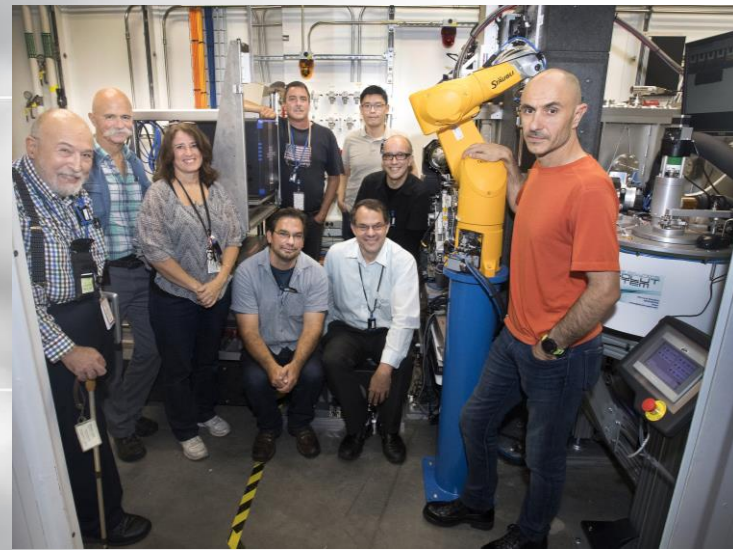
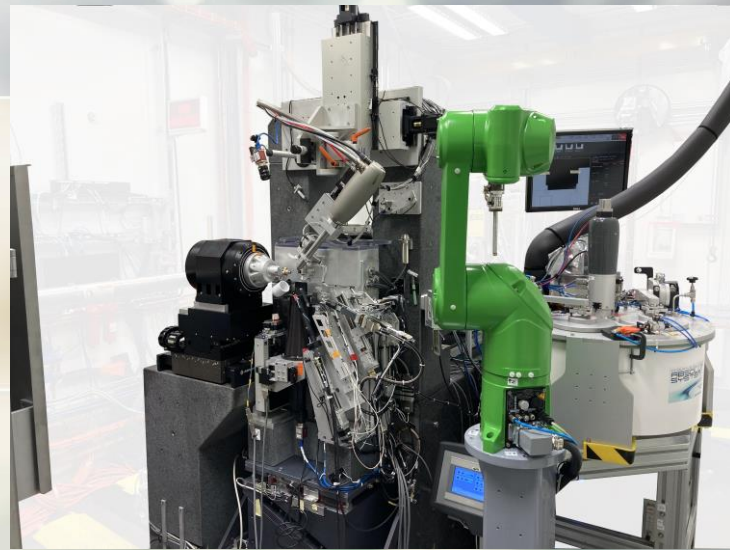
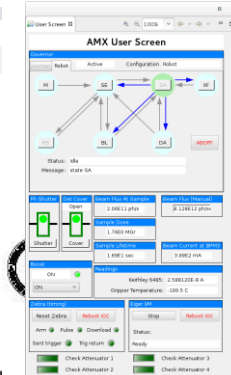
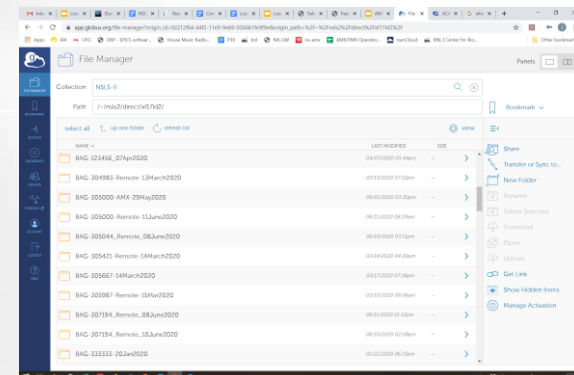
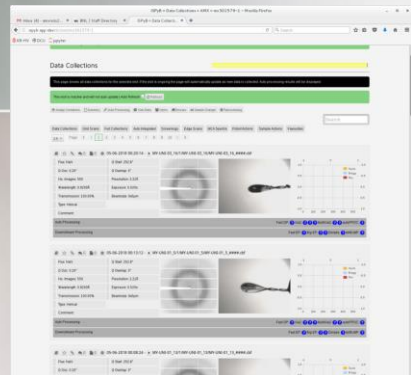
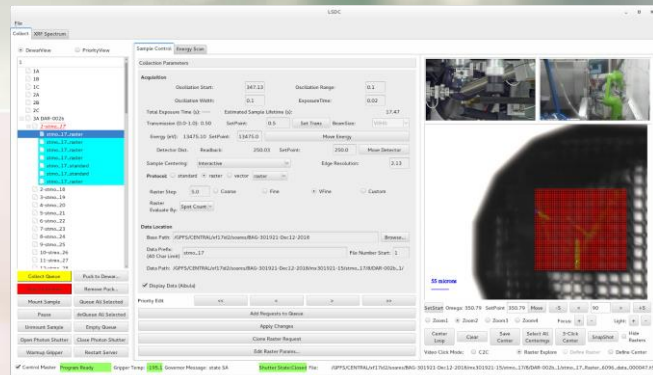


# 3 years of remote access at the 2 NSLS-II MX beamlines focus on Automation



The Remote Experiments Showcase  
Jean Jakoncic, AMX,FMX  
Dec 16, 2020.



