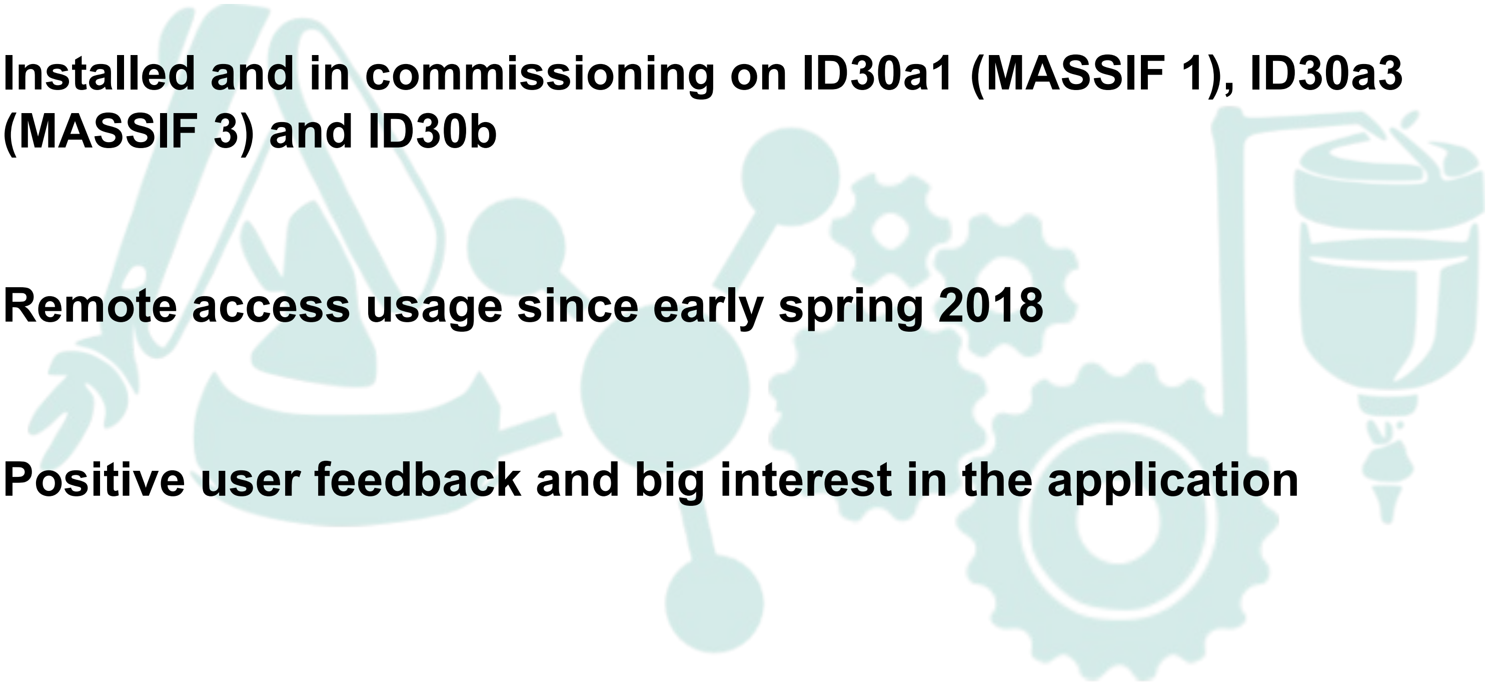
ESRF | The European Synchrotron

Outline

- MXCuBE3 at ESRF
- Remote Access
- Quick Review of 3.0
- New in version 3.0.1
- Future work

MXCuBE3 at ESRF



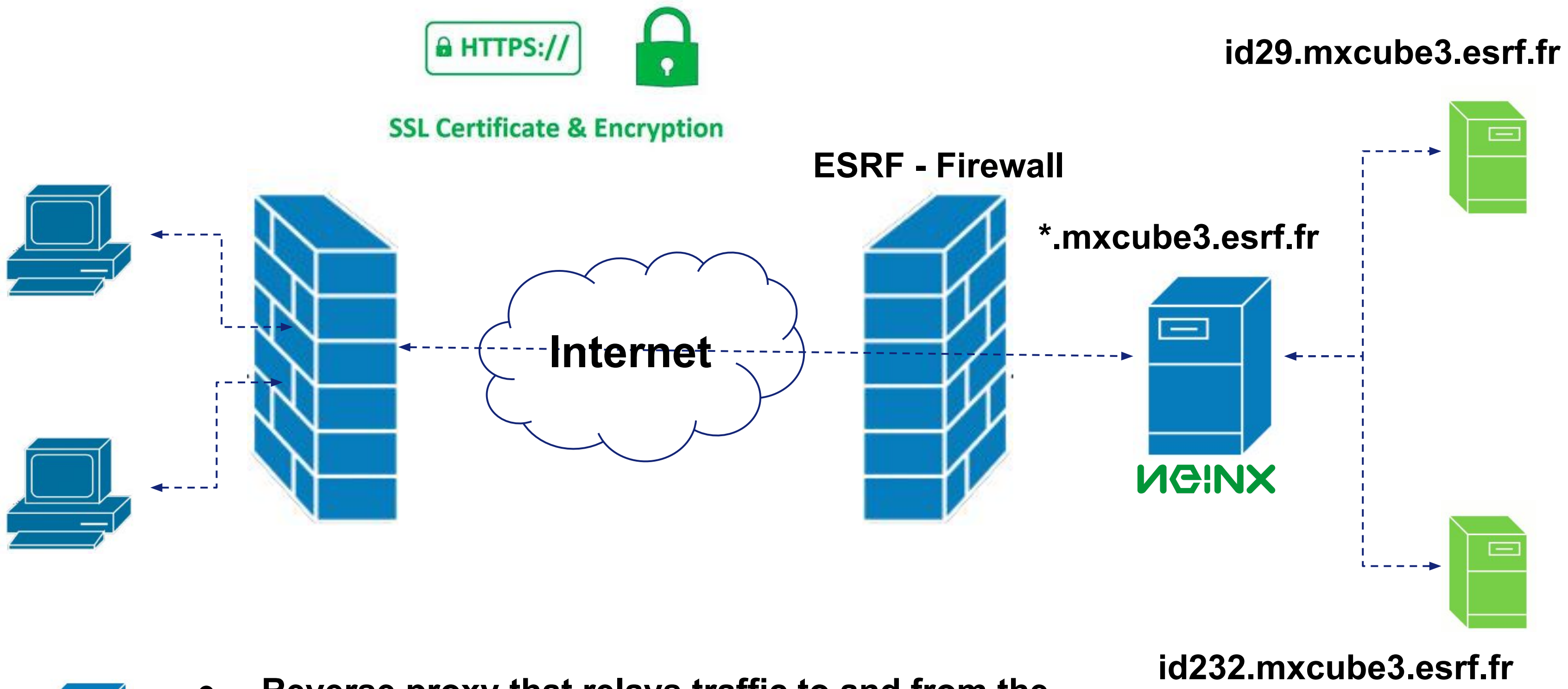
- **Installed and in production on ID29 and ID23-2**
- **Installed and in commissioning on ID30a1 (MASSIF 1), ID30a3 (MASSIF 3) and ID30b**
- **Remote access usage since early spring 2018**
- **Positive user feedback and big interest in the application**

"In general, everyone had a very positive experience with MXCube3. I think most of our crystallographers have now used it and are happy with it. "

- Industrial user

Remote Access

MXCuBE3 - ESRF Remote Access Infrastructure



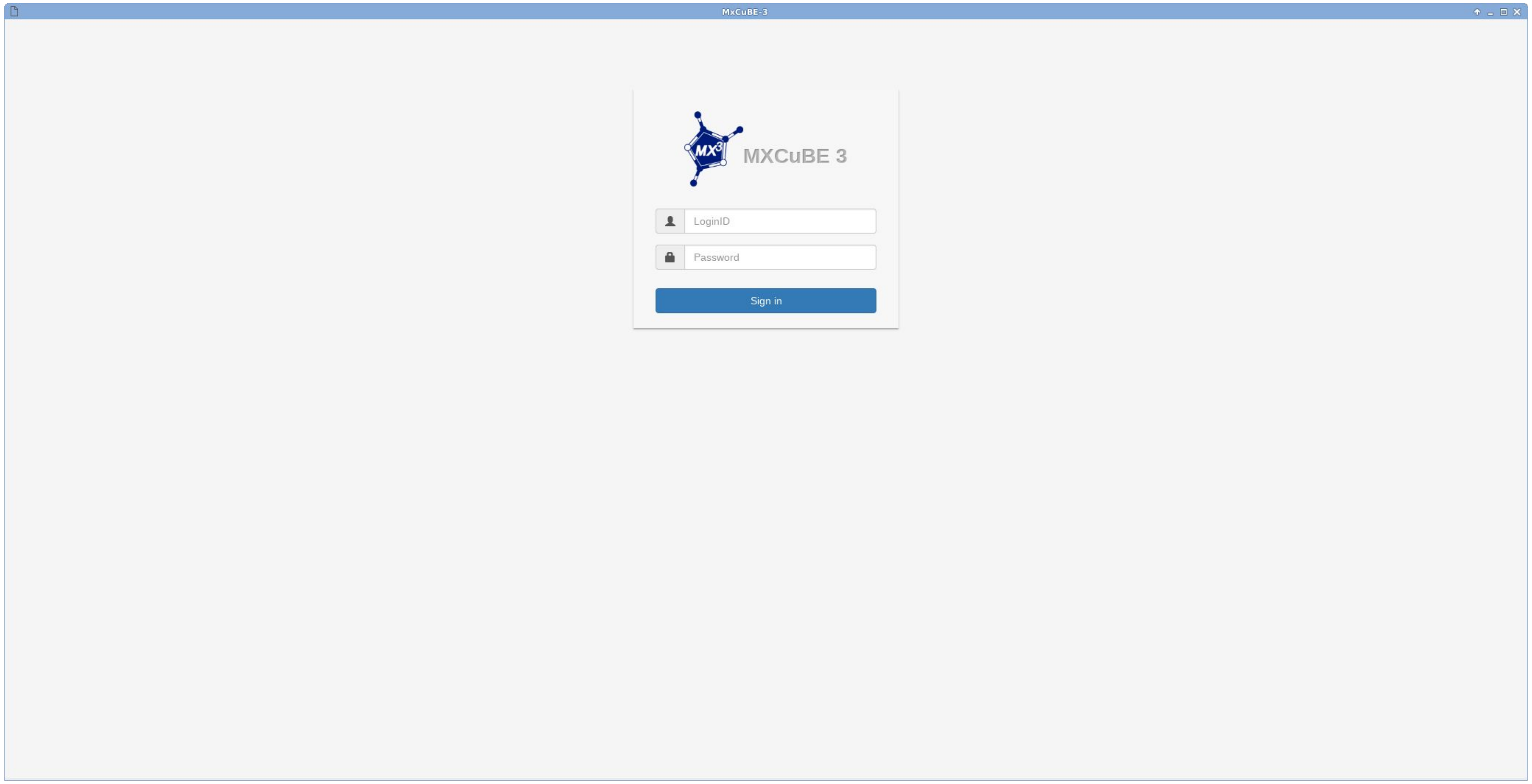
NGINX

- Reverse proxy that relays traffic to and from the MXCuBE3 applacition servers.
- Loading balancing with 3 nodes foreseen

Runs MXCuBE3 Server

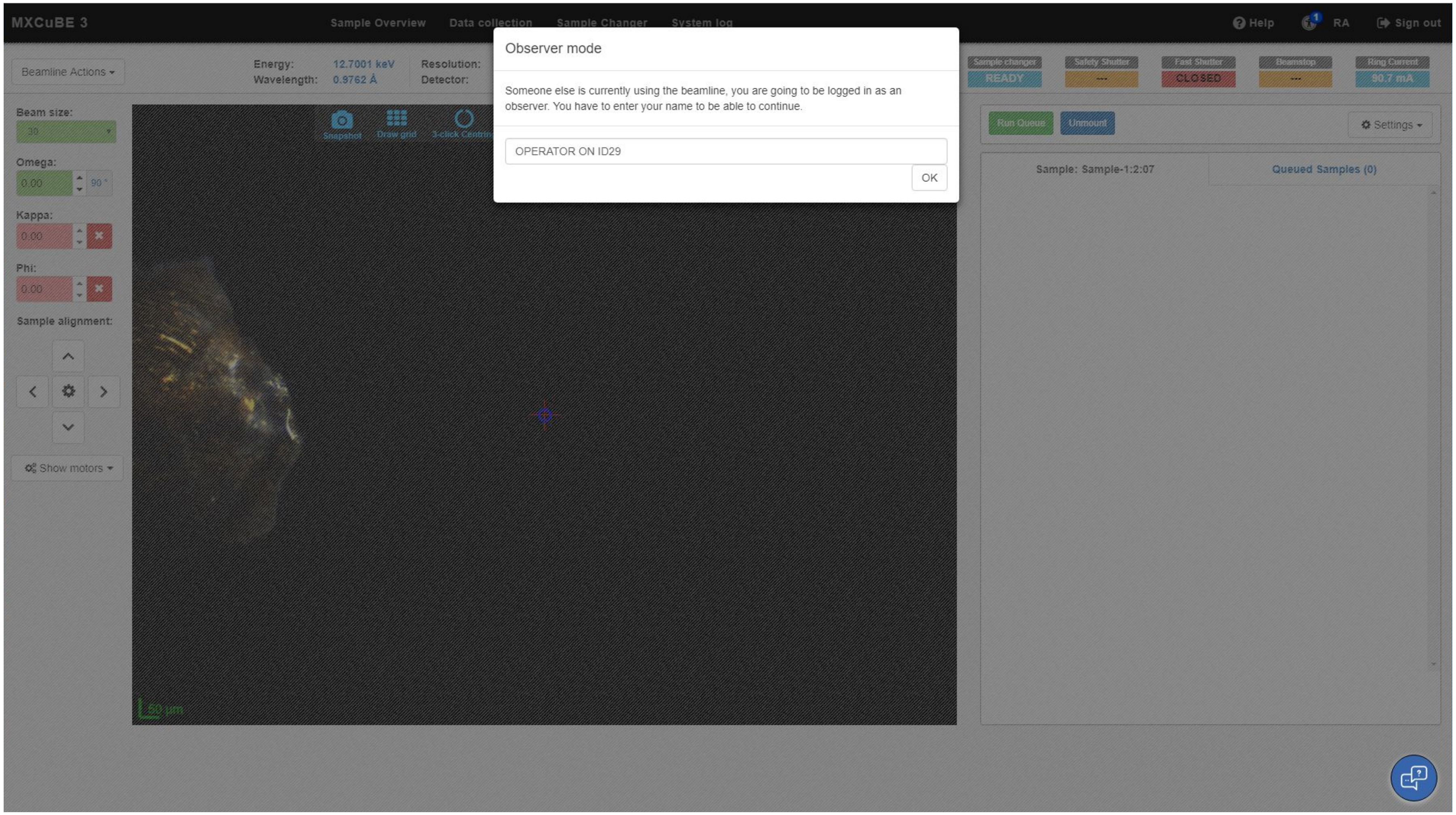
UI

Interface - Login



- Remote users logins at https://idxx.mxcube3.esrf.fr or https://mxcube3.esrf.fr
- Only scheduled users and non beamline operator accounts can login remotely

