MXCuBE3

The European Synchrotron | ESRF

Macromolecular Crystallography Beamline Costumized Beamline Environment

- The first version was deployed at the ESRF in 2005
- Soon after followed by installation/adaptation to other soon-to-be partners
- In 2012 the collaboration is established between

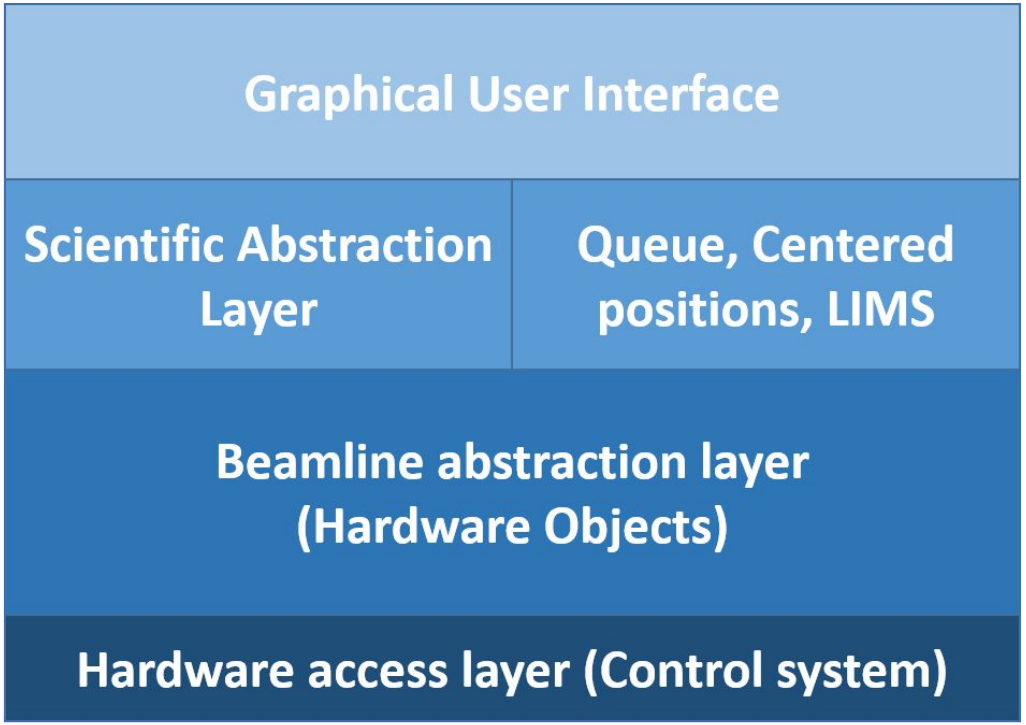
- In 2013 the deployment of **MXCuBE2** at ESRF and soon after at the other sites
- In 2014 two new partners join the collaboration

- In 2016 MAXIV and ESRF start working on the new GUI **MXCuBE3**

- In 2018 **MXCuBE3** is being deployed
- Two new partners are in the process of joining the collaboration

- MXCuBE2 introduced a decoupling of interface and an abstraction layer to boost collaboration

- A GUI independent of the control system
  - Data collection methods, on sample tools (points, grid, lines) and a door for external descriptors
  - An abstraction layer to ease compatibility and deployment at any site



MXCuBE2 was esplicitely designed for:

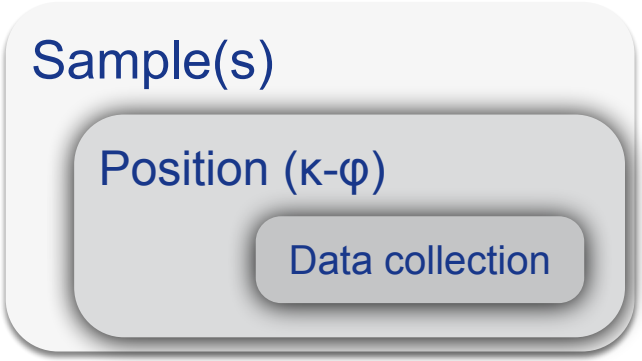
- High-throughput data collection
- Hands-off data collection
- Perform more elaborated data collection for complex experiments

