MX Software Developments at LNLS (Sirius)

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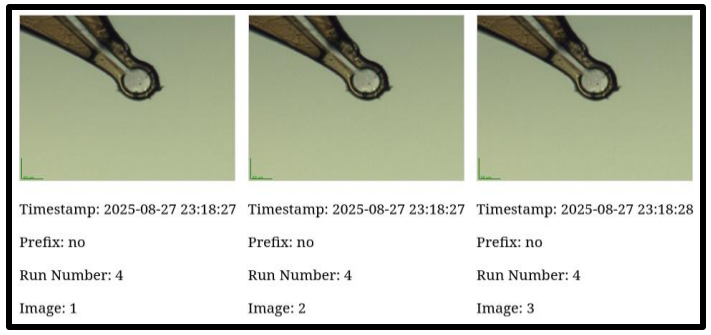
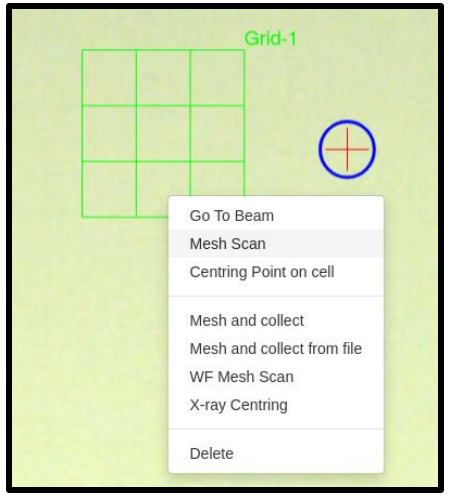
Beamline Support Group/Staff Members
On Behalf of LNLS (Sirius)