# What made us compatible with remote access experiments

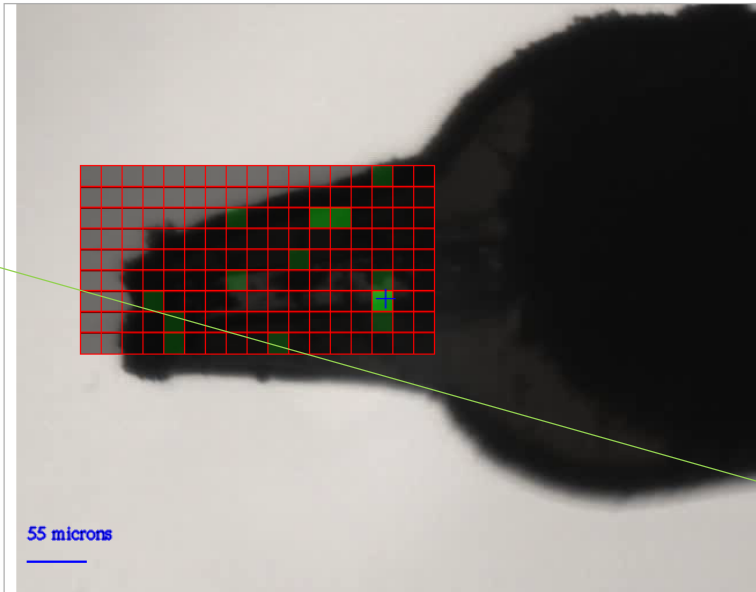
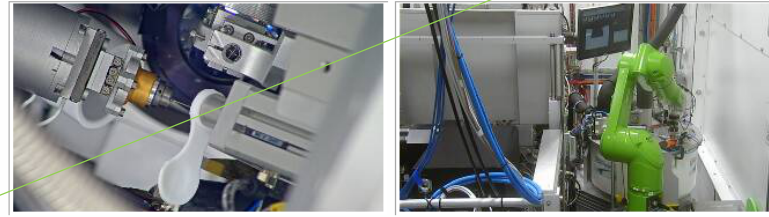
- Robotic sample mounting giving reliable sample exchange (<35 sec)
- Safe operation of the beamline (1 operator; safe transitions from state to state)
- Data collection via a single GUI: LSDC
- Automated experiments (crystal centering and data collection)
- Only ONE sample holder standard :Spine base in Unipuck
- Web access to data collection and processing: SynchWeb/ISPyB
- Automated data processing (pipelines)
- “Streamlined” shipping / receiving of the samples
- Automated data transfer using Globus
- Online material for “simple/common” data collection protocols (MX resources page) To be augmented



# Life Science Data Collection GUI: IsdcGui : one interface

The screenshot displays the LSDC (Life Science Data Collection) GUI. The interface is divided into several sections:

- File Panel (Left):** A tree view showing a collection of samples, including A16\_raster, 7A CDI-20 (with sub-items 1-D1, 2-D2, 3-D3), and 4-D4 (with sub-items 5-D5 to 16-D16).
- Sample Control (Top):** Tabs for 'Sample Control' and 'Energy Scan'. The 'Sample Control' tab is active.
- Collection Parameters (Center):**
  - Acquisition:** Includes fields for Oscillation Start (272.1), Oscillation Range (120.0), Oscillation Width (0.2), Exposure Time (0.01), Transmission (0.050), SetPoint (0.05), BeamSize (VOHO), Energy (eV) (13475.20), SetPoint (13475.0), Detector Dist. (200.00), SetPoint (200.00), Sample Centering (Interactive), and Edge Resolution (1.77).
  - Protocol:** Radio buttons for 'standard', 'raster', and 'vector'. The 'raster' protocol is selected.
  - Raster Step:** Set to 20.0. Options include Coarse, Fine, VFine, and Custom.
  - Vector Start/End:** Buttons for 'Vector Start' and 'Vector End'.
  - Number of Wedges:** Set to 1.
  - Length(microns):** and **Speed(microns/s):** fields.
- Data Location (Center):**
  - Base Path:** /GPFS/CENTRAL/xf17id2/PR-306525\_Remote\_29August2020
  - Data Prefix:** D4
  - File Number Start:** 1
  - Data Path:** /GPFS/CENTRAL/xf17id2/PR-306525\_Remote\_29August2020/mx306525-1/D4/1/CDI-20\_4/
- Control Panel (Bottom):** Includes buttons for 'Collect Queue', 'Stop Collection', 'Mount Sample', 'Unmount Sample', 'Pause', 'Close Photon Shutter', 'Queue All Selected', 'deQueue All Selected', 'User Screen...', 'Empty Queue', 'Warmup Gripper', and 'Restart Server'.
- Status Bar (Bottom):** Shows 'Control Master', 'Program Ready', 'Gripper Temp: -199.7', 'Cryostream Temp: None', 'Ring(mA): 400', 'Beam Available', 'Sample Not Exposed', and 'Governor Message: state SA'.



