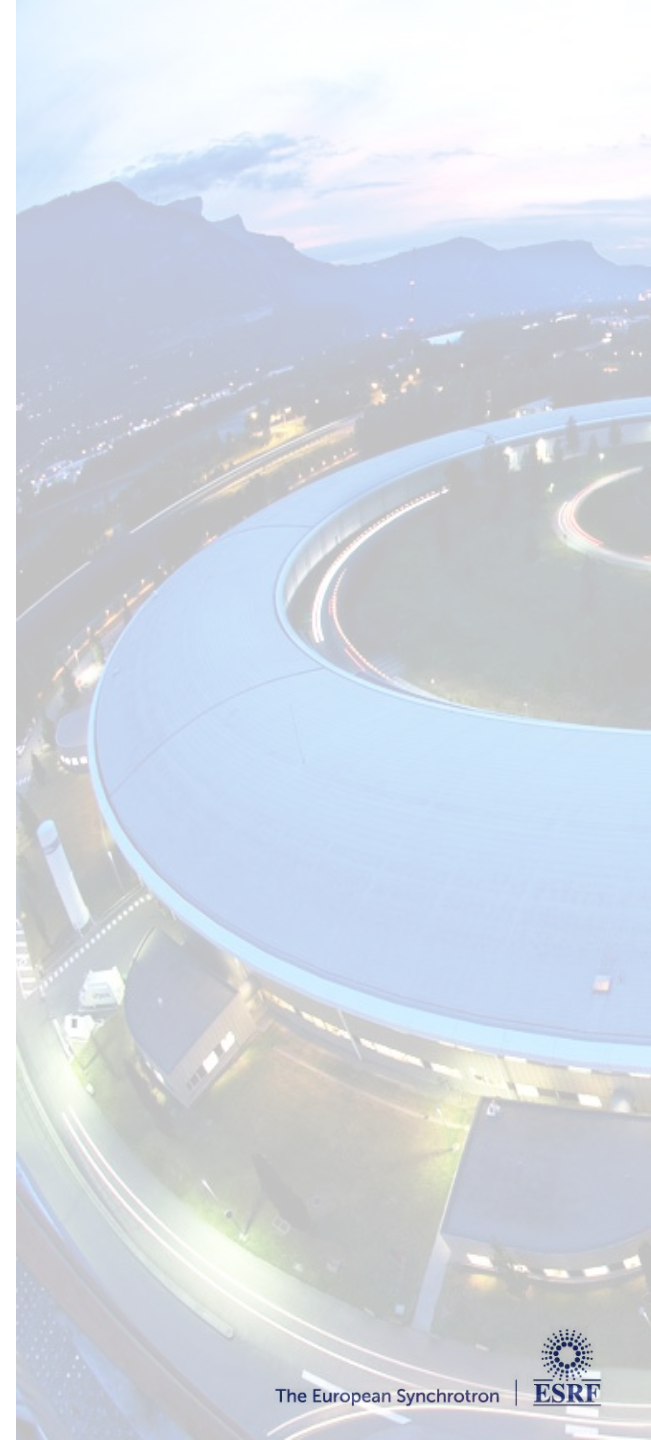




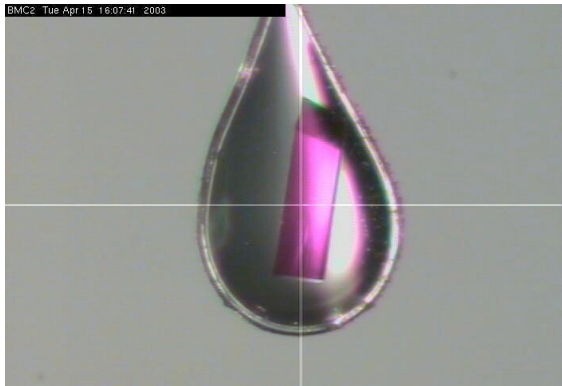
Bringing MX experiments to the web

MXCuBE 3

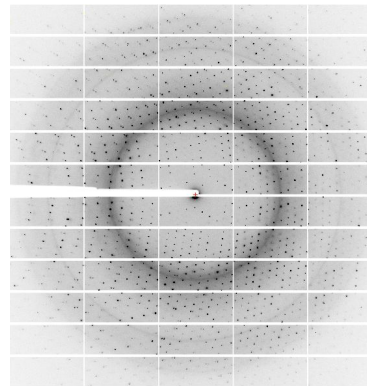
- **An MX Beamline at glance**
- **Project background**
- **Backend, beamline control layer**
- **Web service layer**
- **Frontend Development**
- **Screenshots**