Remote Access - UI



Observer mode

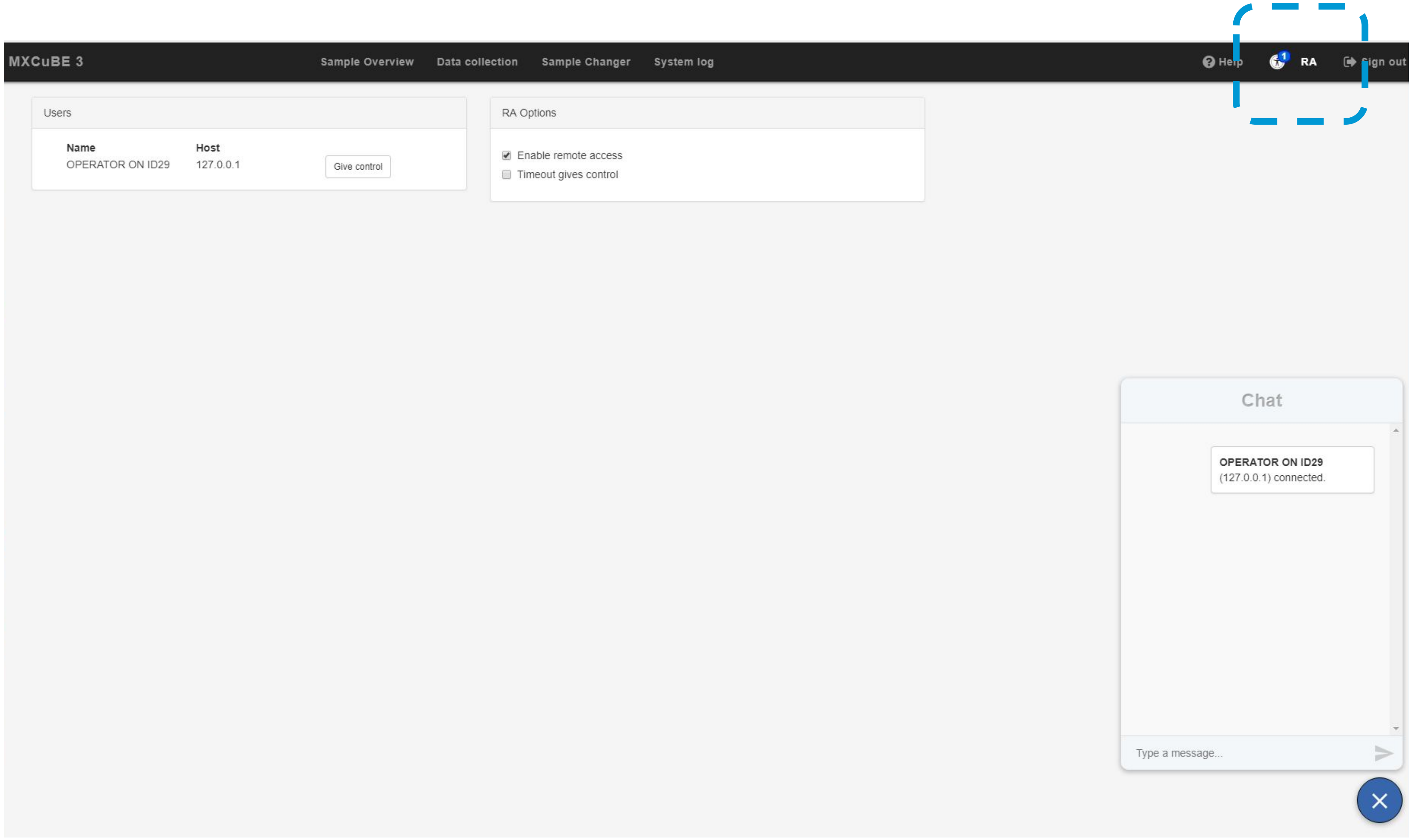
Someone else is currently using the beamline, you are going to be logged in as an observer. You have to enter your name to be able to continue.

OPERATOR ON ID29

OK

- **Remote user is presented with a “Observer mode” dialog**

Remote Access - UI



Users

Name	Host	
OPERATOR ON ID29	127.0.0.1	Give control

RA Options

[✓] Enable remote access
[ ] Timeout gives control

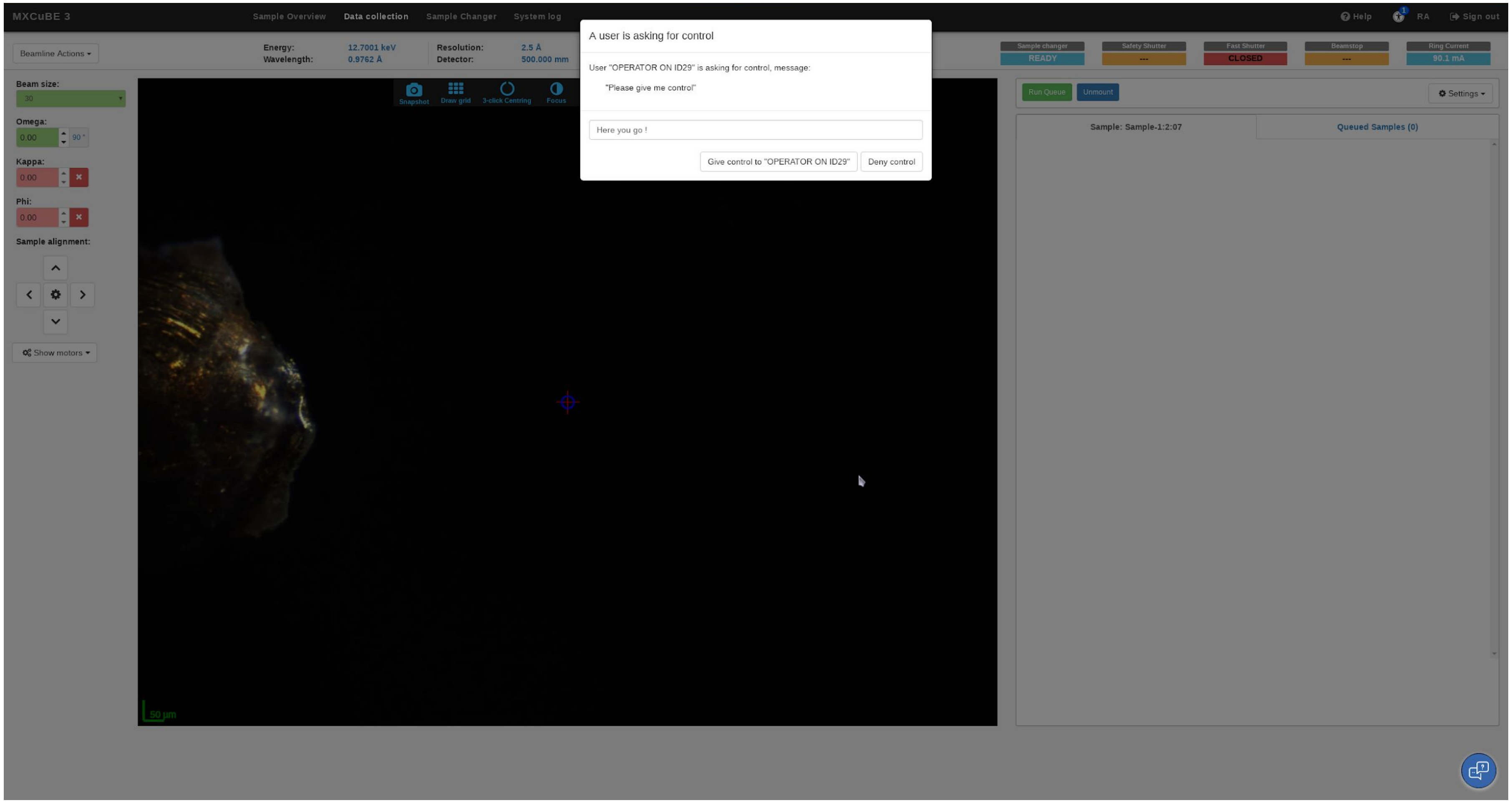
Chat

OPERATOR ON ID29 (127.0.0.1) connected.

Type a message...

- **Goes to RA page to ask for control**
- **User in control can also give away control, like in the screenshot above**

Remote Access - UI



Energy: 12.7001 keV
Wavelength: 0.9762 Å
Resolution: 2.5 Å
Detector: 500.000 mm

Beam size: 30
Omega: 0.00 90 °
Kappa: 0.00
Phi: 0.00

Sample changer READY
Safety Shutter ---
Fast Shutter CLOSED
Beamstop ---
Ring Current 90.1 mA

A user is asking for control

User "OPERATOR ON ID29" is asking for control, message:

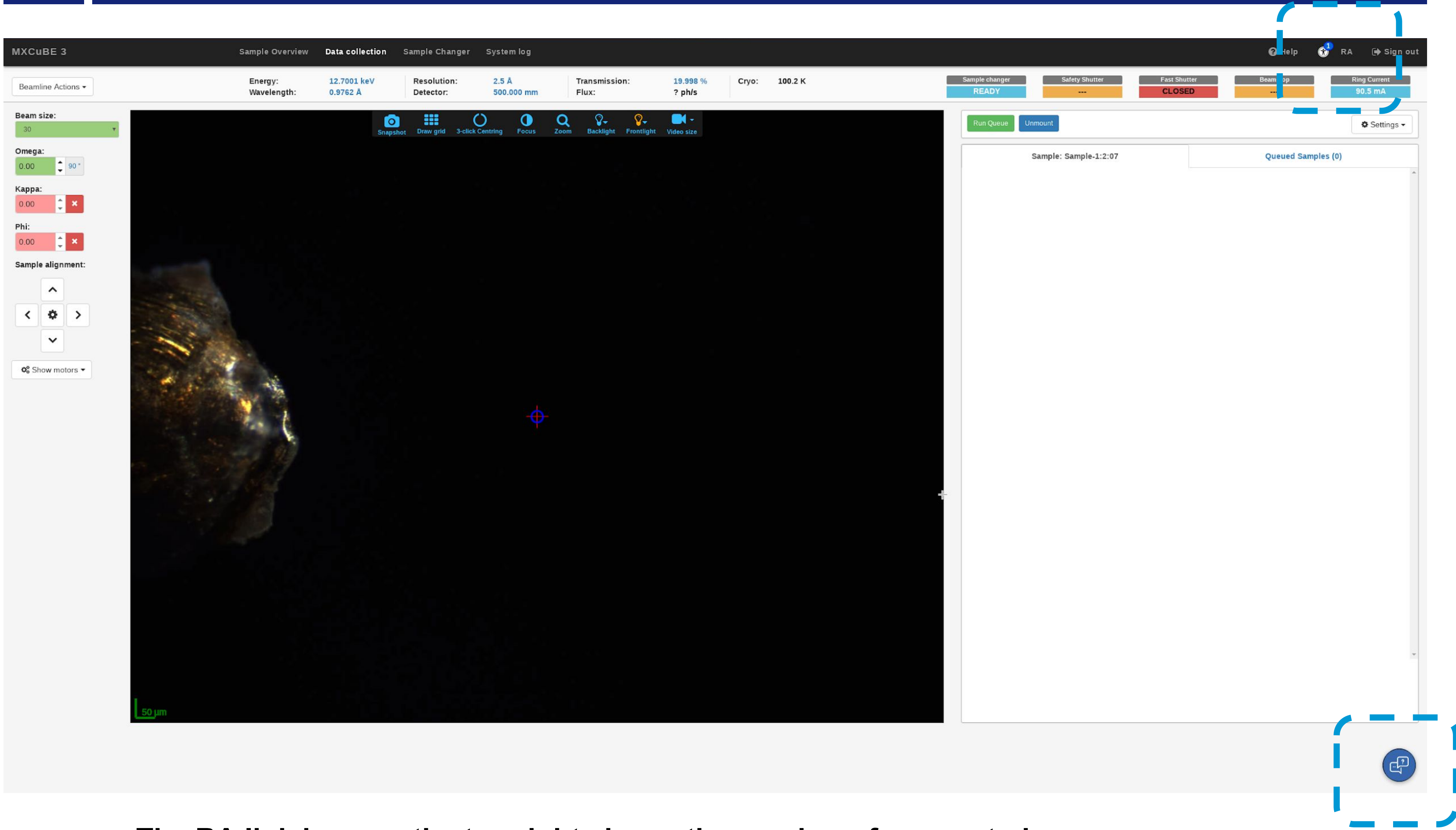
"Please give me control"

Here you go !

Give control to "OPERATOR ON ID29" | Deny control

- **If asked for control the user on control gets a dialog with the possibility to deny or accept request**

Remote Access - UI



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

Energy: 12.7001 keV
Wavelength: 0.9762 Å
Resolution: 2.5 Å
Detector: 500.000 mm
Transmission: 19.998 %
Flux: ? ph/s
Cryo: 100.2 K

Sample changer	Safety Shutter	Fast Shutter	Beamstop	Ring Current
READY	---	CLOSED	---	90.5 mA

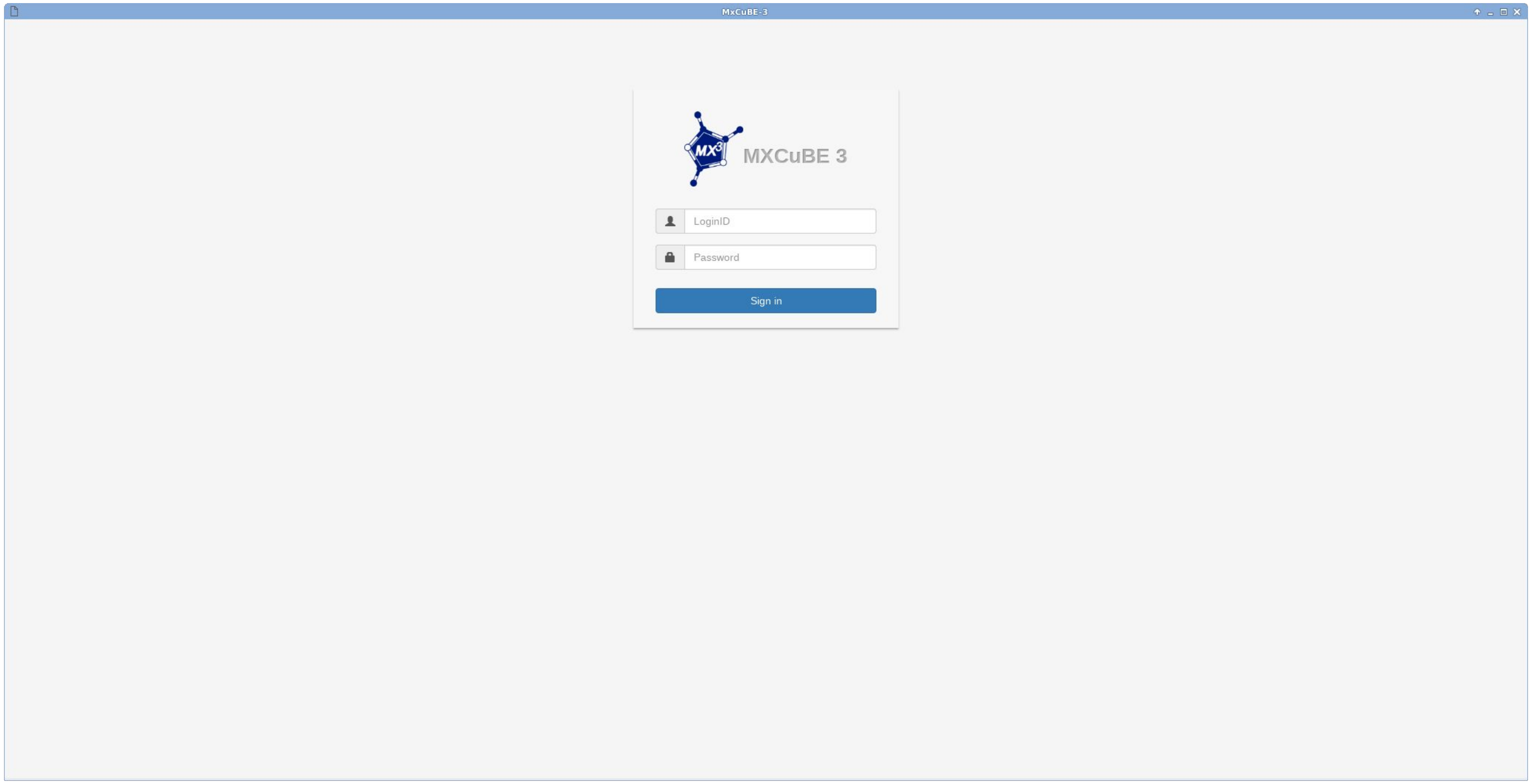
Beam size: 30
Omega: 0.00
Kappa: 0.00
Phi: 0.00

