

MXCuBE at LNLS/Sirius

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October, 2019

Presentation at:

bit.ly/sirius-mx3-2019

Summary

- ▶ **LNLS**
UVX and Sirius
MX2 and MANACÁ
- ▶ **MXCuBE**
Background
Status
- ▶ **Future work**

CNPEM

National Center for Research in Energy and Materials



Campinas, São Paulo - Brazil

4 National Laboratories

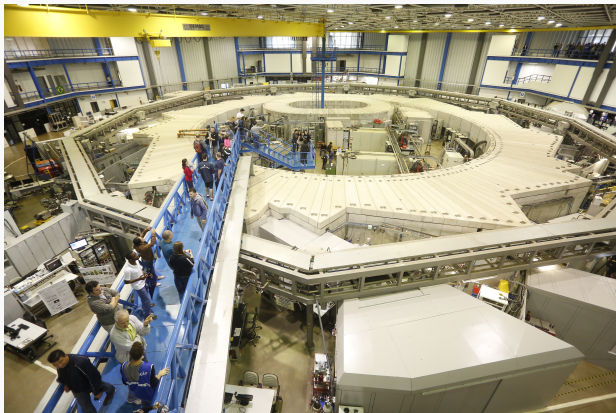


1. LNLS (Synchrotron Light Source)
2. LNBio (Biosciences)
3. LNNano (Nanotechnology)
4. LNBR (Biorenewables)

<http://cnpem.br/>

LNLS

- ▶ Since 1997, Latin America's only synchrotron light source



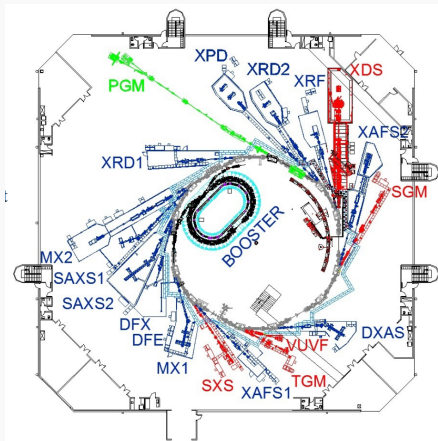
UVX synchrotron

Electron Energy:	1.37 GeV
Current:	250 mA
Circumference:	93 m
Diameter:	29.7 m
Straight sections:	6
Beamlines:	18



<http://www.lnls.cnpe.br/uvx>

UVX



BEAMLINES

XRD1	PGM	XPD	XRD2	XRF
XDS	XAFS2	SGM	IMX	DXAS
TGM	XAFS1	SXS	IR1	SAXS2
SAXS1	MX2			

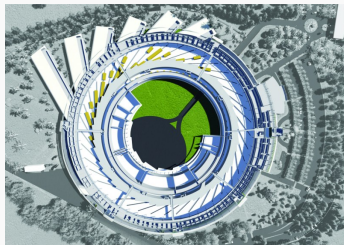
Sirius - The New Brazilian Synchrotron



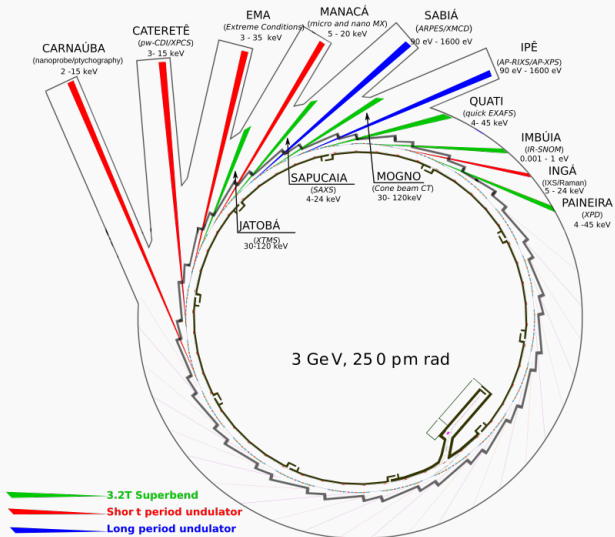


Sirius on Open Science day

Energy:	3 GeV
Current:	350 mA
Circumference:	518.4 m
Diameter:	165 m
Straight sections:	20
Beamlines:	40