- Adaptable to any hardware environment
- Scalable with time

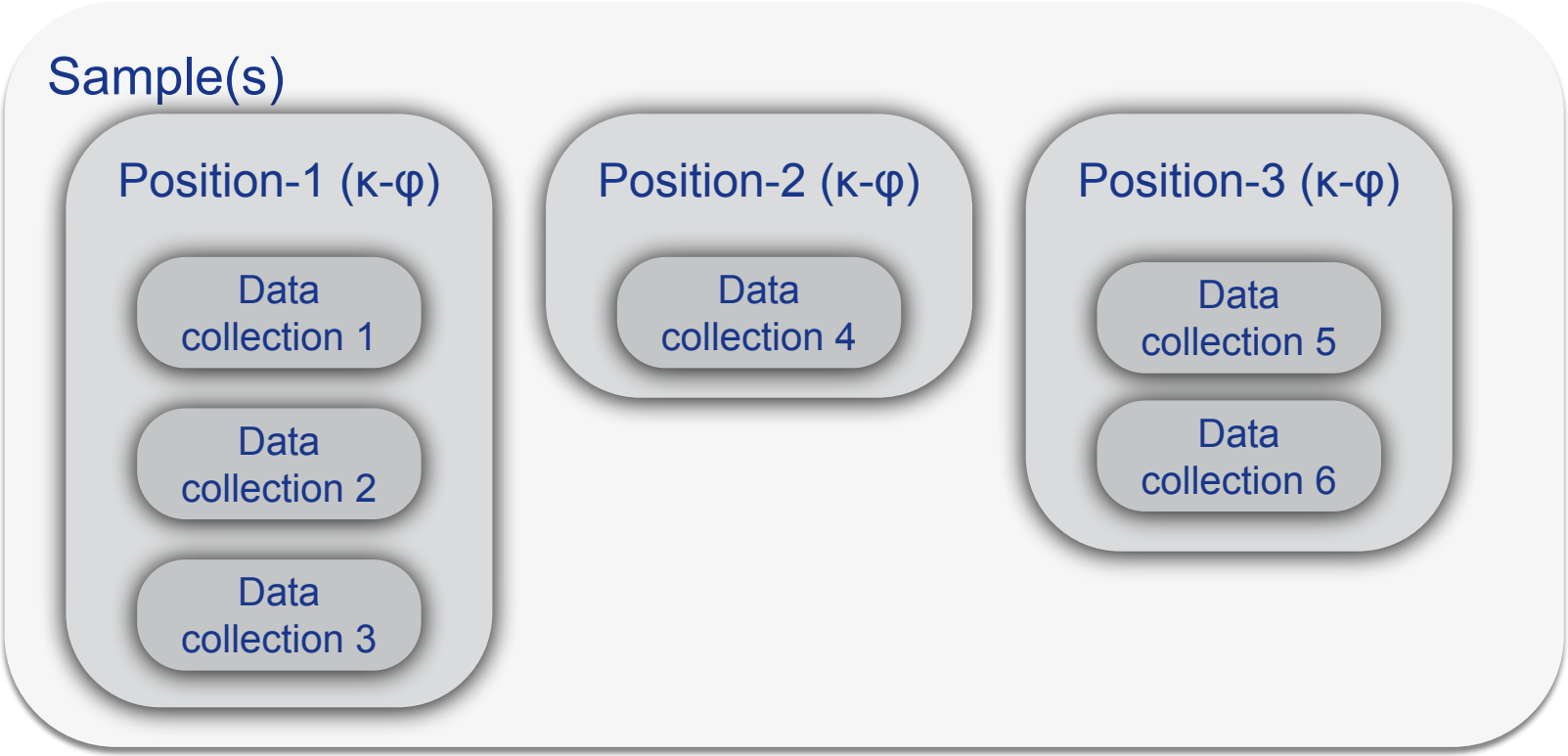
- But the MXCuBE collaboration eventually became not just MXCuBE

- But it stimulates and facilitates collaboration and sharing on EDNA, Workflows, Device servers (CATS), kappa goniometers, automatic centring libraries, autoprocessing pipelines, …

THE MXCUBE2 CONCEPT



- MXCuBE2 works by sample:position:data collection
- Any arbitrary combination is possible