Sample: Sample-1:2:07
Queued Samples (0)

- The RA link icon on the top right shows the number of connected users
- The chat dialog opens when the chat icon, on the lover right, is clicked

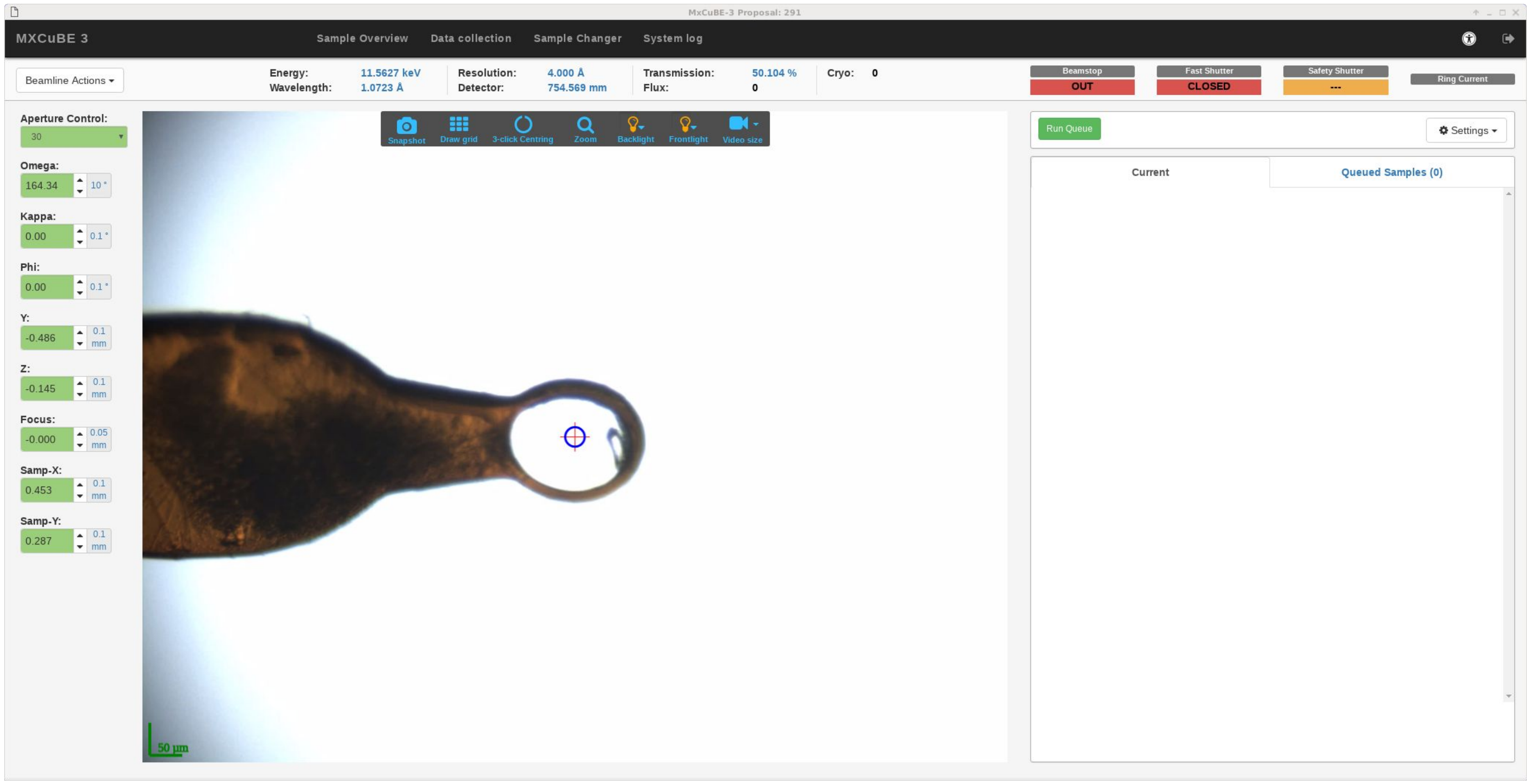
Version 3.0
a review

Interface - Login



- Login view, in the future site and beamline customizable
- Possible to configure login to use either user accounts or proposals directly

MXCuBE 3 - Sample Video with video controls



Energy:	11.5627 keV
Wavelength:	1.0723 Å
Resolution:	4.000 Å
Detector:	754.569 mm
Transmission:	50.104 %
Flux:	0
Cryo:	0
Beamstop	OUT
Fast Shutter	CLOSED
Safety Shutter	---
Ring Current	

Aperture Control:	30	
Omega:	164.34	10 °
Kappa:	0.00	0.1 °
Phi:	0.00	0.1 °
Y:	-0.486	0.1 mm
Z:	-0.145	0.1 mm
Focus:	-0.000	0.05 mm
Samp-X:	0.453	0.1 mm
Samp-Y:	0.287	0.1 mm

Use:

Shift + **DBL Click:** Move to beam

z + **Mouse wheel:** microscope zoom

r + **Mouse wheel:** Rotate sample

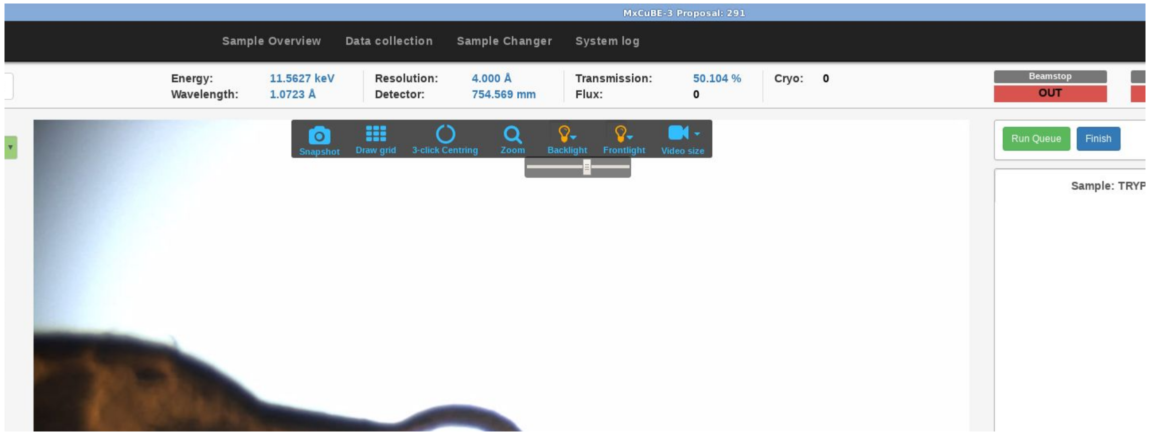
f + **Mouse wheel:** microscope focus

Or, simply motor controls (located to the left)

Video controls

Microscope / video controls:

- Light and zoom intensity changed by slider

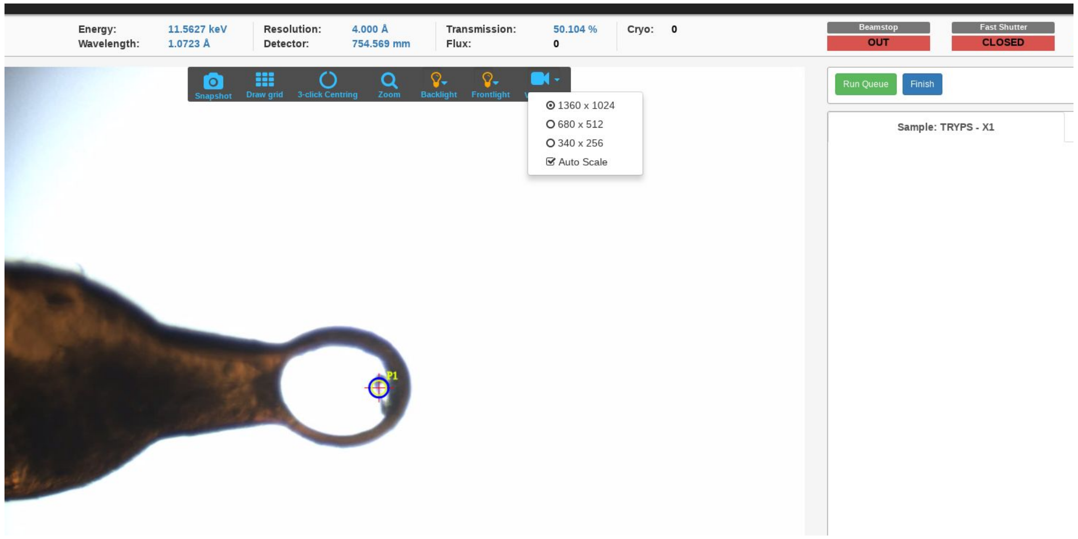


MxCuBE-3 Proposal: 291

Energy: 11.5627 keV
Wavelength: 1.0723 Å
Resolution: 4.000 Å
Detector: 754.569 mm
Transmission: 50.104 %
Flux: 0
Cryo: 0

Beamstop: OUT

Sample: TRYP



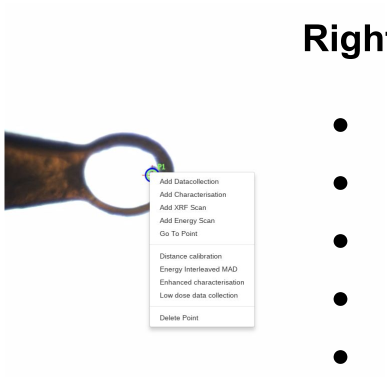
Energy: 11.5627 keV
Wavelength: 1.0723 Å
Resolution: 4.000 Å
Detector: 754.569 mm
Transmission: 50.104 %
Flux: 0
Cryo: 0

Beamstop: OUT
Fast Shutter: CLOSED

Sample: TRYPS - X1

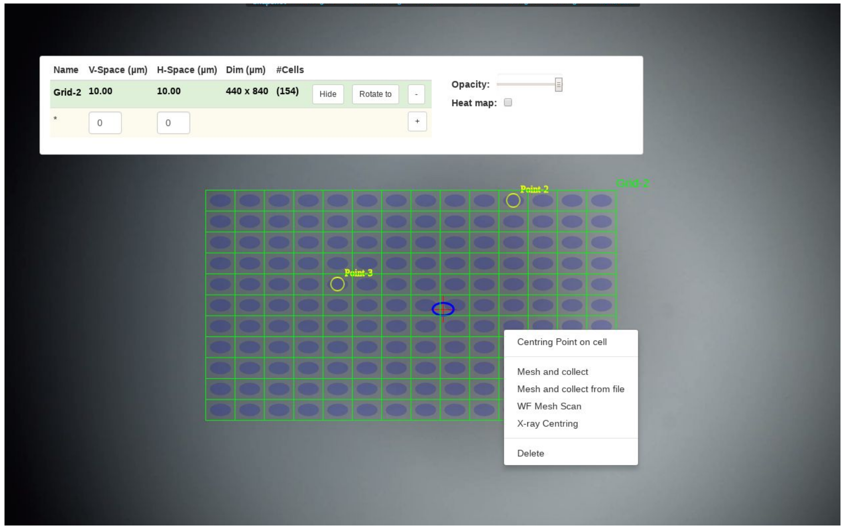
- Video is streamed as MPEG-1, perhaps adaptive MPEG-4 in the future
- Possibility to select video stream size (particularly useful for remote users)
- With auto scale option

Data collection



Right click context menu to add tasks:

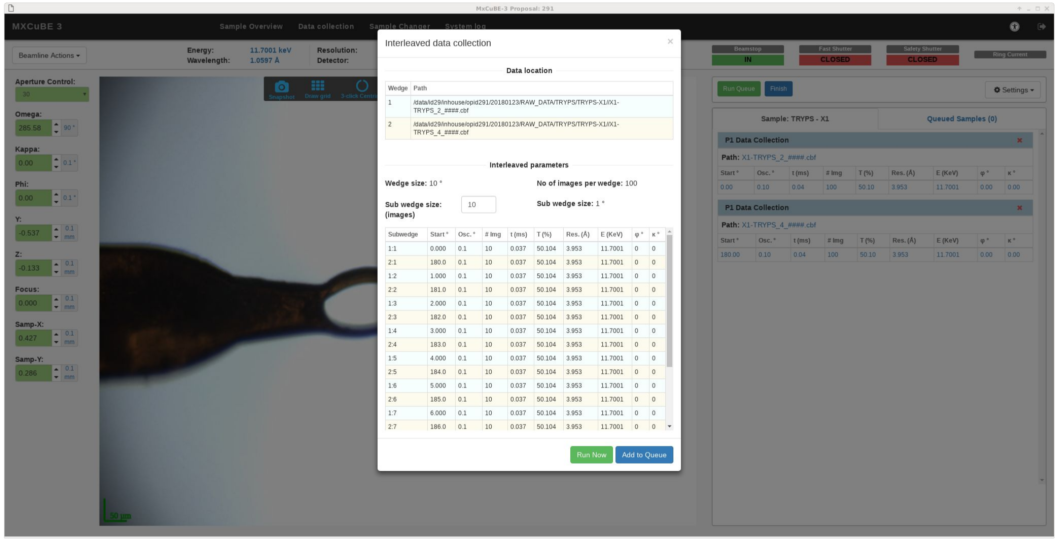
- **Data collection**
- **Helical**
- **Characterisation**
- **XRF**
- **Energy Scan**