<http://www.lnls.cnpem.br/sirius>

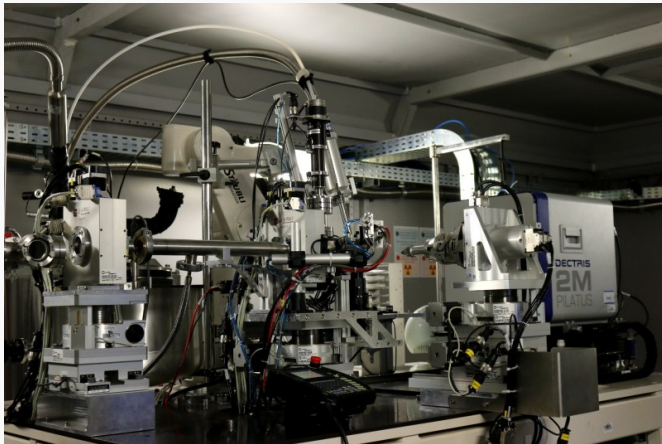


Sirius Beamlines (1st phase)



Sirius beamlines are named after
Brazilian fauna and flora (e.g.: Manacá)

MX2 Beamline (UVX)



MX2 experimental station

MX2 Beamline (UVX)

Energy:	5 - 15 keV
Beam size:	150 x 500 μm
Source:	Wiggler
Area detector:	Dectris Pilatus 2M
XRF detector:	Amptek X-123SDD
Sample changer:	G-Rob
Cryostat:	Oxford Cryojet XL
Camera:	IDS UEye
Goniometer:	Huber air bearing stage + ARINAX mini-kappa (in house)

MX2 Beamline (UVX)



MX2 control station

Distributed control framework:

Experimental GUI:

OS:

Other UIs:

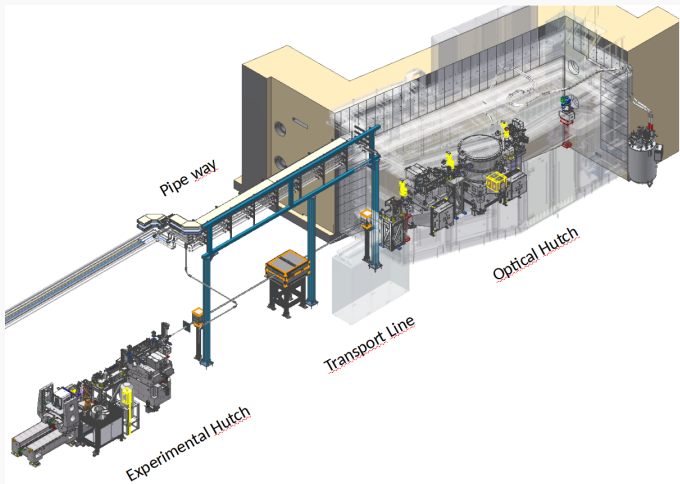
EPICS

MXCuBE 2 (Qt4)

Linux (CentOS 7)

CS-Studio, Py4Syn [2]

MANACÁ Beamline (Sirius)



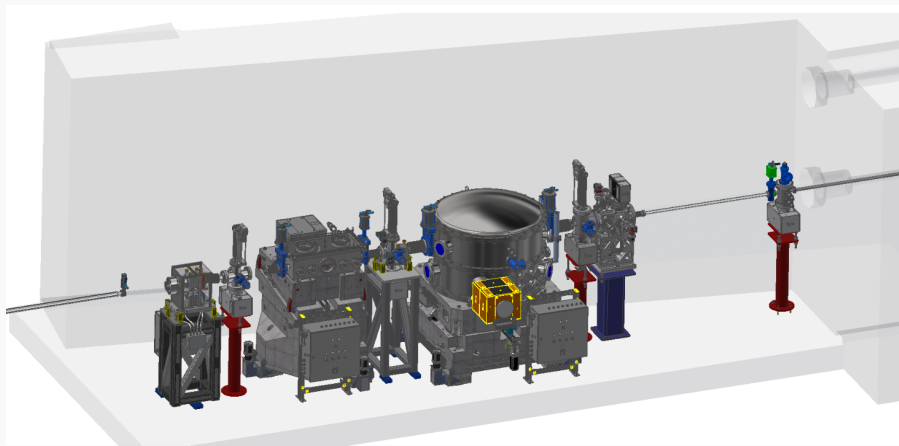
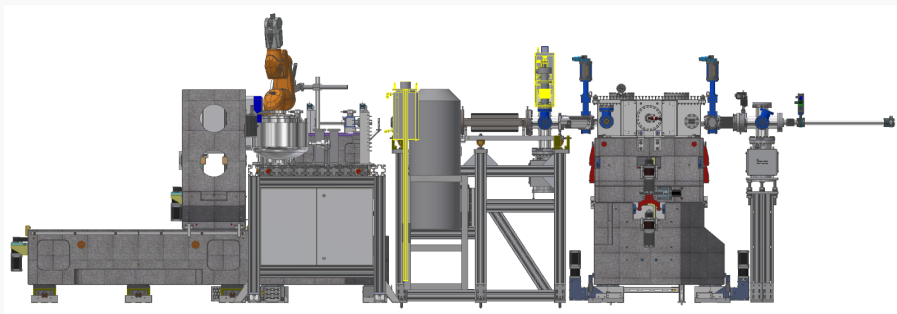


