



MXCuBE 2 @ ALBA status report

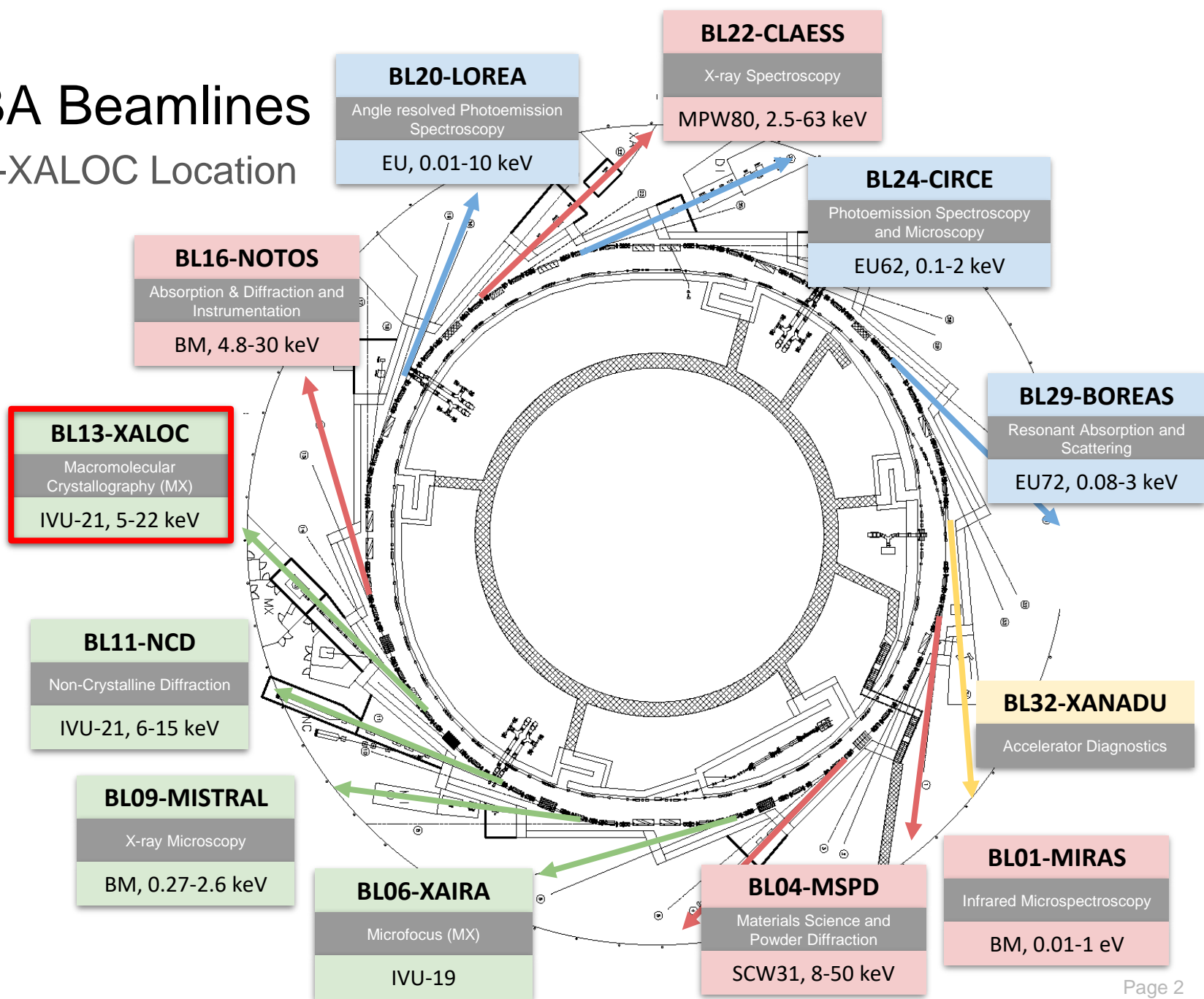
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On behalf of the controls group and BL13-XALOC

MXCuBE meeting, 12 March 2019,
MAX IV (Lund)

ALBA Beamlines

BL13-XALOC Location



BL13 - XALOC Beamline

MX experiments



Detector: Pilatus2 6M (Dectris) LimaCCDs (Core 1.7) OS openSuSE 10.3.

Diffraction: MD2M (Arinax) Icepap driven (no server).

Sample Changer: CATS (Irelec) spine/unipuck (double gripper) + plates.

Instrumentation control: Sardana/Taurus + Tango7.