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

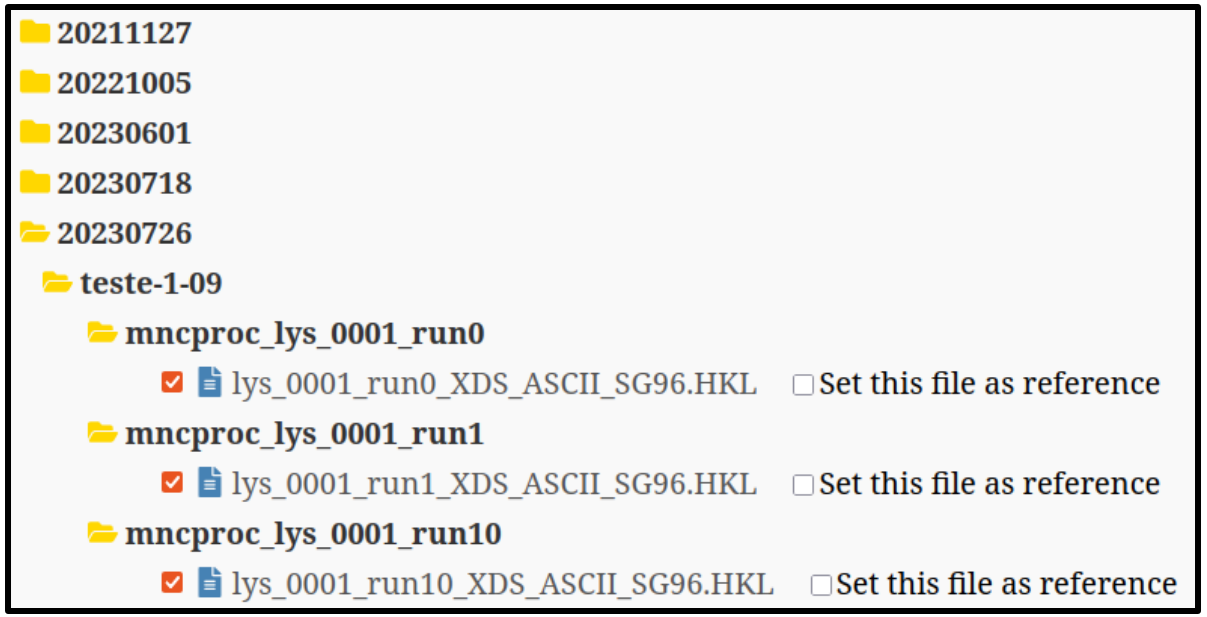




Beamline Developments

Data Collection/Processing

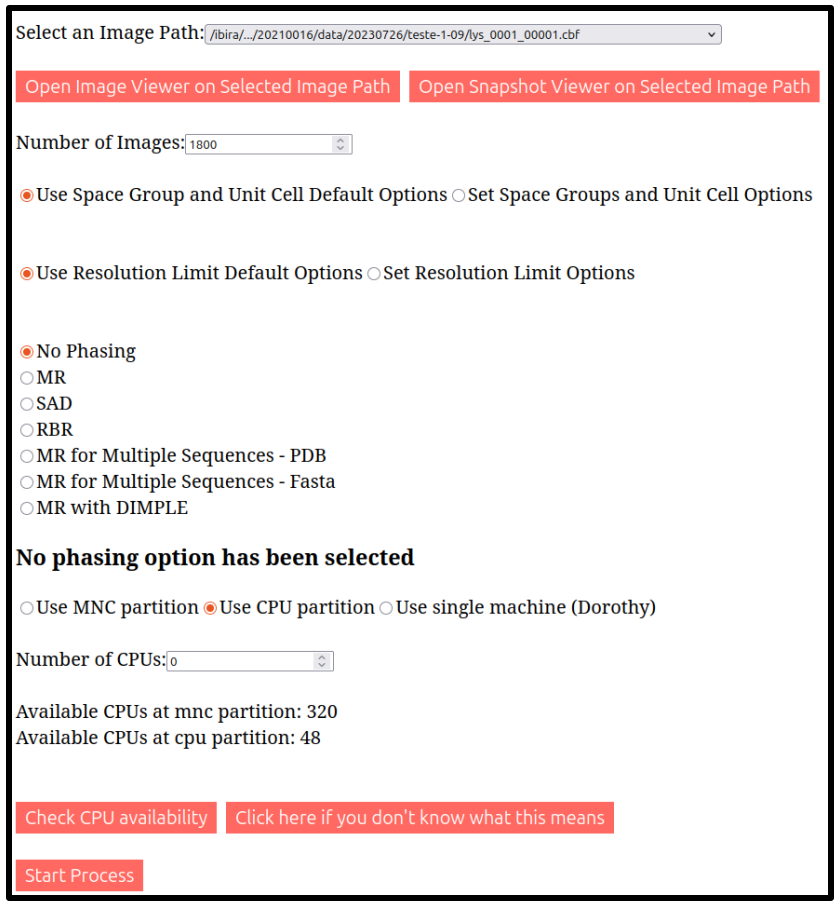
- Initial developments on fragment screening experiments since early 2025
- Data Processing scripts more versatile: phasing, fragment screening pipeline, option for merging HKL files

