Remote experiments at BioMAX

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Overview

- BioMAX characteristics and status
- Remote access implementation
- MXCuBE3 at BioMAX (see also Daniele's talk)

BioMAX

Characteristics

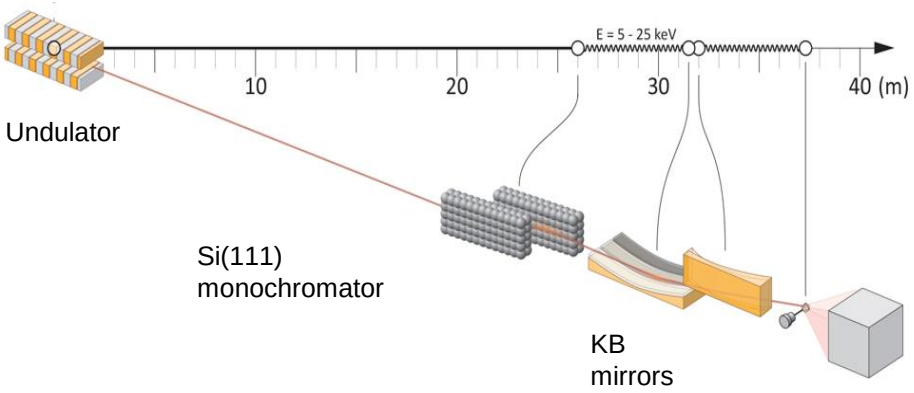
10^{13} photons/s (full unattenuated beam at 12.7 keV)

Energy easily tuneable between 6 and 24 keV

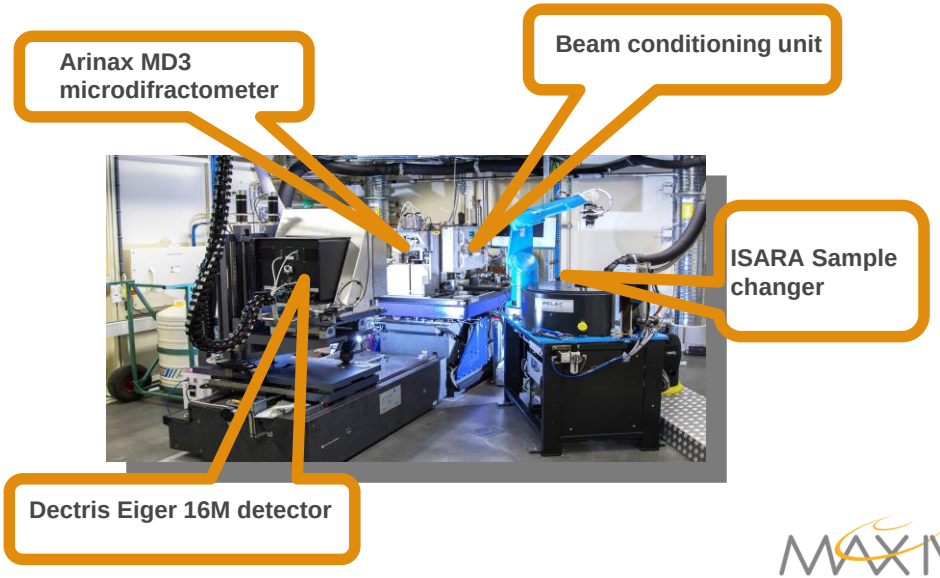
Variable beam focus : 100, 50 and 20 microns in the horizontal and 100, 50 and 5 microns in the vertical

