

# Remote experiments at BioMAX



## Ana Gonzalez on behalf of the MAX IV MX group

Oskar Aurelius, Roberto Appio, Monika Bjelčić, M. Eguiraun, Thomas Eriksson, Ross Friel, Ishkhan Gorgisyan, Andrea Gross, Vahid Haghighat, Elmir Jagudin, Tobias Krojer, Julio Lidon-Simon, Gustavo de Lima, Mirko Milas, Uwe Mueller, Jie Nan, Anastasiia Shilova, Vladimir Talibov, Marjolein Thunnissen, Johan Unge, Thomas Ursby

# 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

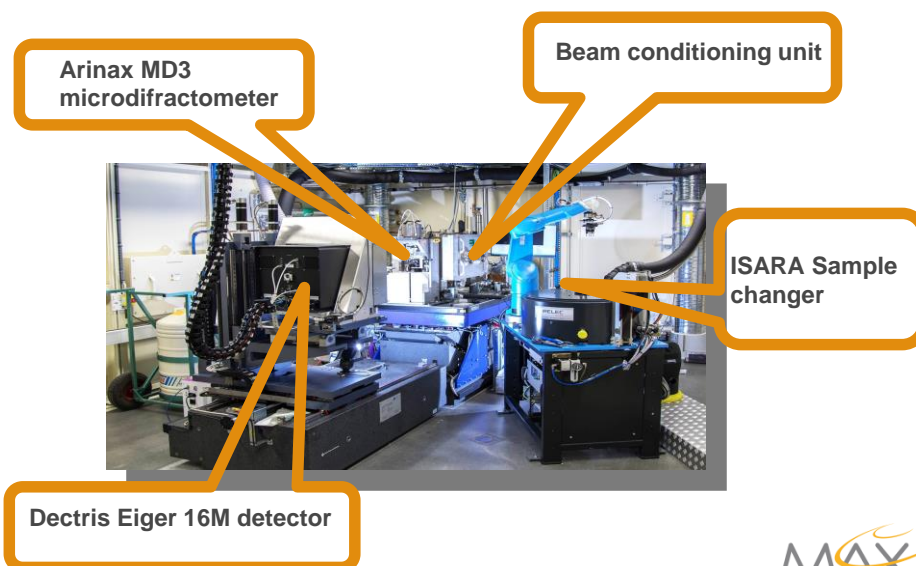
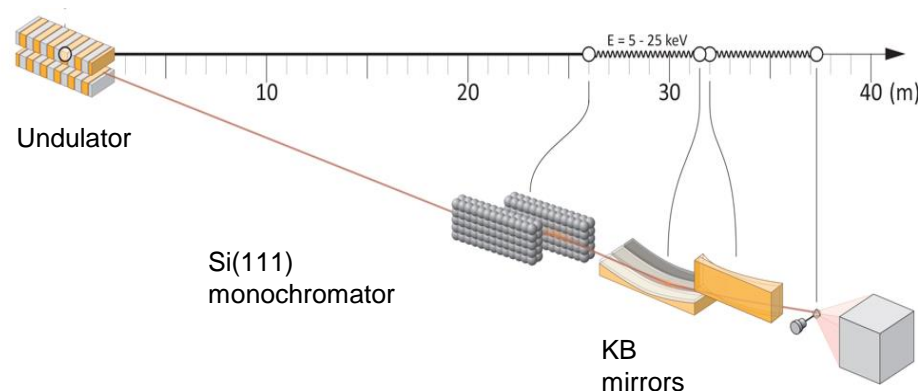
Variable beam focus : 100, 50 and 20 microns in the horizontal and 100, 50 and 5 microns in the vertical