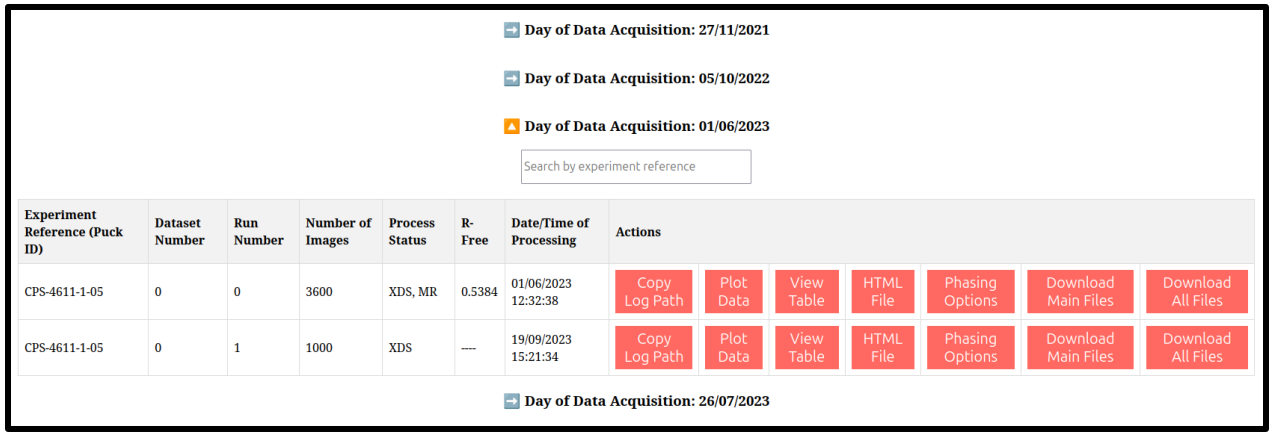


Beamline Developments

Web Applications

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

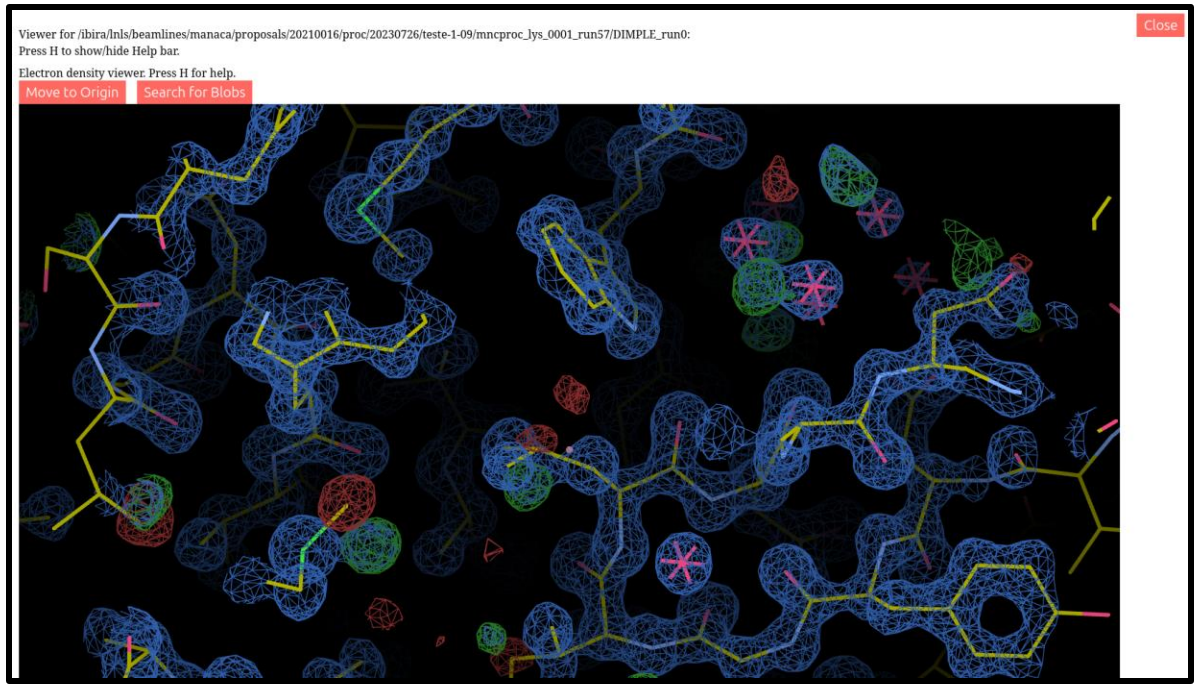


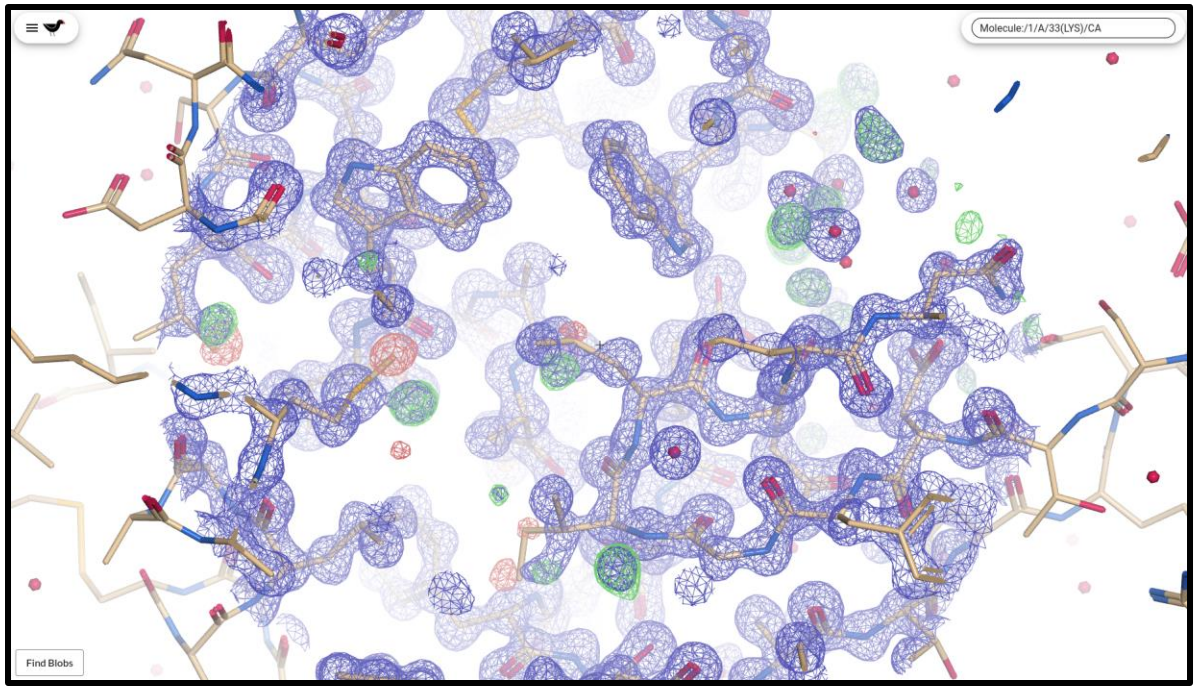