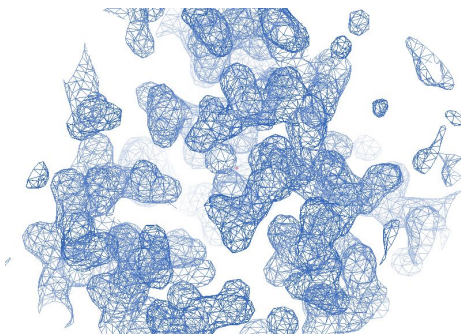
- Aim is to resolve **protein structure**



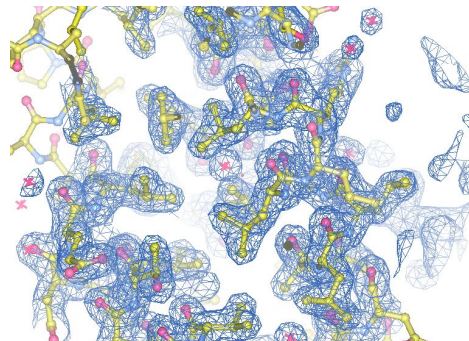
An X-ray beam is focused on a **crystal**



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

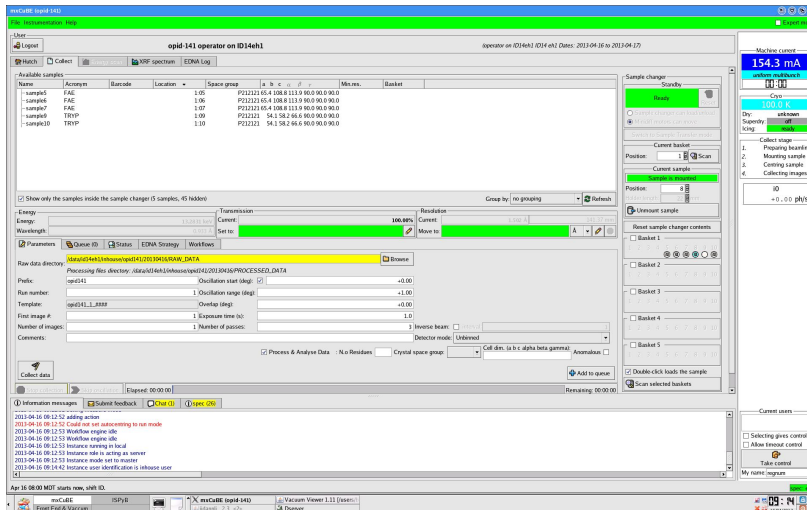


MX-Beamline

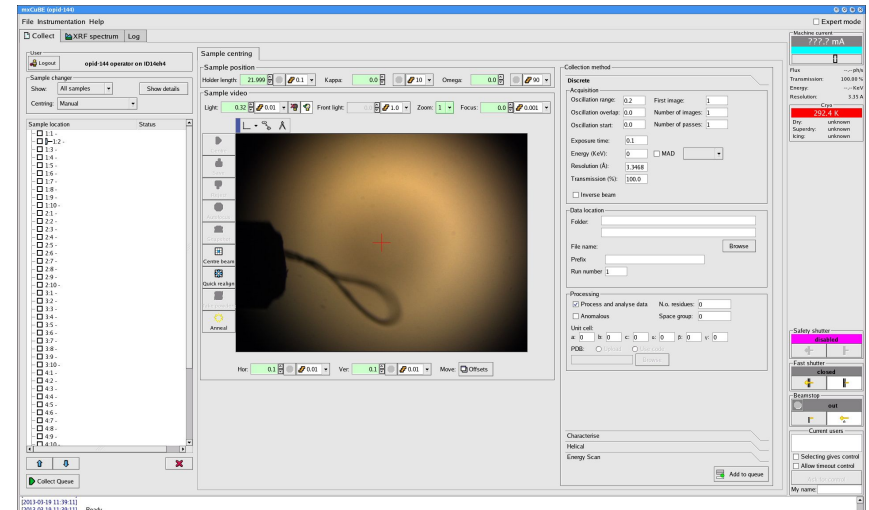
- 2D - Detector
- Diffractometer
- Sample changer
- And various other instruments
 - Monochromator
 - Mirrors
 - Filters
 - Aperture
 - ...