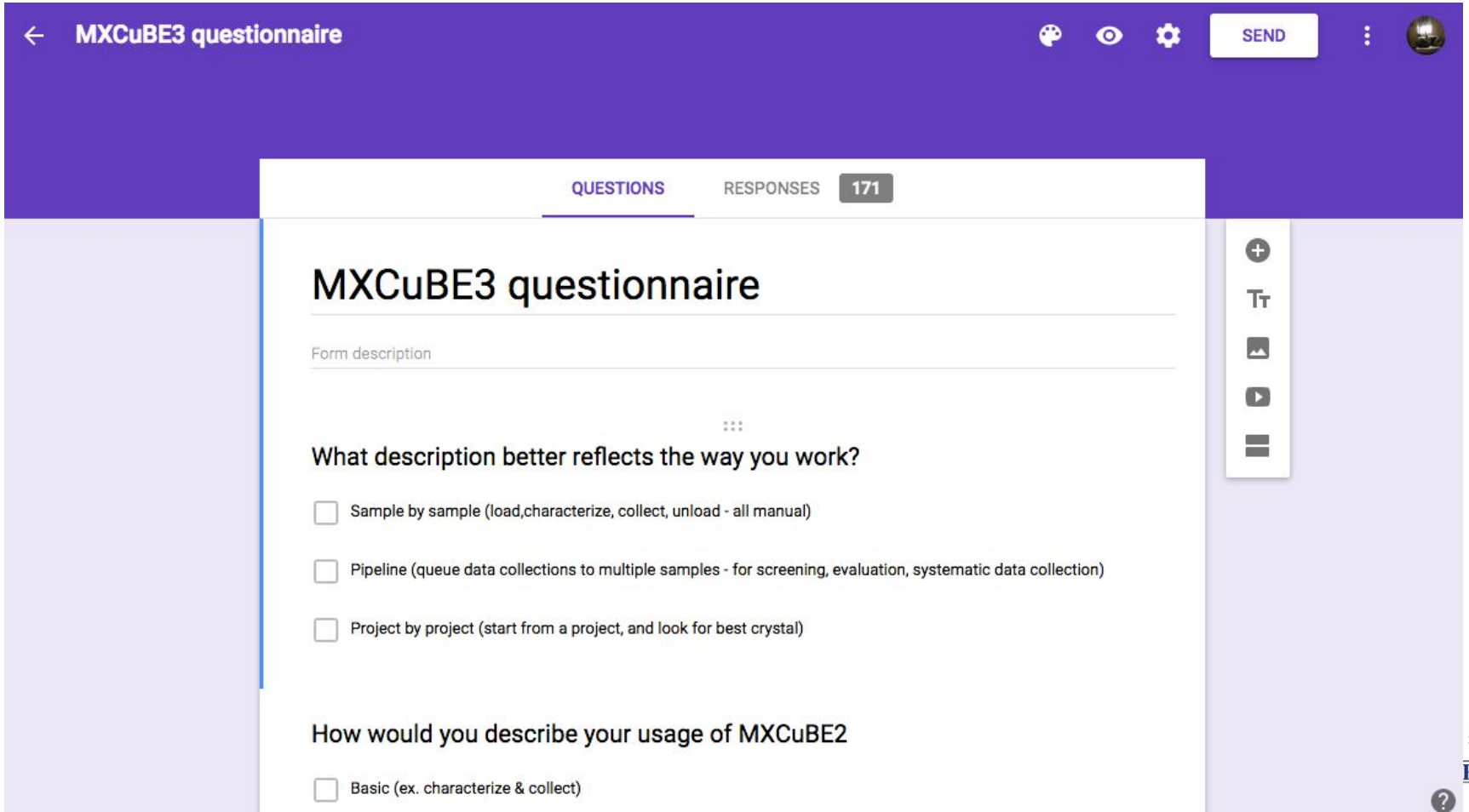
BUT IN THE MEANTIME

- Sample changers got larger capacity
- Data collection got faster and faster
- And experiment sessions shorter
- More demand for Remote Access
- Synergy with LIMS got stronger
- Novel data collection methods need to be implemented

- In other words: MXCuBE2 GUI had to be improved and evolve!

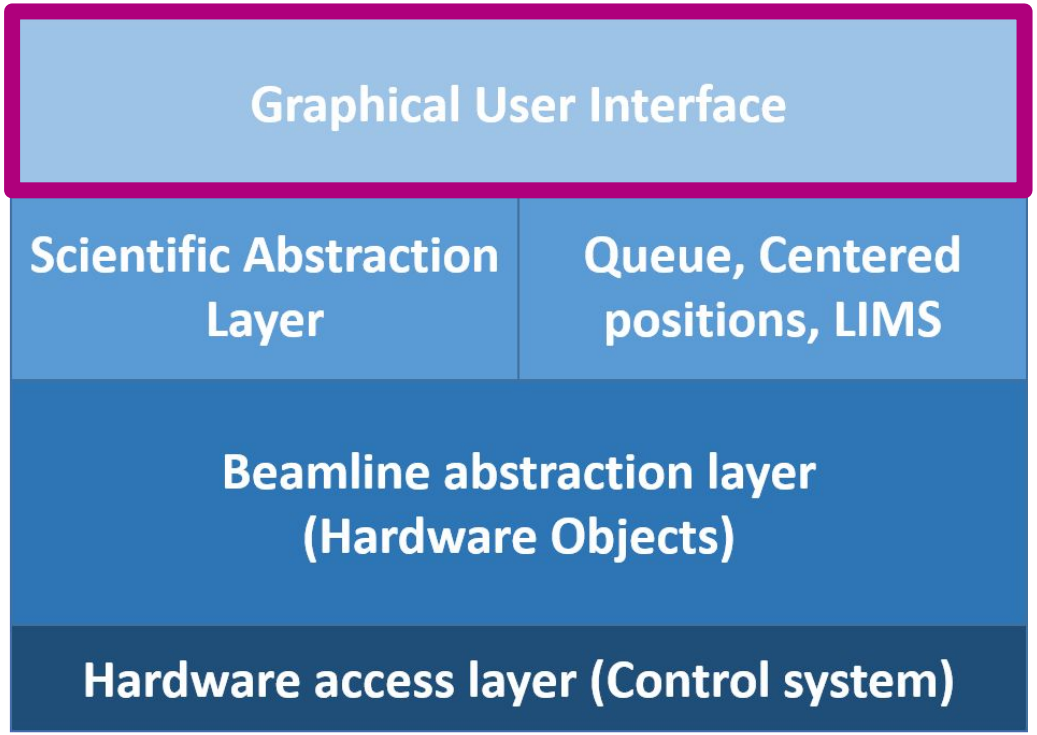
MXCUBE3 SURVEY

- We prepared a survey for the user community to understand (or confirm)
- What users like of MXCuBE2, and what they would improve
- What are their working protocols
- And use the outcome as inspiration for a new GUI



