Status of BL13-XALOC Macromolecular Crystallography beamline

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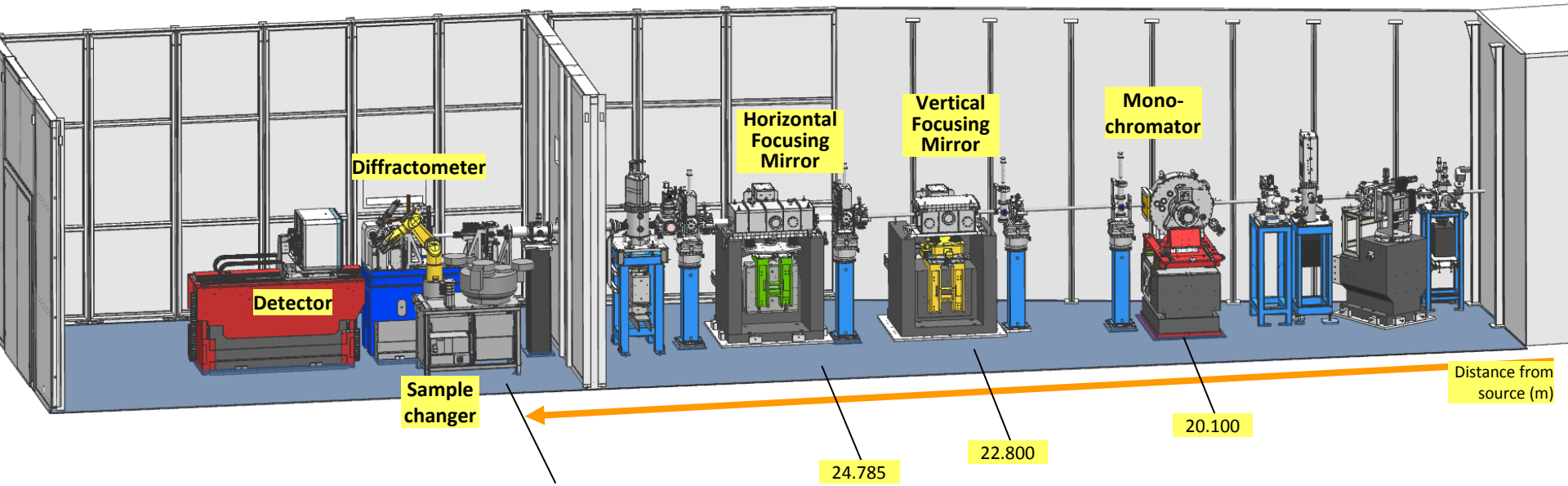
XALOC: Layout reminder

Beamline concept : In-vacuum Undulator IVU21.6 + Channel-cut Si(111) monochromator + KB focusing mirrors