MXCuBE is the application used for instrument control and data acquisition

Project history and background



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

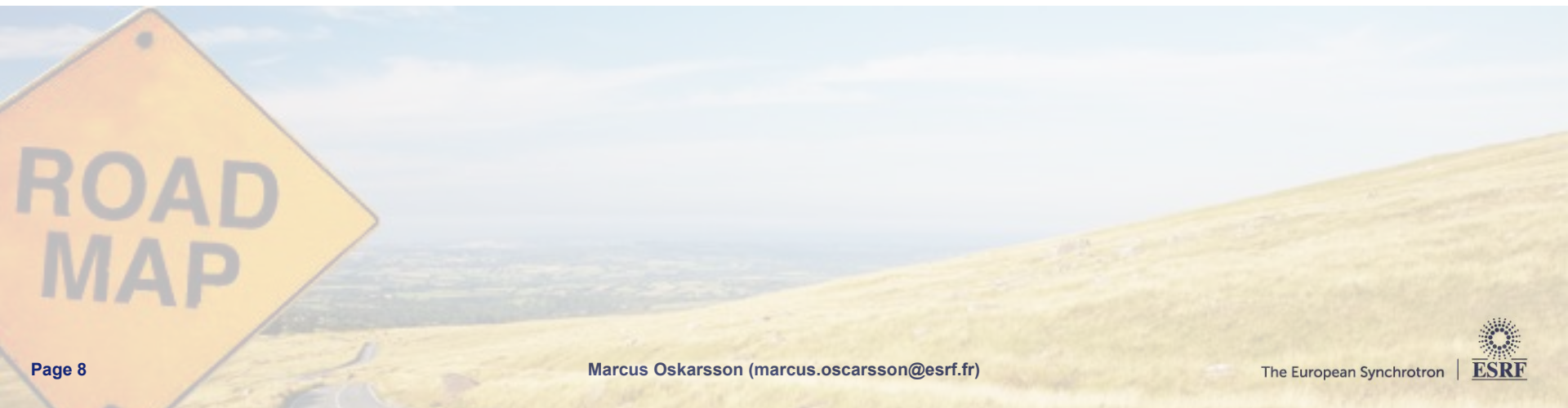
UI gets less user friendly as new functionality is added

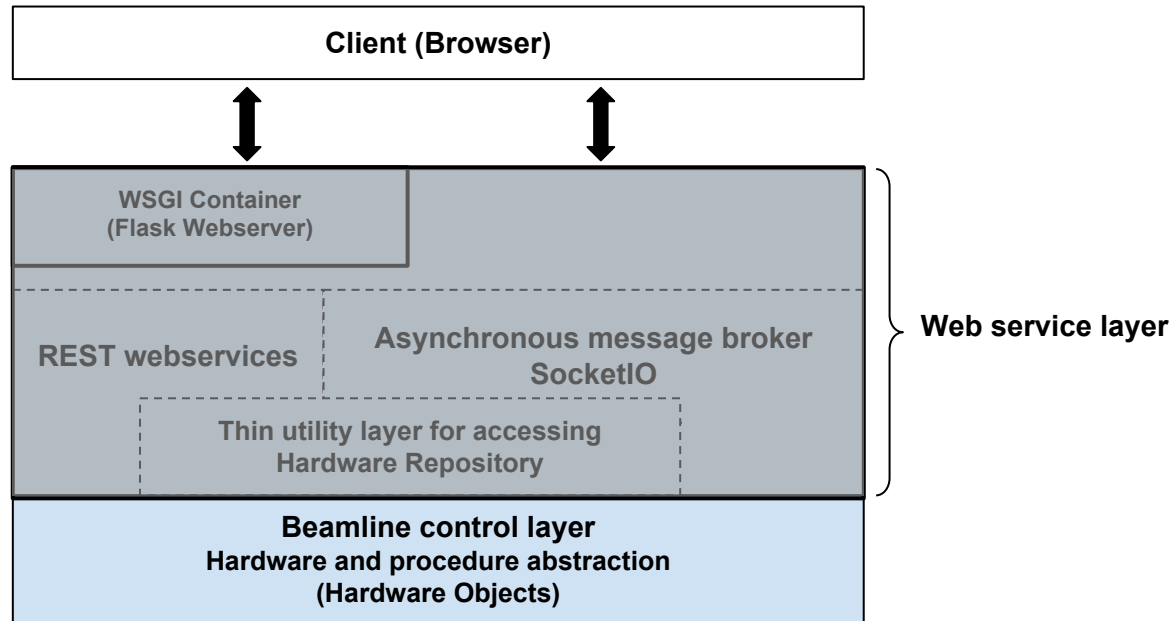
At the same time software industry also evolves