Beamline Developments

Web Applications

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

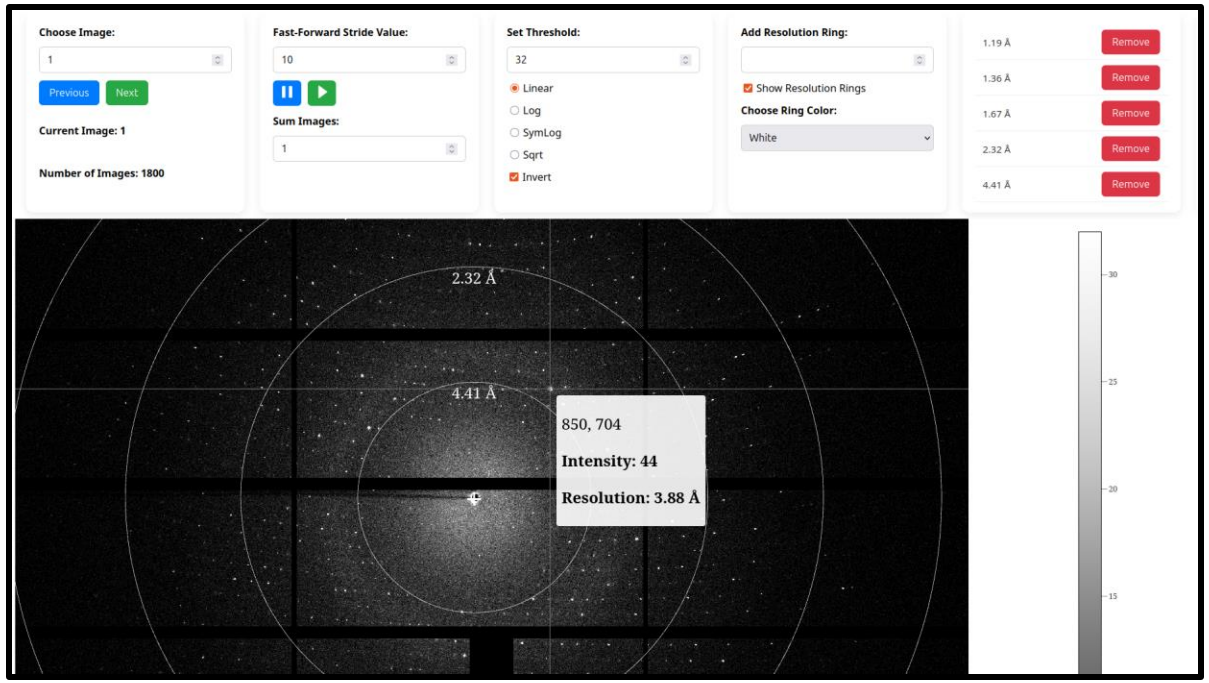


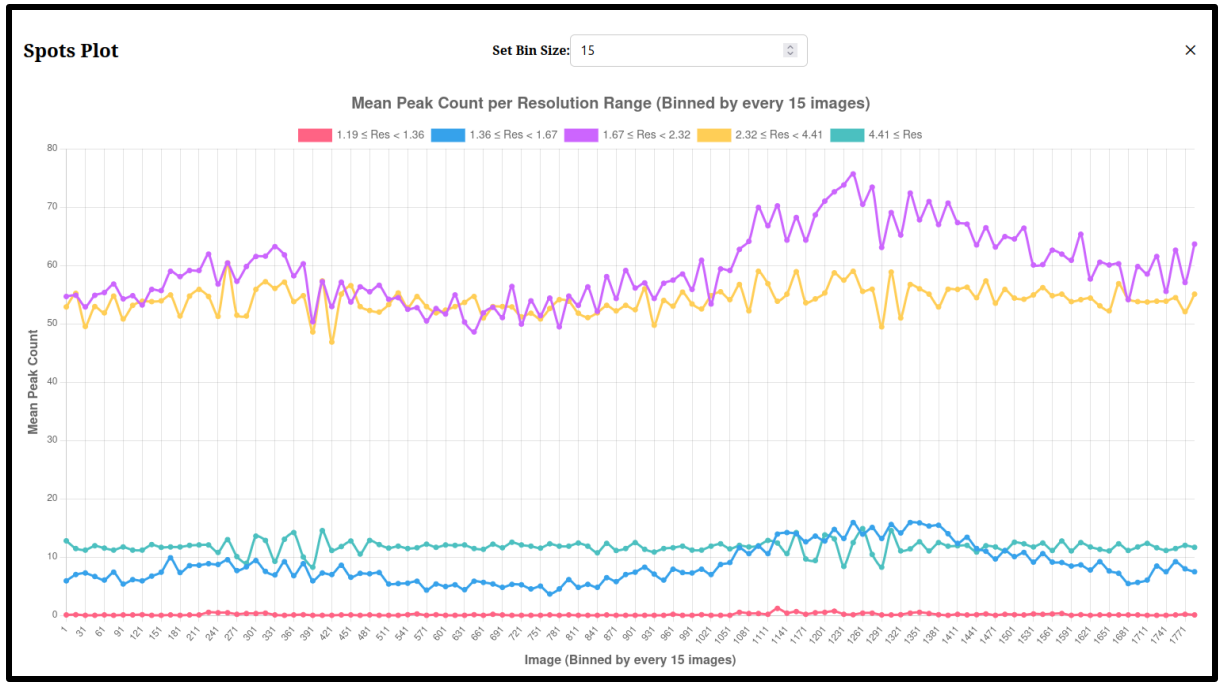


Beamline Developments

Web Applications