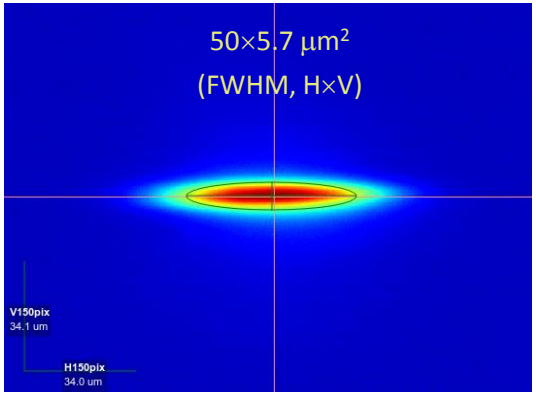
Experimental Hutch

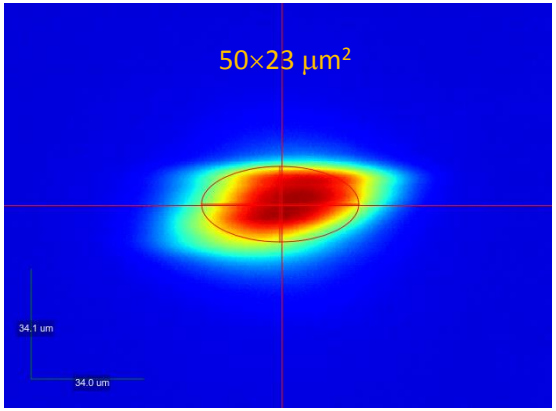
MD2M
CATS
PILATUS 6M

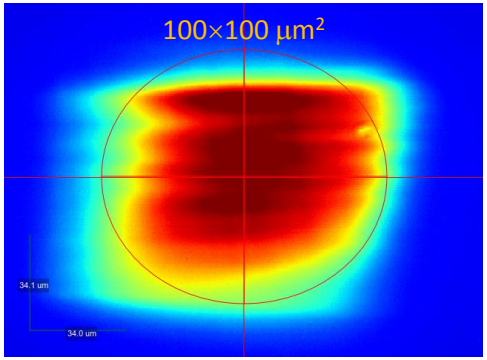
XALOC: Beam Shaping - larger sizes

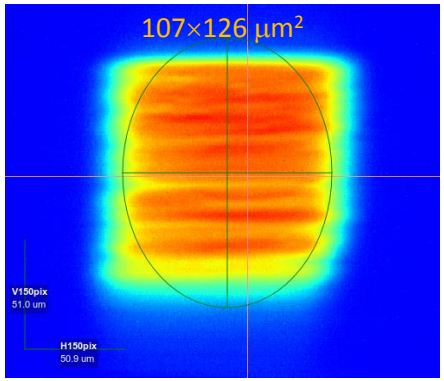
Beam size be expanded by unbending the mirrors and defocusing the beam

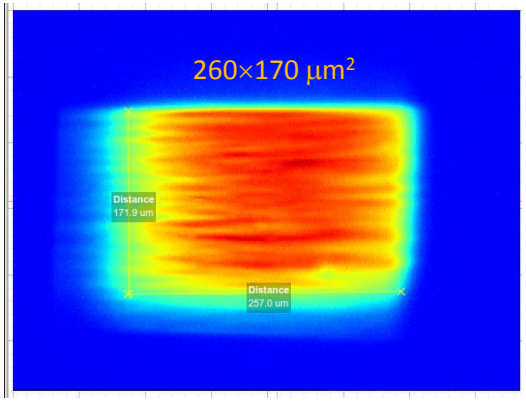
- **From 50×5.7 to 250×250 μm**
- **Increasingly popular for beamtimes with a variety of projects**











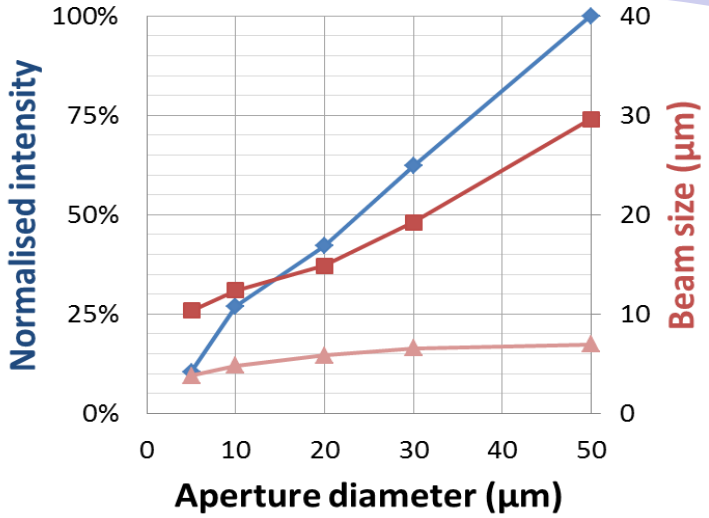
Beam Shaping - smaller sizes

The MD2 penta-aperture consisting in 5 round pinholes is used to reduce the beam size

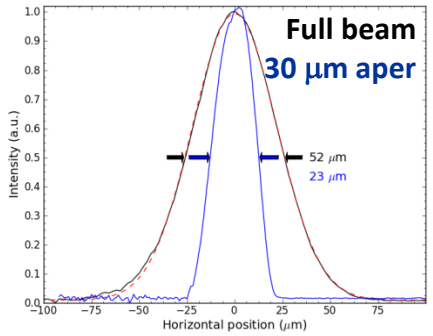
- **Variety of smaller beam sizes for small crystals**
- **More accurate raster scans possible**

BUT:

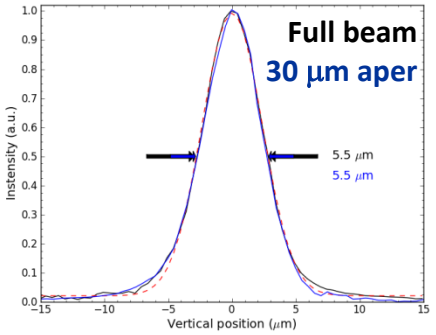
- **Flux is reduced linearly with size**
- **Data have slightly but consistently better quality (ISas) when defocusing the beam**
- **Seeking for beam vibrations…**