New software needed, decision made to implement MXCuBE as a Web Application

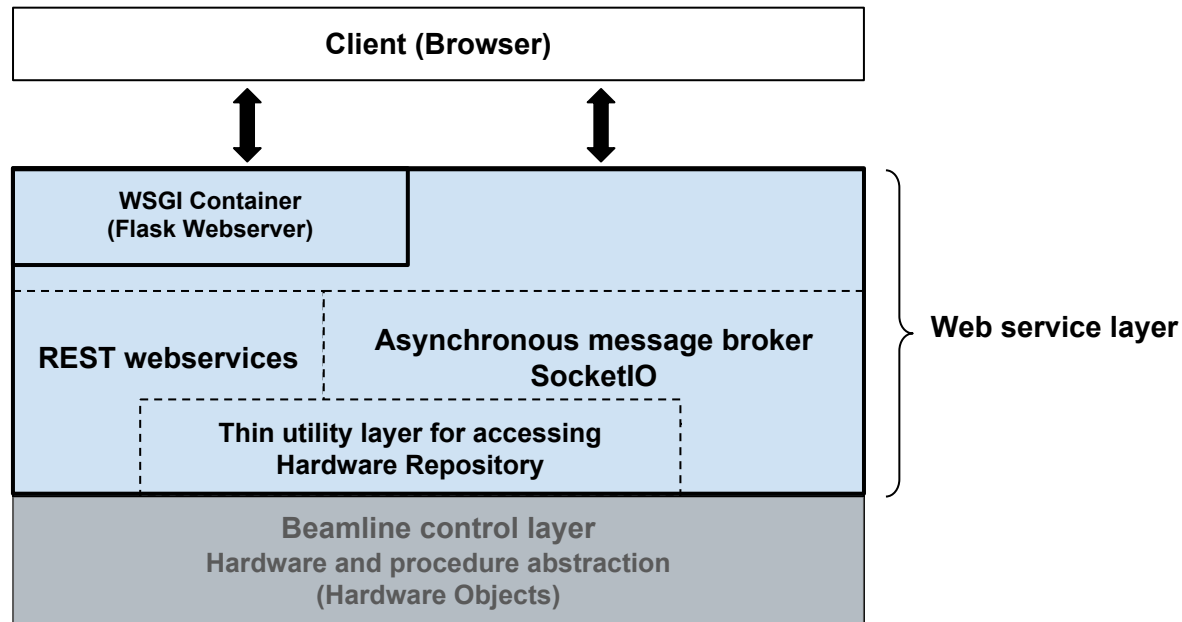
- Better remote access performance
- Keeping up with new instrument capabilities
- Improved user experience
- Easing the maintenance and client install

- MXCuBE 3 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 Eguraun 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**

