

MX Software Developments at LNLS (Sirius)

Rafael Lyra, Pedro Benetton
Beamline Support Group/Staff Members
On Behalf of LNLS (Sirius)



MXCuBE3 Web

Currently in Production

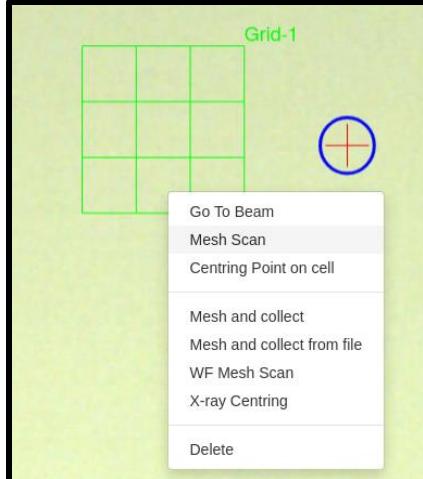
- Bluesky Integration: Gridscan, Flyscan, XRF
- Automatic crystal snapshots saving
- Integration with prefect for post-processing: dozor, PyMca, XDS, Phaser, dimple, PanDDA
- Bug fixes for previous workarounds done in the past





Timestamp: 2025-08-27 23:18:27 Timestamp: 2025-08-27 23:18:27 Timestamp: 2025-08-27 23:18:28

Prefix: no	Prefix: no	Prefix: no
Run Number: 4	Run Number: 4	Run Number: 4
Image: 1	Image: 2	Image: 3



Grid-1

- Go To Beam
- Mesh Scan
- Centring Point on cell
- Mesh and collect
- Mesh and collect from file
- WF Mesh Scan
- X-ray Centring
- Delete

XRF

Path: /ibira/Lnls/beamlines/manaca/proposals/00000000/data/20251104/xrf/xrf/

Filename:

Subdirectory

Prefix

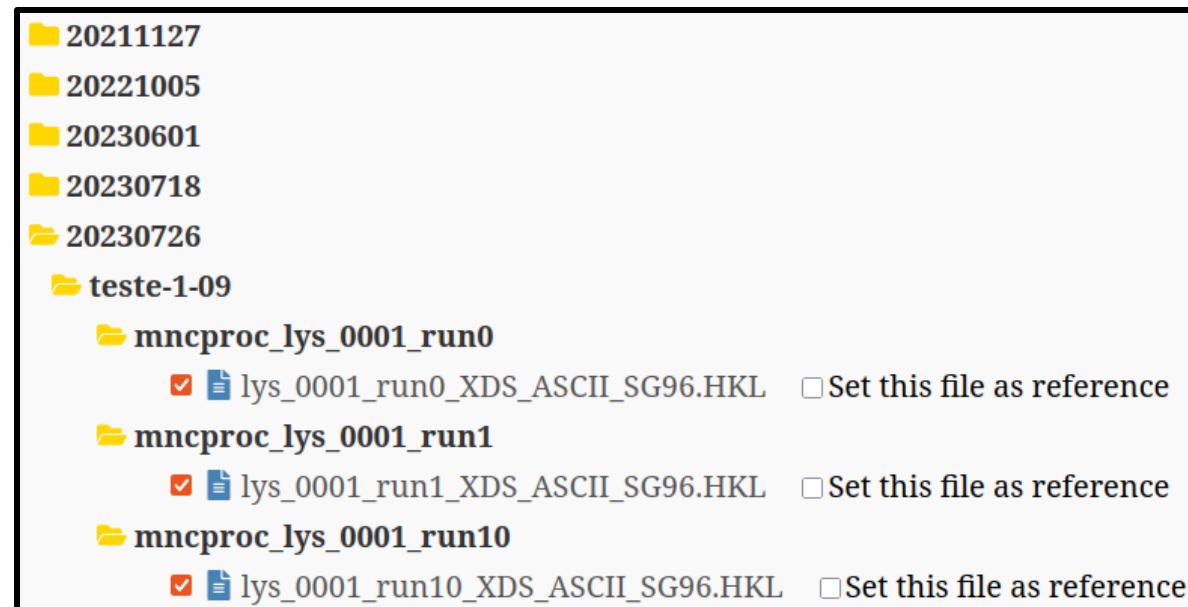
Count time (s)