- standard
- screen
- raster
- vector
- burn
- eScan
- rasterScreen
- stepRaster
- stepVector
- multiCol
- characterize
- ednaCol
- specRaster

protocols

John Skinner  
Jun Aishima



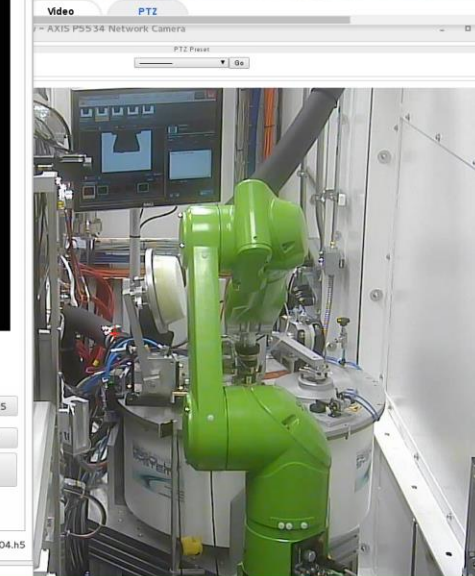
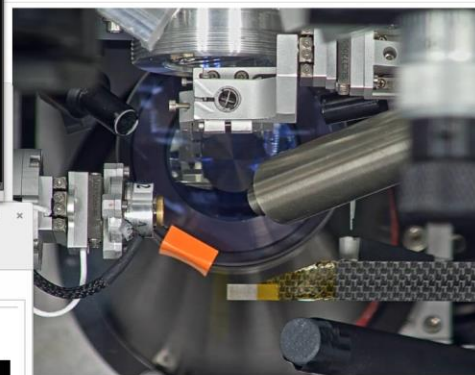
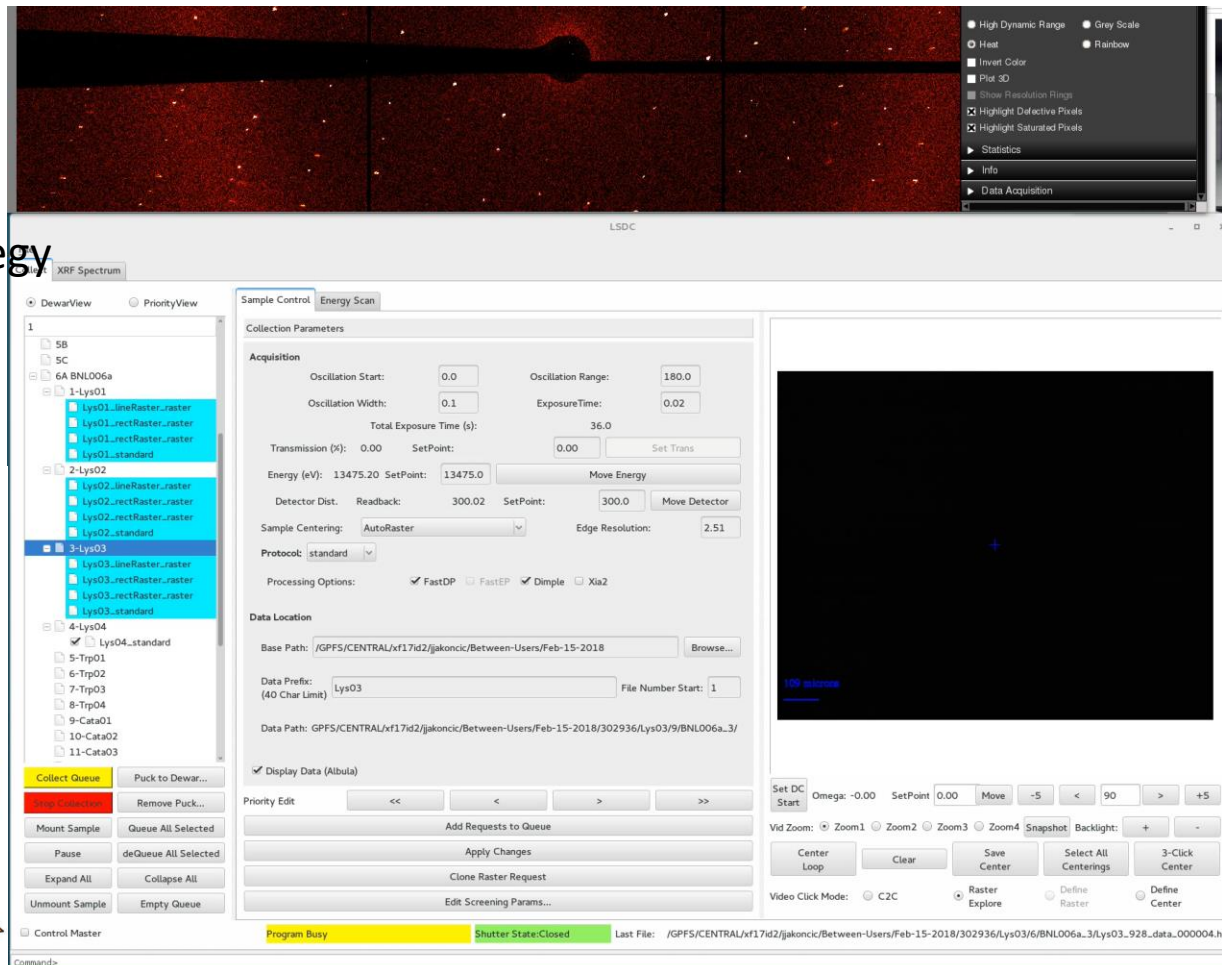
# Fully Automated Data Collection