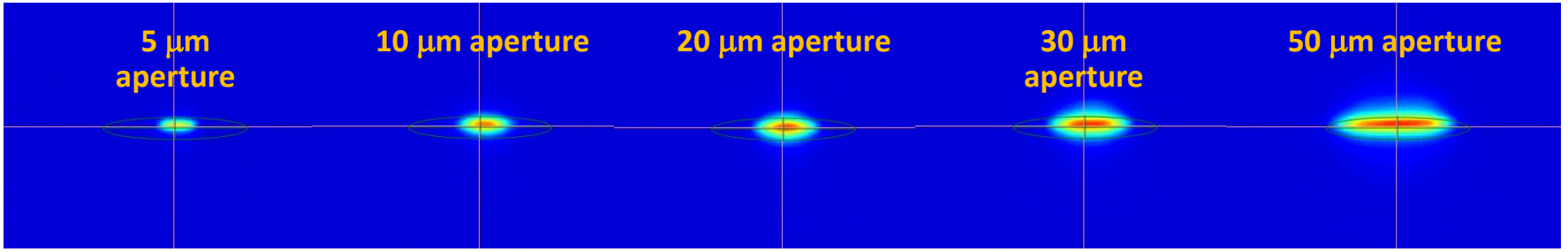


V profile at sample



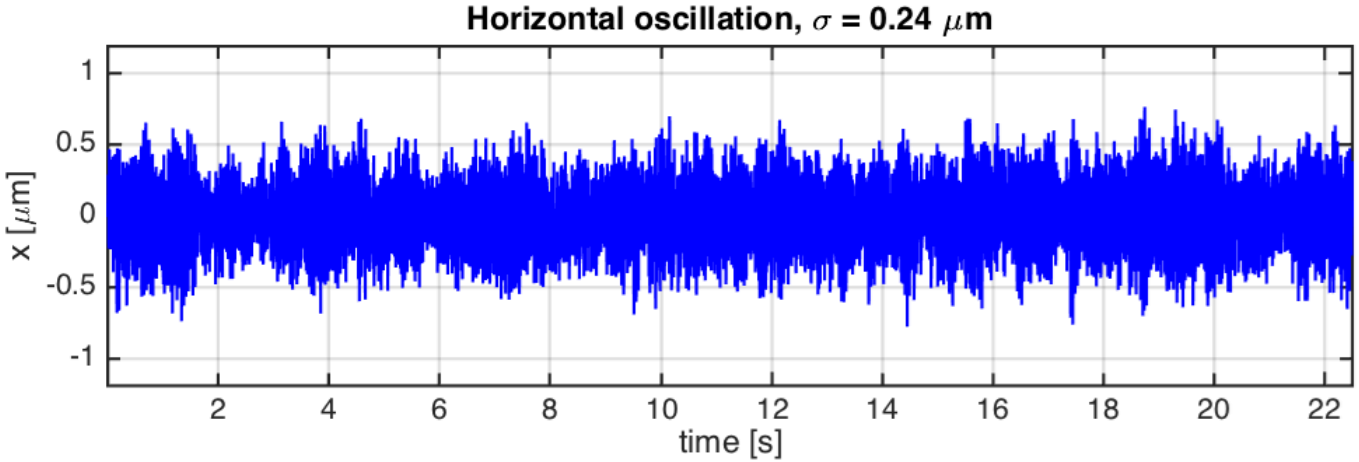
H profile at sample

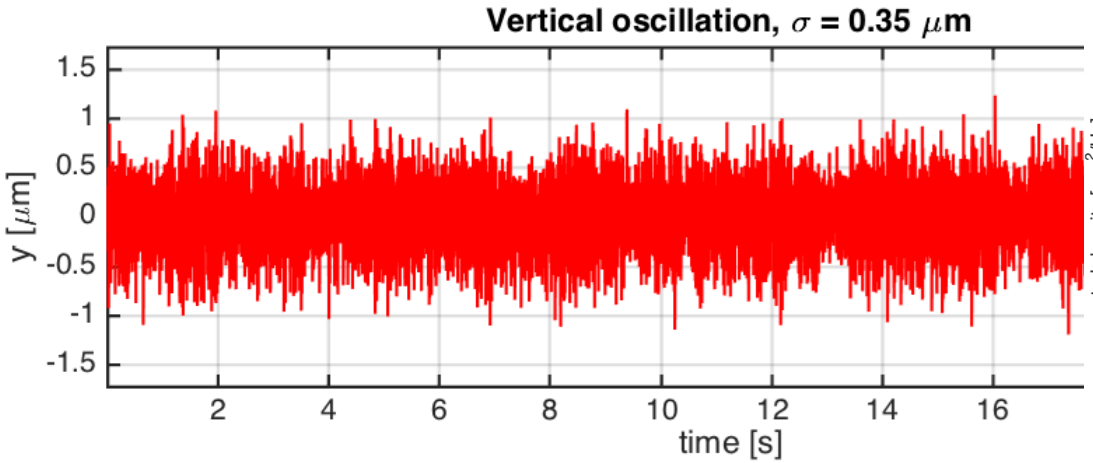


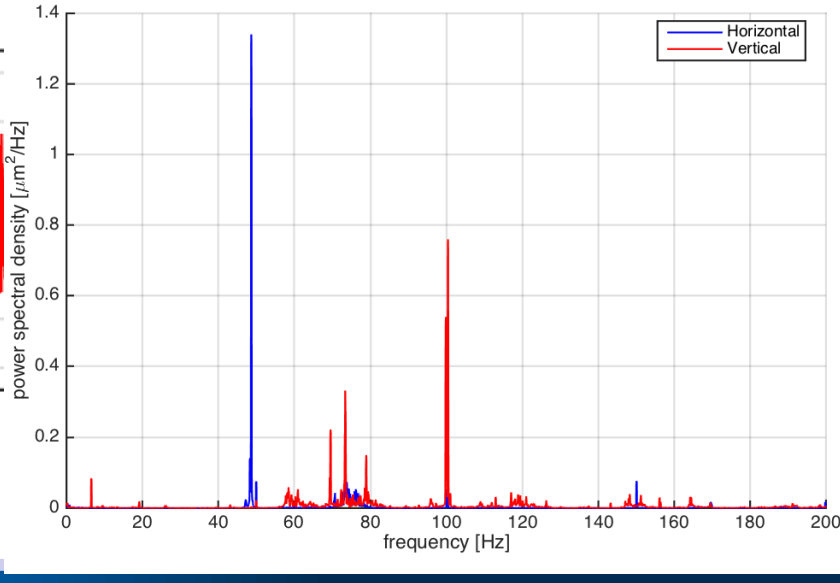


Beam vibrations

- Beam center found by Gaussian fitting of images at focal point recorded at 480 Hz
- High speed camera coupled with a 20 um-thick YAG:Ce screen
- Vibrations with the beamline at rest (no excitations)