Run Now **Add to Queue**

Beamline Developments

Data Collection/Processing

- Initial developments on fragment screening experiments since early 2025
- Data Processing scripts more versatile: phasing, fragment screening pipeline, option for merging HKL files



Beamline Developments

Web Applications

- MANACÁ-Autoproc Web: a Web application for data processing/results visualization

Select an Image Path:

[Open Image Viewer on Selected image Path](#) [Open Snapshot Viewer on Selected image Path](#)

Number of Images:

Use Space Group and Unit Cell Default Options Set Space Groups and Unit Cell Options

Use Resolution Limit Default Options Set Resolution Limit Options

No Phasing
 MR
 SAD
 RBR
 MR for Multiple Sequences - PDB
 MR for Multiple Sequences - Fasta
 MR with DIMPLE

No phasing option has been selected

Use MNC partition Use CPU partition Use single machine (Dorothy)

Number of CPUs:

Available CPUs at mnc partition: 320
Available CPUs at cpu partition: 48

[Check CPU availability](#) [Click here if you don't know what this means](#)

[Start Process](#)

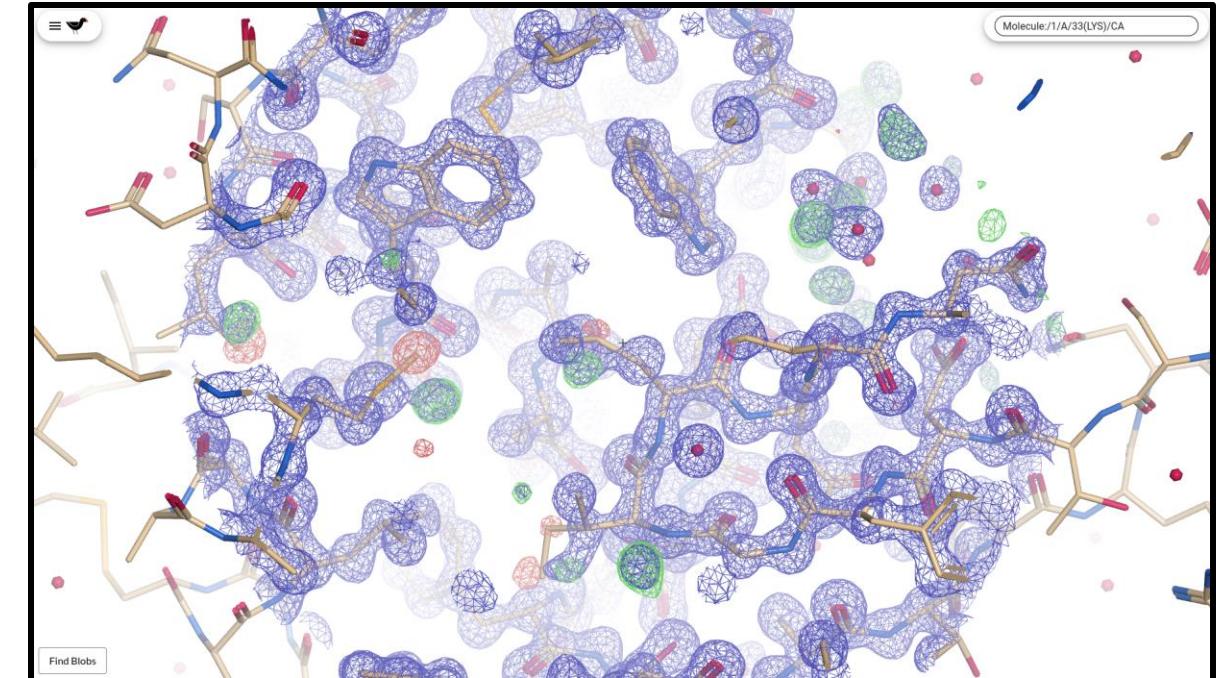
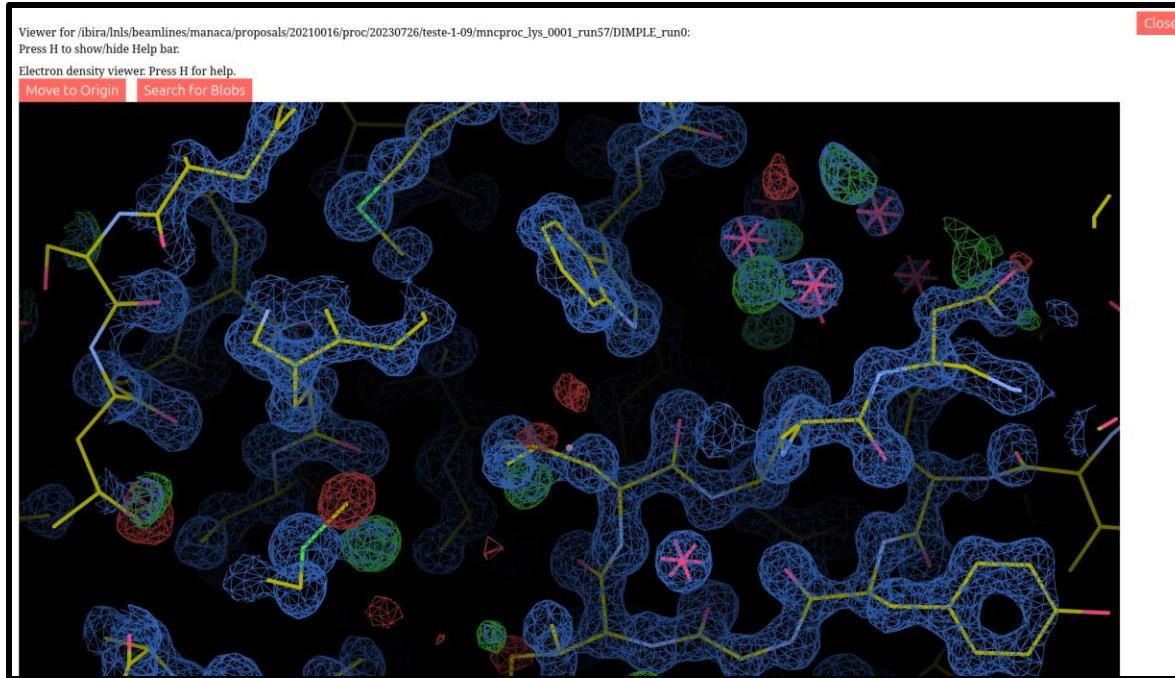
Experiment Reference (Puck ID)										Date/Time of Processing	Actions					
CPS-4611-1-05	0	0	3600	XDS, MR	0.5384	01/06/2023 12:32:38	Copy Log Path	Plot Data	View Table	HTML File	Phasing Options	Download Main Files	Download All Files			
CPS-4611-1-05	0	1	1000	XDS	---	19/09/2023 15:21:34	Copy Log Path	Plot Data	View Table	HTML File	Phasing Options	Download Main Files	Download All Files			

[Day of Data Acquisition: 27/11/2021](#)
[Day of Data Acquisition: 05/10/2022](#)
[Day of Data Acquisition: 01/06/2023](#)