Name	V-Space (µm)	H-Space (µm)	Dim (µm)	#Cells
Grid-2	10.00	10.00	440 x 840	(154)
*	0	0		

- **Mesh interface similar to MXCuBE 2**
- **Possibility to change transparency of grid**
- **Also possible to add centring point to cell**

Interleaved data collection



Interleaved data collection

Data location

Wedge	Path
1	/data/id29/inhouse/opid291/20180123/RAW_DATA/TRYPS/TRYPS-X1//X1-TRYPS_2_####.cbf
2	/data/id29/inhouse/opid291/20180123/RAW_DATA/TRYPS/TRYPS-X1//X1-TRYPS_4_####.cbf

Interleaved parameters

Wedge size: 10 °

No of images per wedge: 100

Sub wedge size: (images) 10

Sub wedge size: 1 °

Subwedge	Start °	Osc. °	# Img	t (ms)	T (%)	Res. (Å)	E (KeV)	φ °	κ °
1:1	0.000	0.1	10	0.037	50.104	3.953	11.7001	0	0
2:1	180.0	0.1	10	0.037	50.104	3.953	11.7001	0	0
1:2	1.000	0.1	10	0.037	50.104	3.953	11.7001	0	0
2:2	181.0	0.1	10	0.037	50.104	3.953	11.7001	0	0
1:3	2.000	0.1	10	0.037	50.104	3.953	11.7001	0	0
2:3	182.0	0.1	10	0.037	50.104	3.953	11.7001	0	0
1:4	3.000	0.1	10	0.037	50.104	3.953	11.7001	0	0
2:4	183.0	0.1	10	0.037	50.104	3.953	11.7001	0	0
1:5	4.000	0.1	10	0.037	50.104	3.953	11.7001	0	0
2:5	184.0	0.1	10	0.037	50.104	3.953	11.7001	0	0
1:6	5.000	0.1	10	0.037	50.104	3.953	11.7001	0	0
2:6	185.0	0.1	10	0.037	50.104	3.953	11.7001	0	0
1:7	6.000	0.1	10	0.037	50.104	3.953	11.7001	0	0
2:7	186.0	0.1	10	0.037	50.104	3.953	11.7001	0	0

Run Now | Add to Queue

P1 Data Collection

Path: X1-TRYPS_2_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.00	0.10	0.04	100	50.10	3.953	11.7001	0.00	0.00

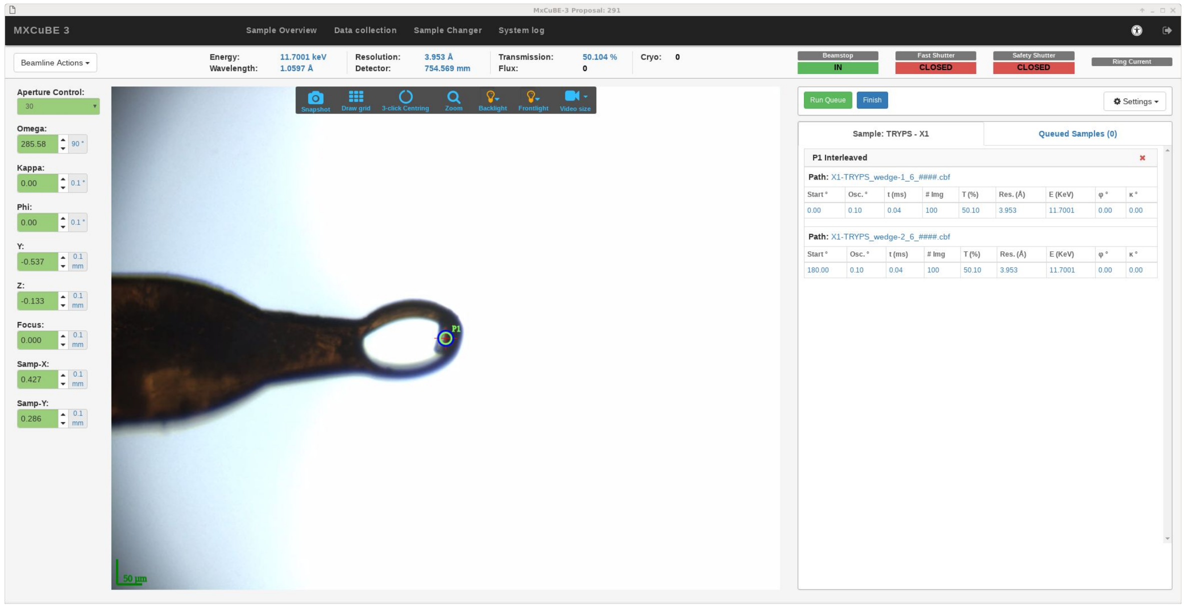
P1 Data Collection

Path: X1-TRYPS_4_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
180.00	0.10	0.04	100	50.10	3.953	11.7001	0.00	0.00

- Now possible to **interleave n data collections**.
- Also possible to interleave **any parameter** such as energy, kappa, omega, resolution …
- In the future **pie chart like display, potentially** with the **possibility to change subwedge order**

- The two (or *n*) principal wedges to be collected are shown in the task



P1 Interleaved

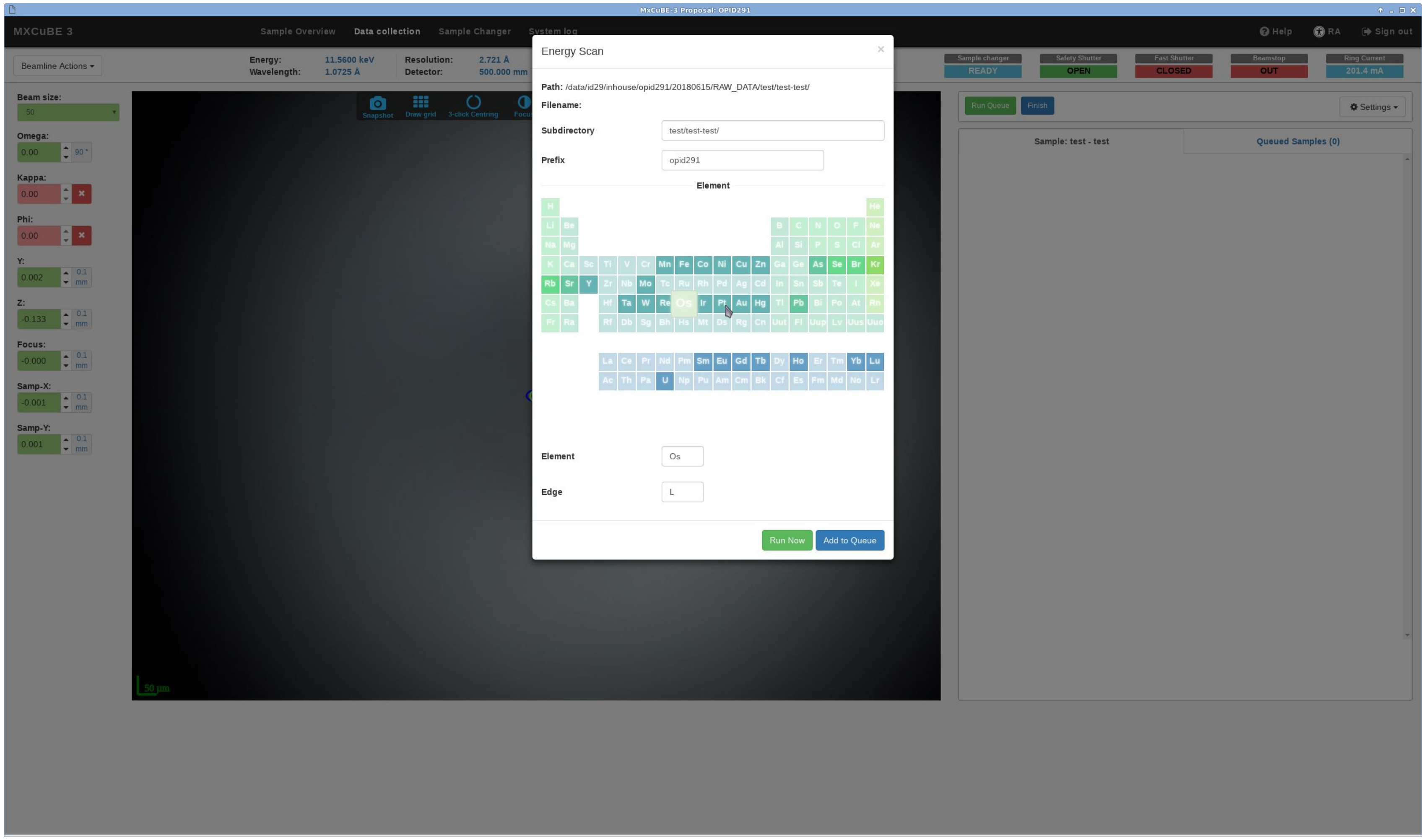
Path: X1-TRYPS_wedge-1_6_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.00	0.10	0.04	100	50.10	3.953	11.7001	0.00	0.00

Path: X1-TRYPS_wedge-2_6_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
180.00	0.10	0.04	100	50.10	3.953	11.7001	0.00	0.00

Energy Scan



Energy: 11.5600 keV
Wavelength: 1.0725 Å
Resolution: 2.721 Å
Detector: 500.000 mm

Sample changer	Safety Shutter	Fast Shutter	Beamstop	Ring Current
READY	OPEN	CLOSED	OUT	201.4 mA

Beam size:	50
Omega:	0.00
Kappa:	0.00
Phi:	0.00
Y:	0.002
Z:	-0.133
Focus:	-0.000
Samp-X:	-0.001
Samp-Y:	0.001

Energy Scan

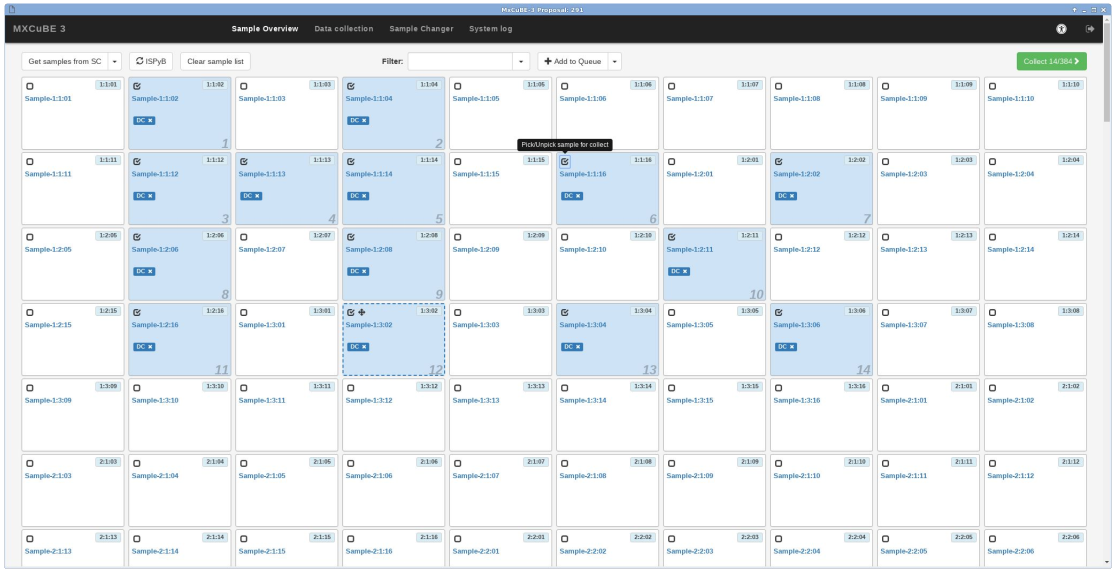
Path: /data/id29/inhouse/opid291/20180615/RAW_DATA/test/test-test/
Filename:

Subdirectory	test/test-test/
Prefix	opid291

Element

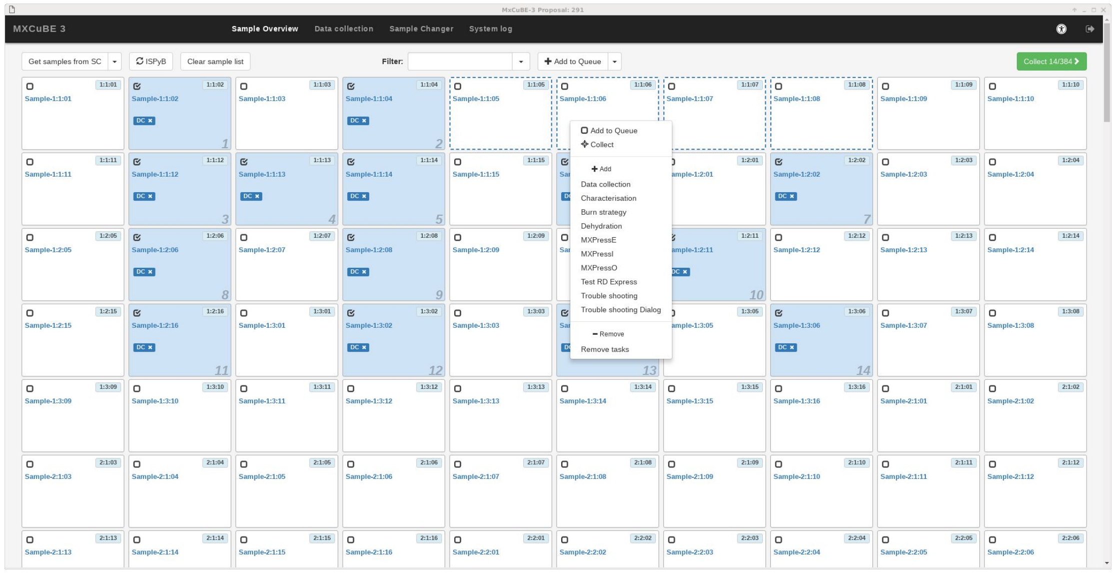
Element	Os
Edge	L

Sample Grid



Sample grid contains available samples

- Synch with LIMS
- Filtering (name, position, LIMS)
- Results view
- Tasks to be executed

