0000	0.00	0.00

Log messages:

- [14:24:31]: Detector ready, continuing
- [14:24:29]: Preparing acquisition
- [14:24:25]: Moving MD2 to Data Collection

Google Chrome mer. mars 17, 14:24

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector RUNNING Sample Changer READY Safety Shutter DISABLE Fast Shutter OPEN Capillary IN Ring Current -0.1 mA

Beam size: 30

Omega: 26.11

Kappa: 0.00

Phi: 0.00

Sample alignment:

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

Point-4

50 µm

Stop Pause Settings

Sample: empty - pin Queued Samples (0)

Point-4: Data Collection

Path: pin-empty\_1\_####.h5

Start °	Osc. °	t (s)	# img	T (%)	Res. (Å)	E (KeV)	$\varphi$ °	$\kappa$ °
360.00	0.10	0.008	100	100.00	5.548	13.0000	0.00	0.00

View Results

Point-4: Data Collection

Path: pin-empty\_2\_####.h5

Start °	Osc. °	t (s)	# img	T (%)	Res. (Å)	E (KeV)	$\varphi$ °	$\kappa$ °
14.44	0.10	0.008	1000	100.00	5.548	13.0000	0.00	0.00

Log messages:

- [14:24:31]: Detector ready, continuing
- [14:24:29]: Preparing acquisition
- [14:24:25]: Moving MD2 to Data Collection

Google Chrome mer. mars 17, 14:23

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: IN Ring Current: -0.1 mA

Beam size: 30

Omega: 14.44 90°

Kappa: 0.00

Phi: 0.00

Sample alignment:

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

Point-4

50 µm

Run Queue Unmount Settings

Sample: empty - pin Queued Samples (0)

Point-4: Data Collection

Path: pin-empty\_1\_####.h5

Start °	Osc. °	t (s)	# img	T (%)	Res. (Å)	E (KeV)	$\phi$ °	$\kappa$ °
360.00	0.10	0.008	100	100.00	5.548	13.0000	0.00	0.00

View Results

Log messages:

- [14:23:48]: Queue execution finished
- [14:23:47]: Not mounting next sample automatically (Auto mount next)
- [14:23:47]: Collection finished

Google Chrome mer. mars 17, 14:20

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: UNKNOWN Ring Current: -0.1 mA

Beam size: 30

Omega: 0.00 90°

Kappa: 0.00

Phi: 0.00

Sample alignment:

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

Grid-1

Point-4

50 µm

Run Queue Unmount Settings

Sample: empty - pin

☐ Automount next sample  
☒ Auto loop centring  
☐ Auto add diffraction plan

Crystal snapshots (4)

Group path: Set

Log messages:

- [14:18:45]: Centring successful
- [14:18:35]: Centring click at, x: 670, y: 482
- [14:18:33]: Centring click at, x: 665, y: 487

Google Chrome mer. mars 17, 14:19

id231.mxcube3.esrf.fr/datacollection

MxCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: UNKNOWN Ring Current: -0.1 mA

Beam size: 30

Omega: 0.00 90°

Kappa: 0.00

Phi: 0.00

Sample alignment:

Show motors

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

Name	Dim (µm)	#Cells	R x C	Ω
*				

Opacity: Heat map: Crystal map:

Point-4

50 µm

Run Queue Unmount Settings

Sample: empty - pin Queued Samples (0)

Log messages:

- [14:18:45]: Centring successful
- [14:18:35]: Centring click at, x: 670, y: 482
- [14:18:33]: Centring click at, x: 665, y: 487



Google Chrome mer. mars 17, 14:18

id231.mxcube3.esrf.fr/datacollection

MXCuBE3 () Samples Data collection SC tools System log Help Remote Sign out

Beamline Actions

Energy: 13.0000 keV Resolution: 5.548 Å Transmission: 100.00 % Cryo: 0.0 K  
Wavelength: 0.9537 Å Detector: 875.000 mm Flux: 0.00E+2 ph/s

Detector: READY Sample Changer: READY Safety Shutter: DISABLE Fast Shutter: CLOSED Capillary: UNKNOWN Ring Current: -0.1 mA

Beam size: 30  
Omega: 0.00  
Kappa: 0.00  
Phi: 0.00  
Sample alignment:   
Show motors