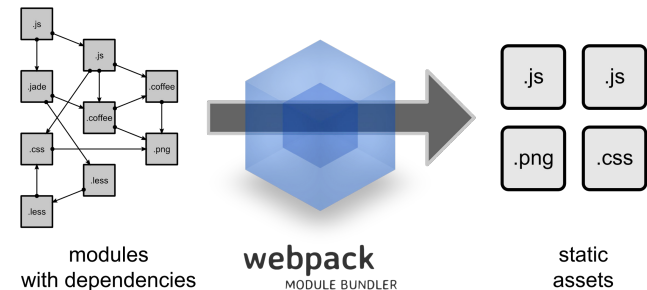
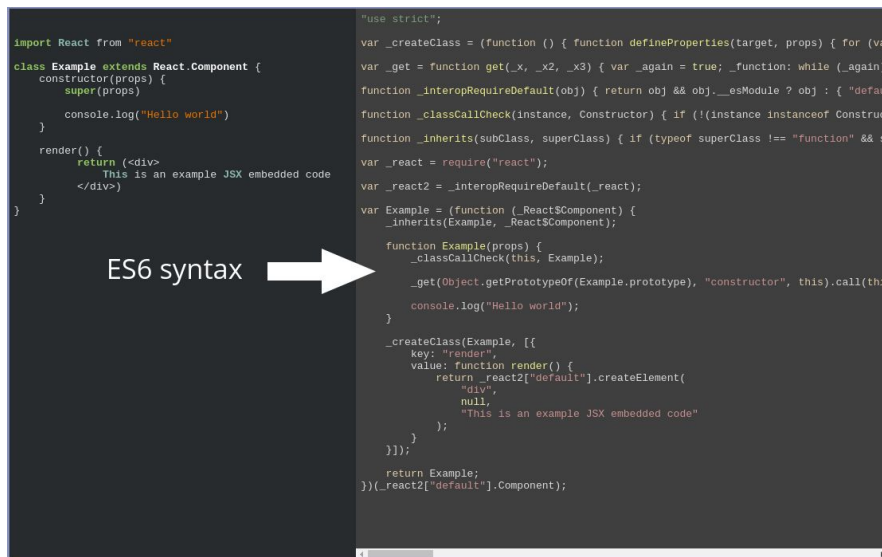


- **Defines an API** for clients to access the HardwareObjects, and relays events between Hardware Objects and clients (**not necessarily a browsers**)
- Thin utility layer for providing new **functionality exclusive to MXCuBE 3** and ease access to Hardware Objects
- Websockets, via SocketIO, **used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



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

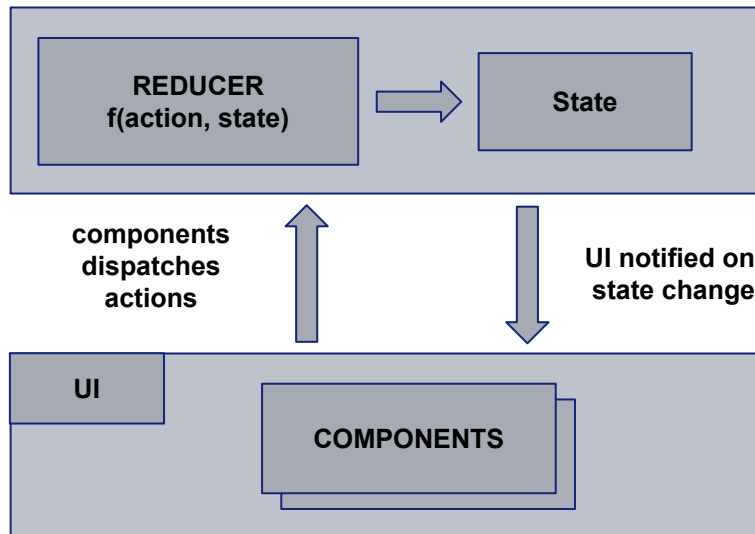
- React is a library for creating user interfaces
- React makes it possible to use widgets like in traditional UI development
- Provides a way to express the UI in a markup language called JSX
- Can be used with state management library, in order to avoid per widget state

```
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>)
  }
}
```



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

Screenshots - Data Collection

The screenshot displays the MXCuBE-3 Data Collection interface. The top navigation bar includes 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. The 'Data collection' tab is active, showing various control panels and a central live image.

Beamline Actions: Beamstop (IN), Fast Shutter (CLOSED), Safety Shutter (OPEN).

Parameters: Energy: 11.5628 keV, Wavelength: 1.0723 Å, Resolution: 1.240 Å, Detector: 169.594 mm, Transmission: 26.01 %, Flux: 1.74e+12, Cryo: 0 K, Ring Current: 193.4 mA.

Phase Control: Omega: 180.00, Kappa: 0.00, Phi: 0.00, Y: -2.27, Z: -0.13, Focus: 0.00, Samp-X: 1.08, Samp-Y: 0.79.