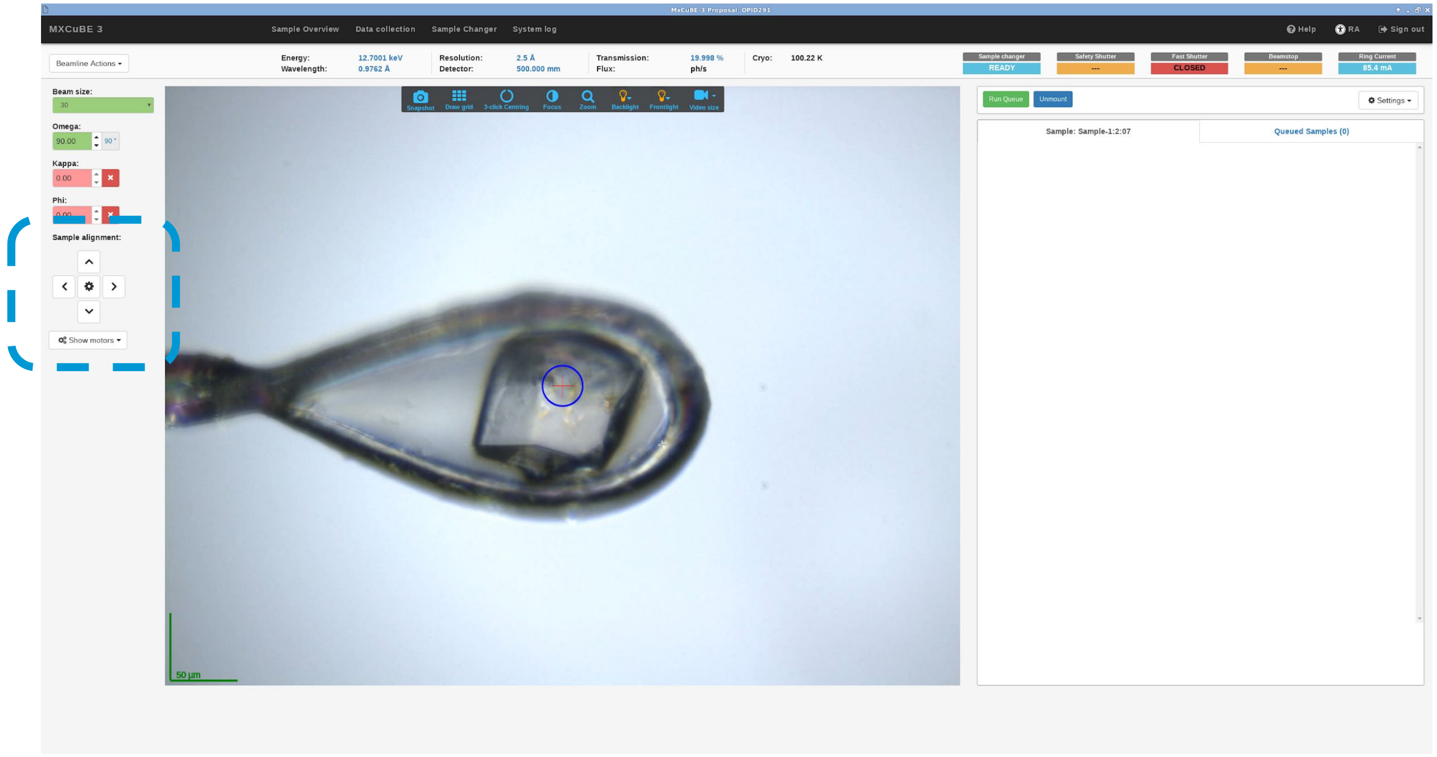


Sample grid context menu

- Preparing for automated execution by selecting multiple samples
- Use context menu to add tasks

New in version 3.0.1

Navigation cross for sample translation



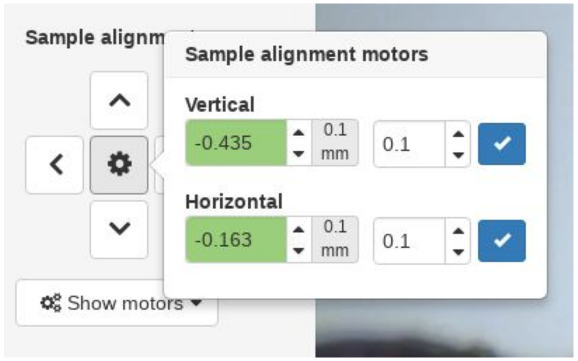
MxCuBE-3 Proposal: OPID291

Energy: 12.7001 keV
Wavelength: 0.9762 Å
Resolution: 2.5 Å
Detector: 500.000 mm
Transmission: 19.998 %
Flux: ph/s
Cryo: 100.22 K

Sample changer	Safety Shutter	Fast Shutter	Beamstop	Ring Current
READY	---	CLOSED	---	85.4 mA

Beam size: 30
Omega: 90.00 90 °
Kappa: 0.00
Phi: 0.00

Sample: Sample-1:2:07
Queued Samples (0)

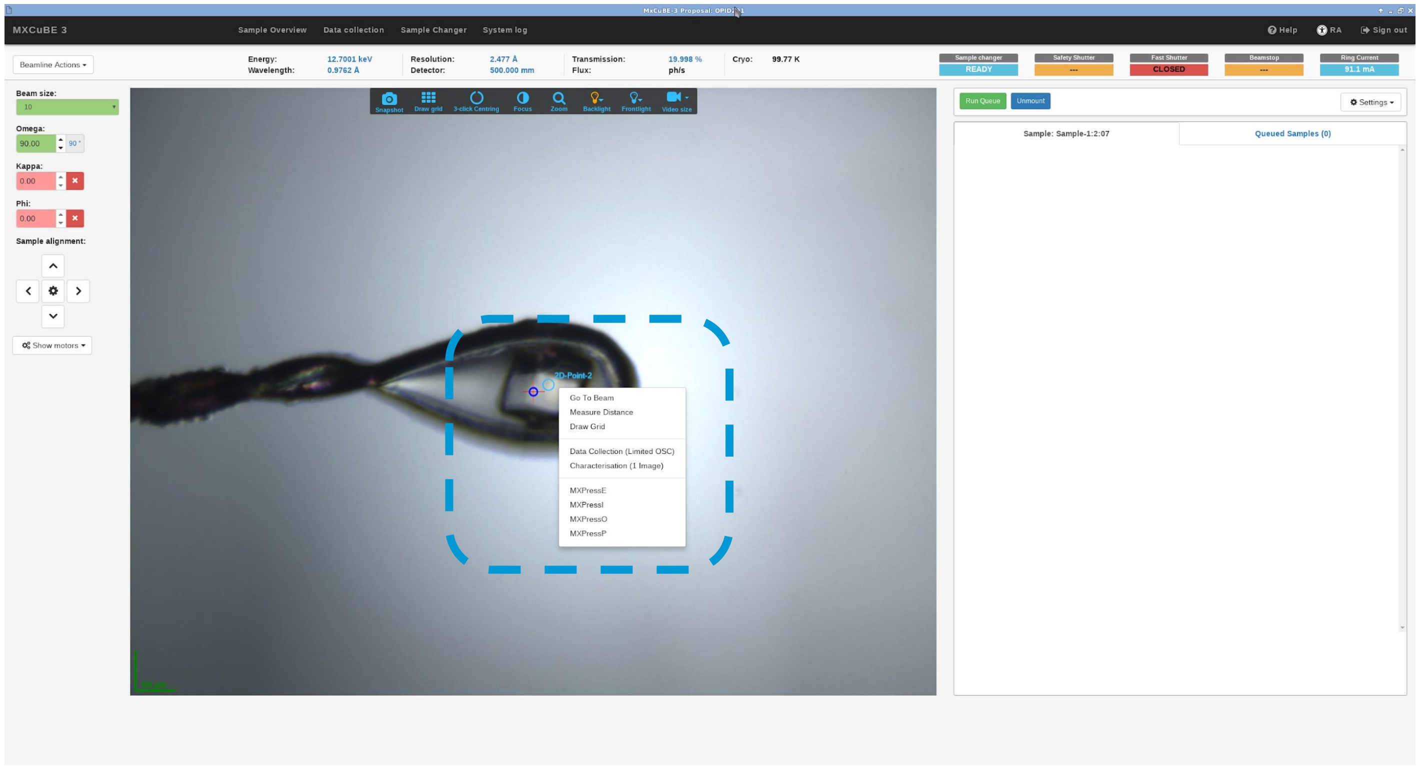


Sample alignment motors

Vertical	-0.435	0.1 mm	0.1
Horizontal	-0.163	0.1 mm	0.1

- New navigation cross (Joystick) control for translating sample
- User does not need to know the diffractometer setup

2D-Points

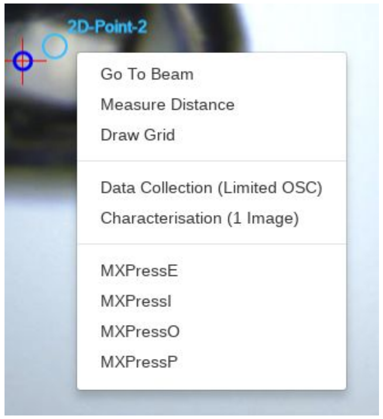

MxCuBE-3 Proposal: OPID

Energy: 12.7001 keV
Wavelength: 0.9762 Å
Resolution: 2.477 Å
Detector: 500.000 mm
Transmission: 19.998 %
Flux: ph/s
Cryo: 99.77 K

Sample changer: READY
Safety Shutter: ---
Fast Shutter: CLOSED
Beamstop: ---
Ring Current: 91.1 mA

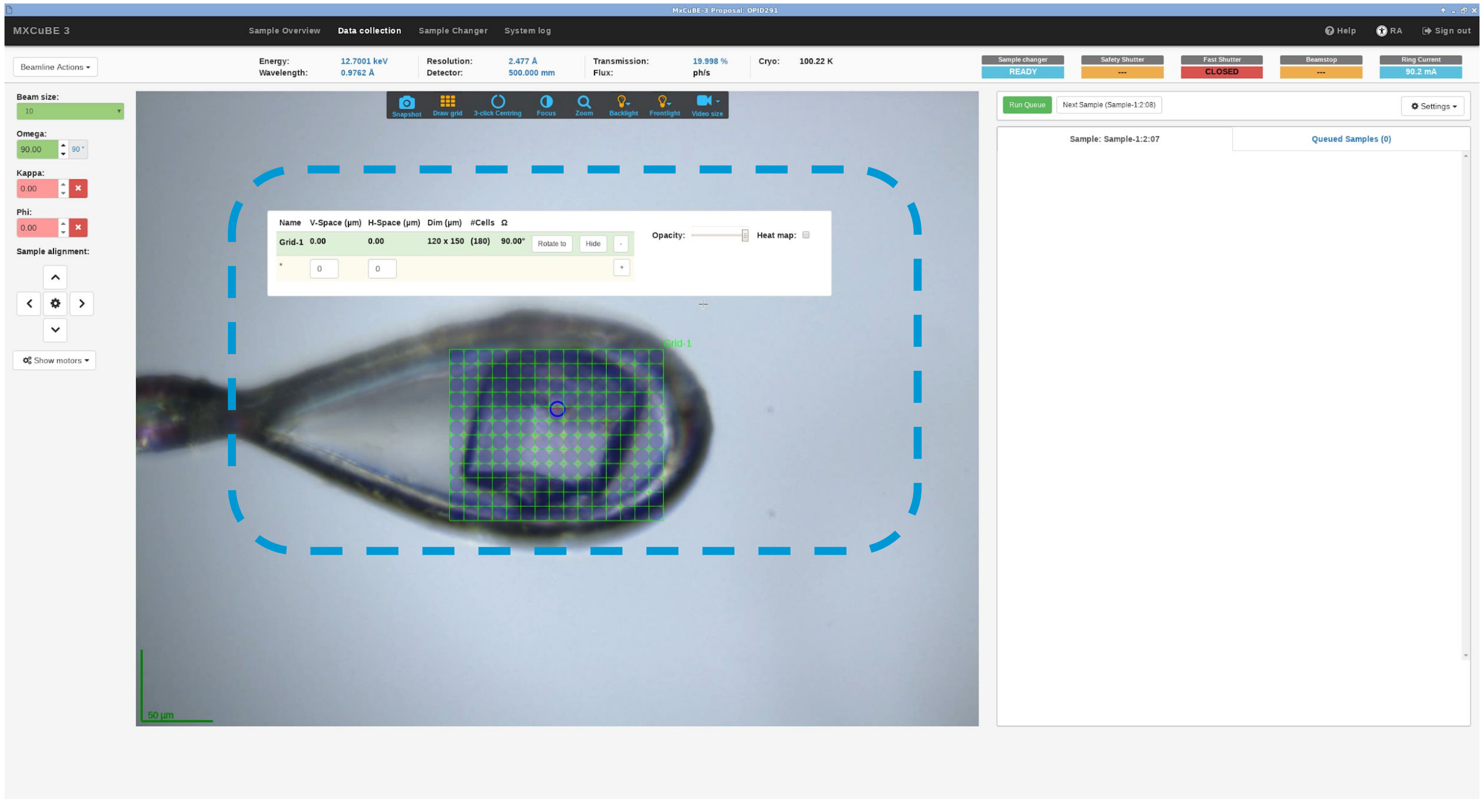
Beam size: 10
Omega: 90.00
Kappa: 0.00
Phi: 0.00

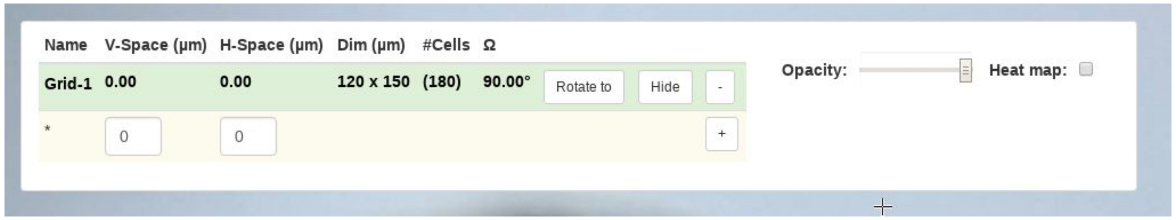
Sample: Sample-1:2:07
Queued Samples (0)



- **2D Centered position, centring that is only valid for a limited rotation range +- 5 degrees by default**
- **Useful for experiments that are fixed in a certain plane**
- **Allows for “quick characterisation”**
- **Valid range to be specified by external event, i.e read from or set by diffractometer**