OS platform: Linux (openSuSE 11.1/12.1)

Remote connection: NX Enterprise (No Machine)

MXCuBEv2: Debian9/Tango9

MXCuBE 2 @ BL13-XALOC

MXCuBE development and features

- Development on Hardware Repository Qt4/2.3.0 branch.
- ISPyB and EDNA in production stage.
- Prepare migration of ALBA-Specific Hardware Objects to 3.0 version.

Done

Optical Centring procedures.
Standard Data Collection.
LDAP authentication.
EDNA postprocessing optimized for the
ALBA cluster.
ISPyB database.
Remote Access (No Machine).
Migration to Debian9/taurus4.
Merge to 2.3.0 version.

Future Work

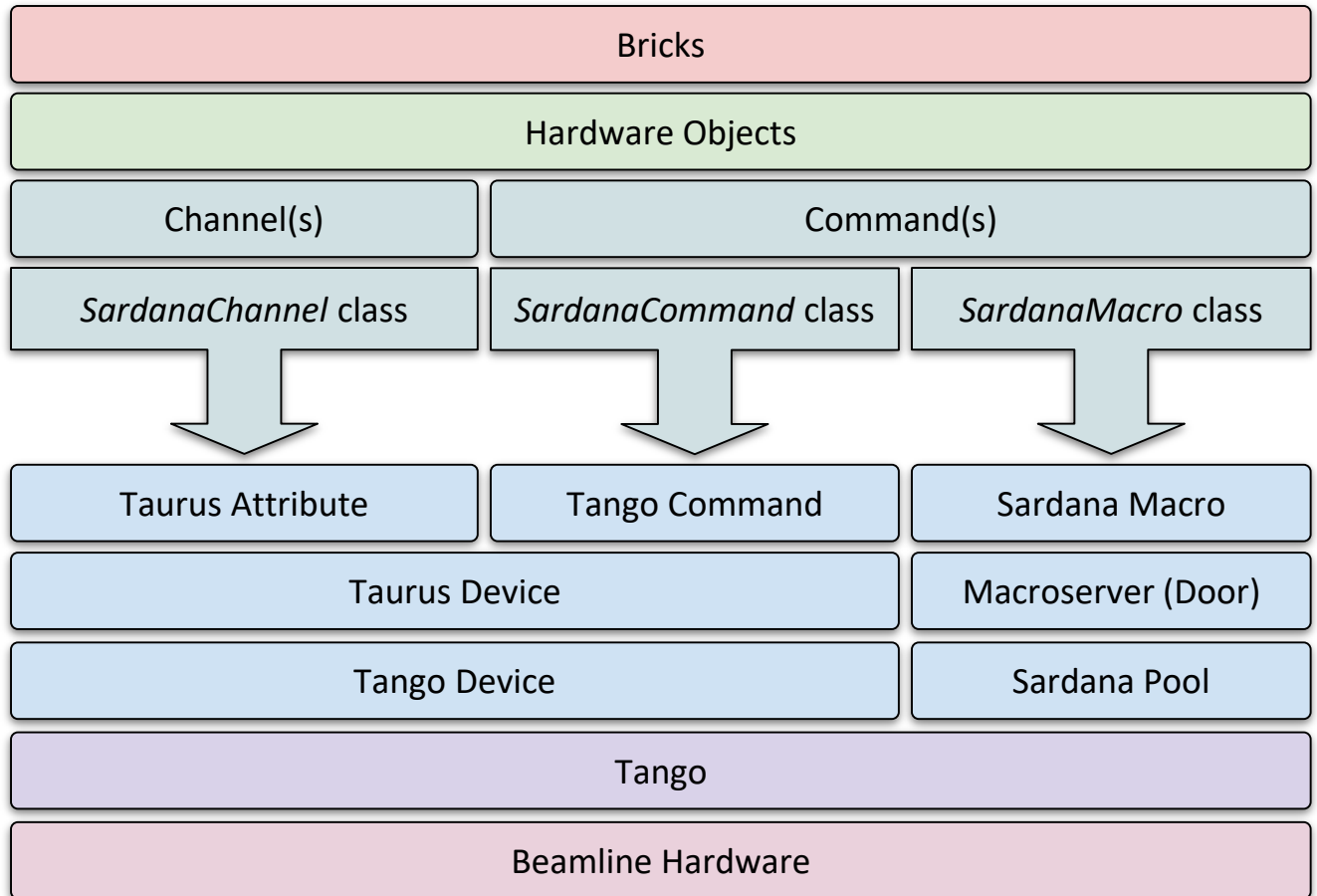
Integrate new collection methods to
Sardana Scan Framework
(trigger by position)

- Standard Data Collection.
- Energy Scan.
- Helical Data Collection.
- Mesh Data Collection.
- X-ray Centring.