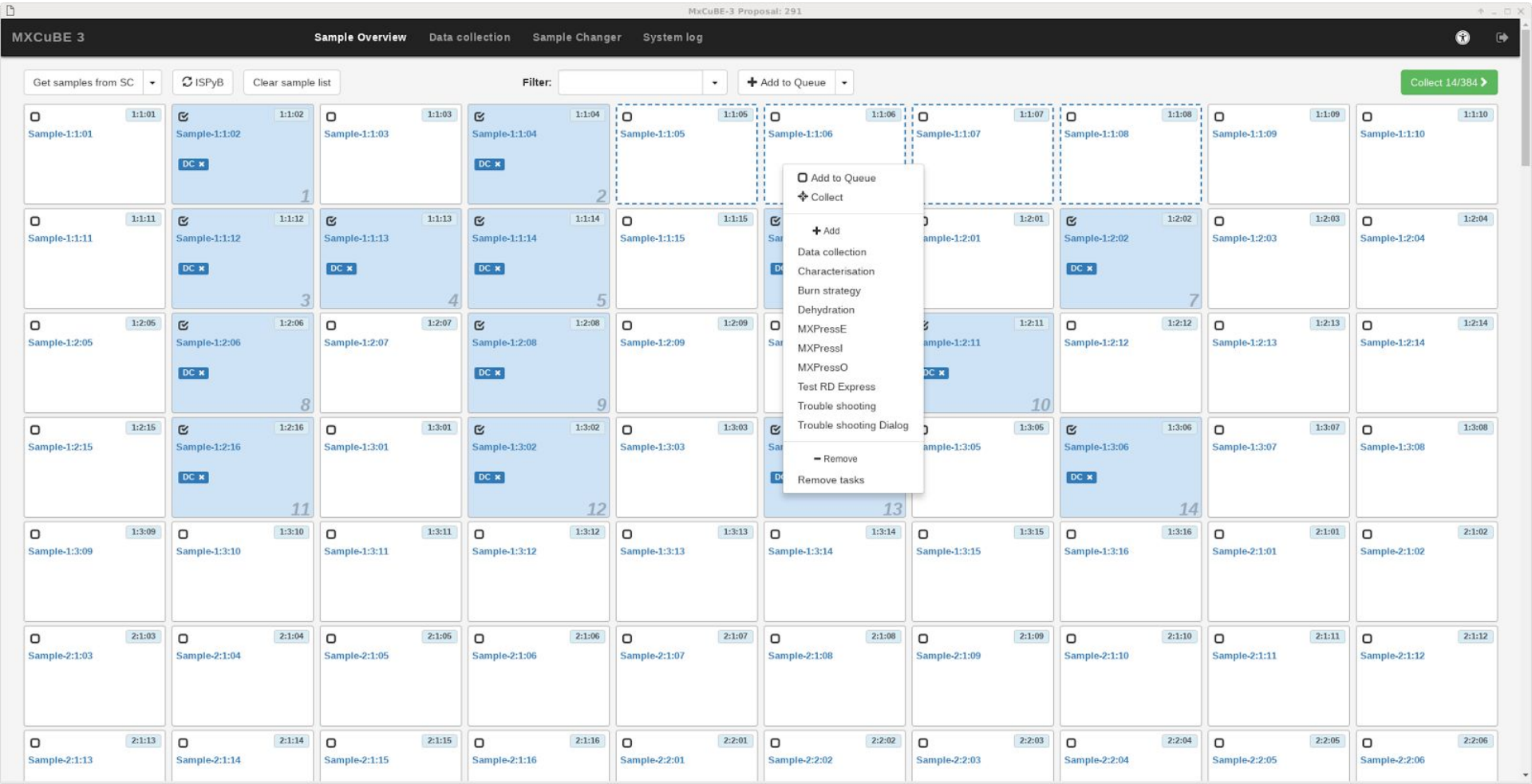
- In close collaboration with MAXIV we started the MXCuBE3 project
- Design a new GUI, with minimal adaptation to the other parts
- This ensures back-compatibility and facilitates transition to the new interface to every partners

- Qt3 was becoming obsolete
- Design the new interface in web technology: MXCuBE3 as a web app!