Diffraction image collection at near 100 Hz

Automated sample exchange at cryotemperature in less than 25 seconds

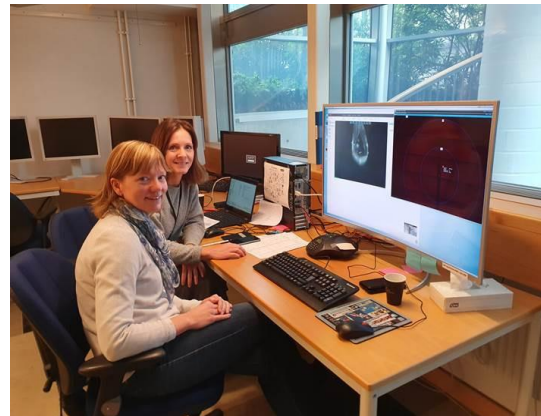
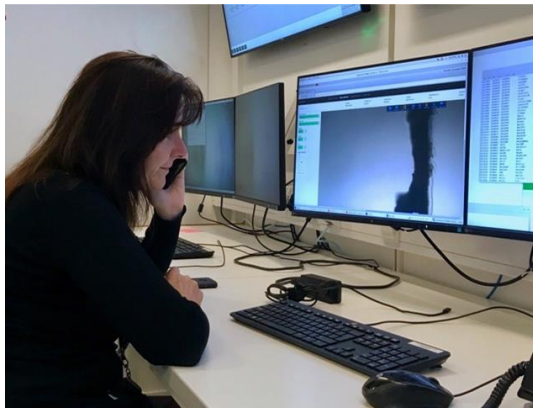


Sample changer dewar with capacity for 464 samples



# 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

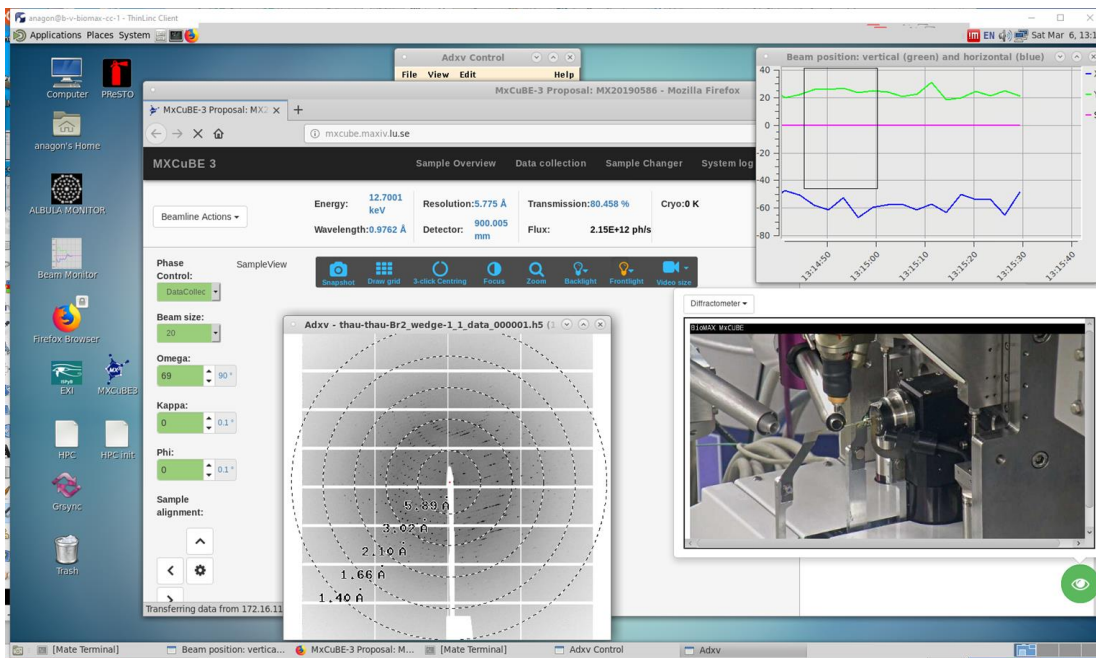
- Web browser applications for the user office (DUO) and sample management (Extended ISPyB or EXI)
- Remote desktop connection to HPC cluster for data inspection and manual data processing