Figure: Optical Hutch



Experimental Hutch

Sirius - MANACÁ Beamline

- ▶ Micro and Nano MX (2 experimental stations)

Energy: 5 - 20 keV

Beam size: 10 x 7 μm (focused)
100-10 x 80-7 μm (adjustable)
0.5 x 0.5 μm (nano station)

Sirius - MANACÁ Beamline

Source:	Ondulator
Area detector:	Pi-Mega (based on Medipix chip) [3]
XRF detector:	Amptek Fast SDD
Sample changer:	Stäubli TX60 (Unipuck + Plate Gripper)
Cryostat:	Oxford Cryojet
Camera:	ARINAX B-Zoom
Goniometer:	Huber air bearing stage + ARINAX mini-kappa (in house)

Sirius - MANACÁ Beamline



Distributed control framework:

Experimental GUI:

OS:

Other UIs:

EPICS

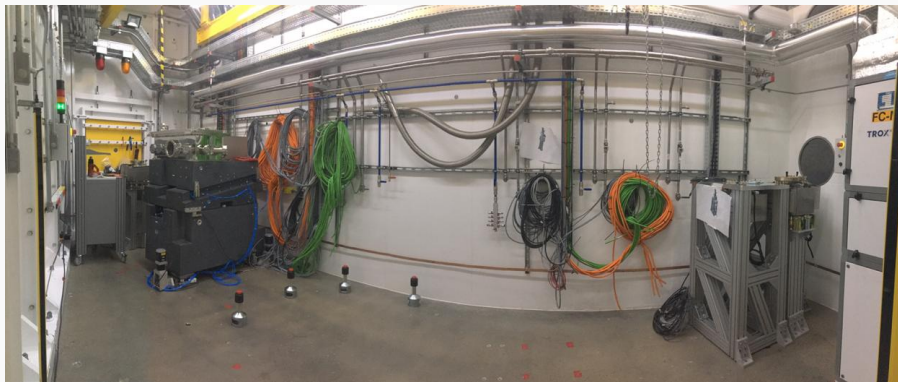
MXCuBE 3 + HR 2.2

Debian 9

PyQt, PyDM, Py4Syn



MANACÁ overview



Optical Hutch (Mirror 1 on the left)



Experimental Hutch (Table and Mirror 2)

Sirius / MANACÁ - Milestones

2019

- ▶ **Jan** – Sirius building delivered
- ▶ **Aug** – UVX Shutdown (for tests only, full focus on Sirius)

2020

- ▶ **Jan** – MANACÁ components installed
- ▶ **1st sem.** – MANACÁ in commissioning
- ▶ **2nd sem.** – MANACÁ open for users

MXCuBE - Background

UVX

- ▶ 2016: **MXCuBE 2 (at MX2)**
LNLS HOs classes dev, commissioning (Python 3.4)
- ▶ Reasons: Python, EPICS, community support
- ▶ Mid 2017: Open to the first users

MXCuBE Qt4

File View Graphics tools Help
Collect | Log |

Sample centering | Beam centering | EPICS KDCs |

Omega: 90.0 | Phi: 90.0 | Kappa: 0.00 | Beam stopper: 20.01

Zoom: 1.5 | Lights: 50 | 30 | 0 | Samples: Horizontal: -0.50 | Focus: 0.00

Collection method

▼ Standard Collection

Acquisition

Oscillation start: 90.00
 Number of images: 1800
 Exposure time (s): 1.0
 Oscillation range: 0.2
 Energy (keV): 8.5001
 resolution (Å): 1.800
 First image: 1
 Kappa: 0.0
 Transmission (%): 100.0
 Detector mode:
 MAD
 MAD
 Subwedge size:
 Shutterless
 Inverse beam