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

Point-4

- Add Datacollection
- Add Characterisation
- Add XRF Scan
- Add Energy Scan
- Burn strategy
- Dehydration
- Energy Interleaved MAD
- Enhanced characterisation
- Kappa Re-orientation
- Low dose data collection
- TestCenterOfRotationAxis
- TestInversedLineScans
- Save Point
- Delete Point

Run Queue Unmount Settings

Sample: empty - pin Queued Samples (0)

Log messages:

- [14:18:35]: Centring click at, x: 670, y: 482
- [14:18:33]: Centring click at, x: 665, y: 487
- [14:18:31]: Centring click at, x: 665, y: 515

50 µm

# CHARACTERISATION

MXCuBE 3

Sample Overview

Data collection

Sample Changer

System log

Help RA Sign out

Get samples from SC

ISPyB

Clear sample list

Filter:

+ Add to Queue

Settings

Collect 1/317

Sample-1:101

Sample-1:102

Sample-1:103

Sample-1:104

Sample-1:105

Sample-1:106

Sample-1:107

Sample-1:108

Sample-1:109

Sample-1:110

Sample-1:2:01

Sample-1:2:02

Sample-1:2:03

Sample-1:2:04

Sample-1:2:05

Sample-1:2:06

Sample-1:2:07 (MOUNTED)

Sample-1:2:08

Sample-1:2:09

Sample-1:2:10

Sample-1:3:01

Sample-1:3:02

Sample-1:3:03

Sample-1:3:04

Sample-1:3:05

Sample-1:3:06

Sample-1:3:07

Sample-1:3:08

Sample-1:3:09

Sample-1:3:10

Sample-1:3:11

Sample-1:3:12

Sample-2:1:01

Sample-2:1:02

Sample-2:1:03

Sample-2:1:04

Sample-2:1:05

Sample-2:1:06

Sample-2:1:07

Sample-2:1:08

Sample-2:1:09

Sample-2:1:10

Sample-2:1:11

Sample-2:1:12

Sample-2:1:13

Sample-2:1:14

Sample-2:1:15

Sample-2:1:16

Sample-2:2:01

Sample-2:2:02

Sample-2:2:03

Sample-2:2:04

Sample-2:2:05

Sample-2:2:06

Sample-2:2:07

Sample-2:2:08

Sample-2:2:09

Sample-2:2:10

Sample-2:2:11

Sample-2:2:12

Sample-2:2:13

Sample-2:2:14

Sample-2:3:01

Sample-2:3:02

Sample-2:3:03

Sample-2:3:04

Sample-2:3:05

Sample-2:3:06

Sample-2:3:07

Sample-2:3:08

Sample-2:3:09

Sample-2:3:10

Sample-2:3:11

Sample-2:3:12

Sample-3:1:01

Sample-3:1:02

Sample-3:1:03

Sample-3:1:04

Sample-3:1:05

Sample-3:1:06

Sample-3:2:01

Sample-3:2:02

Sample-3:2:03

Sample-3:2:04

Sample-3:2:05

Sample-3:2:06

Sample-3:2:07

Sample-3:2:08

Sample-3:3:01

Sample-3:3:02

Sample-3:3:03

Sample-3:3:04

Sample-3:3:05

Sample-3:3:06

Sample-3:3:07

Sample-3:3:08

Sample-3:3:09

Sample-3:3:10

Characterisation (Collected)

Indexing summary

Selected spacegroup	a [Å]	b [Å]	c [Å]	alpha [°]
P4	77.350	77.350	37.390	90.000

Best has detected that the sample can diffract to 1.44 Å

Move the detector to collect 1.44 Å data and re-launch the EDNA characterisation.

