

MX Software Developments at LNLS (Sirius)

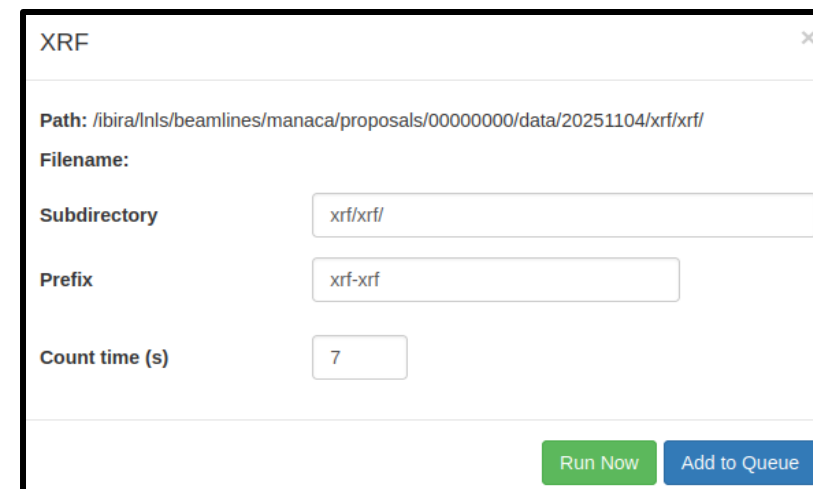
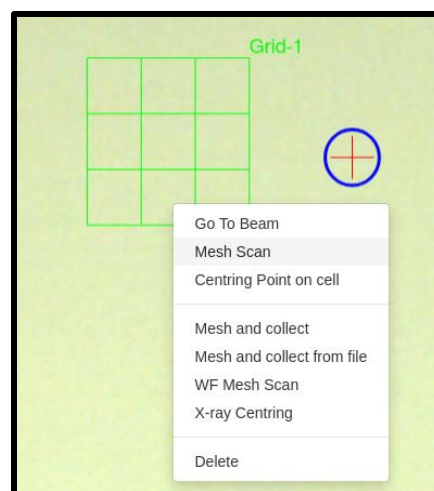
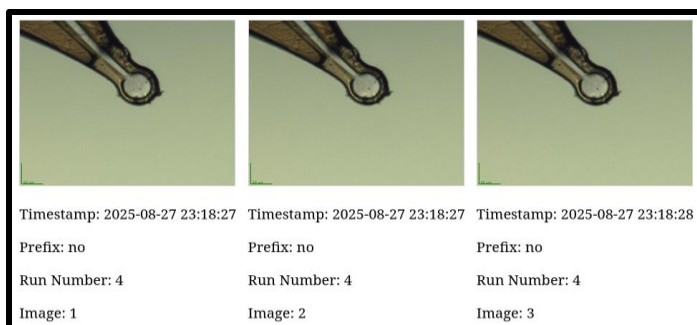
Rafael Lyra, Pedro Benetton
*Beamline Support Group/Staff Members
On Behalf of LNLS (Sirius)*



MXCuBE3 Web

Currently in Production

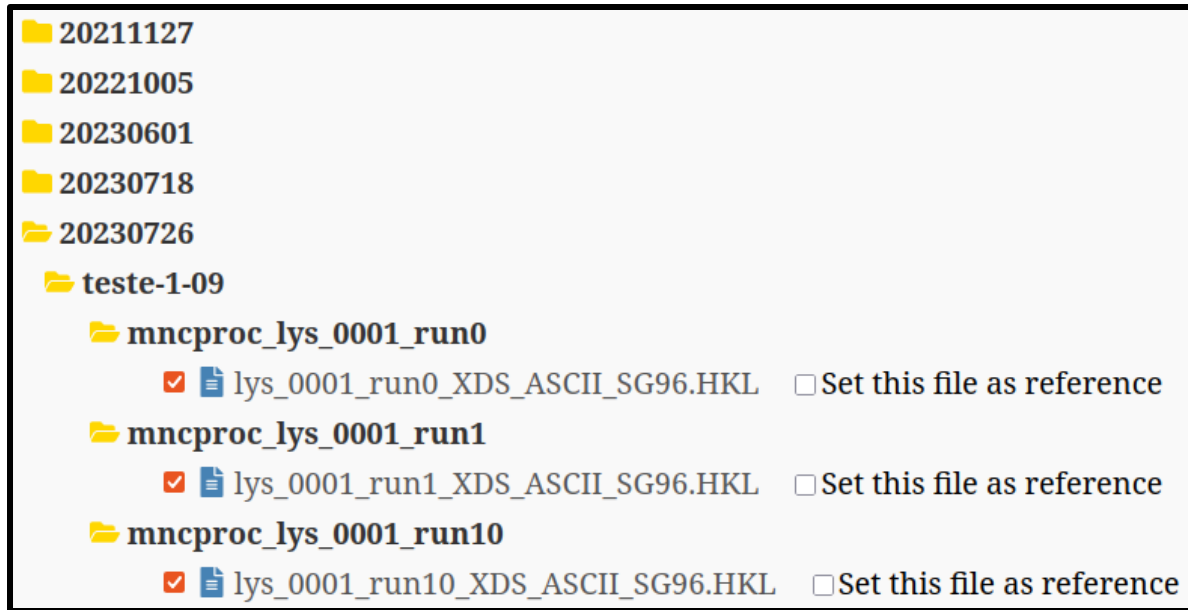
- Bluesky Integration: Gridscan, Flyscan, XRF
- Automatic crystal snapshots saving
- Integration with prefect for post-processing: dozor, PyMca, XDS, Phaser, dimple, PanDDA
- Bug fixes for previous workarounds done in the past