Grid auto hide



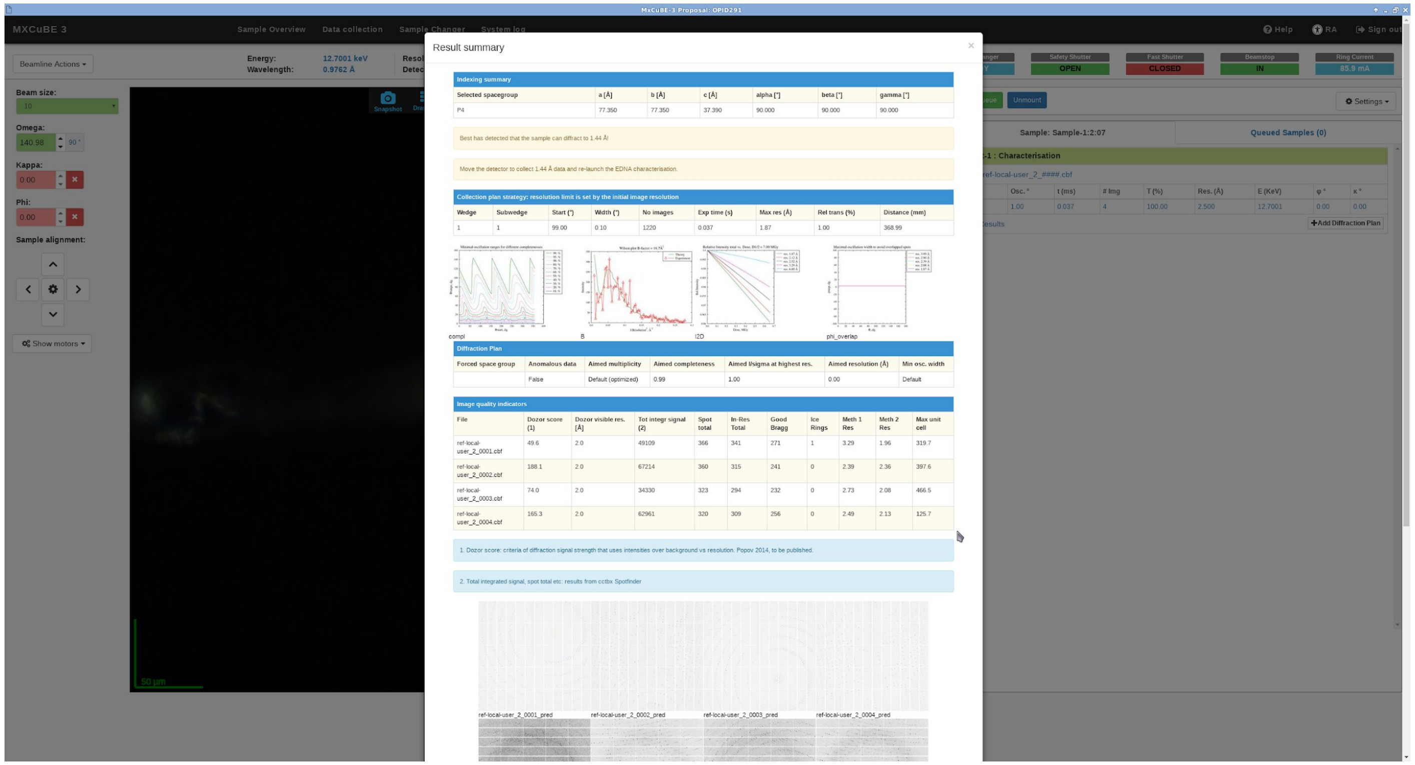


Name	V-Space (µm)	H-Space (µm)	Dim (µm)	#Cells	Ω			
Grid-1	0.00	0.00	120 x 150	(180)	90.00°	Rotate to	Hide	-
*	0	0						+

Opacity: Heat map: ☐

- A grid is automatically hidden when it's not considered to be valid, +-5 degrees by default
- Omega angle at which the grid was defined is shown in the table

LIMS - Results



Result summary

Indexing summary

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

Collection plan strategy: resolution limit is set by the initial image resolution

Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	99.00	0.10	1220	0.037	1.87	1.00	368.99

compl B I2D phi_overlap

Diffraction Plan

Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed I/sigma at highest res.	Aimed resolution (Å)	Min osc. width
	False	Default (optimized)	0.99	1.00	0.00	Default

Image quality indicators

File	Dozor score (1)	Dozor visible res. [Å]	Tot integr signal (2)	Spot total	In-Res Total	Good Bragg	Ice Rings	Meth 1 Res	Meth 2 Res	Max unit cell
ref-local-user_2_0001.cbf	49.6	2.0	49109	366	341	271	1	3.29	1.96	319.7
ref-local-user_2_0002.cbf	188.1	2.0	67214	360	315	241	0	2.39	2.36	397.6
ref-local-user_2_0003.cbf	74.0	2.0	34330	323	294	232	0	2.73	2.08	466.5
ref-local-user_2_0004.cbf	165.3	2.0	62961	320	309	256	0	2.49	2.13	125.7

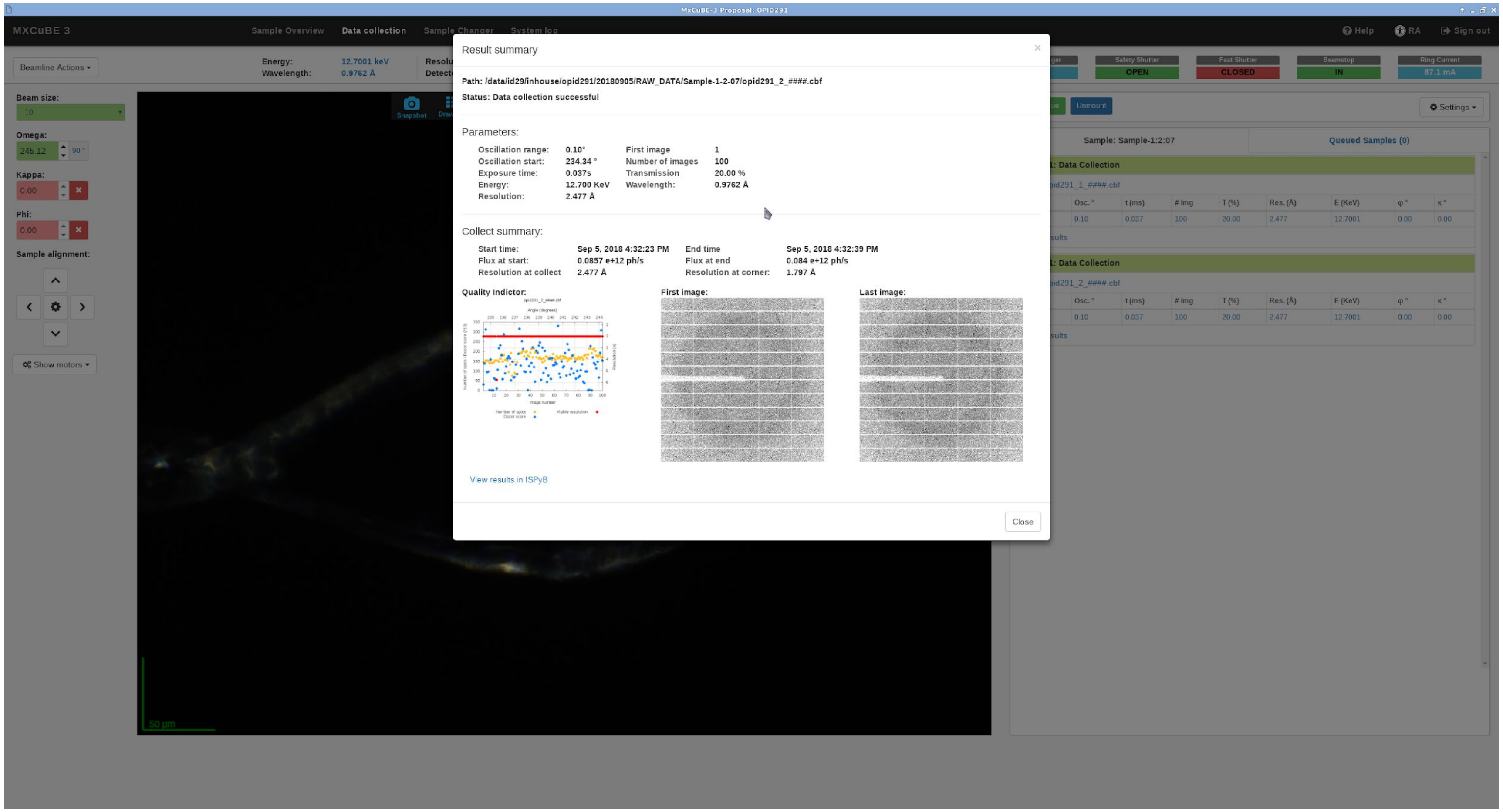
1. Dozor score: criteria of diffraction signal strength that uses intensities over background vs resolution. Popov 2014, to be published.

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

ref-local-user_2_0001_pred ref-local-user_2_0002_pred ref-local-user_2_0003_pred ref-local-user_2_0004_pred

- Using "server side rendering" to display LIMS (ISPyB) results
- Template directory that contain the either pure HTML templates or logic that uses the already existing LIMS UI code to generate HTML
- LIMS Independent
- Enables reuse of already existing LIMS views

LIMS - Results



Energy: 12.7001 keV
Wavelength: 0.9762 Å

Beam size: 10
Omega: 245.12 90°
Kappa: 0.00
Phi: 0.00
Sample alignment:

Safety Shutter: OPEN
Fast Shutter: CLOSED
Beamstop: IN
Ring Current: 87.1 mA

Result summary

Path: /data/id29/inhouse/opid291/20180905/RAW_DATA/Sample-1-2-07/opid291_2_####.cbf

Status: Data collection successful

Parameters:

Oscillation range:	0.10°	First image	1
Oscillation start:	234.34 °	Number of images	100
Exposure time:	0.037s	Transmission	20.00 %
Energy:	12.700 KeV	Wavelength:	0.9762 Å
Resolution:	2.477 Å		

Collect summary:

Start time:	Sep 5, 2018 4:32:23 PM	End time	Sep 5, 2018 4:32:39 PM
Flux at start:	0.0857 e+12 ph/s	Flux at end	0.084 e+12 ph/s
Resolution at collect	2.477 Å	Resolution at corner:	1.797 Å

Quality Indictor: **First image:** **Last image:**

Sample: Sample-1:2:07 | Queued Samples (0)

1: Data Collection
opid291_1_####.cbf

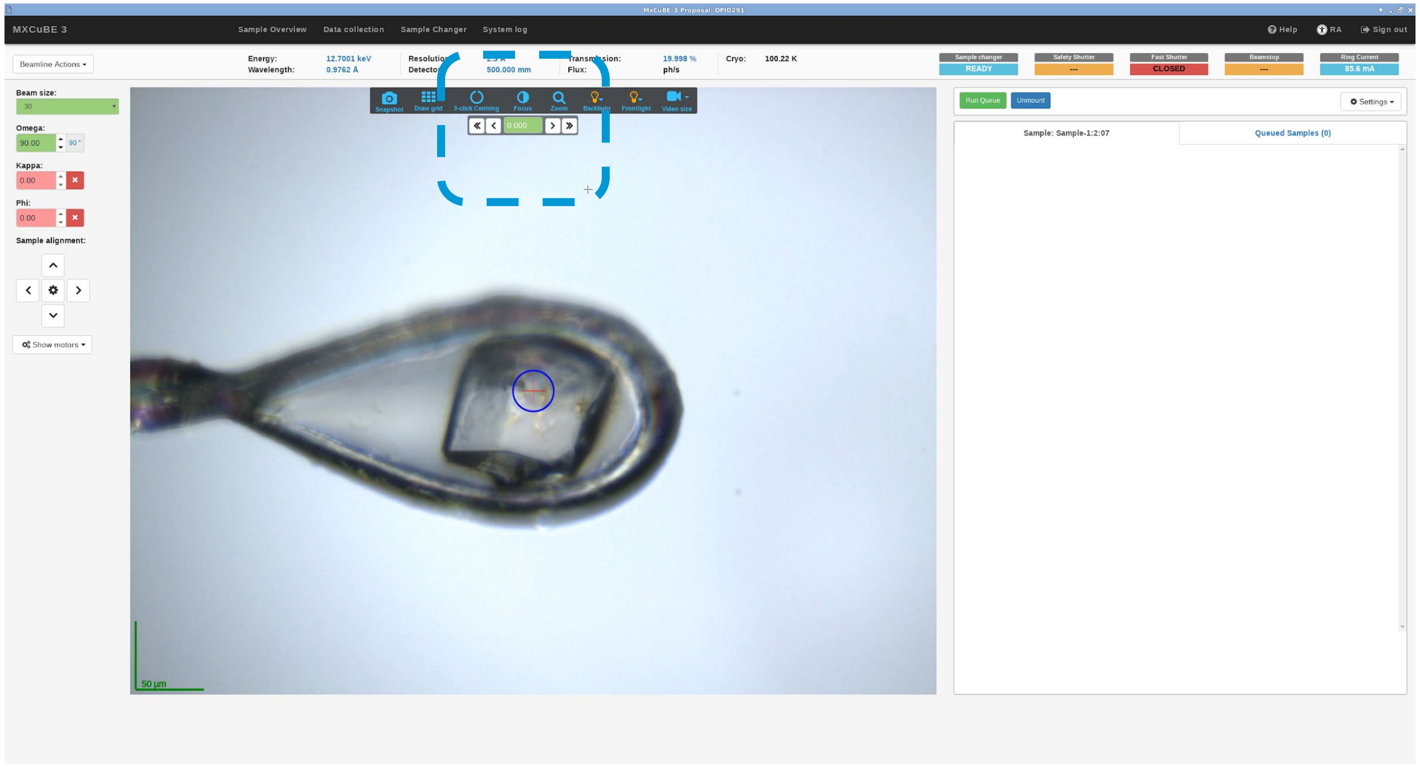
Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.10	0.037	100	20.00	2.477	12.7001	0.00	0.00

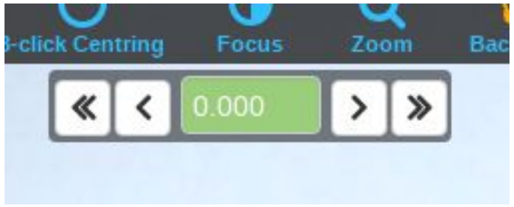
1: Data Collection
opid291_2_####.cbf

Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.10	0.037	100	20.00	2.477	12.7001	0.00	0.00

Data collection results using a pure HTML template

New focus control



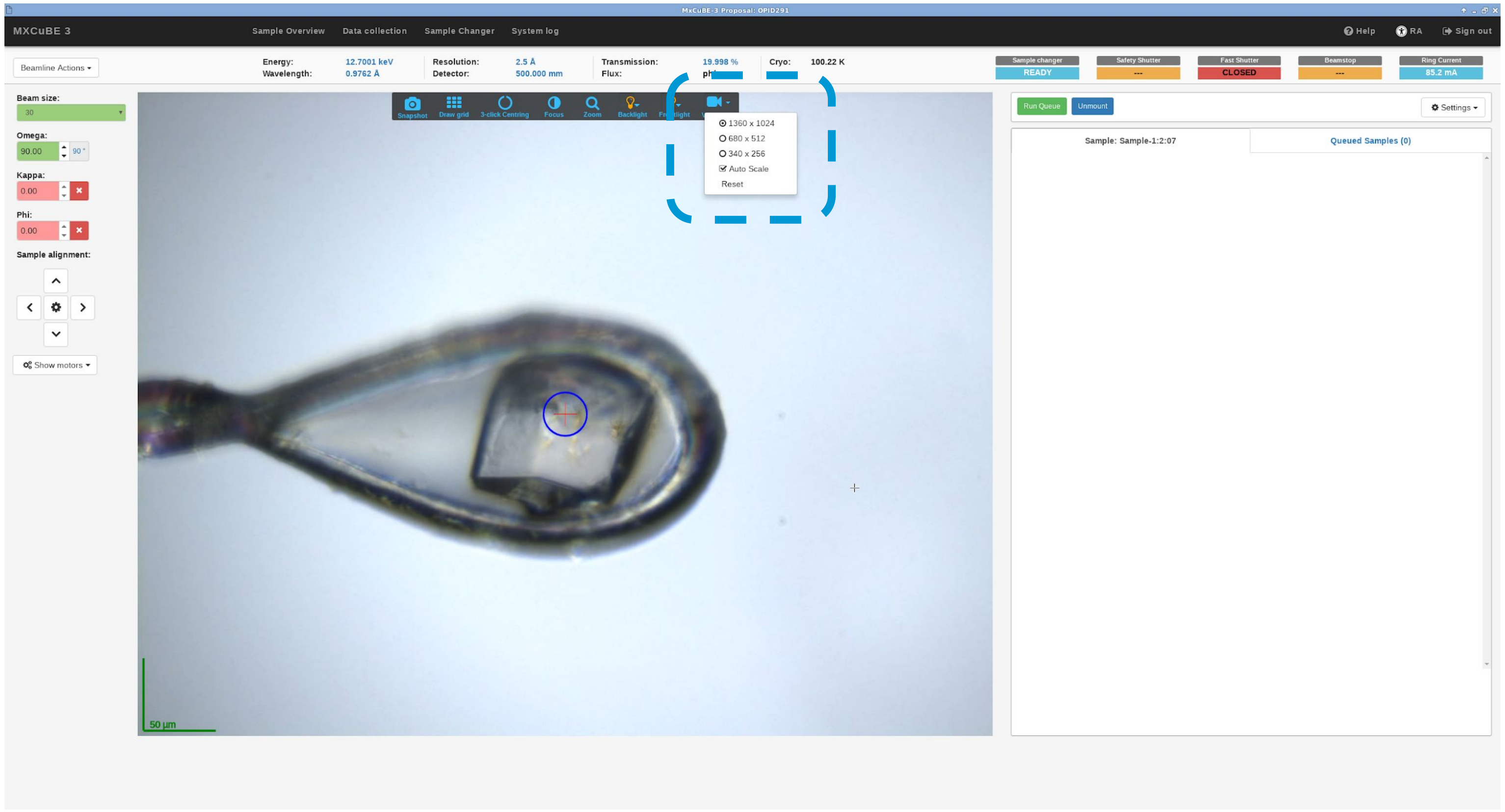


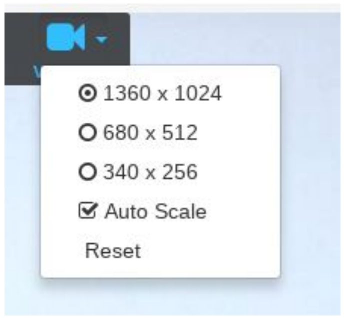
- Focus with step controls instead of slider