Wedge	Subwedge	Start [°]	Width [°]	No. Images	Exp time (s)	Max res (Å)
1	1	99.00	0.10	1220	0.037	1.87

Based on average image to different conditions

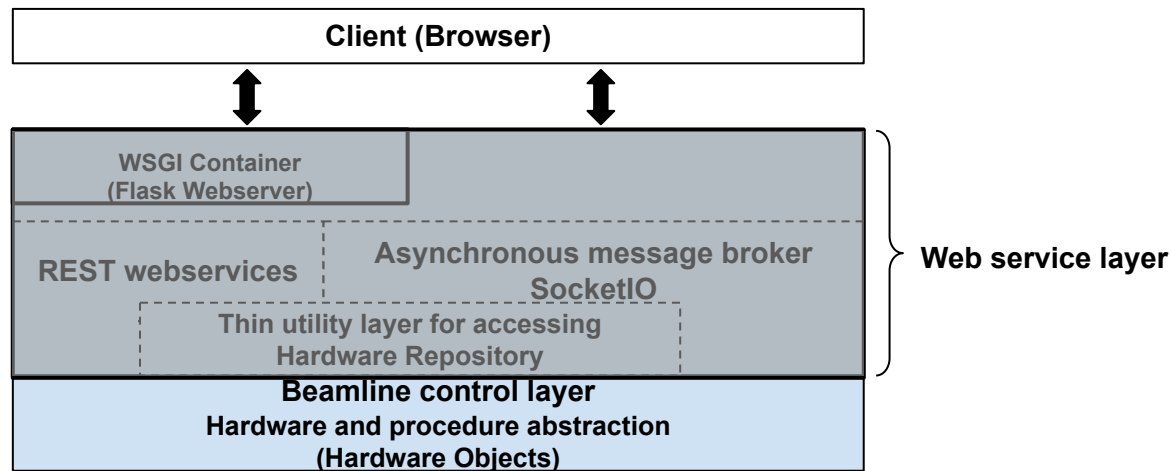
Diffraction Plan

Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed fwhm at highest res.
P4	False	Default (optimized)	0.99	1.00

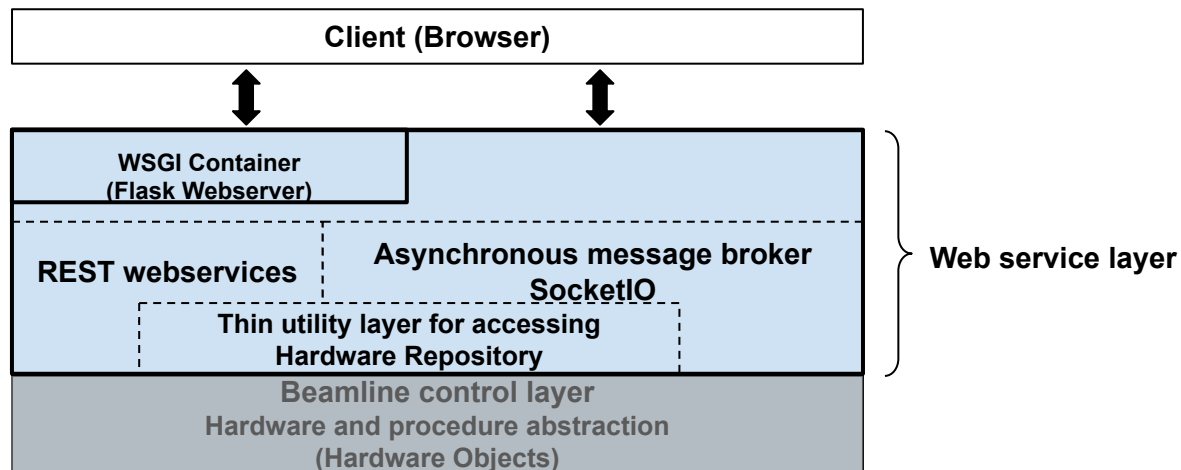
File	Dozor score (1)	Dozor visible res. (Å)	Test integr. signal (2)	Spot total	In-files Total	Good Bragg	h f
ref local user_2_0001.csf	49.6	2.0	49109	366	341	271	1
ref local user_2_0002.csf	188.1	2.0	67214	360	315	241	0
ref local user_2_0003.csf	74.0	2.0	34330	323	294	232	0
ref local user_2_0004.csf	165.3	2.0	62961	320	309	256	0

1. Dozor score: criteria of diffraction signal strength that uses intensities over background vs resolution. Pappe 2014, to be published.