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



CNPEM

- 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](#)

→ Day of Data Acquisition: 27/11/2021

→ Day of Data Acquisition: 05/10/2022

🔦 Day of Data Acquisition: 01/06/2023

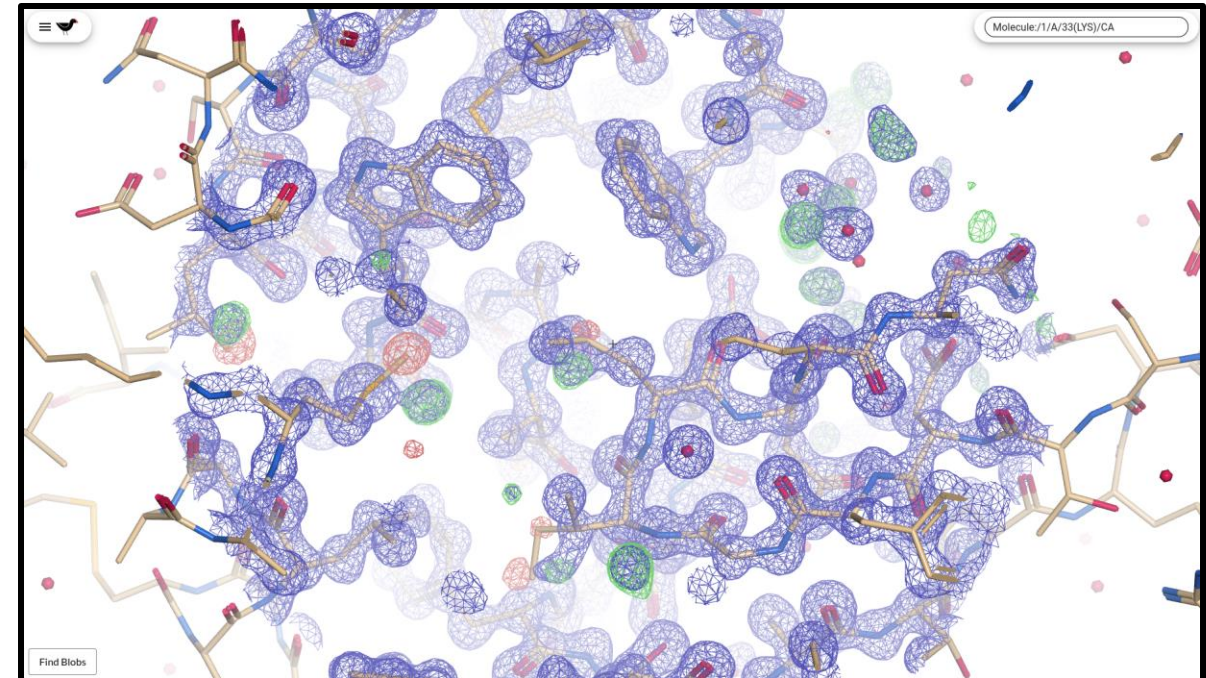
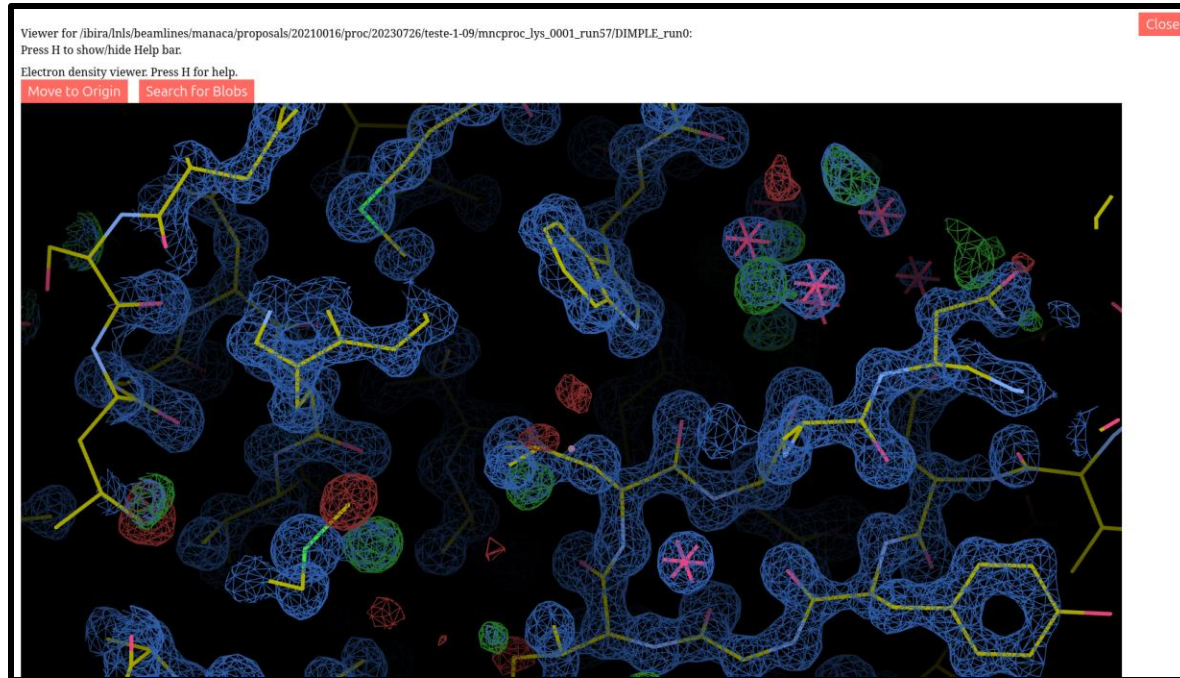
Experiment Reference (Puck ID)	Dataset Number	Run Number	Number of Images	Process Status	R-Free	Date/Time of Processing	Actions						
CPS-4611-1-05	0	0	3600	XDS, MR	0.5384	01/06/2023 12:32:38	Copy Log Path	Plot Data	View Table	HTML File	Phasing Options	Download Main Files	Download All Files
CPS-4611-1-05	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: 26/07/2023