Diffraction image collection at near 100 Hz

Automated sample exchange at cryotemperature in less than 25 seconds

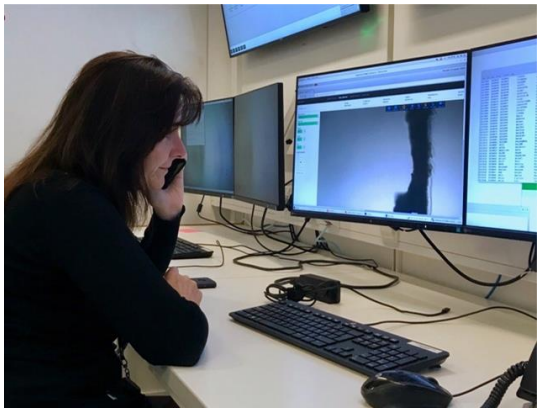


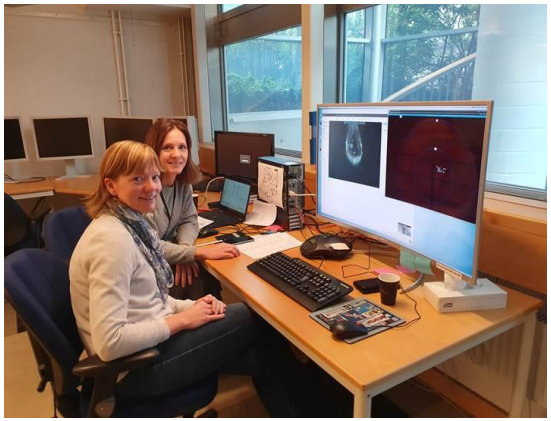
Sample changer dewar with capacity for 464 samples



Status

- In user operation since 2017, full functionality in 2020
- Conventional MX experiments and techniques (oscillation, XRF scans, energy scans, optimized SAD/MAD, helical data collection)
- SSX experiments: simple fixed target (using grid scan), injector based, as part of technique development for MicroMAX (in construction)
- Full remote experiments (only for cryo experiments with Sample Changer)





Remote access requirements

- The user has full control of the experiment, can interact with all the required beamline components from their local computer
- All users belonging to the same proposal and staff can collaborate in preparing the experiment and collecting data
- Users have access to the beamline only during beamtime
- Restrict direct control of beamline components
- Two-step authentication with VPN