2 protocols tested and offered to user groups: Auto Collect & Auto Raster  
 loop centering (~140 secs/sample) / crystal centering (~240 sec / sample)  
**Or 25 samples per hour (loop) / 15 samples per hour (crystal)**

Staubli TX60 TX60L  
 Inhouse Gripper  
 24 Unipucks (384 samples)  
 Dewar: (AbsolutSystem)

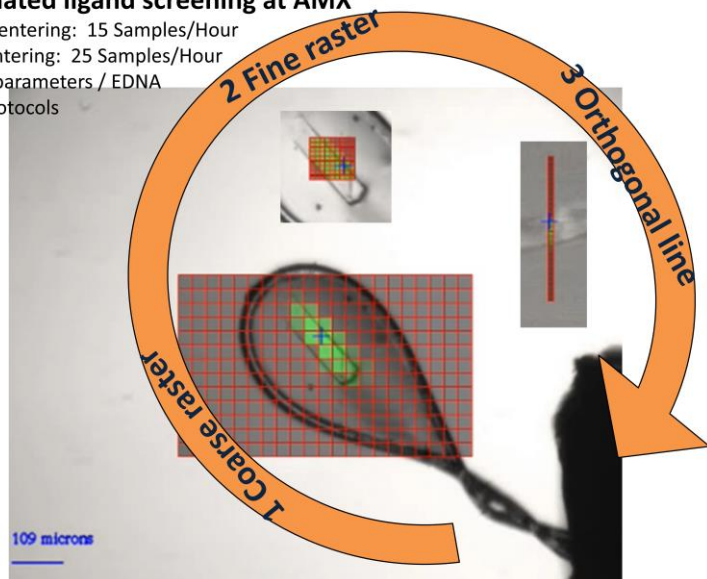
Tons of Data ; Fast file system required  
 Fast feedback required to achieve high  
 throughout

Needs: Better spot finder (**dozor**: done)  
 More protocols (**vector**) / Sorting / Strategy



## Automated ligand screening at AMX

- Crystal centering: 15 Samples/Hour
- Loop centering: 25 Samples/Hour
- Pre-Set parameters / EDNA
- More protocols



Leveraging existing codes:  
 Xrec & C3D; dozor

Movie recorded in 02/2018 National Synchrotron Light Source II

# Automated Data Processing (raster, edna, data reduction, dimple, phasing ...)

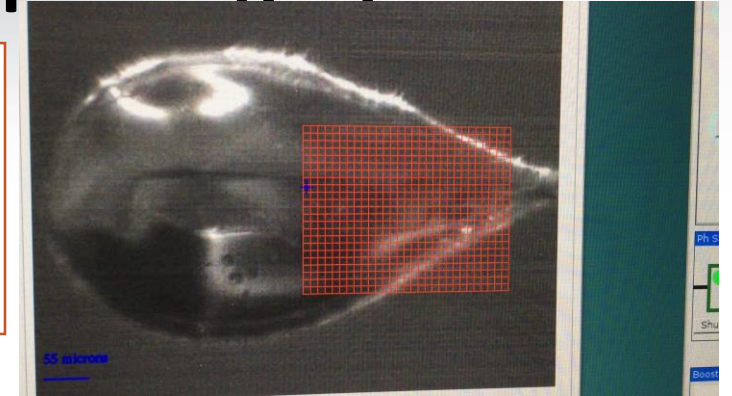
EIGER 9/16M  
(750 Hz 4M ROI)  
AMX / FMX  
Fast buffer (NFS)  
 $\frac{1}{2}$  reduced day (4 TB)  
OC (5 GHz WS)

x40 Gb/s



NSLS-II Computing Facility (august 2018)  
Scalable Storage and Processing Nodes: sustaining growth

Dec 2020  
+  
2 high density nodes  
16 CPUs  
512 cores/1024 threads  
AMD (4 U total)



Optimizing computing hardware and software (inhouse improvements):

3x time speed up for data reduction and ligand binding studies.

