



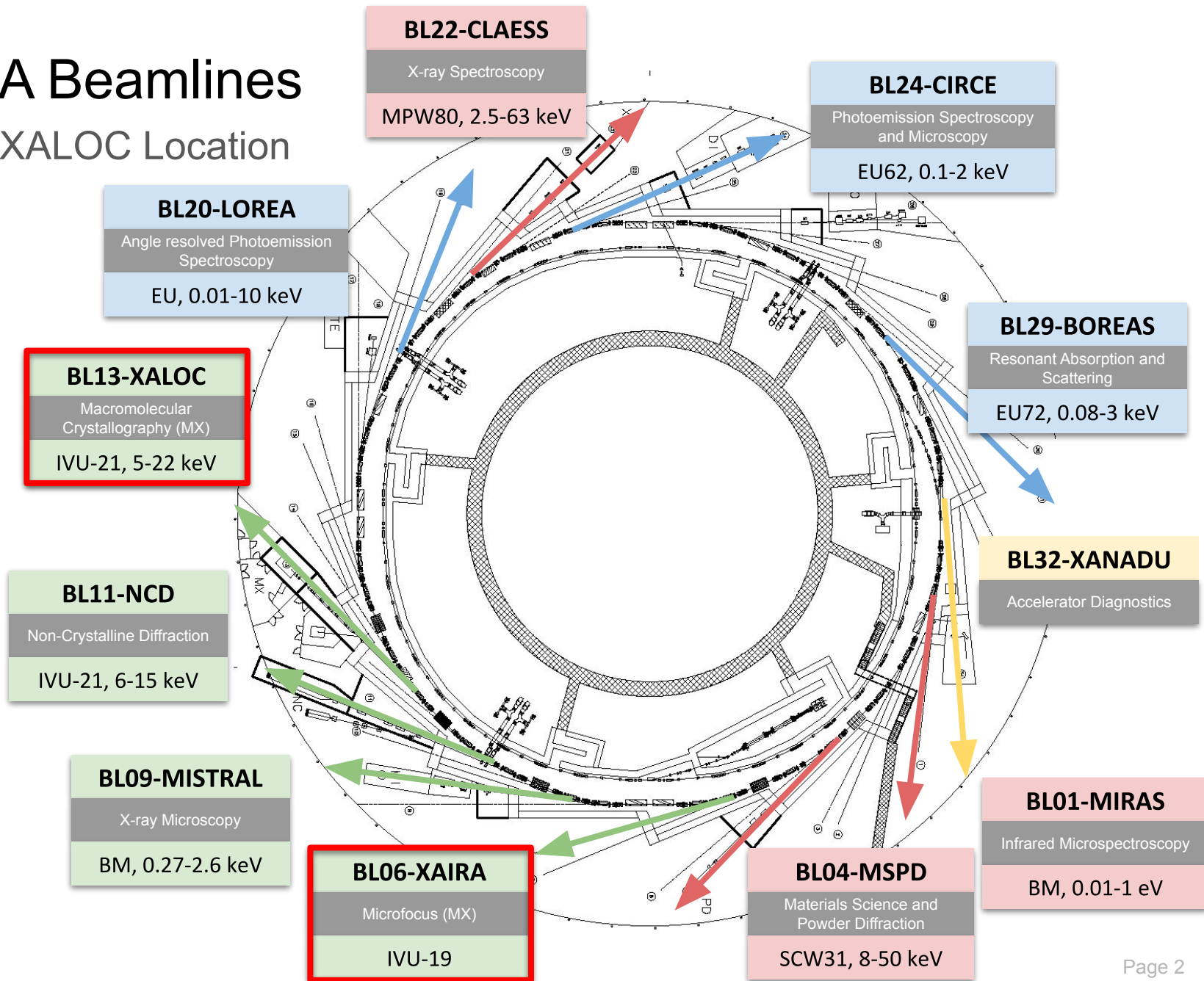
MXCuBE 2 @ ALBA status report

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On behalf of the controls group

MXCuBE meeting, 29 October 2019,
Berlin

ALBA Beamlines

BL13-XALOC Location



BL13 - XALOC Beamline

MX experiments



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

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

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

Instrumentation control: Sardana/Taurus + Tango 7/9.