Beamline Developments

Web Applications

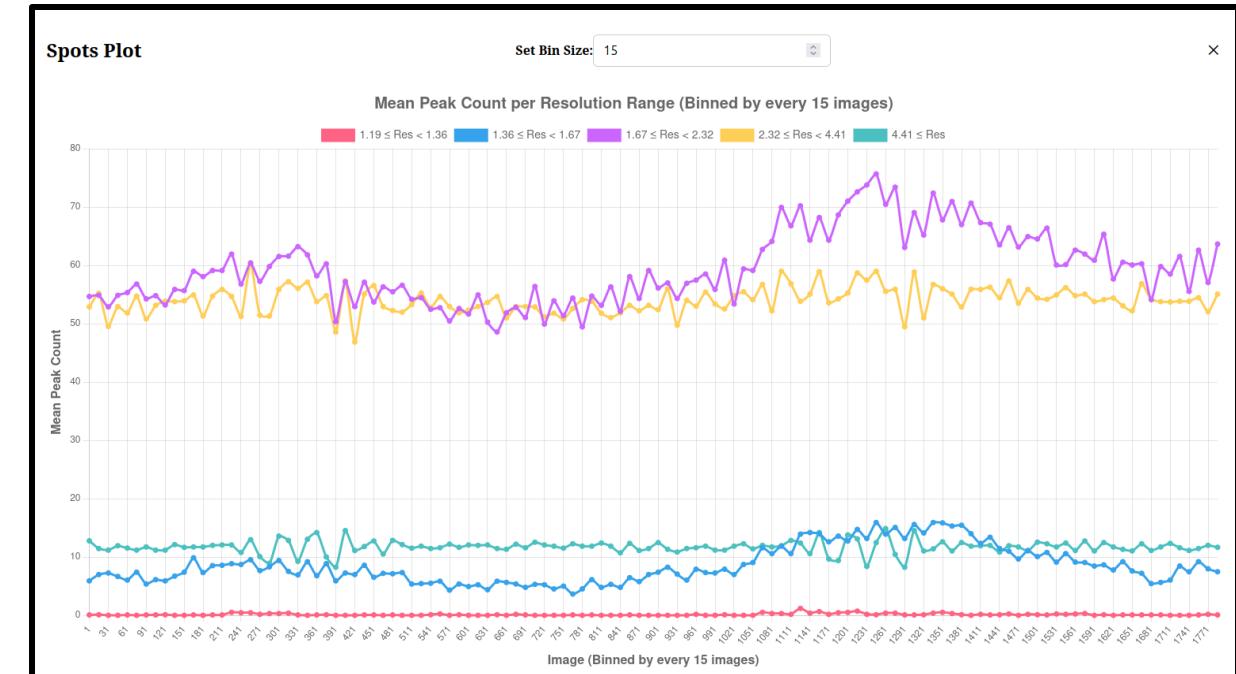
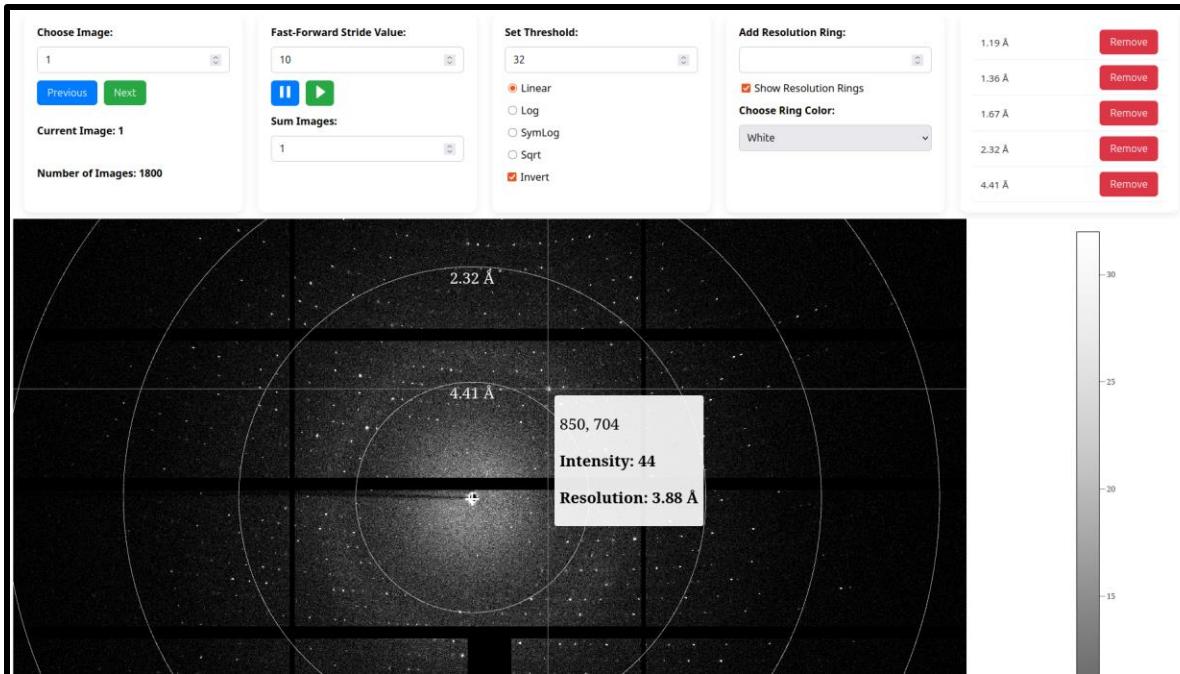
- MANACÁ-Autoproc Web: Uglymol and Moorhen for results validation/refinement