Remote access implementation

Mixed approach combining web browser based interfaces and remote desktop clients

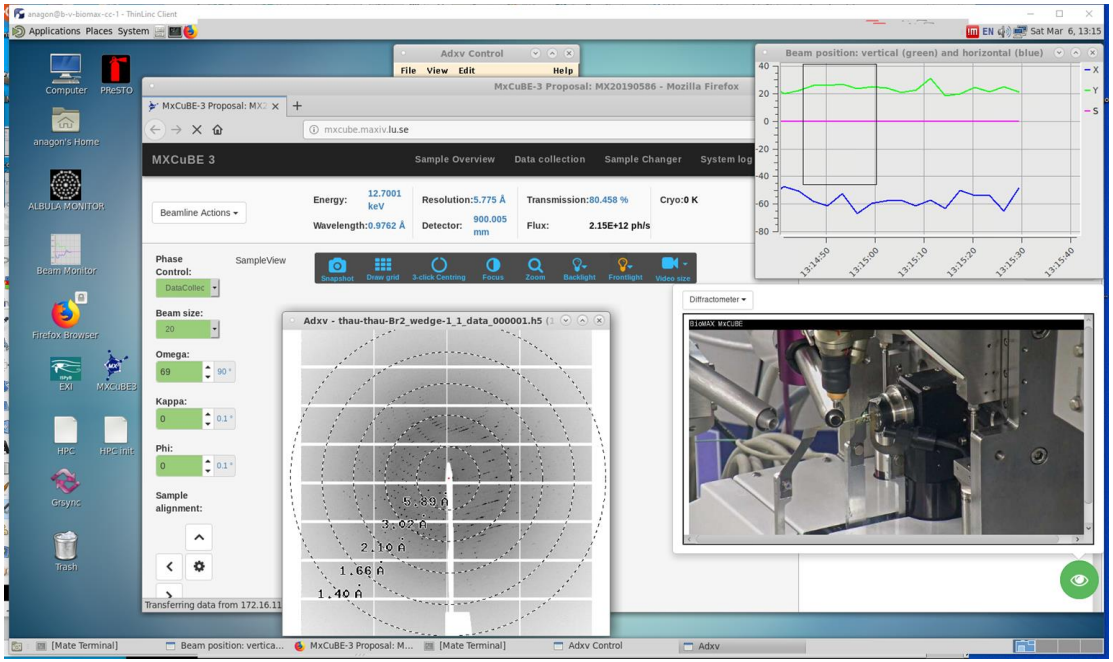
Outside beamtime

- Web browser applications for the user office (DUO) and sample management (Extended ISPyB or EXI)
- Remote desktop connection to HPC cluster for data inspection and manual data processing

During beamtime

- Remote desktop to virtual dedicated server in the BioMAX network, VPN only enabled for scheduled users for the duration of the experiment
  - Single point of access for MXCuBE3, diffraction image inspection and online data processing
  - Multiuser access management in MXCuBE3. User support facilitated by differentiating between staff and user roles.

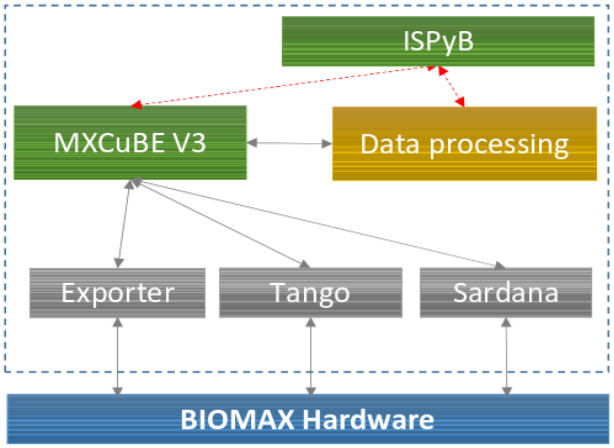
Remote desktop



- Cendio Thinlinc client (similar to NX Nomachine)
- Configurable to look exactly like beamline workstations
- Software keeps on running during internet glitches
- Customized software installation (no “dangerous” beamline control software available)
- No access to other machines - except online HPC cluster for data processing