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

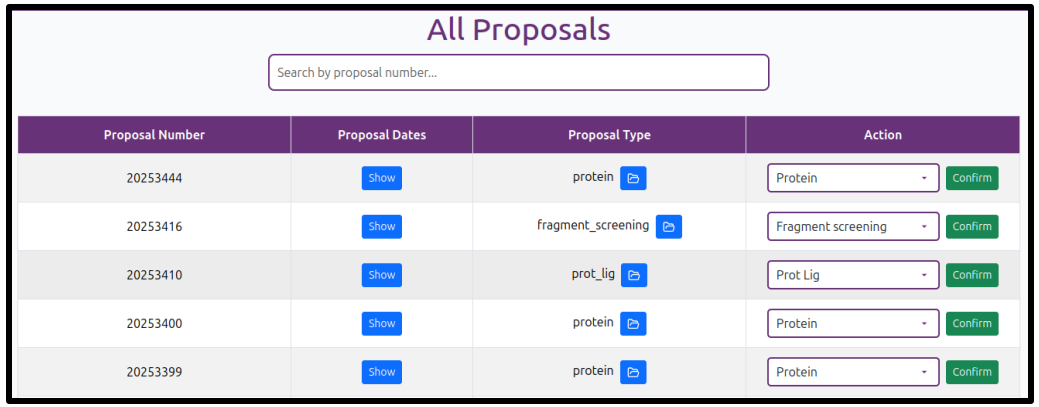


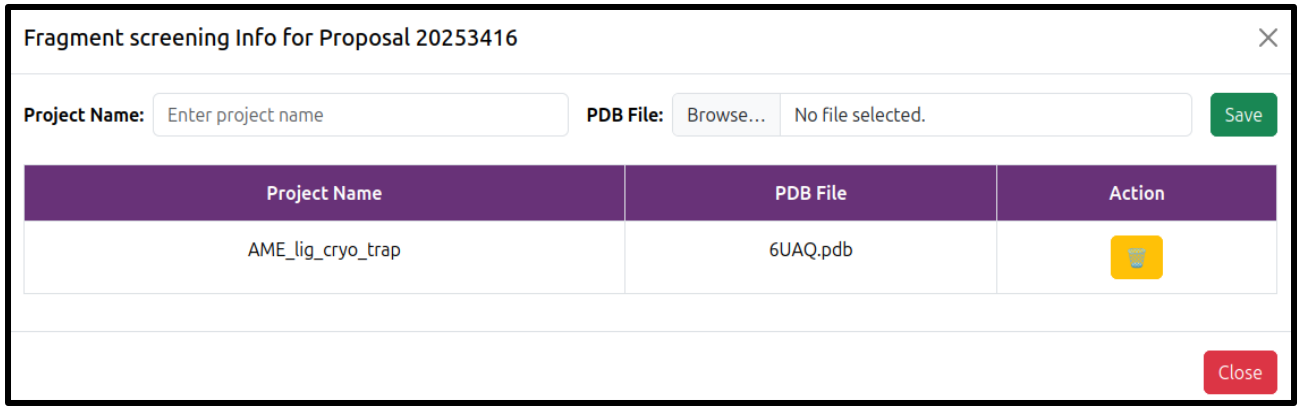


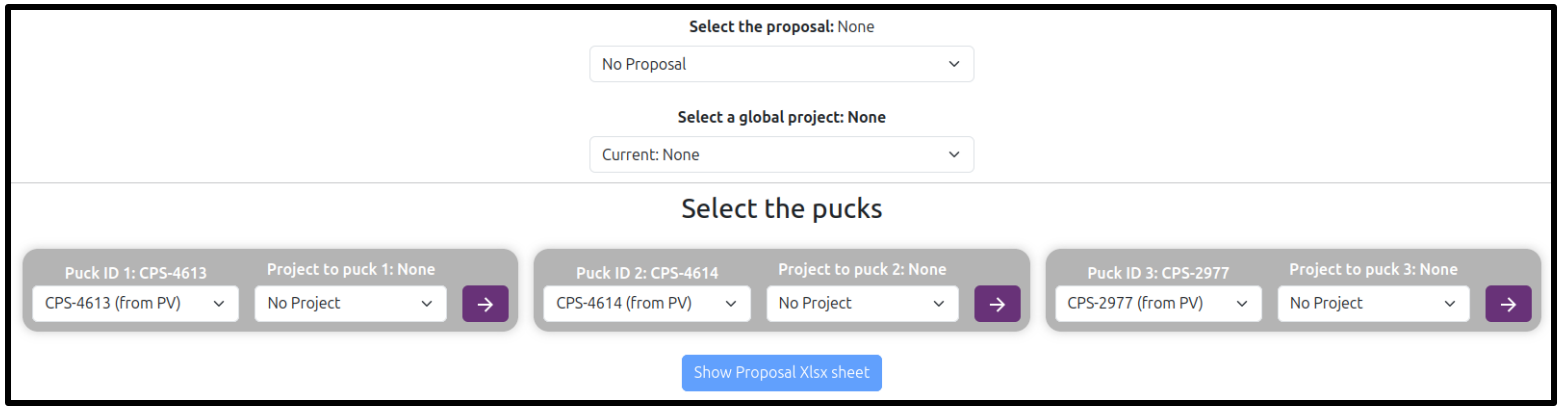
Beamline Developments