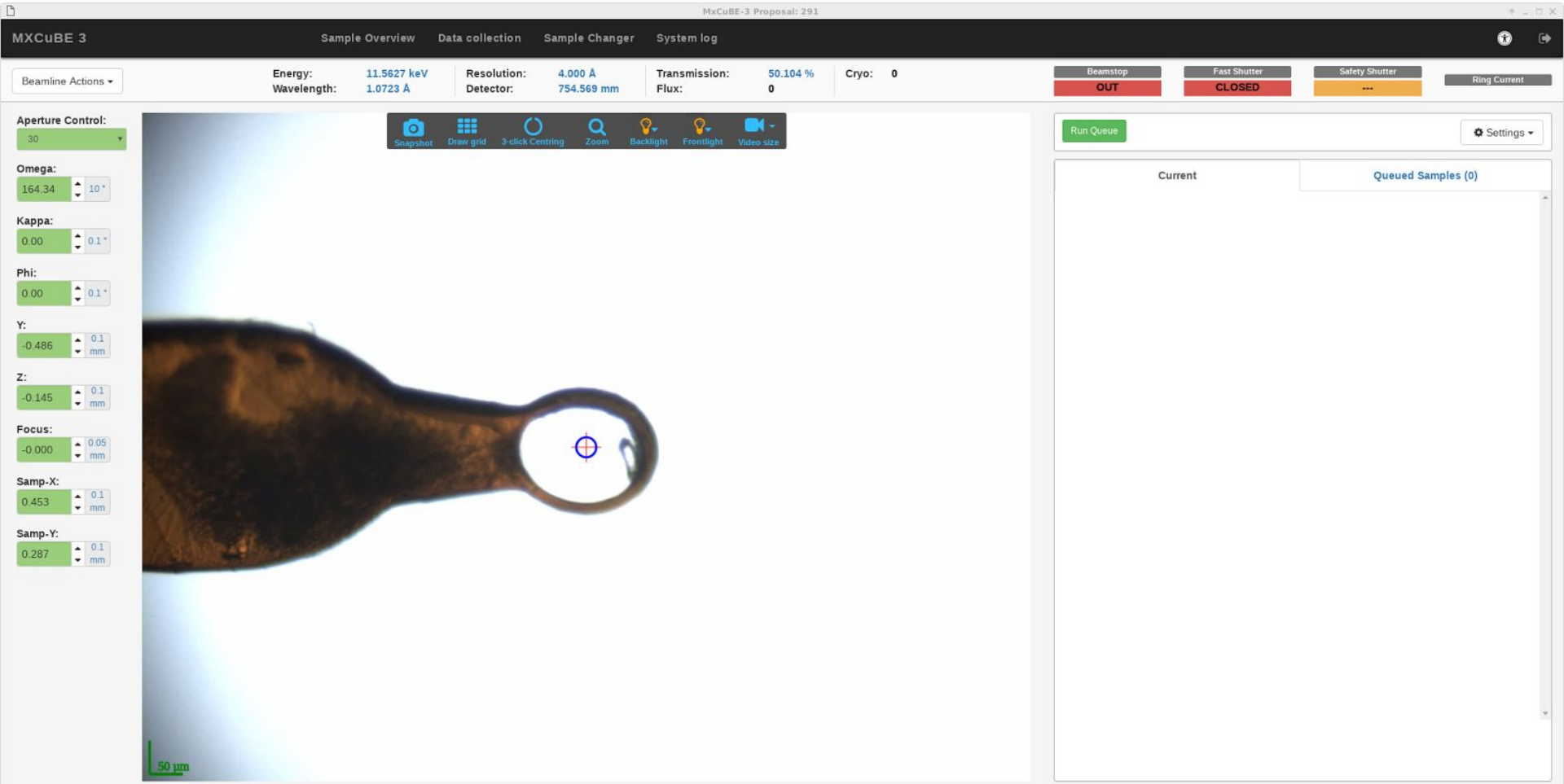


- The advantages of a web application:
- Remote by design
- No need to install extra software but a recent browser
- Large developer community
- Use of modern Library developed and maintained by large IT companies
- Faster to modify, test, maintain
- See Marcus' talk for technical details

- An overview on all the projects present in the sample changer robot, with smart filtering and sorting
- Synchronized with ISPyB