2. Total integrated signal, spot total etc.: results from cctbx.Spotfinder



- 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**
- Base classes define a common API for a particular instrument or procedure, which **facilitates cross site adaptation**



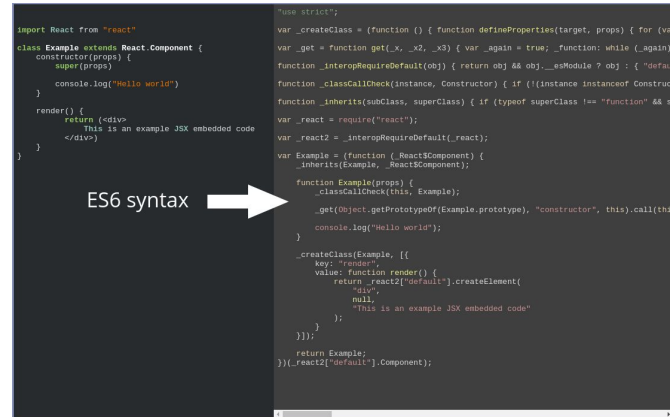
- **Defines an API** for clients to access the HardwareObjects, and relays events between Hardware Objects and clients (**not necessarily a browsers**)
- Thin utility layer for providing new **functionality exclusive to MXCuBE 3** and ease access to Hardware Objects
- Websockets, via SocketIO, **used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



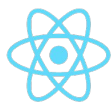
- Application written in HTML 5, Javascript 6 (JS6) and CSS
- JS6 gives us the possibility to use **reusable components and modules**
- Problem, no browser have full JS6 support



Babel allows us to use reusable modules and classes via ES6 syntax  
(<https://babeljs.io/>)



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



## React

<https://facebook.github.io/react/>

- 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

```
import React from "react"

class Example extends React.Component {
  constructor(props) {
    super(props)

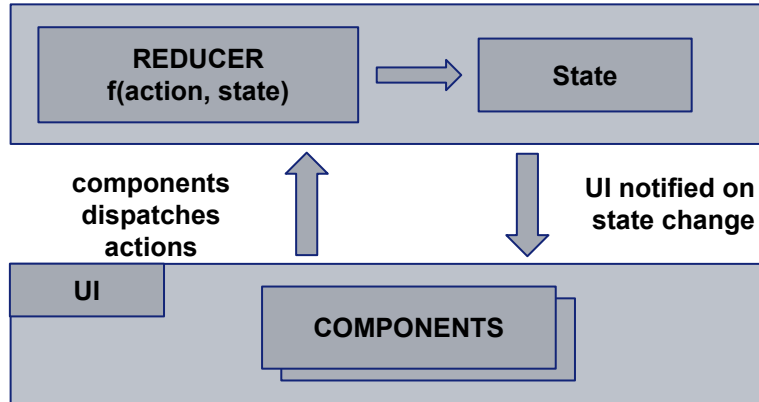
    console.log("Hello world")
  }

  render() {
    return (<div>
      This is an example JSX embedded code
    </div>)
  }
}
```





<http://redux.js.org/>



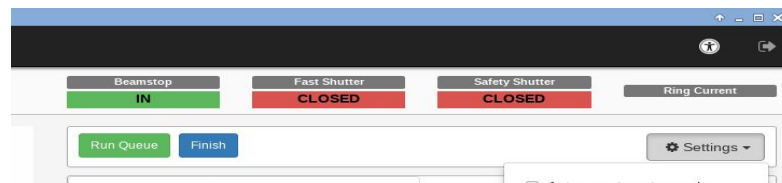
- Application wide state, only source of data for components.
- The redux store is an immutable data structure and can only be updated (replaced) by a pure function, a reducer
- The reducer function is called by dispatching an action for instance when user interacts with UI
- Provides data flow which is easy to debug

# Frontend development - React and Redux

```
1 import React from 'react';
2 import { Button, ButtonGroup, OverlayTrigger, Popover } from 'react-bootstrap';
3
4 import './style.css';
5 import './input.css';
6
7
8 export default class InOutSwitch extends React.Component {
9   constructor(props) {
10     super(props);
11     this.setIn = this.setIn.bind(this);
12     this.setOut = this.setOut.bind(this);
13   }
14
15   shouldComponentUpdate(nextProps) {
16     return nextProps.data !== this.props.data;
17   }
18
19   setIn() {
20     if (this.props.onSave !== undefined) {
21       this.props.onSave(this.props.pkey, 'in');
22     }
23   }
24
25   setOut() {
26     if (this.props.onSave !== undefined) {
27       this.props.onSave(this.props.pkey, 'out');
28     }
29   }
30 }
31
32
33
34
```