Beamline Developments

Web Applications

- ARARA: image viewer with @h5web/lib, image analysis tools (xds, dials)
- github.com/cnpem/arara



Beamline Developments

Web Applications

- Manacá-Proposals: defining experiment type and submitting pdb files
- Web Puck ID: monitoring data collection and setting a pdb file to a puck/sample, so that the processing pipeline can perform phasing methods

All Proposals

Search by proposal number...

Proposal Number	Proposal Dates	Proposal Type	Action
20253444	Show	protein	Protein Confirm
20253416	Show	fragment_screening	Fragment screening Confirm
20253410	Show	prot_lig	Prot Lig Confirm
20253400	Show	protein	Protein Confirm
20253399	Show	protein	Protein Confirm

Fragment screening Info for Proposal 20253416

Project Name: Enter project name PDB File: Browse... No file selected.

Project Name	PDB File	Action
AME_lig_cryo_trap	6UAQ.pdb	

Select the proposal: None

No Proposal

Select a global project: None

Current: None

Select the pucks

Puck ID 1: CPS-4613 Project to puck 1: None
CPS-4613 (from PV) No Project

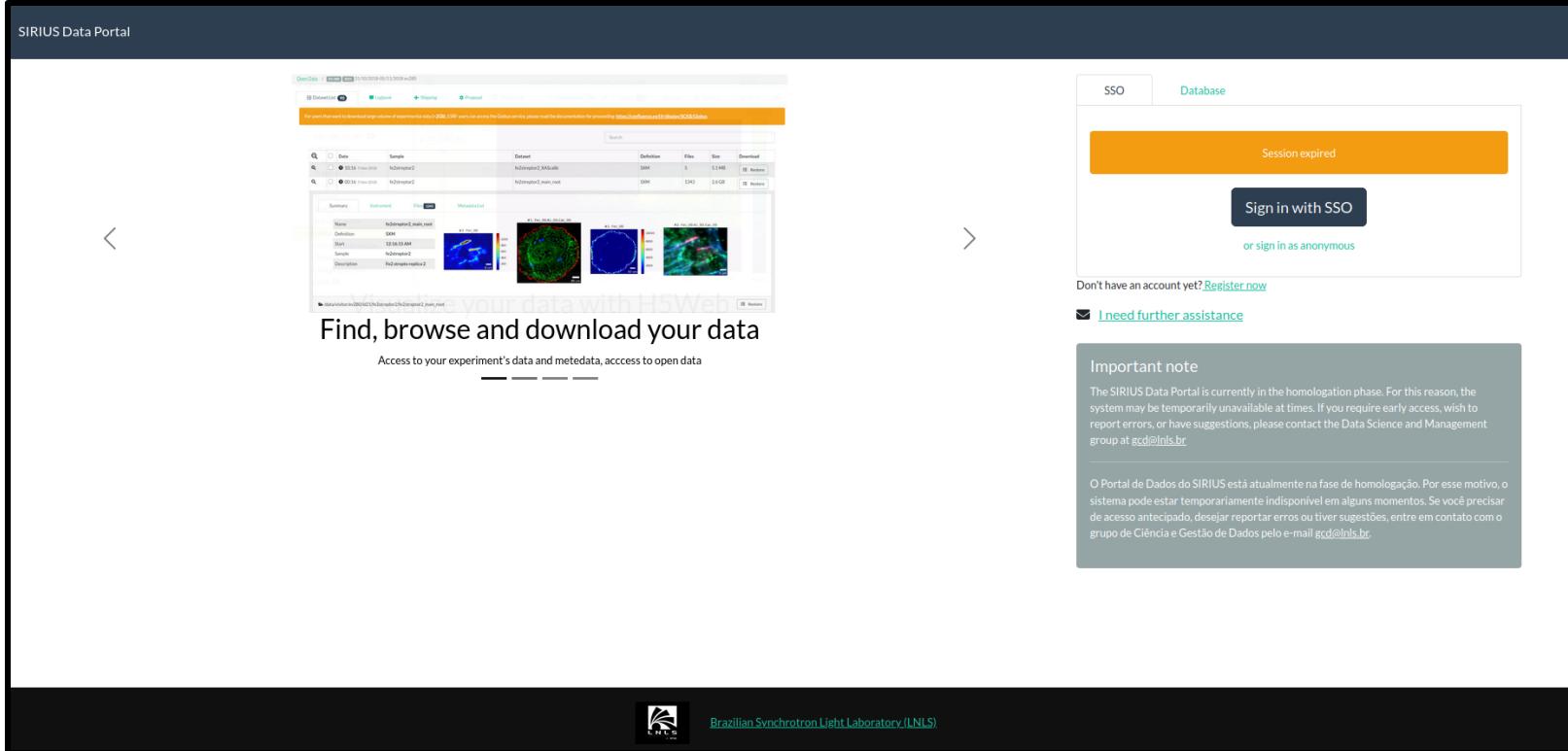
Puck ID 2: CPS-4614 Project to puck 2: None
CPS-4614 (from PV) No Project