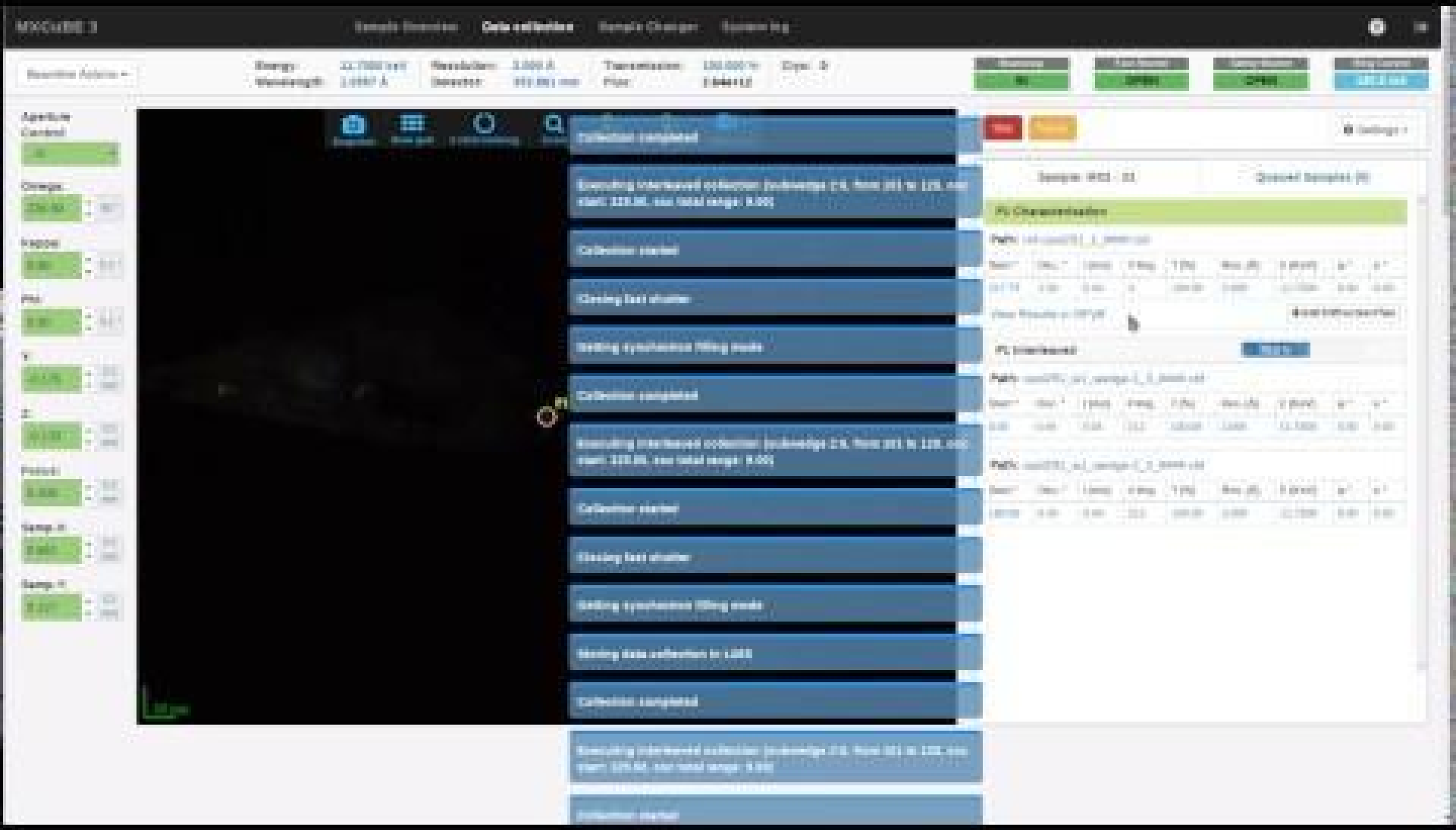


- A Data collection view, with interactive operation on the crystal
- Only pertinent options presented to users (if a mesh only mesh data collection types, if a line helical data collections are proposed, etc)