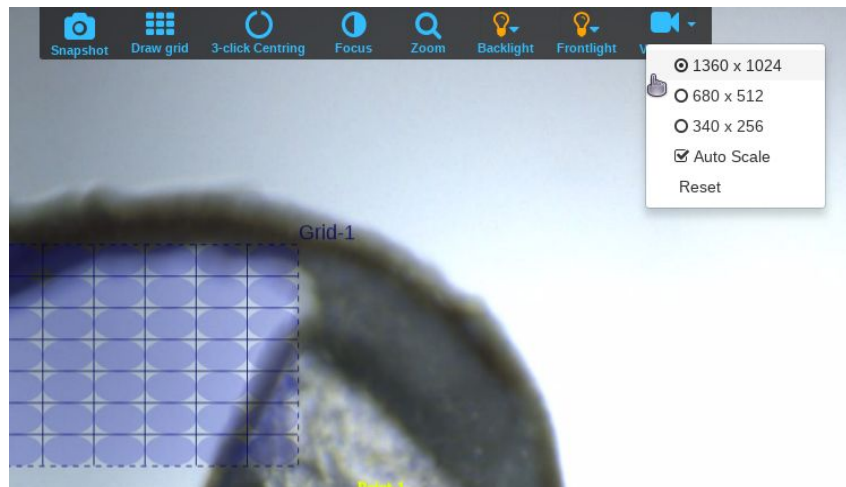
```
46 createActuatorComponent() {
47   const acts = [];
48   for (let key in this.props.data.attributes) {
49     if (this.props.data.attributes[key].type === 'DUOSTATE') {
50       acts.push({ col: key, sm: {1: smPush={2}}});
51       <InOutSwitch
52         onText={ this.props.data.attributes[key].commands[0] }
53         offText={ this.props.data.attributes[key].commands[1] }
54         labelText={ this.props.data.attributes[key].label }
55         pkey={ key }
56         data={ this.props.data.attributes[key] }
57         onSave={ this.setAttribute }
58       />
59     </Col>
60   );
61 }
62 }
63 return acts;
64
```

```
35 render() {
36   const isIn = this.props.data.state === 'in';
37   const inButtonStyle = isIn ? 'success' : 'default';
38   const outButtonStyle = !isIn ? 'default' : 'success';
39   let msgBgStyle = 'input-bg-moving';
40
41   if (this.props.data.state === 'in') {
42     msgBgStyle = 'input-bg-ready';
43   } else if (this.props.data.state === 'out') {
44     msgBgStyle = 'input-bg-fault';
45   }
46
47   return (
48     <div>
49       <div className="inout-label">
50         {this.props.labelText}
51       </div>
52       <OverlayTrigger
53         placement="bottom"
54         overlay={
55           <Popover id={this.props.labelText}>
56             {this.props.labelText} is:
57             <div className={msgBgStyle}>
58               {this.props.data.msg}
59             </div>
60           </Popover>
61         }
62       </OverlayTrigger>
63       <ButtonGroup>
64         <Button
65           className=""
66           bsStyle={inButtonStyle}
67           bsSize="small"
68           onClick={this.setIn}
69           active={isIn}
70         >
71           {this.props.onText}
72         </Button>
73         <Button
74           bsStyle={outButtonStyle}
75           bsSize="small"
76           className=""
77           onClick={this.setOut}
78           active={!isIn}
79         >
80           {this.props.offText}
81         </Button>
82       </ButtonGroup>
83     </div>
84   );
85 }
86
87
```





- **Webpack is used as a build tool to bundle the various assets, JS, CSS, LESS, Fonts and images to a set of static files that can be loaded by the browser.**
- **Provides a development server with “hot reloading” (changes are automatically built and app updated)**
- **Runtime for Javascript development provided by node.js**



- **Video is streamed as MPEG-1, perhaps adaptive MPEG-4 in the future**
- **Possibility to select video stream size (particularly useful for remote users)**
- **With auto scale option**

**Context based navigation, options depends on selection**