Integration of MXCuBE 2 @ ALBA

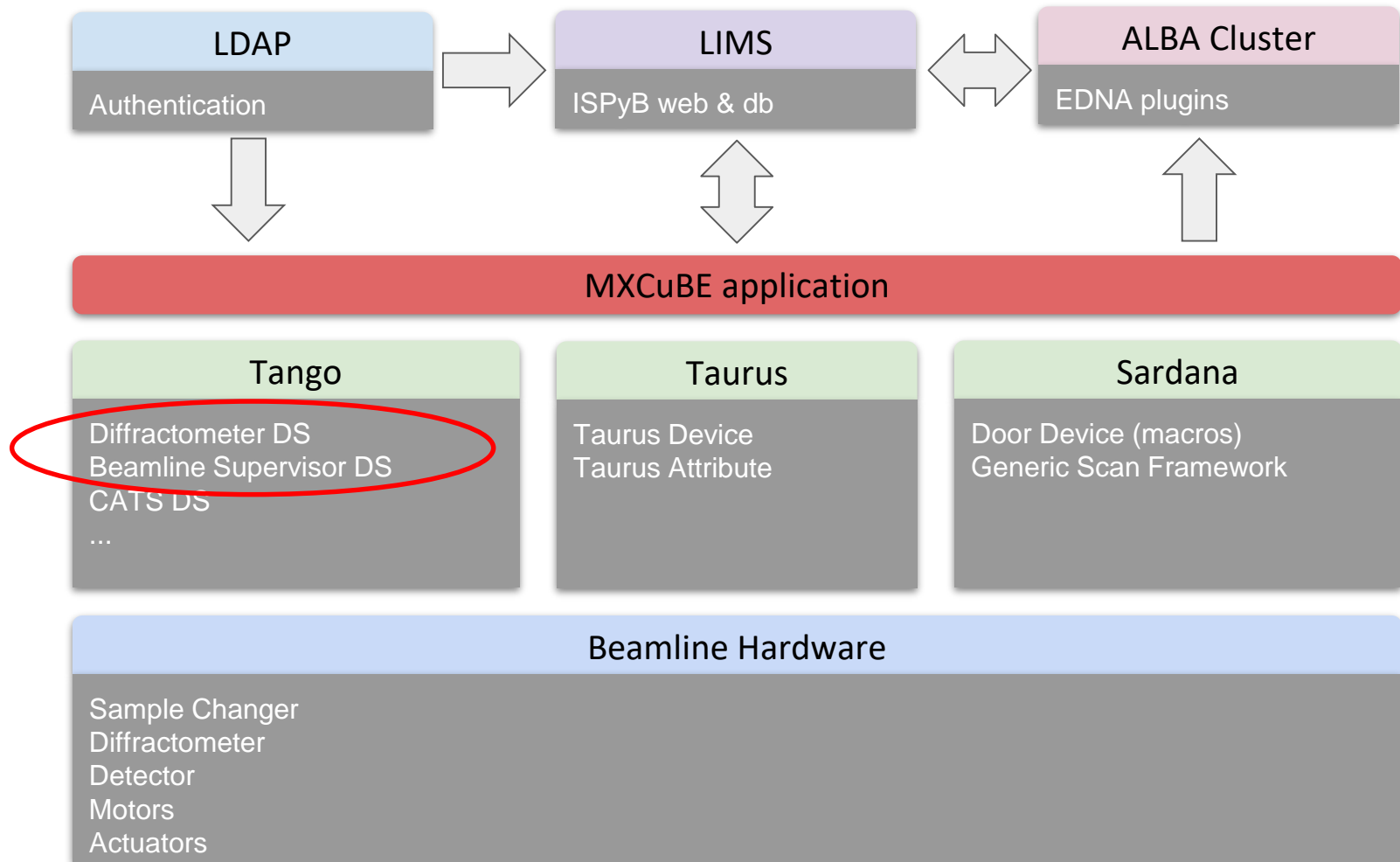
Sardana Support for BlissFramework

BlissFramework
Hardware Repository



Integration of MXCuBE 2 @ BL13-XALOC

Architecture



MXCuBE 2 @ BL13-XALOC

MXCuBE app snapshot

ISPyB proposal
Code: mx Password: Login

Sample tree
Mode: Sample changer Show SC-details
Sample: ISPyB
Centring: Manual 3-click
Filter: No filter

Sample centring
Omega: 0.00 Kappa: 0.00 KappaPhi: 0.00

Sample video
Zoom 21

Acquisition
Sample: 7:3 Standard Collection
Oscillation start: 0 Osc. range per frame: 0.1
Number of images: 1 Total osc. range: 0
First image: 1 Full range
Exposure time (s): 0.1 Detector mode:
Kappa: -0 Phi: 0
Energy (keV): 12.661 MAD
Resolution (Å): 1.748
Transmission (%): 39.795
Shutterless