Data location

Folder:

File name:

File:

▼ Energy Scan

Machine current: 243.0 mA

Machine state read

Intensity monitor (1) open
 Intensity monitor (2) open
 Intensity monitor (3) open
 Intensity monitor (4) open
 Hatch temperature: 0.0 C
 Hatch humidity: 0.0 %
 Storage disk space: 740.50G
 Free: 293.10G (39%)

Current: 8.5001 keV
 Wavelength: 1.458 Å
 Set to:

Detector distance: 1.800 Å
 Resolution: 1.800 Å
 Distance: 132.05 mm
 Set to:

Safety shutter: closed

MCA control: out

Attenuators: 10 50 100 200 400

Sample list

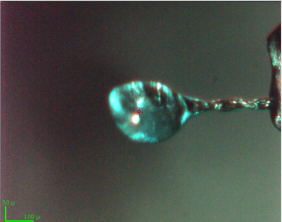
Mode: Manually mounted

Centring: Manual

Riten:

- Manually-mounted
 - Standard_1 Collection done
 - Standard_2 Collection done
 - Standard_3 Stopped
 - Standard_4 Stopped
 - Standard_5 Stopped
 - allenv2_5 (Point - not d...)
 - allenv2_5 (Point - not d...)
 - allenv2_5 (Point - not d...)

Sample video



x: 581 y: 261

Beam size

	Sits 1	Sits 2
Horizontal	Horizontal: 1400.0 µm 1400.0 µm	Horizontal: 500.0 µm 500.0 µm
Vertical	Vertical: 300.0 µm 400.0 µm	Vertical: 200.0 µm 200.0 µm

2018-11-30 12:37:48 Preparing acquisition, start=90.000000, wedge size=1800
 2018-11-30 13:00:08 User requested the end of collection!
 2018-11-30 13:00:08 Beamline acquisition was aborted, queue stopped by user
 2018-11-30 13:00:08 Closing safety shutter at: 3011/2018 13:00:08

MXCuBE 2 (with EPICS) at MX2

MXCuBE Qt4

File View Graphics tools Help
Collect | Log

Sample centering Beam centering EPICS IOCs

2nd slit pitch: 0.00203 SR 1 base X: 5.22 SR 1 base Z: 1.53 SR 2 base X: 30.50 SR 2 base Z: 30.36

Use default optimization parameters

Optical hatch		1st Slits		2nd Slits	
Center 2nd slit		Center 1st slits		Center 2nd slit	
Inclination angle (mrad): 0.005	Inclination position: 0.00204	Horizontal distance (mm): 3.0	Horizontal position: 5.22	Horizontal distance (mm): 1.75	Horizontal position: 30.502
Step width (mm): 0.5405	Intensity: 3.866E+00	Vertical distance (mm): 1.25	Vertical position: 1.533	Vertical distance (mm): 0.5	Vertical position: 30.363
		Step width (mm): 0.025	Intensity: 2.523E+00	Step width (mm): 0.01	Intensity: 6.976E+00

Full path
Go to centroid

Start Cancel

Rocking (2nd slit) Translation horizontal (SR 1) Translation vertical (SR 1) Translation horizontal (SR 2) Translation vertical (SR 2)

x=0.941747 y=0.856398

Code: [] Password: [] Logout

Sample list
Mode: Manually mounted Show SC Details

Centering: Manual SPY

Filter: [] No filter

- Manually-mounted
 - Standard - 1 Collection done
 - Standard - 2 Collection done
 - Standard - 3 Stopped
 - Standard - 4 Stopped
 - Standard - 5 Stopped
 - afw0.5 0'arrk - not d... Stopped

Energy
Current: 8.5000 keV
Wavelength: 1.450 Å
Set to: [] keV [] Å

Detector distance
Resolution: 1.800 Å
Distance: 132.05 mm
Set to: [] mm [] Å

Safety shutter
closed
Open Close

MCA control
out
Connect Disconnect

Attenuators
10 100 200 400
0 0 0 0

Machine current: 235.9 mA
Machine state: led
Intensity monitor (I1): open
Intensity monitor (I2): open
Storage disk usage: 7.95e+08 V
Hatch temperature: 0.0 C
Hatch humidity: 0.0 %
Storage disk space: 704M 740.50E
Free: 293.10E (39%)