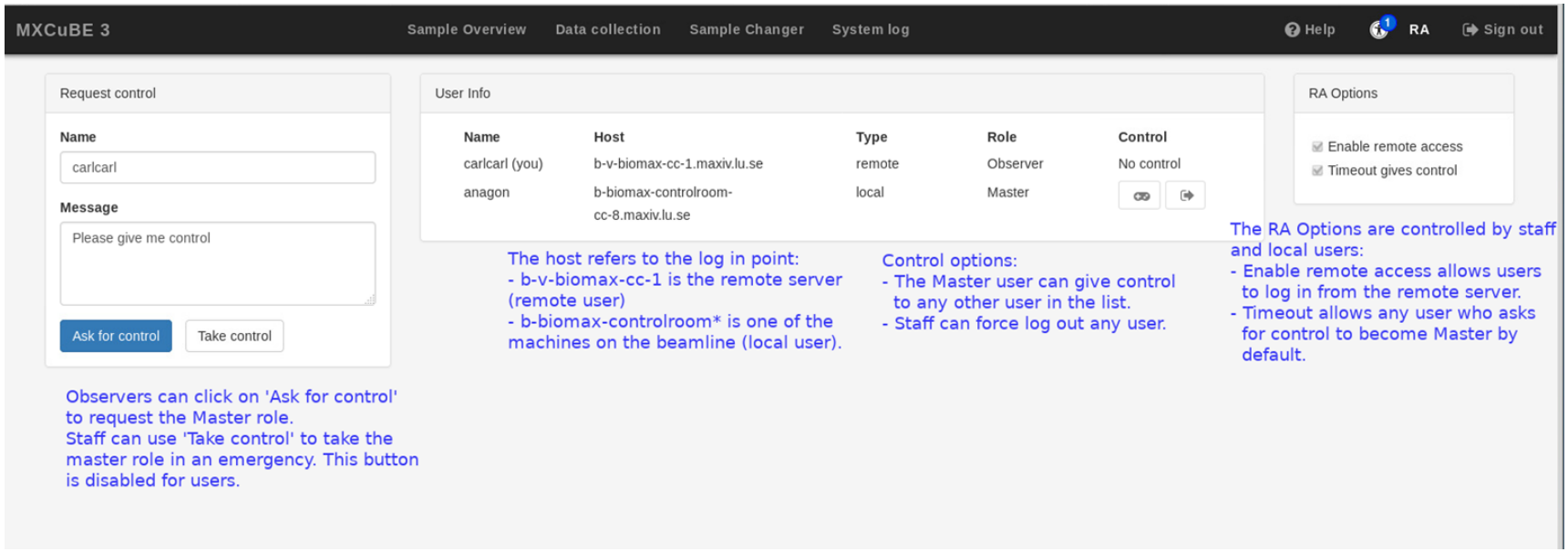
Experiment control with MXCuBE 3

- Beamline instrument control mainly through Tango controllers (eg, Sample changer, Eiger detector, different beamline motor controllers) the Exporter protocol (Arinax microdiffractometer). It is possible to run Sardana (beamline control) scripts
- Launches automated processing pipelines (EDNA 2) after data collection



Remote access control with MXCuBE 3

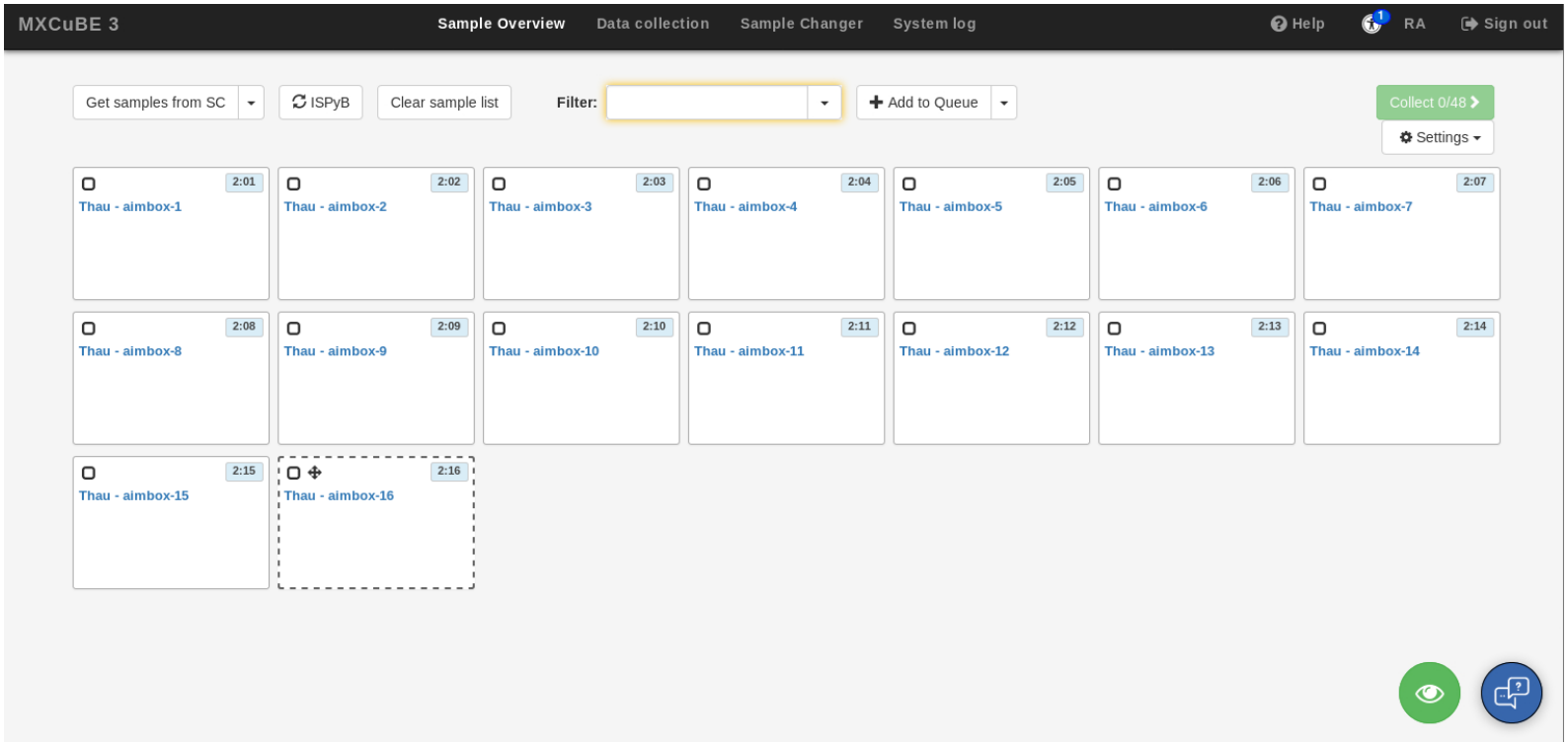
- Master user has active control of the interface, other users are observers.
- All the users can see who else is logged in and who is the active user
- Button to request active status (granted by default)
- Staff can set access parameters and kick out users
- Automated login reject for users not belonging to the proposal