Data Reduction: from ~ 90 secs to 30 secs: **fast\_dp\_nslsii** (H. Bernstein, D. Kreitler et al. et JJ)

Dimple: from ~50 secs to 12 secs: **dimple\_nslsii** (H. Bernstein et al. et JJ)

fast\_ep\_nslsii (E. Lazo et al. et JJ)

SDCC  
**Globus** EndPoint  
Jupyter Hub  
Controls Compute Nodes  
Transfer to cloud services ?

Github: <https://github.com/nsls-ii-mx>

- @ NSLS-II central facility: 23 nodes: ~ 720 cores (**56 Gb/s IB** to **GPFS**; 10 Gbs/ node to node)
- @ NSLS-II central facility: 2 x 16 TB SSD fast buffer (NSDs) **GPFS**

Happily share compute resources when AMX and or FMX not in operation **slurm** (D. Hidas):

Accelerator Division, covid-19 (DOE), vina (CBMS work), radiation simulations, SAXs: feel free to reach out if you need access.

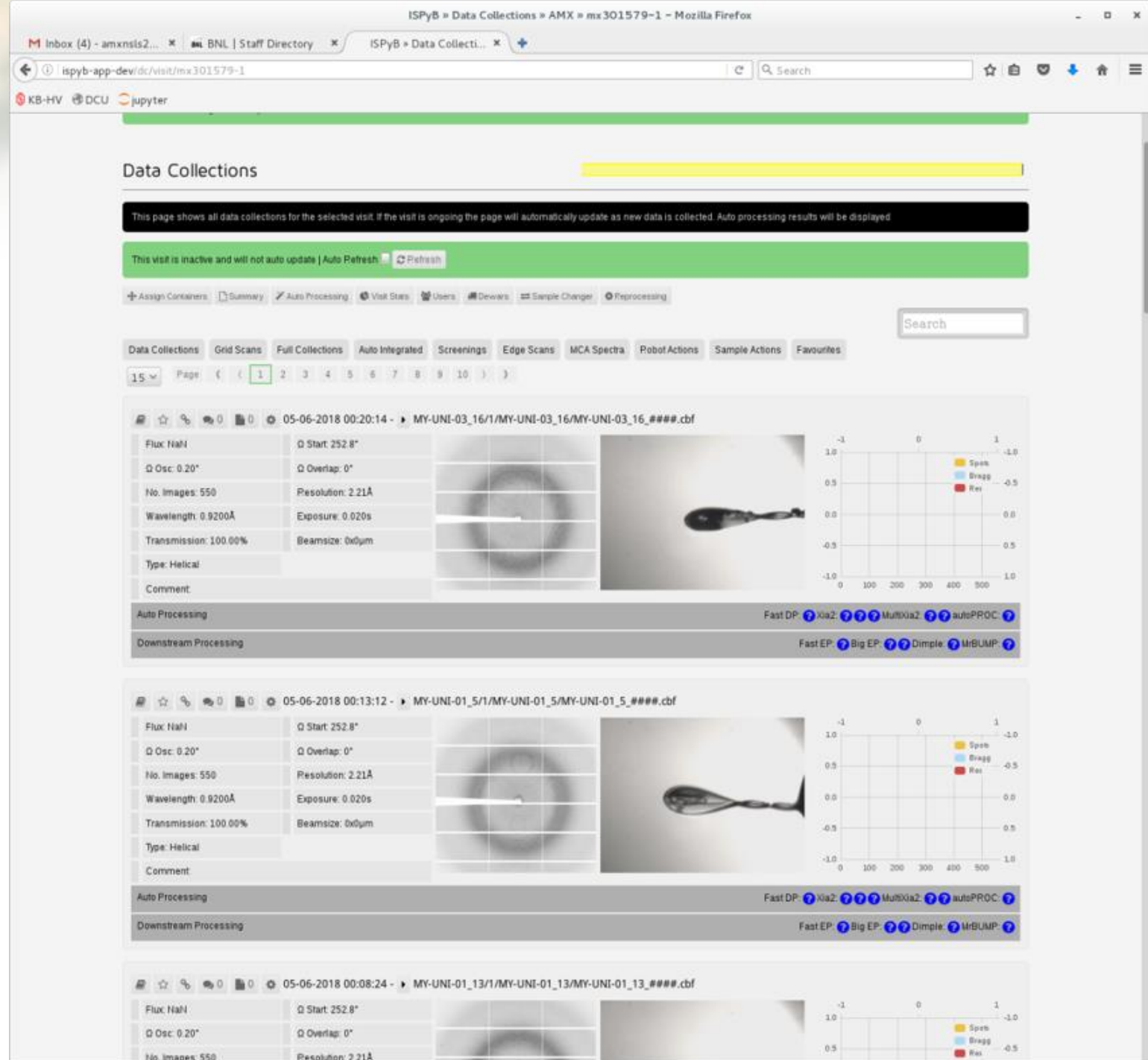


# ISPyB/SynchWeb

- ESRF / DLS
- Monitor data processing results (samples, data)
- Will implement more functions soon

(shipping, reporting ...)