2018-11-30 12:37:46 Preparing acquisition, start=90.00000, wedge size=1000
2018-11-30 13:00:08 User requested the end of collection
2018-11-30 13:00:08 Beamline resolution was aborted, queue stopped by user
2018-11-30 13:00:08 Closing safety shutter at: 3011/2018 13:00:08

Beam Centering widget at MX2 [1]

MXCuBE - Background

Sirius

- ▶ Good feedback from users (and staff) about MXCuBE
- ▶ 2018: Online meetings, remote test with ESRF, Trieste Meeting
- ▶ **MXCuBE 3, Web (for MANACÁ)**
Interest to adopt **ISPyB** too
- ▶ **2019:** LNLS joins MXCuBE collaboration

MXCuBE - Status

Focus on MANACÁ

- ▶ **MXCuBE 3 + HR 2.2 + EPICS + Docker**
(Dev / Test)
- ▶ **Migration of LNLS Hardware Objects (classes)**
to this setup
- ▶ **EPICS IOCs developments:**
Motor (Delta Tau), Camera (Arinax B-Zoom), Det (Pi-Mega)

MXCuBE - Status

Done:

Tested classes for MXCuBE3 + EPICS:

- ▶ Epics Command
- ▶ LNLS Motor
- ▶ LNLS Camera (UEye, B-Zoom)
- ▶ Machine info (e.g.: ring current and similiar PVs)

Aplicativos Locais Sistema MxCuBE-3 Proposal: IDTEST0 - Mozilla Firefox

manaca.lns.br/mxcube

MxCuBE 3 Sample Overview Data collection Sample Changer System log Help RA Sign out

Beamline Actions Energy: 12.0000 keV Resolution: 3.000 Å Transmission: 100.000 % Cryo: 0 K
Wavelength: 1.0332 Å Detector: 277.382 mm Flux: 0 ph/s

Beam size: 5
Omega: 20
Kappa: 34.24
Phi: -43.9

Sample alignment: Show motors

READY CLOSED CLOSED WAIT 1.0 nA

Real Queue Waitlist Settings

Sample: Sample-1.01 Queued Samples (0)

Point-1: Data Collection
Path: local-user_1_www.cdf

Start	Disc.	T (ms)	# img	T (h)	Res. (Å)	E (KeV)	ω °	κ °
20.00	1.00	10.000	1	100.00	3.000	12.0000	-43.90	34.24

MxCuBE-3 Proposal: ID...

MxCuBE 3 developments at MANACÁ

MXCuBE - Status

Done:

ISPyB:

- ▶ Docker container for learning and testing
- ▶ Improvements discussed with the community
- ▶ All merged and available at:

<http://github.com/ispyb/ispyb-docker>

MXCuBE - Status

Doing (WIP):

Rebase our code to **MXCuBE3 (master) + HR 3.0**

- ▶ Align with upstream
- ▶ Python 3 compatibility

More dev/tests on MXCuBE3 + EPICS:

- ▶ LNLS Detector (Pilatus, Pi-Mega)
- ▶ LNLS MultiCollect

MXCuBE - Status

Repositories?

- ▶ <http://github.com/lnls-sol/mxcube3>
- ▶ <http://github.com/lnls-sol/HardwareRepository>
- ▶ <http://github.com/lnls-sol/mx3docker>

Stable code on branch: **lnls-manaca**

Future work

MXCuBE

- ▶ Auto centering routines
- ▶ Cateretê (SAXS bl) also interested (BSXCuBE?)
- ▶ Serial MX
- ▶ Remote access

ISPyB

- ▶ 2020: Developments and tests for MANACÁ

Acknowledgments

Beamline Operation Software (SOL group)

Allan Serra Braga Bugyi

Dawood Awny Dawood Alnajjar

Douglas Henrique C. de Araújo

Gabriel Previato de Andrade

George Nicolas Kontogiorgos

Gustavo Henrique Ornaghi Aranha

James Rezende Piton

Laís Pessine do Carmo

Luciano Carneiro Guedes

Marcelo Alexandre Leite de Moraes

Pedro Junji Hirasawa



MX Group

Ana Carolina de Mattos Zeri

Ana Carolina Rodrigues

Andrey Fabricio Ziem Nascimento

Carlos Yujiro Hagio

Evandro Ares de Araujo

MXCuBE and ISPyB community

References



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Accessed: 2019-10-01.

Meeting in Brazil? :)



MXCuBE at LNLS/Sirius

Thank you!

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Questions?