## 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.



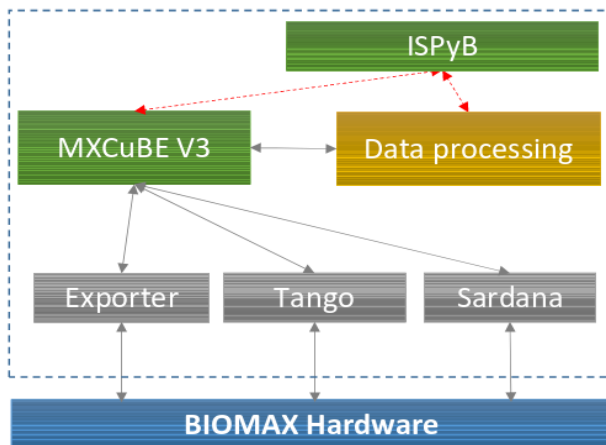
# Remote desktop



- 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

The screenshot displays the MXCuBE 3 web interface. At the top, a navigation bar includes 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. On the right, there are links for 'Help', 'RA' (with a notification icon), and 'Sign out'.

The main content area is divided into three panels:

- Request control:** Contains a 'Name' input field with 'carlcarl', a 'Message' text area with 'Please give me control', and two buttons: 'Ask for control' (highlighted in blue) and 'Take control'.
- User Info:** A table listing active users.
- RA Options:** A panel with two checked options: 'Enable remote access' and 'Timeout gives control'.

Name	Host	Type	Role	Control
carlcarl (you)	b-v-biomax-cc-1.maxiv.lu.se	remote	Observer	No control
anagon	b-biomax-controlroom-cc-8.maxiv.lu.se	local	Master	 

**Annotations:**

- Request control:** Observers can click on 'Ask for control' to request the Master role. Staff can use 'Take control' to take the master role in an emergency. This button is disabled for users.
- User Info:** The host refers to the log in point:
  - b-v-biomax-cc-1 is the remote server (remote user)
  - b-biomax-controlroom\* is one of the machines on the beamline (local user).
- Control options:**
  - The Master user can give control to any other user in the list.
  - Staff can force log out any user.
- RA Options:** The RA Options are controlled by staff and local users:
  - Enable remote access allows users to log in from the remote server.
  - Timeout allows any user who asks for control to become Master by default.

# Sample overview

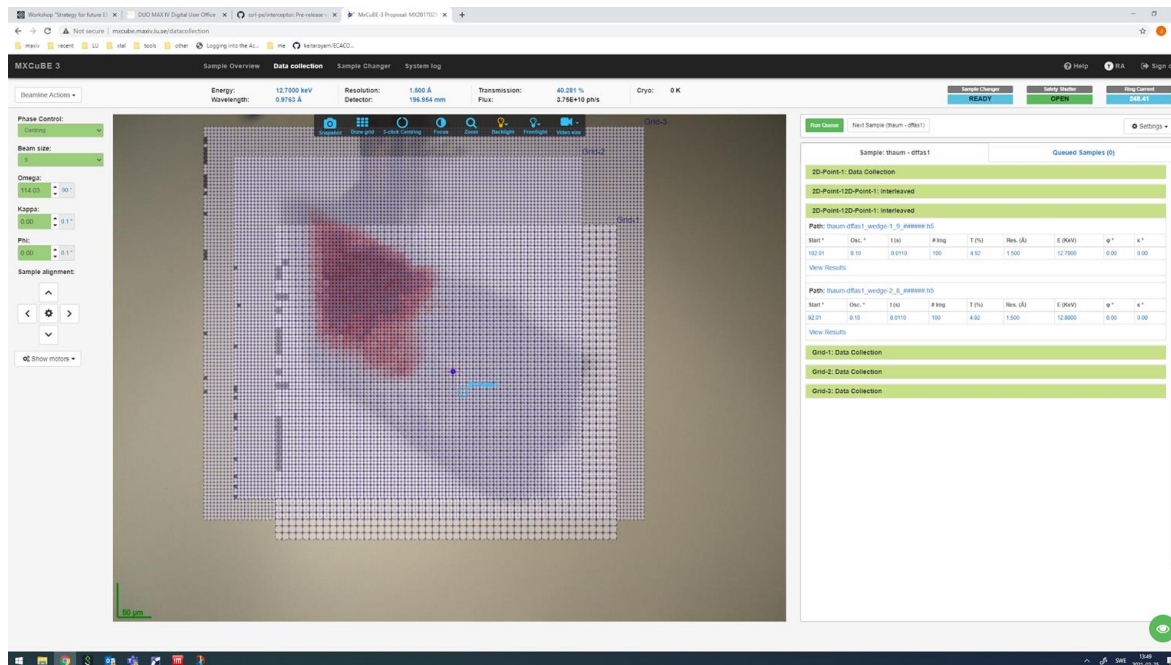
Sample information handling:

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

The screenshot displays the 'Sample Overview' window of the MXCuBE 3 software. The interface features a dark top bar with the title 'MXCuBE 3' and navigation links for 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. On the right of the top bar are links for 'Help', 'RA', and 'Sign out'. Below the top bar, there is a control area with buttons for 'Get samples from SC', 'ISPyB', 'Clear sample list', a 'Filter:' dropdown menu, and an 'Add to Queue' button. A green 'Collect 0/48' button and a 'Settings' dropdown are also present. The main area contains a grid of 16 sample boxes, each labeled 'Thau - aimbox-1' through 'Thau - aimbox-16' with corresponding timestamps from 2:01 to 2:16. The box for 'Thau - aimbox-16' is highlighted with a dashed border and a plus icon, indicating it is the selected sample. At the bottom right, there are two circular icons: a green eye and a blue speech bubble.

# Data collection

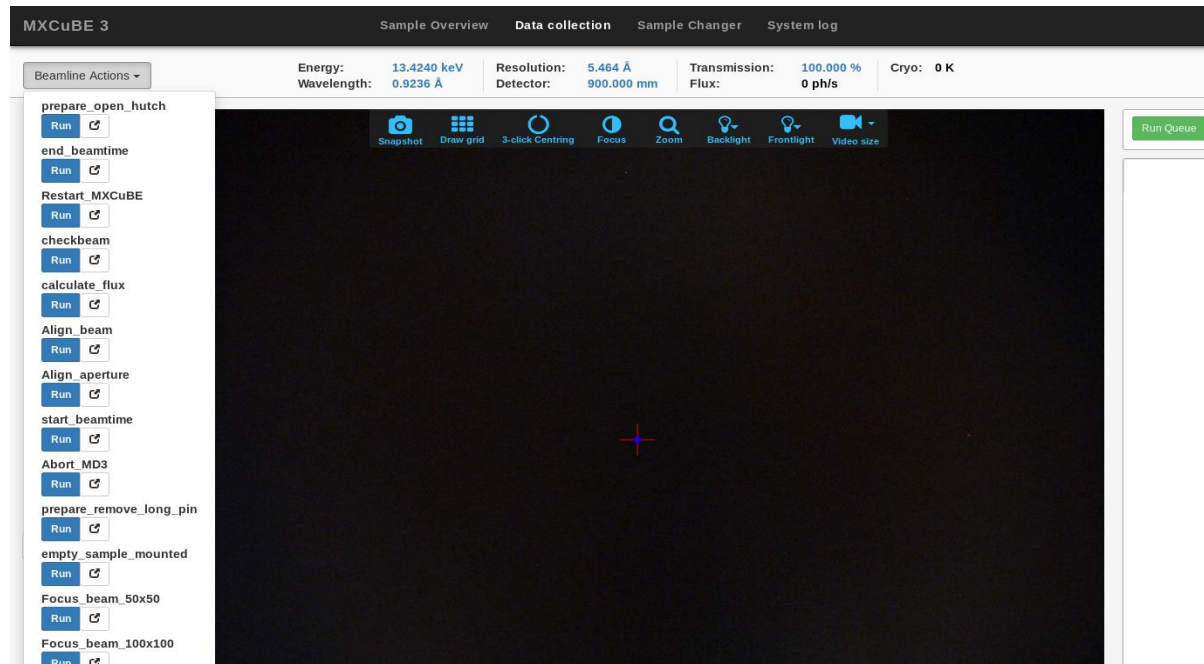
- Interaction with sample, centring and data collection setup
  - Oscillation data collection
  - Characterization
  - XRF scan
  - Energy scan
  - Helical data collection
  - Mesh scans (adapted for fixed target)
  - Primitive support for injector based experiments (not remote yet)
- Interaction with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