Sample overview

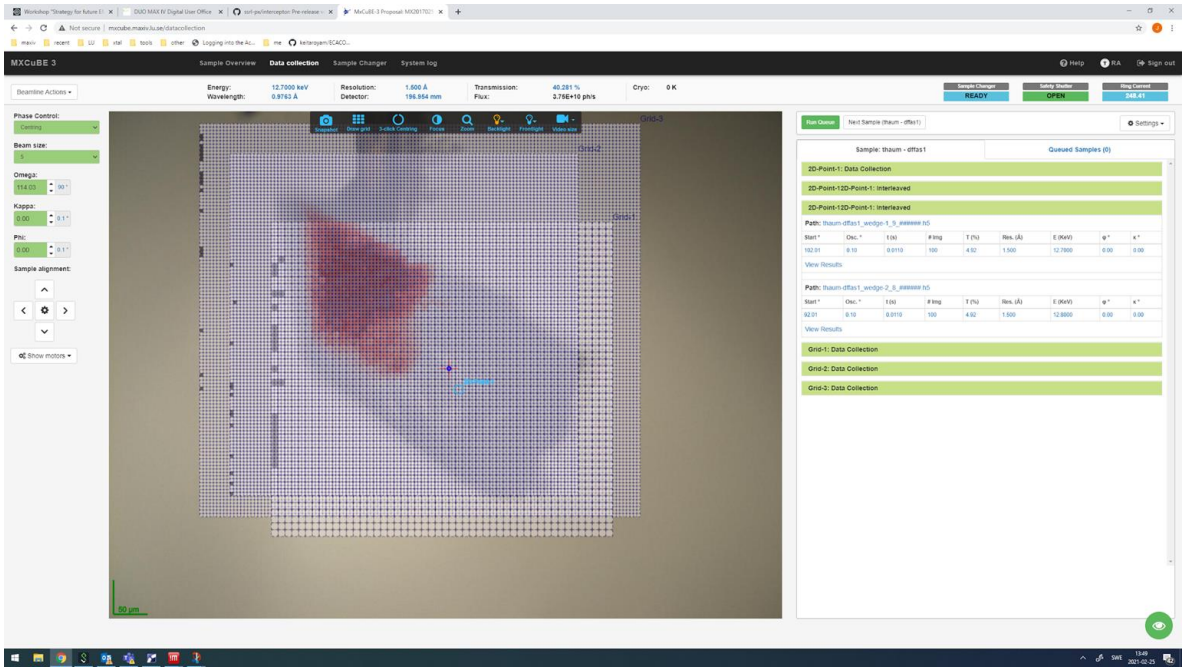
Sample information handling:

- ➢ Displays sample list entered in ISPyB for the current beamtime and proposal
- ➢ Sample selection for data collection



Data collection

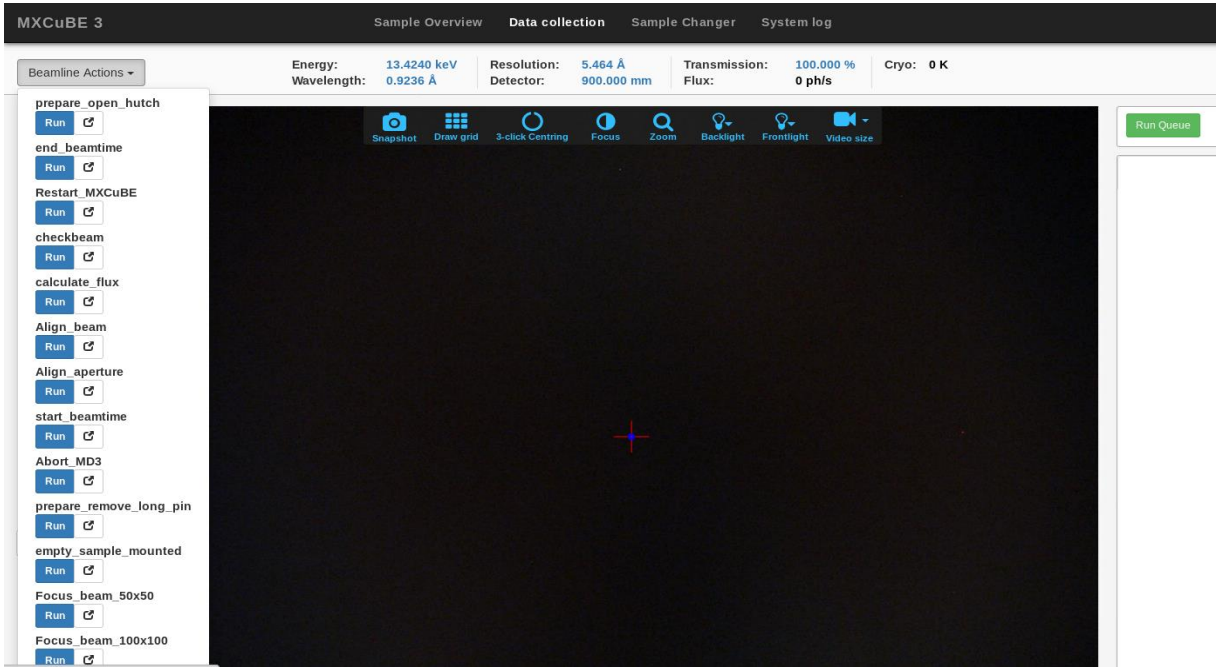
- Interaction with sample, centring and data collection setup
  - Oscillation data collection
  - Characterization
  - XRF scan
  - Energy scan
  - Helical data collection
  - Mesh scans (adapted for fixed target)
  - Primitive support for injector based experiments (not remote yet)
- Interaction with beamline instrumentation