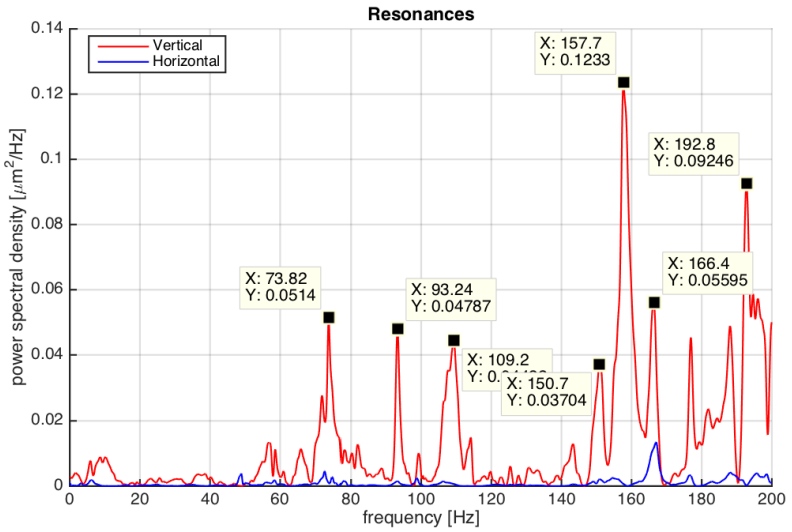




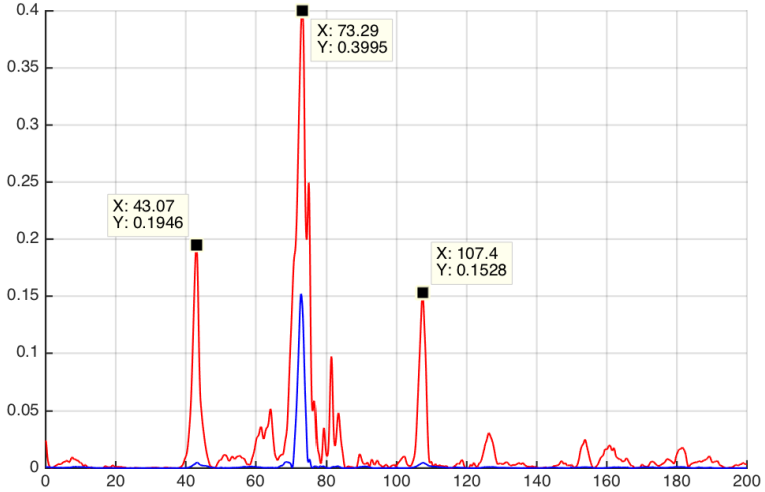


Beam vibrations

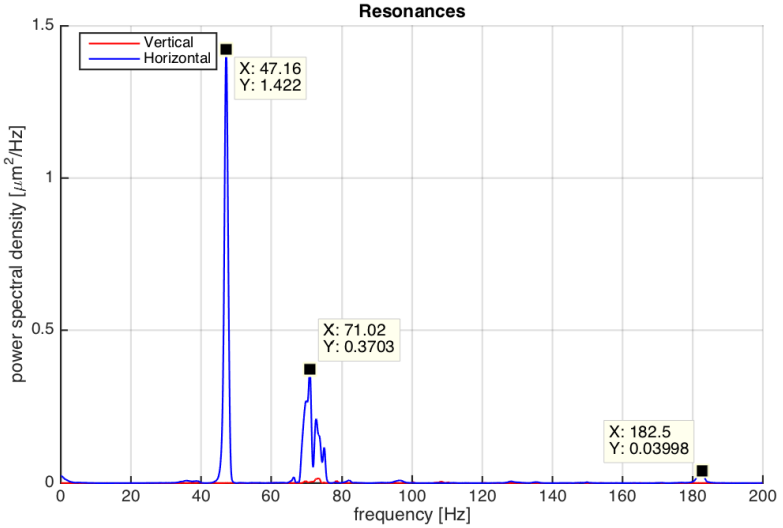
- The origin of the resonances can be found by hitting the vacuum vessels of the critical elements
- All resonances have frequencies higher that the maximum detector frame rate (12 Hz)



Mono eigenfrequencies

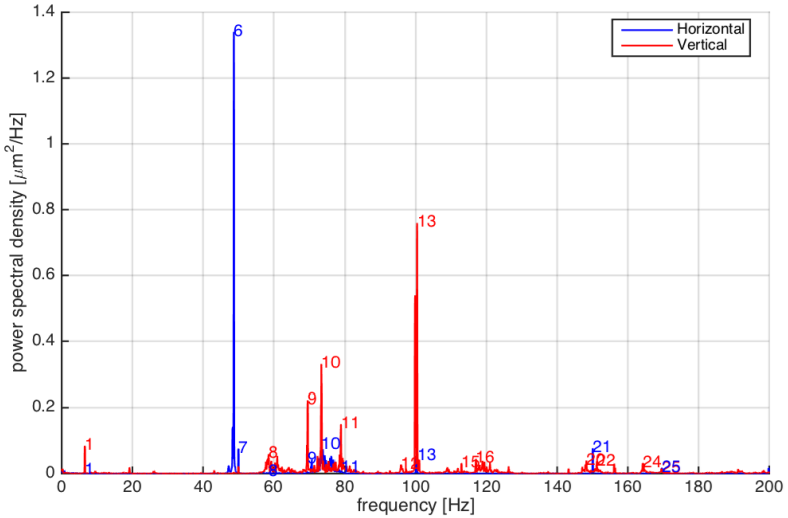


VFM eigenfrequencies



HFM eigenfrequencies

Beam vibrations



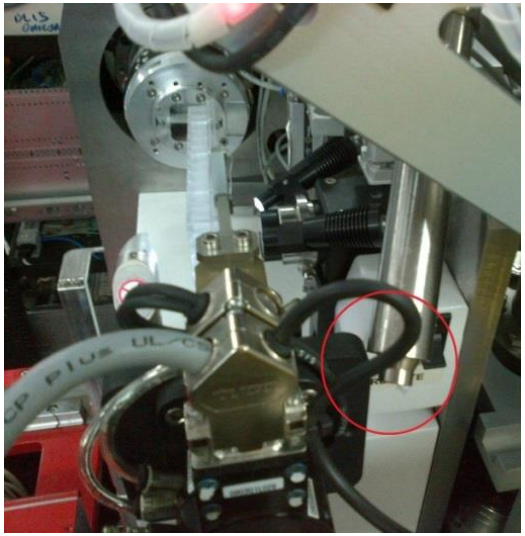
Spectrum of the beam motion at detector position (no-excitation): Amplitudes