Reminder:

f + **Mouse wheel:** microscope focus

Reset video stream



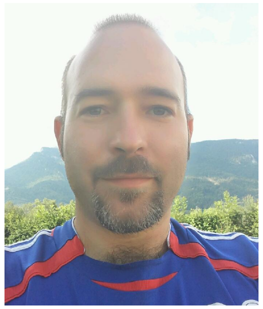


Possibility to reset video stream remotely

Coming soon

- Integration of new MESH-BEST results
- Diffraction images for grid cells
- Hutch camera view
- Diffraction image viewer
- Plate support, UI control for plate navigation
- Serial crystallography data collection methods

Big thanks to everyone involved



Matias Guijarro:
MXCuBE and
BLISS Development and support

Daniele de Sanctis:
Scientific coordination

Antonia Beteva:
BLISS Support and development,
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Didier Nurizzo:
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Workflow integration

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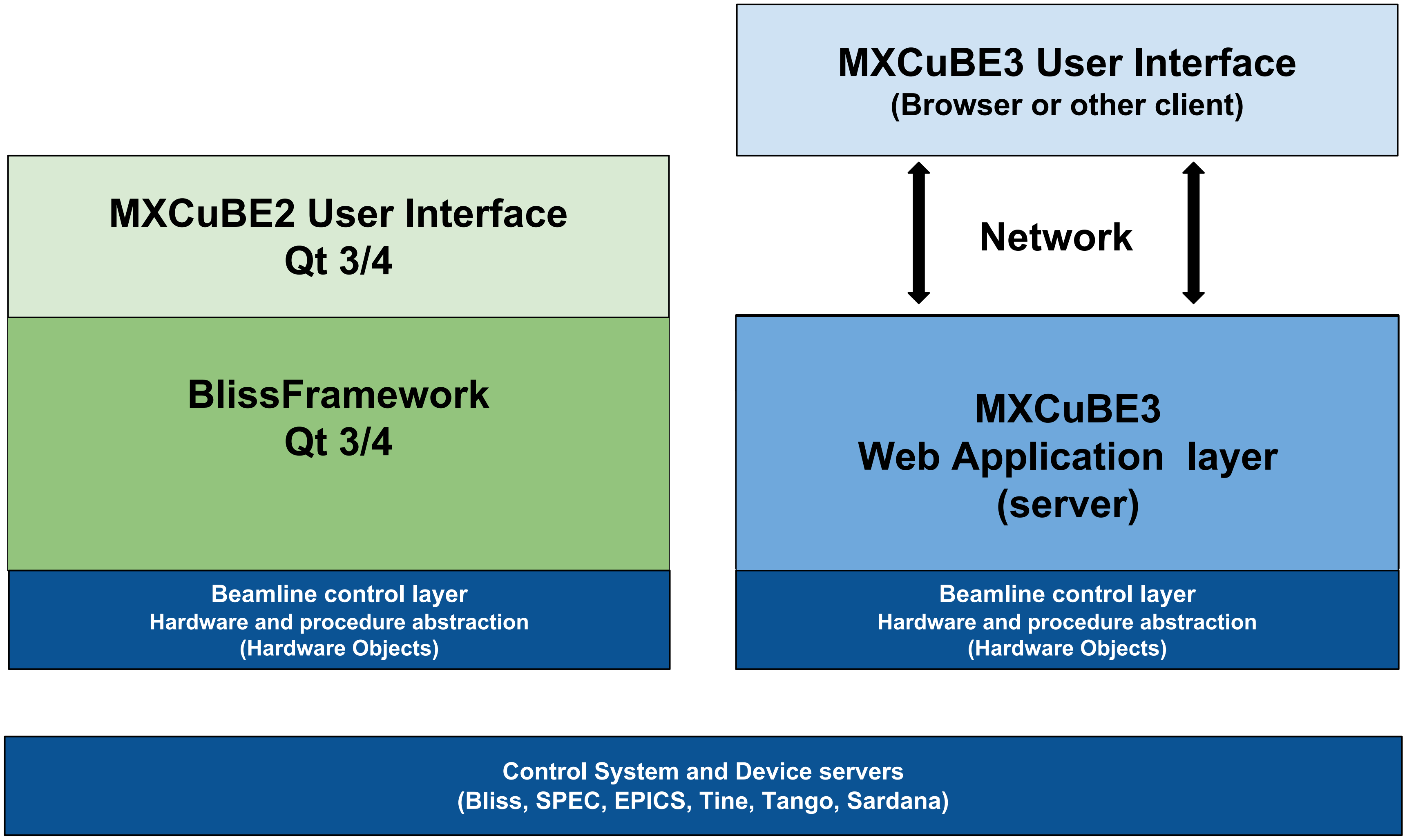
Thank you for your attention !

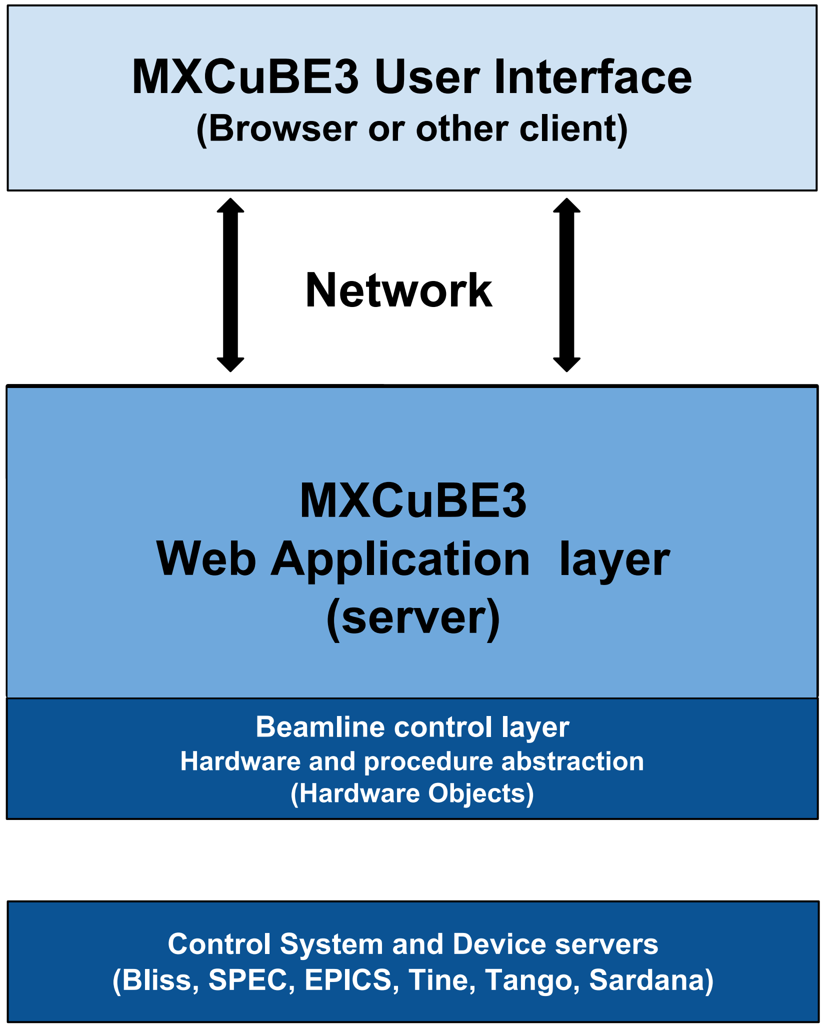
MXCuBE3 Appendix - Development

Marcus Oskarsson (marcus.oscarsson@esrf.fr)

MXCuBE3 - Design Overview



MXCuBE3 - Tech stack


MXCuBE3 User Interface
(Browser or other client)
Network
MXCuBE3
Web Application layer
(server)
Beamline control layer
Hardware and procedure abstraction
(Hardware Objects)
Control System and Device servers
(Bliss, SPEC, EPICS, Tine, Tango, Sardana)

HTML CSS JS

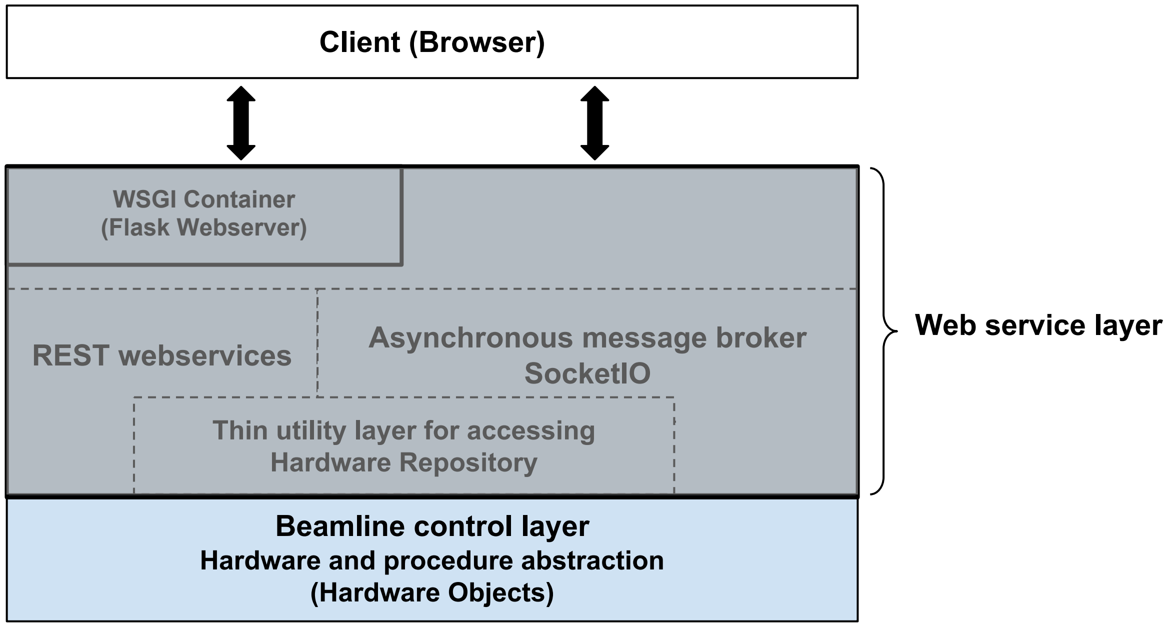
React
Redux

node JS

Flask
web development, one drop at a time

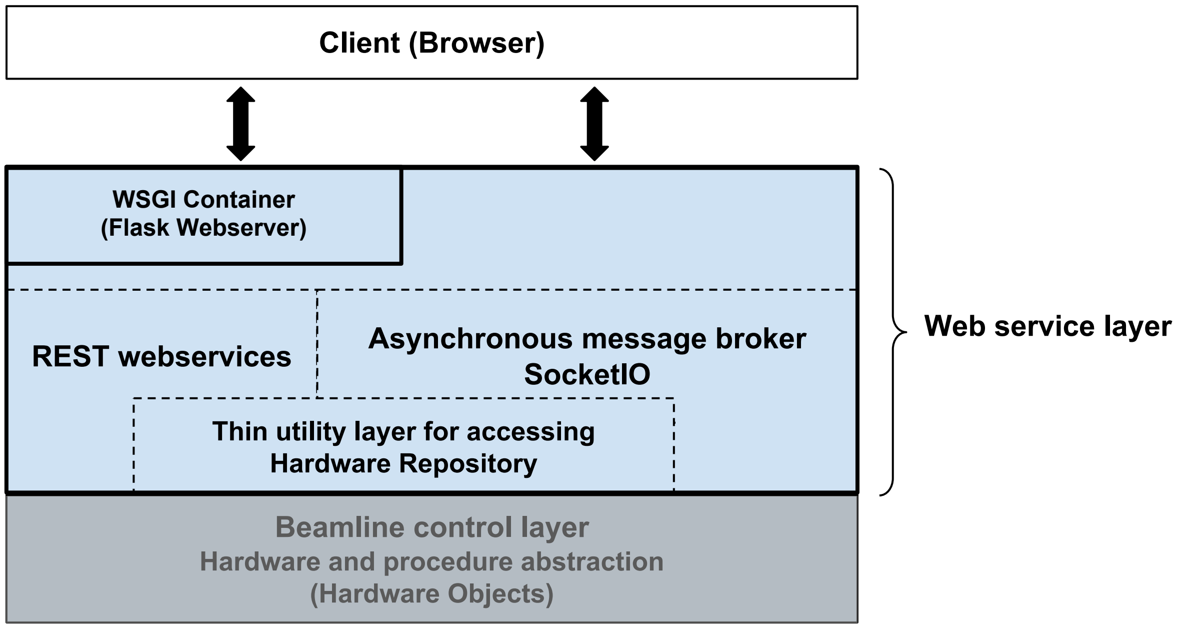
Websockets

Backend


Client (Browser)
WSGI Container (Flask Webserver)
REST webservices
Asynchronous message broker SocketIO
Thin utility layer for accessing Hardware Repository
Web service layer
Beamline control layer
Hardware and procedure abstraction
(Hardware Objects)

- 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**

Web Service Layer


Client (Browser)
WSGI Container (Flask Webserver)
REST webservices
Asynchronous message broker SocketIO
Thin utility layer for accessing Hardware Repository
Web service layer
Beamline control layer
Hardware and procedure abstraction
(Hardware Objects)

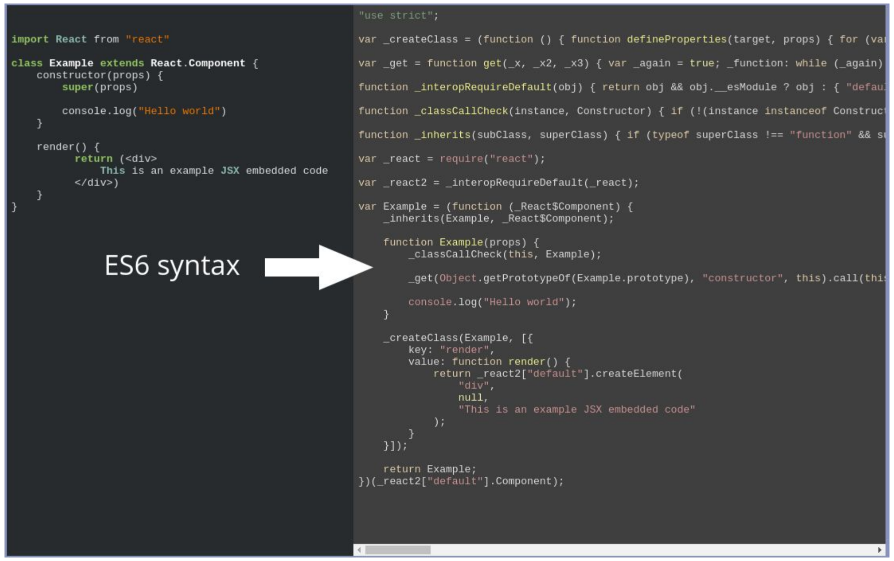
- **Defines an API** for clients to access the HardwareObjects, and relays events between Hardware Objects and clients **(not necessarily a browsers)**
- Thin utility layer for providing new **functionality exclusive to MXCuBE 3** and ease access to Hardware Objects
- Websockets, via SocketIO, **used 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 is a JavaScript compiler.
Use next generation JavaScript, today.