# Data collection

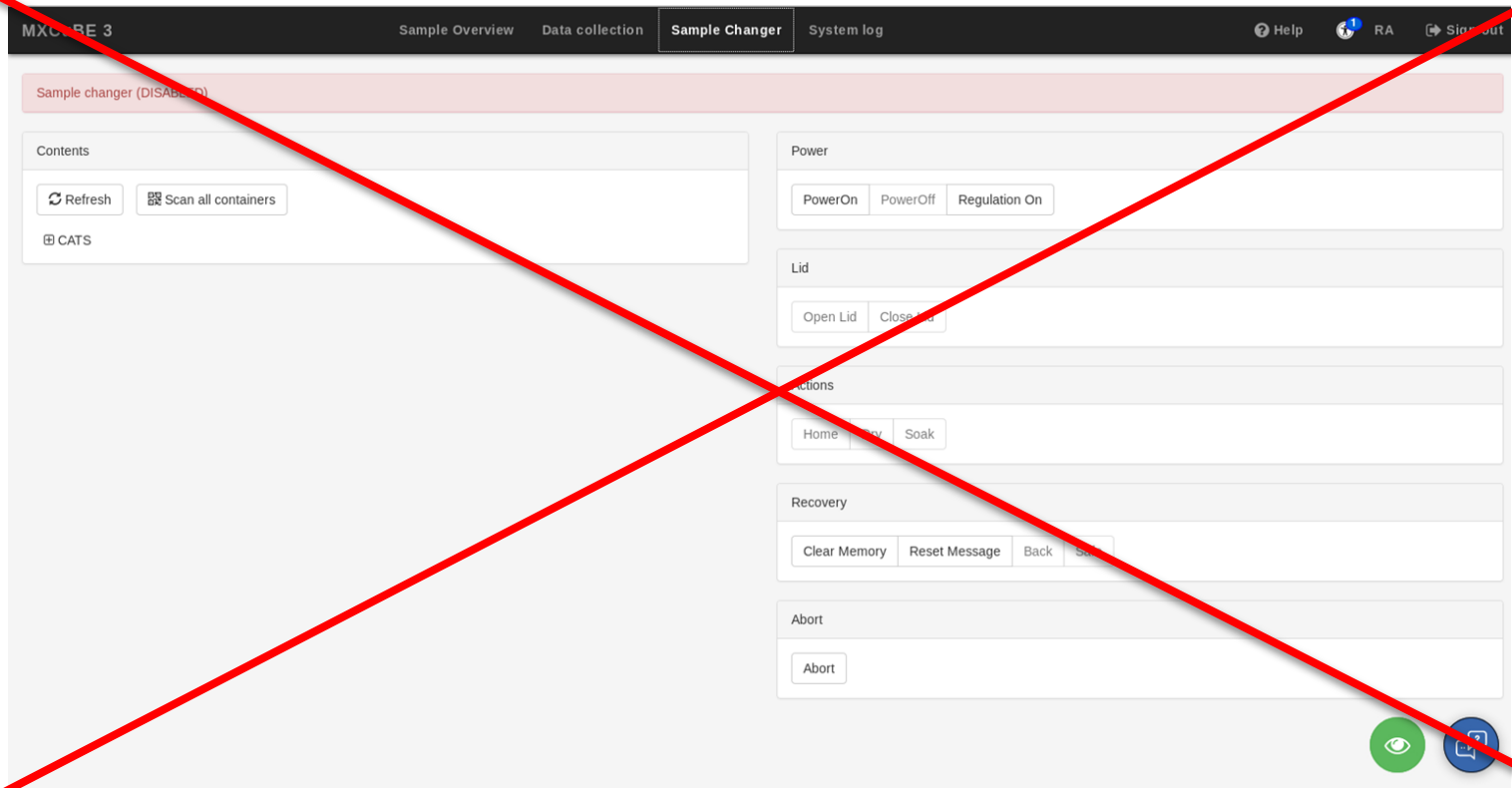
Scripts to control beamline instruments

- 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