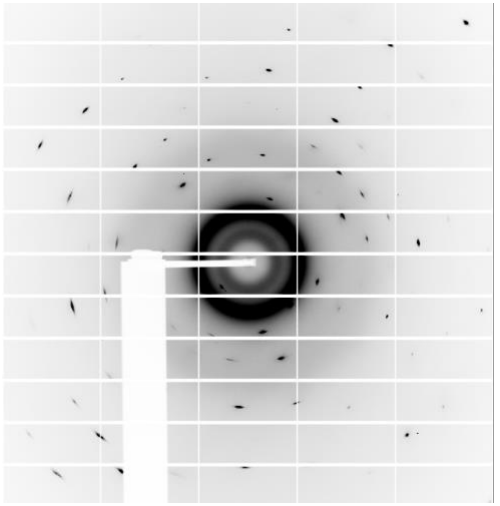
ID	frequency interval (Hz)	frequency (Hz)	x-amplitude (um rms)	ratio to total amplitude (%)	y-amplitude (um rms)	ratio to total amplitude (%)		Resonance
1	0.00-15.00	6.53	0.034	2.08	0.06	3.05		
2	15.00-22.00	19.16	0.01	0.17	0.029	0.71		
3	22.00-35.00	26.13	0.011	0.22	0.026	0.55		
4	35.00-41.00	39.42	0.011	0.21	0.014	0.15		
5	41.00-45.00	43.2	0.014	0.35	0.019	0.31		VFM
6	45.00-49.60	48.71	0.164	47.66	0.017	0.23	H	HFM
7	49.60-52.00	50.04	0.038	2.55	0.021	0.38		
8	52.00-67.00	58.53	0.042	3.14	0.113	10.73		
9	67.00-72.00	69.6	0.048	4.05	0.092	7.15		
10	72.00-78.00	73.47	0.121	25.83	0.131	14.37	Both	HFM, VFM, MONO
11	78.00-88.00	78.8	0.036	2.25	0.102	8.78		
12	88.00-98.00	95.82	0.016	0.43	0.058	2.82		Mono
13	98.00-106.00	100.36	0.036	2.25	0.165	22.9	V	
14	106.00-110.00	108.93	0.009	0.15	0.043	1.57		VFM
15	110.00-116.00	112.93	0.01	0.18	0.054	2.4		
16	116.00-124.00	116.98	0.013	0.31	0.09	6.82		
17	124.00-129.00	126.27	0.009	0.13	0.038	1.18		
18	129.00-142.00	137.42	0.017	0.48	0.035	1.04		
19	142.00-145.00	143.2	0.008	0.11	0.02	0.32		
20	145.00-149.00	148.27	0.009	0.15	0.053	2.33		
21	149.00-150.50	150.04	0.037	2.4	0.029	0.71		
22	150.50-154.00	151.24	0.011	0.21	0.049	2.05		
23	154.00-160.00	156.13	0.012	0.26	0.038	1.24		Mono
24	160.00-168.00	164.18	0.021	0.75	0.056	2.66		
25	168.00-200.00	169.6	0.046	3.74	0.082	5.7		

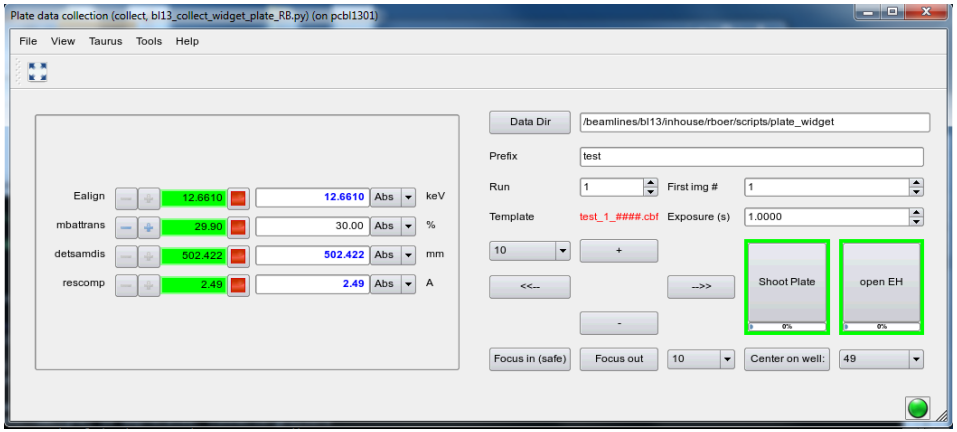
- **Horizontal beam vibrations are dominated by a 48 Hz coming from HFM**
- **Vertical beam vibrations are dominated by a series frequencies at ~75 Hz and one at 100 H from Mono and VFM**
- **Still no conclusions on the effect on the quality of data.**

XALOC: Crystallization plates

- Plates are mounted on the robot, using the plates tool
- The new XYZ moveable beam stop required for plates is already installed
- The cryostream is swung out remotely
- A special widget is used for collection. Integration in the standard collection widget is foreseen before Summer 2016
- A TRIS crystal was positioned in the beam using manual operation of the robot
- An still image was recorded using an exposure of 0.5 s
- Now able to scan plates, but not ready for users