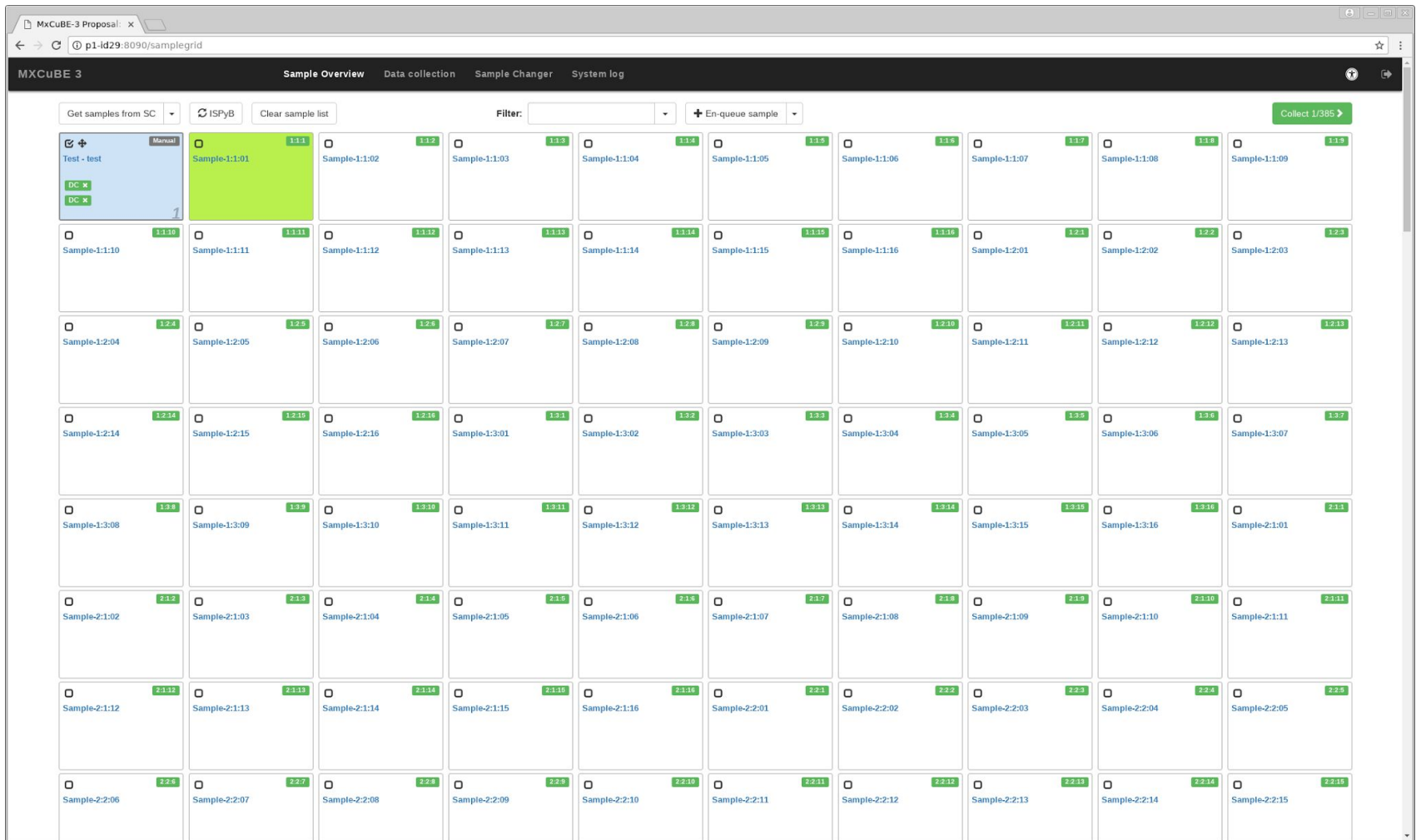
Central Image: A live X-ray image of a sample with a grid overlay. The grid is labeled 'G1' and shows a 10x10 grid of points. The grid is centered on the sample, and the spacing between points is 0.00 mm.

Right Panel: Sample: Sample-1:1:01 (). Upcoming (0). P1 Characterisation: 100 %. Path: ref-opid291_1_###.cbf. Table with columns: Start, Osc., t (ms), # Img, T (%), Res. (Å), E (KeV), φ°, κ°. Data Collection: G1 X-ray Centring: 100 %.

Start	Osc.	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ°	κ°
360	1	0.037	4	100	1.5	11.5628	0	0

Data collection view, for interactive data collection and sample alignment

Screenshots - Sample overview



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**

Questions ?



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