Puck ID 3: CPS-2977 Project to puck 3: None
CPS-2977 (from PV) No Project

Beamline Developments

LIMS

- Sirius Data Portal (Local instance of ICAT Project)
- Initial developments by the data science management group (allan.pinto@lnls.br)



The screenshot displays two main sections of the SIRIUS Data Portal. On the left, the 'Dataset' page shows a table of datasets with columns for Date, Sample, Dataset, Definition, File, Size, and Download. One dataset is highlighted: 'h2Sirius2_main' with a 'SOM' definition, 5 files, 1.14MB size, and 16 downloads. Below the table are four thumbnail images of microscopy images. A banner at the bottom reads 'Find, browse and download your data'. On the right, a 'Session expired' message is shown, with a 'Sign in with SSO' button and an 'or sign in as anonymous' link. Below this, there's a 'Register now' link and an 'Important note' section. The 'Important note' section states: 'The SIRIUS Data Portal is currently in the homologation phase. For this reason, the system may be temporarily unavailable at times. If you require early access, wish to report errors, or have suggestions, please contact the Data Science and Management group at gcd@lnls.br'. At the bottom, the LNLS logo and the text 'Brazilian Synchrotron Light Laboratory (LNLS)' are visible.

MXCuBE4 Web

Under Development

- Early stages of development
- Emphasis on much cleaner code and proper collaboration with the community
- Integration with our local instance of ICAT
- Single Sign-On Login implemented
- Improved version of EPICSMotors and EPICSActuator classes
- Usage of YAML configuration files
- Suggestion: .env files at core/configuration folders?
- Suggestion: flowcharts for documentation (we did it while studying MXCuBE and it was very useful)
- Mxcubeweb repository is crashing for us if pulled beyond a certain commit

Conclusion

- Major implementations and bug fixes at MXCuBE3, which should, on the next few months, reach a stable version
- Web Applications that can help with data visualization/processing while ICAT is not fully implemented
- Early stages of Sirius Data Portal for our participation in the ICAT Project
- Early stages of development of MXCuBE4, maintaining code quality and collaboration standards

Thank You

Pedro Benetton

pedro.benetton@lnls.br

+55 (19) 99736-1104

MANACÁ beamline

Ana Júlia Zangrandi (XRF)
Guilherme Aun (LIMS)

cnpem.br

Control Software

Ana Clara Souza
Rafael Lyra

Data Science Management

Allan da Silva Pinto
Paulo Baraldi Mausbach



CNPEM
Brazilian Center for Research
in Energy and Materials

MINISTRY OF
SCIENCE TECHNOLOGY
AND INNOVATION