- DLS staff helped install
- ALS installing on MX and SAXs
- **Post Processing ?**



# Overnight with limited support

MONTH	DATE	WeekDay	Operation	AMX morning 9 am - 3 pm	AMX afternoon 4 pm-10 pm	AMX overnight 10 pm - 7 am	FMX morning 9 am - 3 pm	FMX afternoon 4 pm-10 pm	FMX overnight 10 pm - 7 am		
AUGUST	14	Fri	M								
	15	Sat	UO								
	16	Sun	UO								
	17	Mon	S/O								
	18	Tue	O	BAG 305036	DK RA 307462-Training-?)	JJ		BAG 305069 WS	BAG305000-K WS		
	19	Wed	O	BAG 305036 (end@noon)	AS RA 307474 (start@11am)	AS RA 307474 AS	PR 306522	BA BAG 304983	BA BAG 304983		
	20	Thur	O	RA 307474 AS	PR 306519	EL PR 306519	BAG 305000-K, 12 WS	BAG 305043	WS		
	21	Fri	O	BAG 305987	JJ	BAG 305041 JJ	BAG 305037 WS	PR 305587 MF	PR 305587		
	22	Sat	O	BAG 305133	AS/V	BAG 305044 AS/VS	BAG 305990 WS	RA 307474 MF	RA 307474		
	23	Sun	O	GU 306108	EL		RA 307474 until n MF	PR 306519 until 6 MF	RA 307474		
	24	Mon	O		BAG 305000-DK/AS	DK		PR 305587	BA		
	25	Tue	M	Maintenance 6:00 am to 6:00 pm							
	26	Wed	O		BAG 305000-DK	DK	BAG 305000 AS	WS	RA 307504-training - 2h/BAG 30500-QL - 4h		
	27	Thur	O	RA 307484 / PR 306525training	PR 307505	AS	BAG 305000-BA	BA	RA 307504 WS RA 307504		
	28	Fri	O	PR 303851 AS/V	PR 303851	AS	PR 303851 AS	BAG 305046 BA(M)	PR 305587 BA(MF) PR 305587		
	29	Sat	O	PR 306525	JJ		JJ	BAG 305007 WS	BAG 305007 WS		
	30	Sun	O	RA 307484	JJ	PR 303851(?)	JJ	RA 307474 MF	RA 307474 MF		
	31	Mon	O	RA 306558	AS/V	PR 306519	AS	PR 306519 AS	BAG 305069 BA(W) BAG 305013(?) MF		

## NLS-II AMX & FMX User Resources

**How-To and Manuals**

Data collection

- Introduction to the LSDC GUI
- Introduction to data analysis software
- Center a crystal with "Click to Center /C2C"
- Center a crystal with assistance from automated "Center Loop"
- Setup and do a mesh raster scan
- Center a crystal with X-ray (with rasters)
- Do a vertical line raster scan and "Raster Explorer"
- Setup a standard data collection
- Vector scans
  - Setup and do a vector /helical data collection (w/rasters)
  - Setup and do a vector collection with 2 rasters 90 degrees apart
- Energy scans
  - Do an energy edge scan
  - Detailed video

Remote connection

- Remote connection at AMX & FMX using the NX client: Preferred
- Remote connection at AMX & FMX using the web browser

**Tools**

Data processing tools

- NLS-II MX tools on GitHub - fast\_dp, eiger2cif, duple, etc
- Processing Data, re-Processing data from home institutions: slides
- AMX/FMX Data Directory Tree: file
- HKL2000 site definition files
  - AMX def file
  - FMX def file

Sample mounting robot tools

- Spreadsheet template
- Spreadsheet instructions
- Supported picks: Uni-Picks
- Supported sample holders: SPINE caps - these are the only holders supported

Shipping Form

- Shipping instructions and form to be included into your dry shipper

Reporting publications and beamline acknowledgement

- NLS-II Publications
- Please use the CBMS beamline acknowledgement to acknowledge research projects

**Feedback forms**

Give us feedback about your experience at our beamlines: [Structural Biology feedback](#)

**Useful Links**

- AMX (17-ID-1)
- FMX (17-ID-2)
- Center for Biomolecular Structure at Brookhaven National Laboratory

**User Extras** - □ ×

Set Governor State: SE SA DA BL

Current Governor State: state DA

Open Photon Shutter

**Robot**

Unmount Cold Test Robot Recover Robot Dry Gripper

**Zebra (Timing)**

Reset Zebra Reboot Zebra IOC

Arm  Pulse  Downloading  Trigger Sent  Trigger Returned

**Eiger Detector**

Stop Reboot Det IOC

Detector Status: Ready

**Beam**

Sample Flux 2.061410E+11

OK

- Increased demand (academia and PR)
- More online documentations including videos
- Support from home (local contact discretion ~ 10 PM)
- Special overnight manual with most common issues and steps for recovery
- UserScreen functions on LSDC
- FloCos trained to recover robot from collision (part of user training)



# Local Vs Remote NoMachine-NX





# Local Vs Remote

This screenshot shows a local workstation environment. On the left, a terminal window displays the output of a command, listing various system parameters and their values. In the center, a Gmail inbox is visible, showing several email messages with their subjects and senders. On the right, a file explorer window shows the contents of a directory, including files and subdirectories.