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



```
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>)
    }
}
```

ES6 syntax

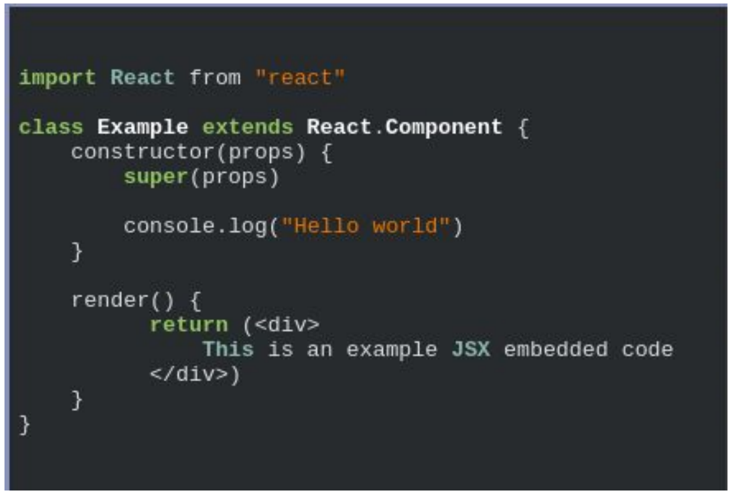
```
"use strict";

var _createClass = (function () { function defineProperties(target, props) { for (va

var _get = function get(_x, _x2, _x3) { var _again = true; _function: while (_again)

function _interopRequireDefault(obj) { return obj && obj.__esModule ? obj : { "defau

function _classCallCheck(instance, Constructor) { if (!(instance instanceof Construc

function _inherits(subClass, superClass) { if (typeof superClass !== "function" && s

var _react = require("react");

var _react2 = _interopRequireDefault(_react);

var Example = (function (_React$Component) {
    _inherits(Example, _React$Component);

    function Example(props) {
        _classCallCheck(this, Example);

        _get(Object.getPrototypeOf(Example.prototype), "constructor", this).call(thi

        console.log("Hello world");
    }

    _createClass(Example, [{
        key: "render",
        value: function render() {
            return _react2["default"].createElement(
                "div",
                null,
                "This is an example JSX embedded code"
            );
        }
    }]);

    return Example;
})(_react2["default"].Component);
```

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

Frontend development - React and Redux

React https://facebook.github.io/react/

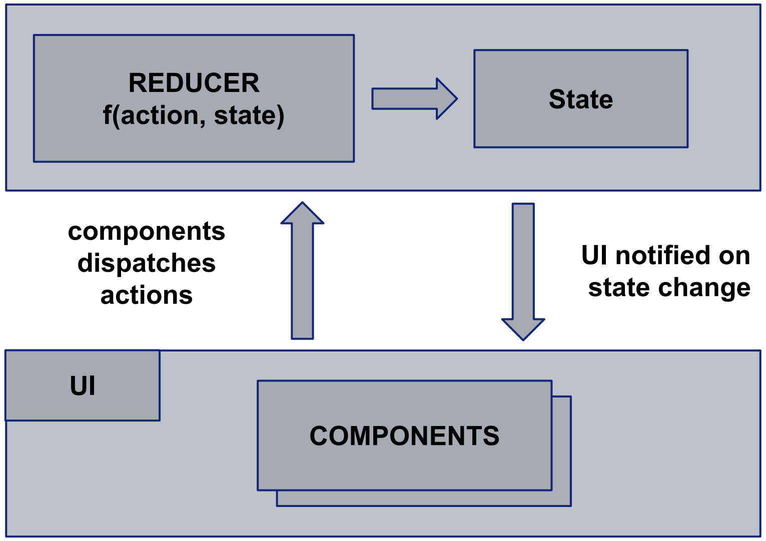
- React is a library for creating user interfaces
- React makes it possible to use widgets like in traditional UI development
- Provides a way to express the UI in a markup language called JSX
- Can be used with state management library, in order to avoid per widget state



```
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>)
    }
}
```

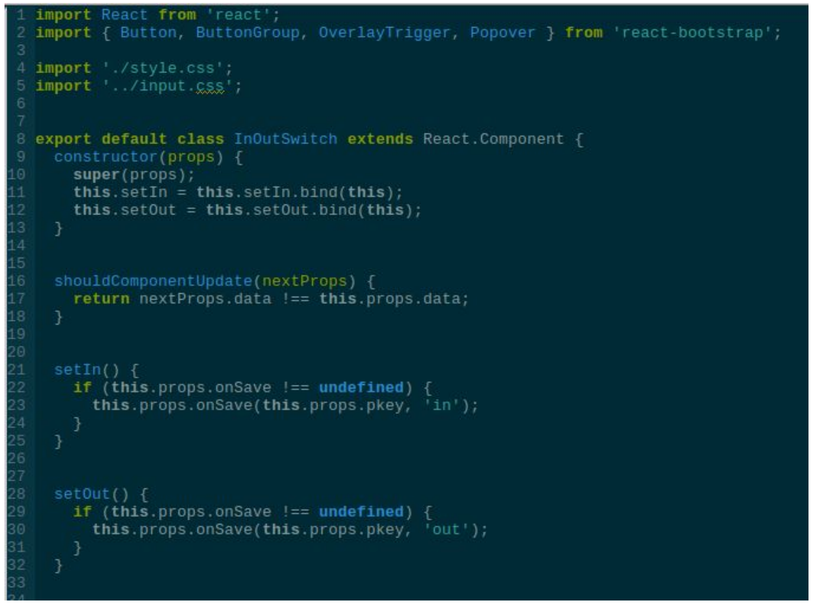
Frontend development - React and Redux

Redux http://redux.js.org/

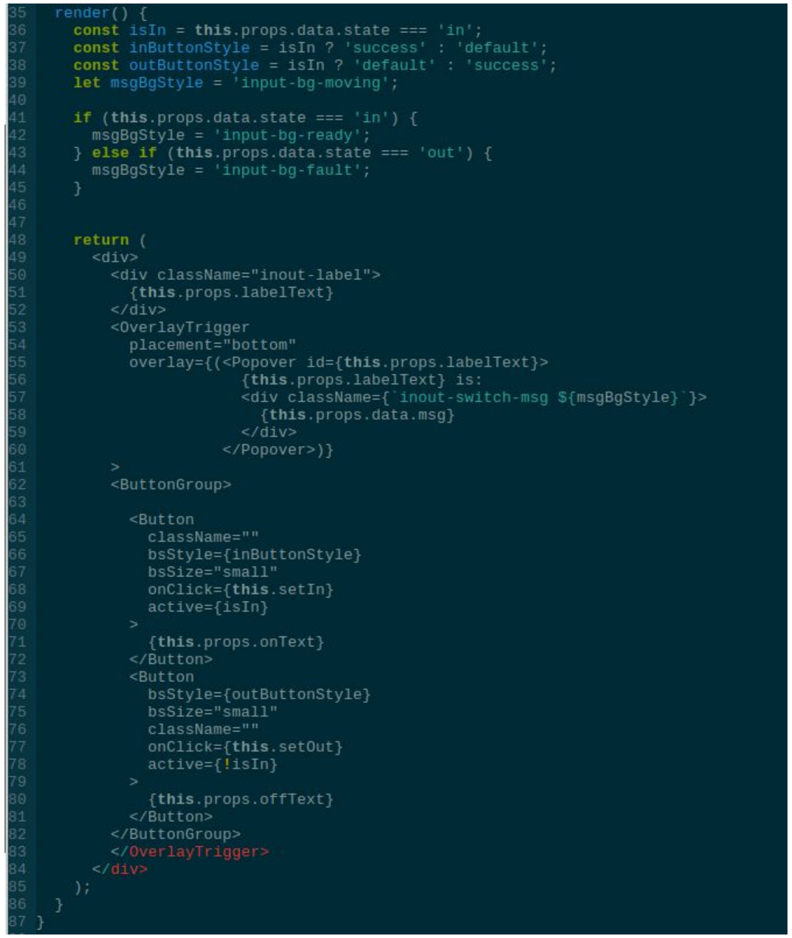


- Application wide state, only source of data for components.
- The redux store is an immutable data structure and can only be updated (replaced) by a pure function, a reducer
- The reducer function is called by dispatching an action for instance when user interacts with UI
- Provides data flow which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

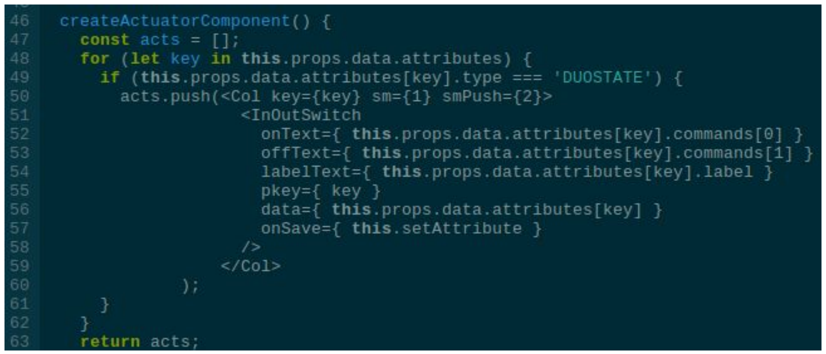
Frontend development - React and Redux



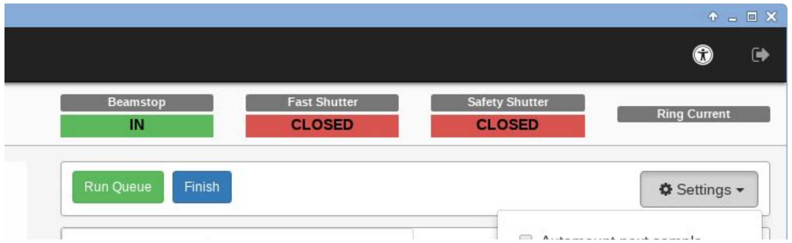
```
import React from 'react';
import { Button, ButtonGroup, OverlayTrigger, Popover } from 'react-bootstrap';

import './style.css';
import '../input.css';


export default class InOutSwitch extends React.Component {
  constructor(props) {
    super(props);
    this.setIn = this.setIn.bind(this);
    this.setOut = this.setOut.bind(this);
  }


  shouldComponentUpdate(nextProps) {
    return nextProps.data !== this.props.data;
  }


  setIn() {
    if (this.props.onSave !== undefined) {
      this.props.onSave(this.props.pkey, 'in');
    }
  }


  setOut() {
    if (this.props.onSave !== undefined) {
      this.props.onSave(this.props.pkey, 'out');
    }
  }

```



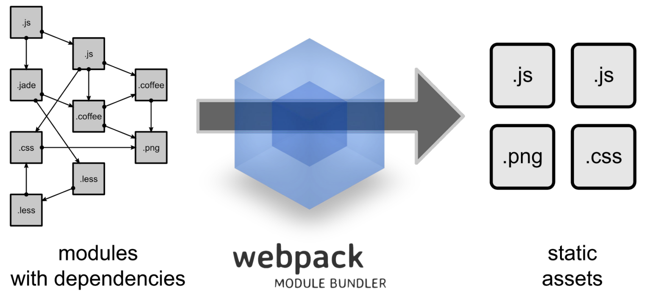
```
  render() {
    const isIn = this.props.data.state === 'in';
    const inButtonStyle = isIn ? 'success' : 'default';
    const outButtonStyle = isIn ? 'default' : 'success';
    let msgBgStyle = 'input-bg-moving';

    if (this.props.data.state === 'in') {
      msgBgStyle = 'input-bg-ready';
    } else if (this.props.data.state === 'out') {
      msgBgStyle = 'input-bg-fault';
    }


    return (
      <div>
        <div className="inout-label">
          {this.props.labelText}
        </div>
        <OverlayTrigger
          placement="bottom"
          overlay={(<Popover id={this.props.labelText}>
                      {this.props.labelText} is:
                      <div className={`inout-switch-msg ${msgBgStyle}`}>
                        {this.props.data.msg}
                      </div>
                    </Popover>)}
        >
        <ButtonGroup>

          <Button
            className=""
            bsStyle={inButtonStyle}
            bsSize="small"
            onClick={this.setIn}
            active={isIn}
          >
            {this.props.onText}
          </Button>
          <Button
            bsStyle={outButtonStyle}
            bsSize="small"
            className=""
            onClick={this.setOut}
            active={!isIn}
          >
            {this.props.offText}
          </Button>
        </ButtonGroup>
        </OverlayTrigger>
      </div>
    );
  }
}
```



```
  createActuatorComponent() {
    const acts = [];
    for (let key in this.props.data.attributes) {
      if (this.props.data.attributes[key].type === 'DUOSTATE') {
        acts.push(<Col key={key} sm={1} smPush={2}>
                      <InOutSwitch
                        onText={ this.props.data.attributes[key].commands[0] }
                        offText={ this.props.data.attributes[key].commands[1] }
                        labelText={ this.props.data.attributes[key].label }
                        pkey={ key }
                        data={ this.props.data.attributes[key] }
                        onSave={ this.setAttribute }
                      />
                    </Col>
                );
      }
    }
    return acts;
```



Frontend development - Webpack



- 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.

webpack
webpack Dev Server

- Provides a development server with “hot reloading” (changes are automatically built and app updated)

- Runtime for Javascript development provided by node.js