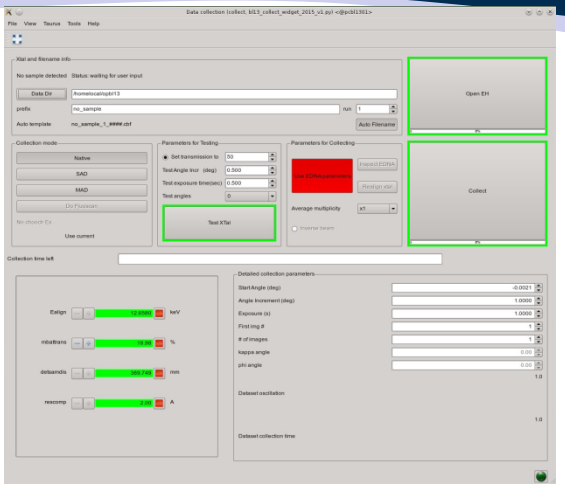


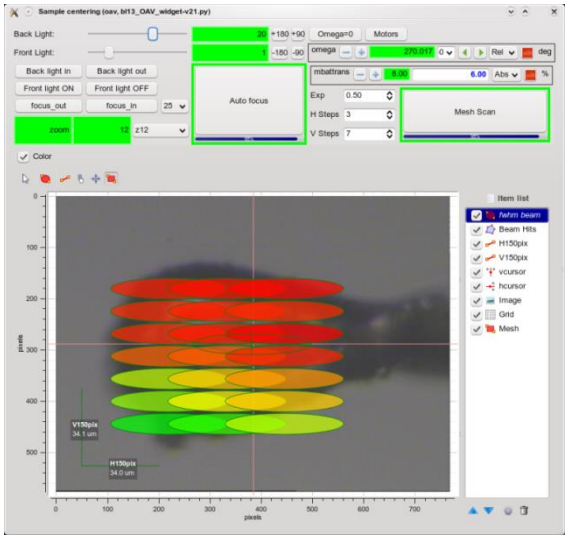


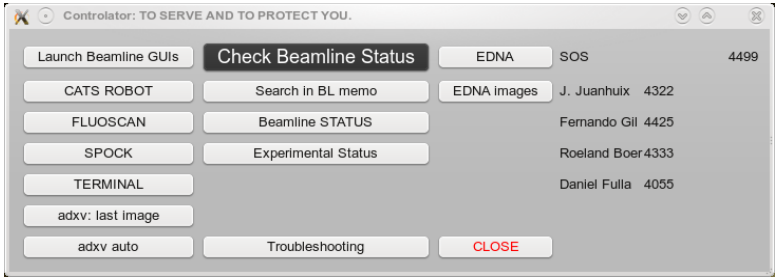


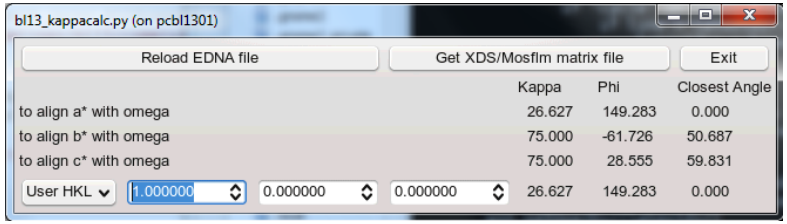
XALOC: Controls upgrades

- **EDNA** implemented and integrated in the experiment pipeline
- **Automatic data processing**
  - Using the cluster
  - AutoPROC (Global Phasing Ltd) implemented
  - Implementing Phaser in the pipeline
- Diffraction **data queues** ready.
  - **Inverse beam** (wedged) anomalous data collection
  - Many others to be implemented
- Multiple crystal position data collection: **crystal cartography**
- **Reorientation of the crystal** after indexing with EDNA
- **Beamline diagnostic** tool
- **sftp service for users**