This screenshot displays the AMX Staff Screen interface on a remote workstation. The interface is divided into several sections: a central control panel with buttons for 'Start', 'Stop', and 'Reset'; a data readout section on the right showing various parameters like 'DCM Prog', 'DCM Risk', and 'DCM Risk'; and a bottom section with a 'Monitor Detail' panel and a 'Status' panel. The background features a heatmap visualization.

This screenshot shows the AMX User Screen interface on a local workstation. The interface includes a control panel with buttons for 'Start', 'Stop', and 'Reset'; a data readout section on the right showing parameters like 'Energy Int', 'Sample Counting', and 'Edge Resolution'; and a video feed on the left showing a close-up of a component. The interface also includes a 'Sample Control' section and a 'Data Location' section.

This screenshot displays a large heatmap visualization on a remote workstation. The heatmap shows a distribution of values across a grid, with a color scale ranging from blue (low) to red (high). The interface also includes a control panel with buttons for 'Start', 'Stop', and 'Reset'; a data readout section on the right showing parameters like 'Energy Int', 'Sample Counting', and 'Edge Resolution'; and a 'Monitor Detail' panel at the bottom.





# Local Vs Remote

QHD: 2560x1440

The screenshot displays the LSDC (Local Synchrotron Data Collection) interface. The main window is titled "LSDC" and shows various control panels. On the left, there is a "Collect" panel with a list of sample positions (1A-8C) and buttons for "Collect Queue", "Mount Sample", "Pause", "Queue All Selected", "User Screen...", "Warmup Gripper", "Stop Collection", "Unmount Sample", "Close Photon Shutter", "deQueue All Selected", "Empty Queue", and "Restart Server". The central panel is "Sample Control | Energy Scan" and contains "Collection Parameters" for Acquisition (Oscillation Start, Range, Width, Exposure Time, Stills, Transmission, Energy, Sample Centering, Protocol, Vector Start/End, Number of Wedges, Length, Speed, AutoProcessing, FastDP, FastEP, Dimple) and "Data Location" (Base Path, Data Prefix, File Number Start, Data Path). Below this are "Priority Edit" buttons and a "Control Master" status bar. The right side of the interface shows a "Movie Mode" window titled "EIGER Monitor" displaying a grid of diffraction patterns with labels for different wavelengths: 2.1 Å, 2.5 Å, 3.4 Å, and 6.3 Å. The bottom of the screen shows a terminal window with a shell prompt and commands like "ls" and "lsdcGuiLog.txt".



# Local Vs Remote

UHD: 3840x2160

Applications Menu ALBULA LSC jjakoncic@xf17id2-ws... jjakoncic@xf17id2-ws... LSC

Collect | XRF Spectrum

Sample Control | Energy Scan

Collection Parameters

Acquisition

Oscillation Start: [ ] Oscillation Range: 180.0

Oscillation Width: [ ] ExposureTime: [ ]

Transmission (0.0-1.0): 0.251 SetPoint: 0.6 BeamSize: v0+0

Energy (eV): 13475.30 SetPoint: 13475.00 Detector Dist.: 250.00 SetPoint: 250.00

Sample Centring: Interactive Edge Resolution: [ ]

Protocol: standard raster vector standard

Vector Start [ ] Vector End [ ] Number of Wedges 1 Length(microns): [ ] Speed(microns/s): [ ]

AutoProcessing On FastDP FWHM Dimple

Data Location

Base Path: /GPFS/CENTRAL/xf17id2/PR-306519\_Remote\_31August2020

Data Prefix: [ ] File Number Start: [ ]

Data Path: [ ]

Display Data (Albula)

Priority Edit << < > >>

Add Requests to Queue

Apply Changes

Clone Raster Request

Edit Raster Params...

SetStart Omega: 0.00 SetPoint: 0.00 -5 < > 90 > +5

Center Loop Clear Save Center Select All Centerngs 3-Click Center Snapshot Hide Rasters

Video Click Mode: C2C Raster Explore Define Raster Define Center

Control Master Program Ready Gripper Temp: 4.00 Cryostream Temp: None Ring(A): 400 Sample Not Exposed Governor Message: state SE

File: /GPFS/CENTRAL/xf17id2/PR-306558\_Remote\_31Aug2020/mx306558-2/impro-Eb54/SBC-007\_Simpro-Eb5\_Raster\_3034\_data\_000007.h5