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



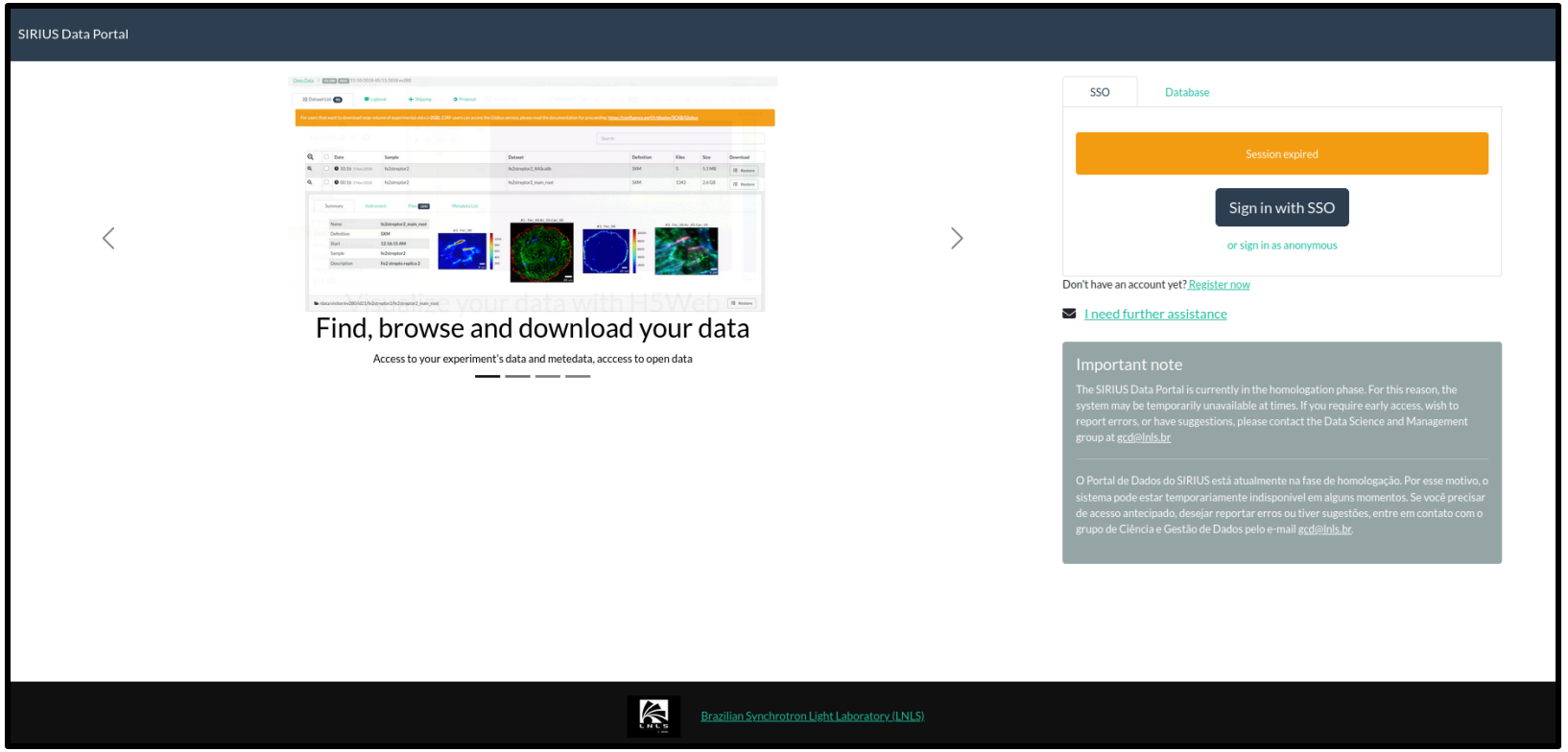




Beamline Developments

LIMS

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



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

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LNLS + sirius

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Brazilian Center for Research in Energy and Materials

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