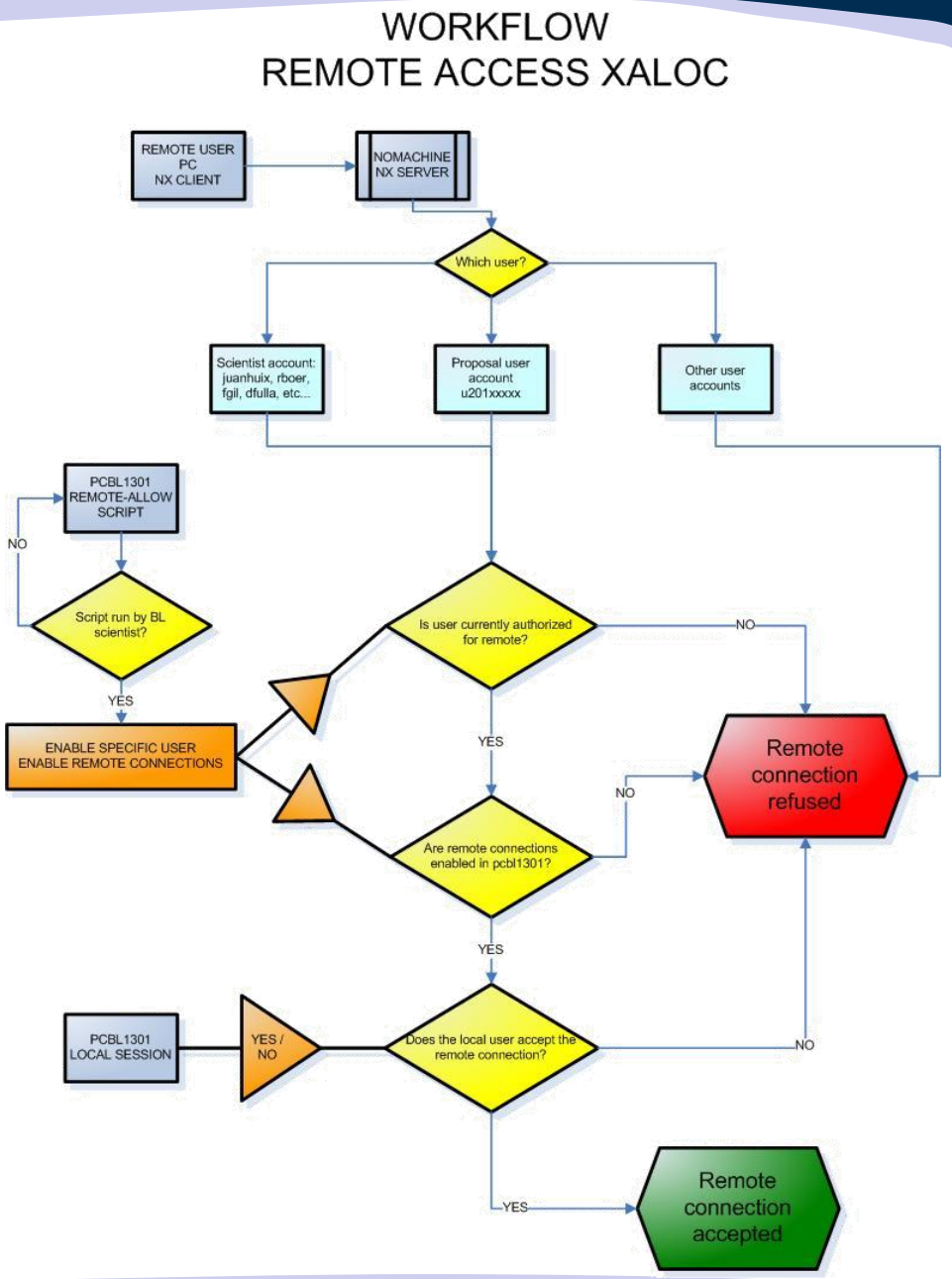


Remote data collection

- **NX based (Server ready)**
- **User needs to install NX Enterprise client for Windows/Linux/Mac (exe file)**
- **Connect to:**

```
Host: remotenx.cells.es
Port: 443
```

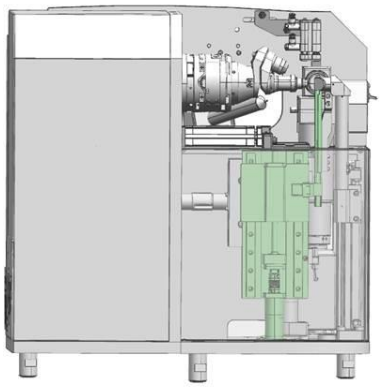
- **Currently in beta testing**
- **Still to be done: script giving user authentication**



XALOC: Future upgrades

Mechanical

- **Installation of a (de)humidifier device**
  - Control system required
- **Mechanized crystal annealing**
- **New viewing camera**



Controls

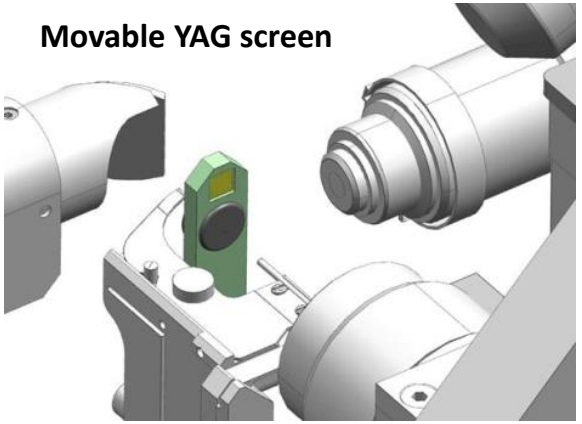
- **Installation of MXCuBE**

- Implementation of (pending MxCUBE??):
  - Helical data collection
  - MAD data collection pipeline
  - Multiple kappa angle data collection
  - Automated crystal centering

- **Automatic beam alignment** to be started when the fluorescence screen can be automatically placed at sample position

- **Automatic loop centering** : waiting for MXCuBE?

Movable YAG screen



The XALOC Team

Engineering

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Carles Colldelram	Mech. Engineer
Robert Oliete	Mech. Technician
Ricardo Valcárcel	Mech. Technician

Computing

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José Ávila	Electronics Engineer
Xavi Fariña	Electronics Tech.
Jorge Villanueva	EPS engineer

Experiments

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Roeland Boer	BL scientist
Jordi Juanhuix	BL responsible
Josep Nicolás	Mirrors, Metrology
Igors Šics	Diagnostics
Inma Hernández	Administration