ALBULA

File Synchroniz Auto Load Help

Movie Mode Watch Series EIGER Monitor

View

View

Histogram

Background: 0.0000 Foreground: 4.0000

# Pixels <= BG: 7193166

BG < # Pixels < FG: 2317895

# Pixels >= FG: 18068

High Dynamic Range Grey Scale

Heat Rainbow

Invert Color

Plot 3D

Show Resolution Rings

Highlight Defective Pixels

Highlight Saturated Pixels

Statistics

Info

Data Acquisition

```
jjakoncic@xf17id2-ws4: /GPFS/CENTRAL/xf17id2/PR-306519_Remote_31August2020
jjakoncic@xf17id2-ws4: /GPFS/CENTRAL/xf17id2/PR-306519_Remote_31August2020 Box10
jjakoncic@xf17id2-ws4: /GPFS/CENTRAL/xf17id2/PR-306519_Remote_31August2020 ls
AMX-Aug31.xls lscGuiLog.txt lscServerLog.txt
jjakoncic@xf17id2-ws4: /GPFS/CENTRAL/xf17id2/PR-306519_Remote_31August2020 lscGuiRemote
jjakoncic@xf17id2-ws4: /GPFS/CENTRAL/xf17id2/PR-306519_Remote_31August2020 Mon Aug 31 15:57:44 2020
importSpreadsheet("/GPFS/CENTRAL/xf17id2/PR-306519_Remote_31August2020/AMX-Aug31.xls")
```

# Communications: training / beamtime

Staff to Staff: teams (various teams, meetings, video chats ...)

Staff to Staff during user beamtime: group SMS (works “well”)

User <-> Staffs: chat ([amxnsls2](#), [fmxnsls2](#)...) + **bnl.gov emails**

All AMX staff have access to chat, all necessary files shared across beamlines (AMX/FMX)

For **training of new users**: video chat using a beamline iPod touch (wifi; teams ...)

zoom on staff laptops (remote connection to collect data etc ...)

All remote users are required to obtain a bnl domain account including bnl email

Could users use teams as well ?

All chats, email used for transferring data in Globus are stored in a spreadsheet shared between the 2 MX beamlines. (future database)

We see significant increased throughput for returning users (“unprecedented number of samples”)



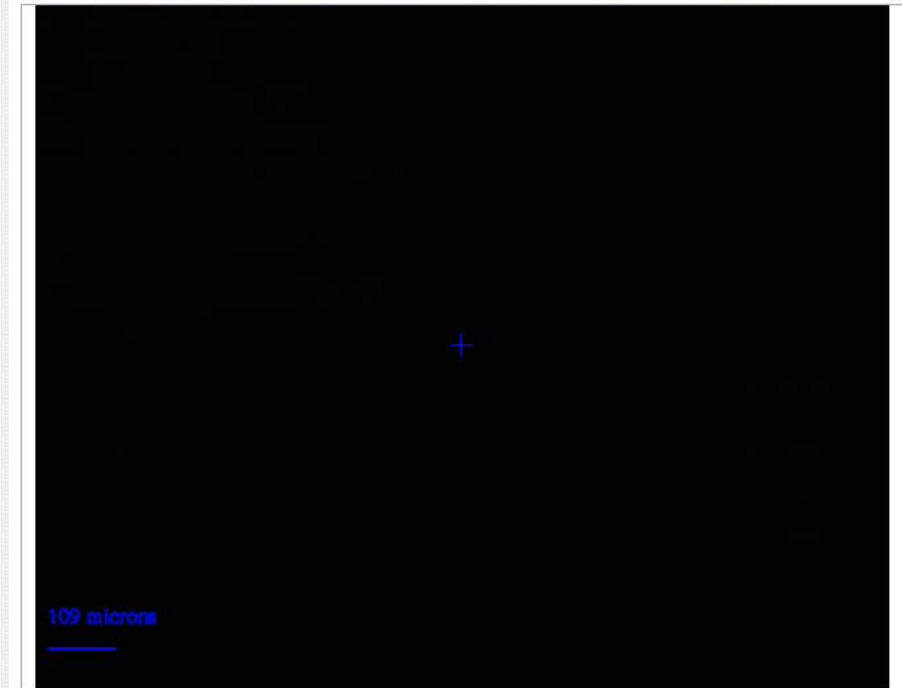
# Remarks & Acknowledgements

Large number of samples (expert PR user)  
High throughput for  $\sim 1 \text{ \AA}$  resolution of SARS-CoV-2 protein target:  
100's of very high resolution

testament that remote access can work and deliver *near* onsite experience

We do see decreased remote access performances (NX limitations / bandwidth)

- LS: AMX, FMX, LIX, CryoEM and all staff
- Herbert (HDRMX)
- Operations support
- ESH group
- ICT group DAMA/SDCC
- Shipping and Receiving 740
- Accelerator staff



SetStart Omega: 0.00 SetPoint 0.00 -5 < 90 > +5

Mag1  Mag2  Mag3  Mag4 Focus + - Light + - Anneal Time 0.5

Center Loop Clear Save Center Select All Centerings 3-Click Center SnapShot  Hide Rasters

Video Click Mode:  C2C  Raster Explore  Define Raster  Define Center