Data collection

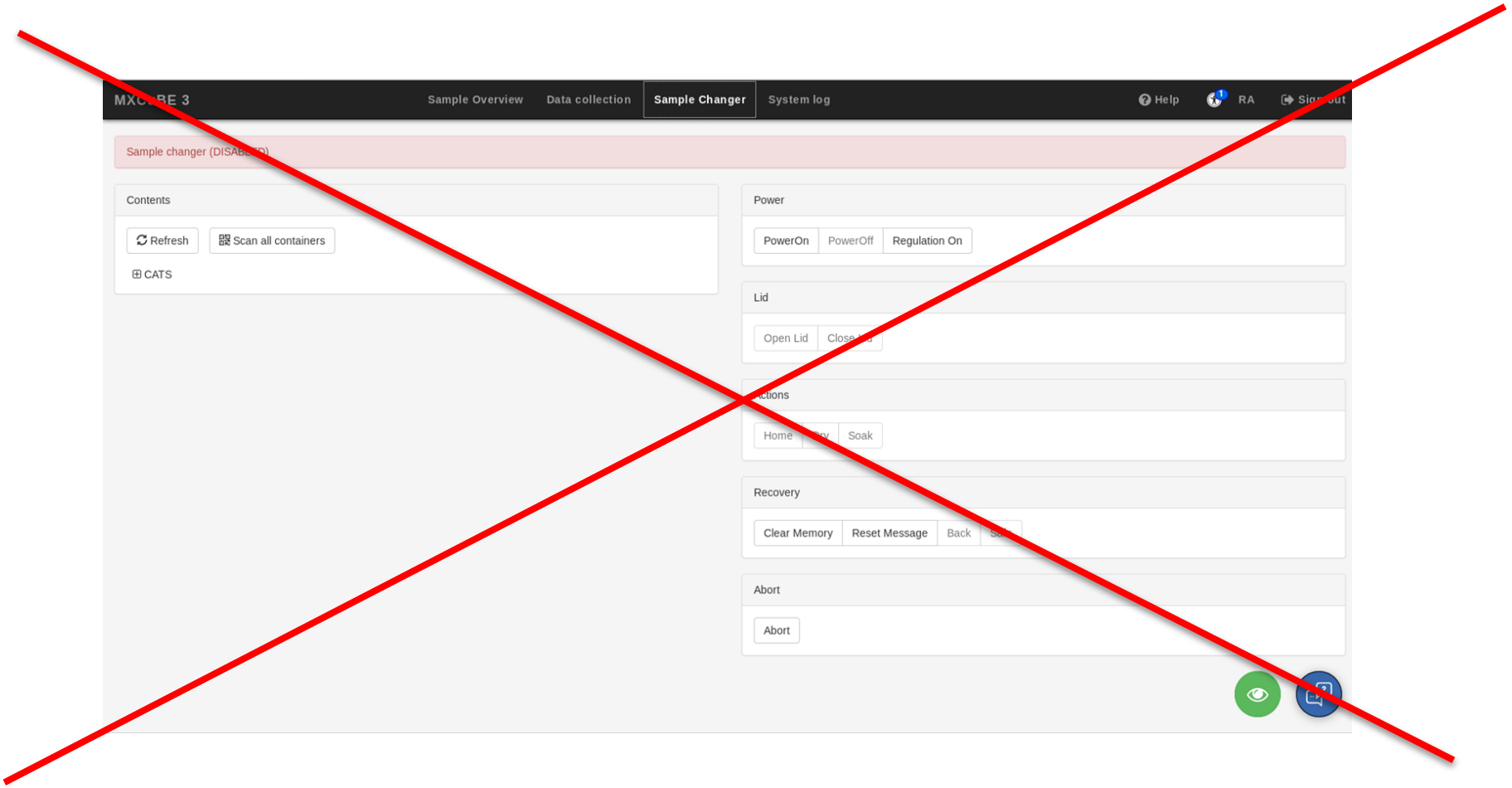
Scripts to control beamline instruments

- Opening and closing front ends, closing the undulator gap
- Changing the beam focus
- Restarting servers
- Beam diagnostics, alignment
- Sample changer troubleshooting



Sample changer control

- Superseded by beamline functions
- Only used by staff, not visible for users



Summary

- BioMAX remote access has been successful, used by a majority of users (100% during covid-19 related access restrictions)
- Combination of web browser tools, thinlinc remote desktop
- Many remote access and automation functionality are enabled via MXCuBE3. Further development for serial crystallography experiments is ongoing