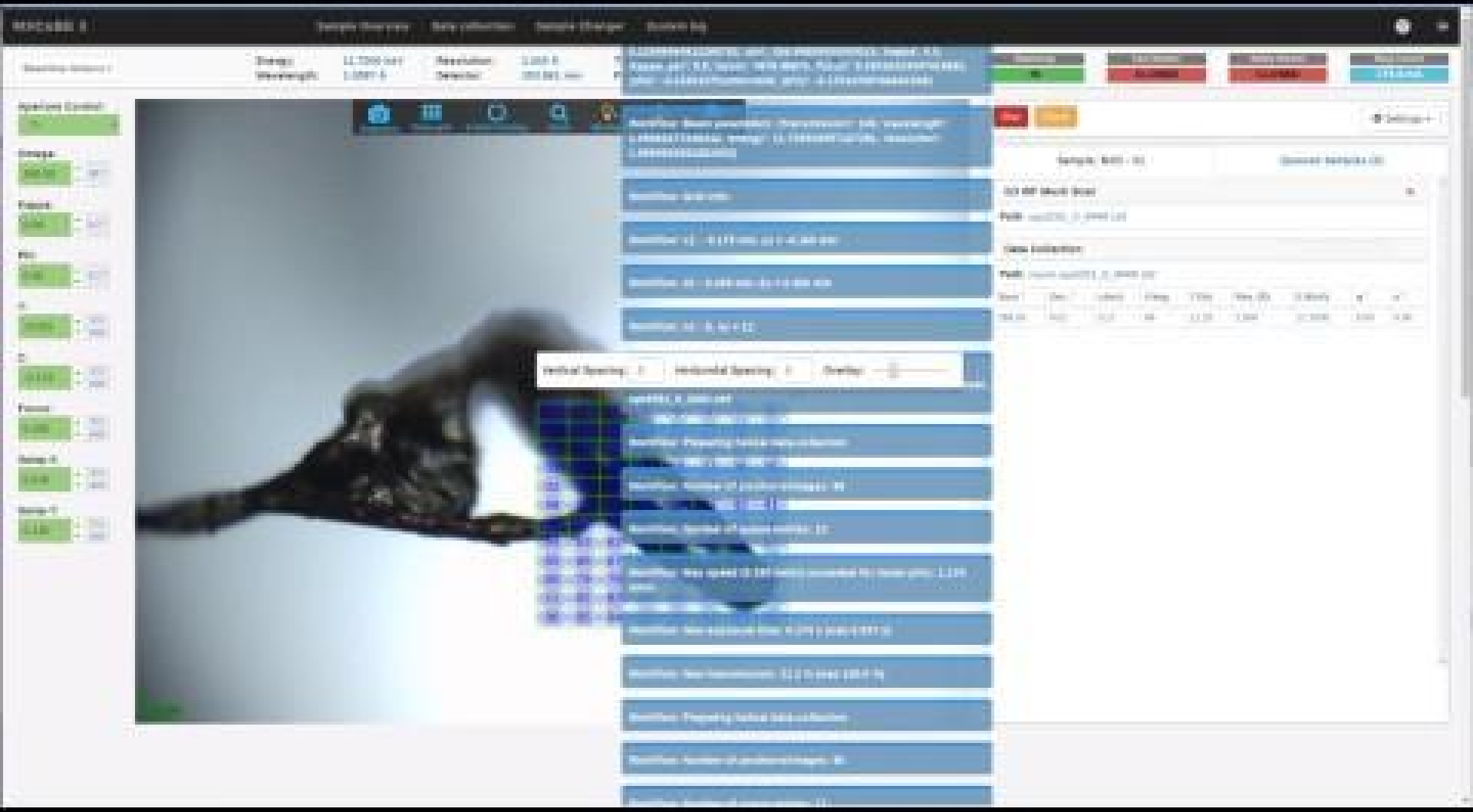


General

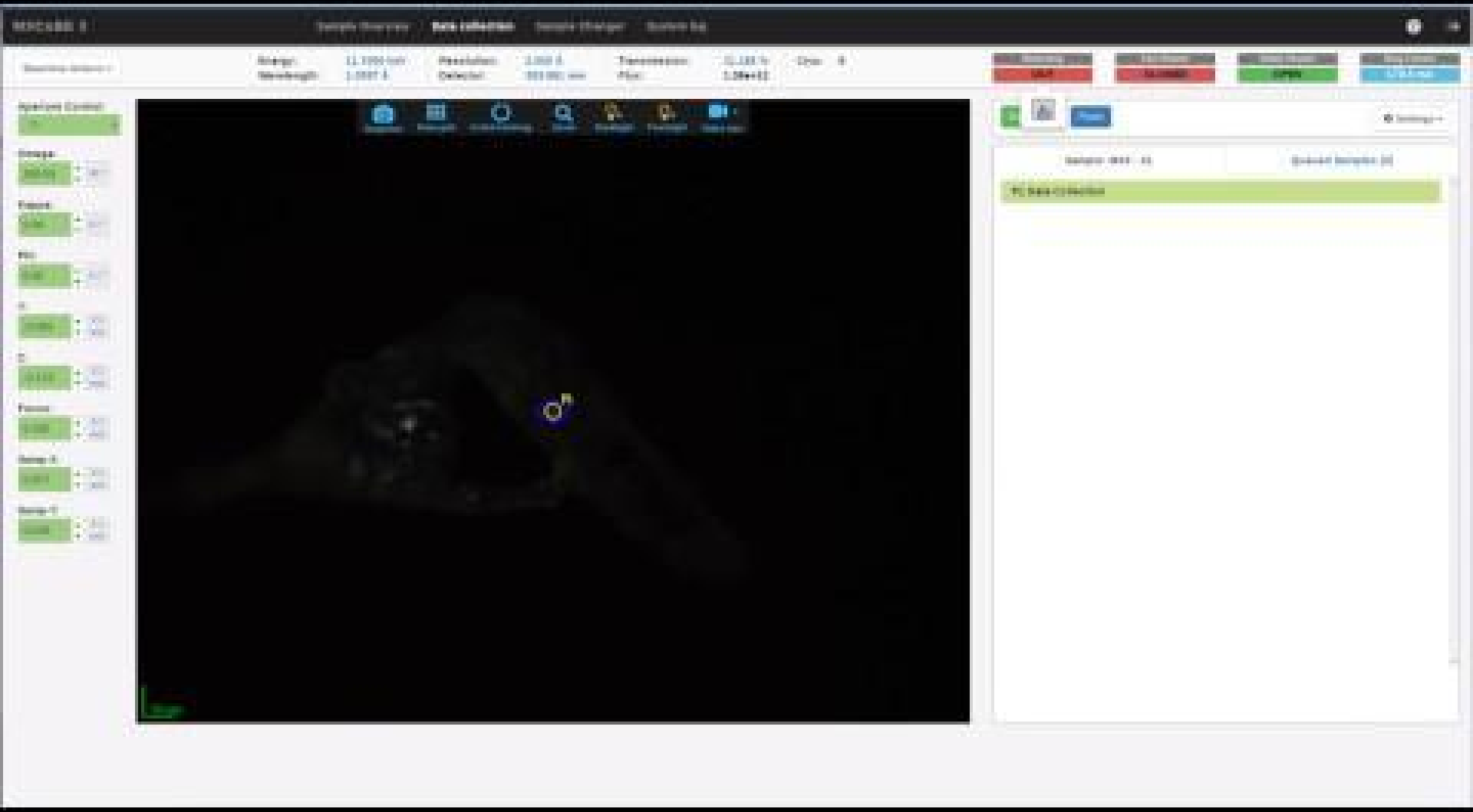
Interleave

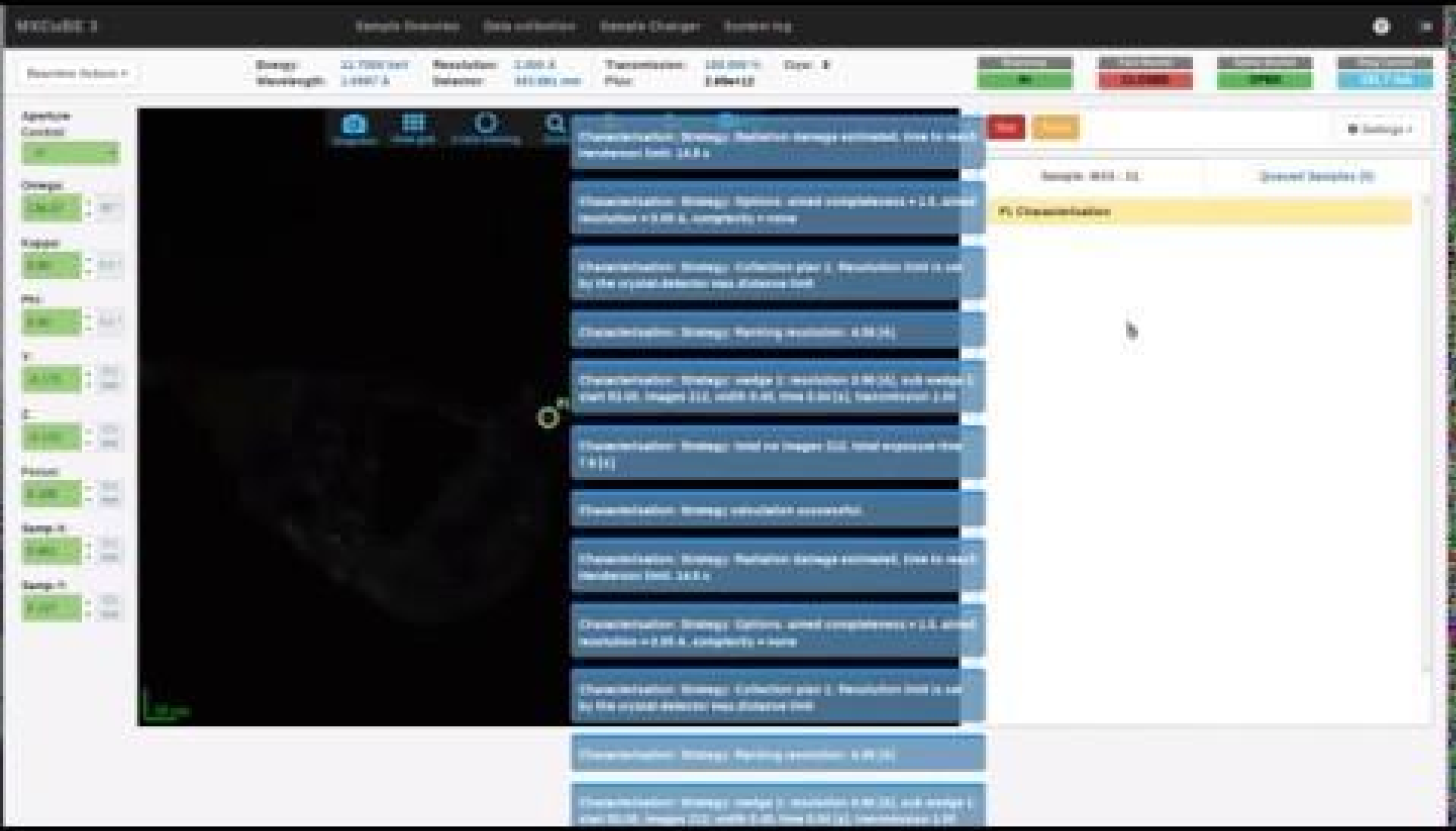


Mesh



Miscellanea




MXCuBE 3
Sample Centring
Data collection
Sample Changer
Energy:
Wavelength:
Resolution:
Detector:
Transmission:
Flux:
Characterisation: Strategy: Radiation damage estimated, time to reach resolution limit: 14.8 s
Characterisation: Strategy: Options: aimed completeness = 1.0, aimed resolution = 0.00 Å, complexity = none
Characterisation: Strategy: Collection plan 1: Resolution limit is set by the crystal-detector max distance limit
Characterisation: Strategy: Ranking resolution: 4.56 (Å)
Characterisation: Strategy: wedge 1: resolution 2.56 (Å), sub wedge 1 start 0.0 (0, images 112, width 0.40, time 0.04 (s), transmission 1.00
Characterisation: Strategy: total no images 112, total exposure time 7.4 (s)
Characterisation: Strategy calculation successful
Characterisation: Strategy: Radiation damage estimated, time to reach resolution limit: 14.8 s
Characterisation: Strategy: Options: aimed completeness = 1.0, aimed resolution = 0.00 Å, complexity = none
Characterisation: Strategy: Collection plan 1: Resolution limit is set by the crystal-detector max distance limit
Characterisation: Strategy: Ranking resolution: 4.56 (Å)
Characterisation: Strategy: wedge 1: resolution 2.56 (Å), sub wedge 1 start 0.0 (0, images 112, width 0.40, time 0.04 (s), transmission 1.00
Sample: 4x4 - 01
Queued Samples (0)
Characterisation

A DUMMY MX3 FOR USER TRAINING

- A docker image is available here

  https://hub.docker.com/r/oscarsso/mxcube3_debian9/
- Install and start docker
- follow the instruction in the page above
- I have tested successfully in windows (where command should be given in powershell), Linux, and others on MacOS

DEPLOYMENT PLAN

- ID29 now
- ID23-2 and MASSIF-1
- ID30B and MASSIF-3
- ID23-1

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- The MXCuBE Collaboration
- The ESRF Structural Biology Group
- The ESRF Beamline Control Unit (M. Oscarsson, M.Guijarro, A.Beteva)
- MAXIV Biomax team