Data location
Folder: /tmp/20190301/RAW_DATA
File name: local-user_1_####.cbf Browse
Prefix: local-user
Run number: 1
Compress data

Processing
N.o. residues: 200 Space group:
Unit cell:
a: 0 b: 0 c: 0

Machine Info
Machine current: 152.0 mA
Machine status: TopUp Remaining: 999.2 s
Energy
Current: 12.6610 keV
Wavelength: 0.979 Å
Transmission
Current: 39.80 %
Resolution
Current: 1.748 Å
331.91 mm
Beam Stop Z: -20.00

Beam on Sample
Photon Shutter Closed
Open Close

Phase Transfer

Collect Now Add to queue

Queue history
Collect Queue Pause

Beam size
Horizontal: 77 μm
Vertical: 25 μm

State: - Diffractometer: Not ready Sample changer: - Last collect: -

File system EDNA ISPyB

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ISPyB portal snapshot : production stage

Selected Session

Proposal: mc2018002222
 Start Date: 12-02-2019
 BeamLine: MX-BL13
[Back to this session](#)
[Back to sessions](#)

Data Collection info...

Reports

General report: [PDF icon] [Word icon] [Excel icon]

Screening report: [PDF icon] [Word icon]

Parameters

Ignore RSymm in the low resolution shell over:
 Ignore I / Sigma in the low resolution shell under:

References

When reporting data collected on MX-BL13 please cite the appropriate references

DataCollections

13 DataCollections

Save Experiment Parameters Rank EDNA Expand All Collapse All Clear Grouping

Image Prefix	Run No	# images	Exp. Param.	Status	Space Group	Completeness	Resolution	Rsymm Inner Outer Overall	Unit_cell a, b, c alpha, beta, gamma	Exp. Type	Protein Acronym	Start time	Sample Ranking	Skip	Comments	Download autoprotos files
B4X5_w1	1	754	1	●●●●	P 4 2 2	99.25 - 6.16 1.65 - 1.59 39.25 - 1.59	4.7 131.4 10.1	78.50, 78.50, 37.17 90.00, 90.00, 90.00	OSC		19:41:53 12-02-2019		<input type="checkbox"/>			
ref-B4X5	1	2	1	●●○○						Characterization		19:40:04 12-02-2019	<input checked="" type="checkbox"/>	<input type="checkbox"/>		
ref-B4X4	3	2	1	●●○○						Characterization		19:29:50 12-02-2019	<input checked="" type="checkbox"/>	<input type="checkbox"/>		
ref-B4X4	2	2	1	●●○○						Characterization		19:25:17 12-02-2019	<input checked="" type="checkbox"/>	<input type="checkbox"/>		
ref-B4X4	1	2	1	●●○○						Characterization		18:44:57 12-02-2019	<input checked="" type="checkbox"/>	<input type="checkbox"/>		
ref-B4X4	1	2	1	●●○○						Characterization		18:29:24 12-02-2019	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Data collection failed! DevFailed[DevError[desc = Exception: Control: prepareAcq(CicControl.cpp, 459): Error: Acquisition not finished origin = File "/home/local/isc/ila/ibpython/site-packages/Lima/Core/v1.7.0/Debug.py", line 52, in real_fn return new_fn("arg", **kw) File "/home/local/isc/ila/ibpython/LimaCCDs/LimaCCDs.py", line 1628, in prepareAcq self.__control.prepareAcq() reason = PyDs_PythonError severity = ERR] DevError[desc = Failed to execute command_inout on device BL13/eh/plasuma, command prepareAcq origin = Connection::command_inout() reason = API_CommandFailed severity = ERR]]	
ref-B4X4	1	2	1	●●○○						Characterization		18:20:00	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Data collection failed! DevFailed[DevError[desc = Exception: Control:	

MXCuBE 2 @ BL13-XALOC

New application for users

Commissioning
from mid 2018

Friendly users
2nd half 2018

Operation since
Feb 2019

Current installation includes:

- Full interoperability with ISPyB
- Autocentering
- Characterization of crystals & calculation of diffraction plan
- Single wedge data collection method
- Autoprocessing using EDNAproc (soon, AUTOproc)

Next features:

- Helical and raster scans (via Sardana macros)
- Fluorescence methods
- Global Phasing pipelines for external BL operation

Highlights:

~80% of current users switched to MXCuBE

Previous system not longer maintained

Acknowledgements

The people

Thank you.

BL13-XALOC

Roeland Boer
Fernando Gil
Barbara Machado
Xavi Carpena

Controls

Guifre Cuni
Jordi Andreu

IT Systems

Sergi Puso
Ramon Escriba

MIS

Daniel Salvat
Daniel Sanchez

Externals

Bixente Rey