Beamline Developments

Web Applications

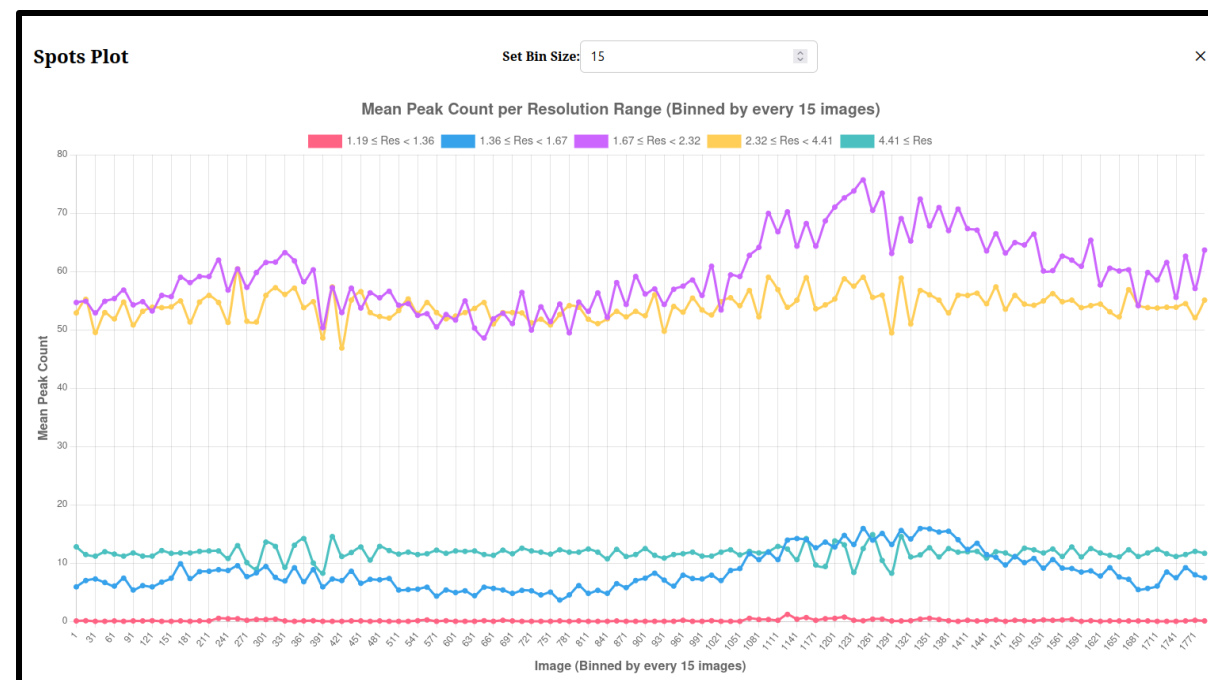
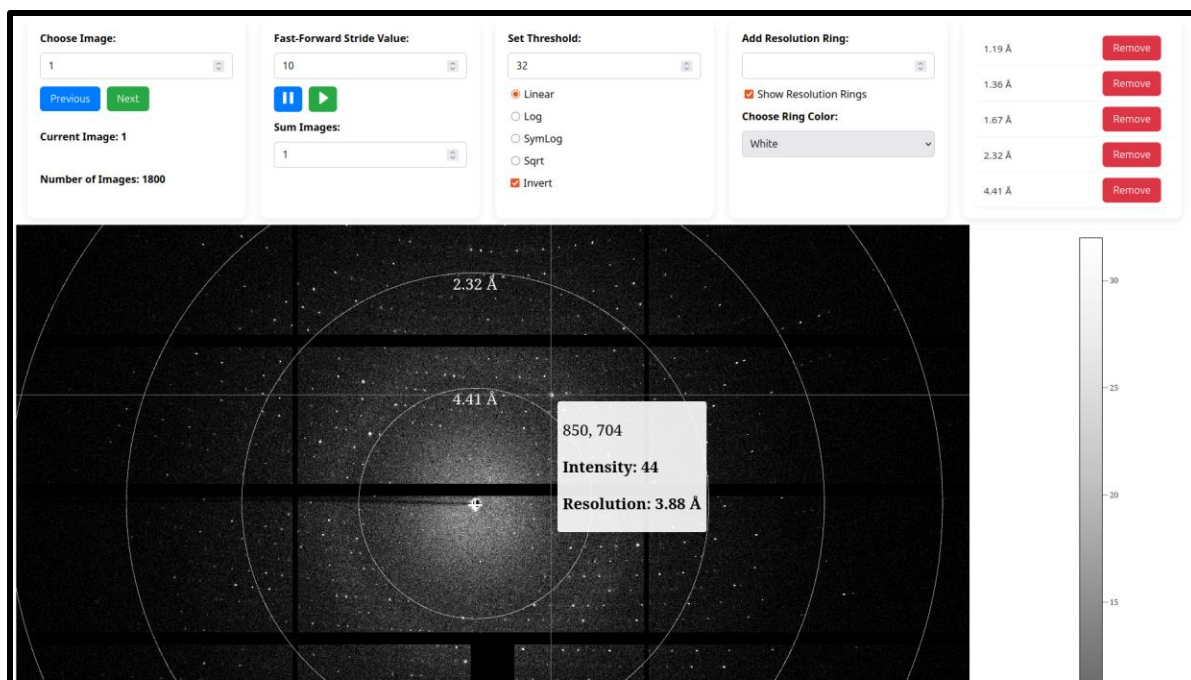
- MANACÁ-Autoproc Web: Uglymol and Moorhen for results validation/refinement



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: PDB File: No file selected. [Save](#)

Project Name	PDB File	Action
AME_lig_cryo_trap	6UAQ.pdb	

[Close](#)

Select the proposal: None

Select a global project: None

Select the pucks

Puck ID 1: CPS-4613

Project to puck 1: None

Puck ID 2: CPS-4614

Project to puck 2: None

Puck ID 3: CPS-2977

Project to puck 3: None

[Show Proposal Xlsx sheet](#)

Beamline Developments

LIMS



CNPEM

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

SIRIUS Data Portal

Find, browse and download your data

Access to your experiment's data and metadata, access to open data

Session expired

Sign in with SSO

or sign in as anonymous

Don't have an account yet? [Register now](#)

[I need further assistance](#)

Important note

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.

O Portal de Dados do SIRIUS está atualmente na fase de homologação. Por esse motivo, o sistema pode estar temporariamente indisponível em alguns momentos. Se você precisar de acesso antecipado, deseja reportar erros ou tiver sugestões, entre em contato com o grupo de Ciência e Gestão de Dados pelo e-mail gcd@lnls.br.

Brazilian Synchrotron Light Laboratory (LNLS)

MXCuBE4 Web

Under Development



CNPq

- 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)

Control Software

Ana Clara Souza

Rafael Lyra

Data Science Management

Allan da Silva Pinto

Paulo Baraldi Mausbach

cnpem.br



CNPem
Brazilian Center for Research
in Energy and Materials

MINISTRY OF
SCIENCE TECHNOLOGY
AND INNOVATION