OS platform: Linux (openSuSE 11.1/12.1/**Debian9**)

Remote connection: NX Enterprise (No Machine)

MXCuBE 2 Qt4 @ BL13-XALOC

MXCuBE app snapshot

The screenshot displays the MXCuBE 2 Qt4 application interface. The main window shows a live video feed of a sample, which appears to be a circular object with a blue and green center. The interface is divided into several sections:

- Top Panel:** Contains menu options (File, Queue, View, Help, Graphics) and a "Logout" button. Below this are input fields for "Group:" and "Set".
- Sample centring:** A row of control buttons for "Omega", "Omega Centring", "Kappa", "KappaPhi", and "Omega X". Each has a numerical value and a "Set" button. Values shown are Omega: 180.00, Omega Centring: 180.00, Kappa: 0.00, KappaPhi: 0.00, and Omega X: -0.32.
- Sample video:** A large central window showing the microscope view. It includes a toolbar with icons for Centre, Save, Line, Grid, Focus, Snapshot, Refresh, Align, Select all, Clear all, and Auto. A scale bar at the bottom left indicates 50 μ and 100 μ . Coordinates X: 869 Y: 551 are shown.
- Sample tree:** A panel on the right showing the current sample as "manually-mounted".
- Standard Collection:** A panel for configuring acquisition parameters. It includes fields for Oscillation start (180), Osc. range per frame (0.1), Number of images (1), Total osc. range (0.1), First image (1), Exposure time (s) (0.1), Detector mode (Full range), Kappa (-0), Phi (0), Energy (keV) (12.661), Resolution (\AA) (3.812), and Transmission (%) (4.991). There is a checkbox for "Shutterless" which is checked.
- Data location:** Fields for Folder (mes/bl13/projects/cycle2018-1/2018002222-ispybtest/20191028/RAW_DATA), File name (mx2018002222_1_####.cbf), Prefix (mx2018002222), and Run number (1). There is a "Browse" button for the file name.
- Processing:** Fields for "N.o. residues" (200) and "Space group".
- Characterisation:** A section with "Helical Collection" and "Energy Scan" options.
- Advanced:** Includes "XRF Spectrum" and "Collect Now" buttons.
- Machine Info:** A panel on the far right showing "Machine current: 1.0 mA", "Machine status: ON", and "TopUp Remaining: 0.0 s". It also displays Energy (12.6610 keV), Wavelength (0.979 \AA), Transmission (4.99%), and Resolution (3.812 \AA , 800.01 mm).
- Beam Stop Z:** A field set to -95.70.
- Beam on Sample:** A row of four indicator lights (grey, green, purple, purple).
- Photon Shutter:** A control panel with "Closed", "Open", and "Close" buttons.
- Bottom Panel:** A status bar showing "mx2018002222@BL13 - XALOC State: - Diffractometer: - Sample changer: Disabled Last collect: -". It also includes a "Queue history" section with "Collect Queue" and "Pause" buttons, and an "Add to queue" button.

MXCuBE 2 @ BL13-XALOC

MXCuBE running in a conda environment

- **mxcube:** (master frozen + local changes)
- **hwr:** (master frozen + local changes)
- **Miniconda3:** 4.6.14

# Name	Version	Build	Channel
python	2.7.13	heccc3f1_16	
pytango	9.2.1	py27he9270ad_0	tango-controls
pyqt	4.11.4	py27_4	
gevent	1.1.2	py27_0	
numpy	1.11.3	py27h3dfced4_4	
scipy	0.18.1	np111py27_1	
pydispatcher	2.0.5	py27_1	
jsonpickle	1.1	py_0	
lxml	4.3.3	pypi_0	pypi
matplotlib	1.5.1	np111py27_0	
pillow	4.2.1	py27_0	
pyyaml	5.1	py27h7b6447c_0	
suds-jurko	0.6	py27_3	
openldap	2.4.36	1	
tabulate	0.8.3	py27_0	
enum34	1.1.6	py27_1	
lucid2	1.0	pypi_0	pypi
opencv-python	4.1.0.25	pypi_0	pypi
sardana	2.5.0	pypi_0	pypi
taurus	4.5.1	pypi_0	pypi
bl13-modules	1.9.0	pypi_0	pypi
albaclusterclient	2.0.0	dev_0	<develop>

MXCuBE 2 @ BL13-XALOC

General controls system issues

Controls System General Update:

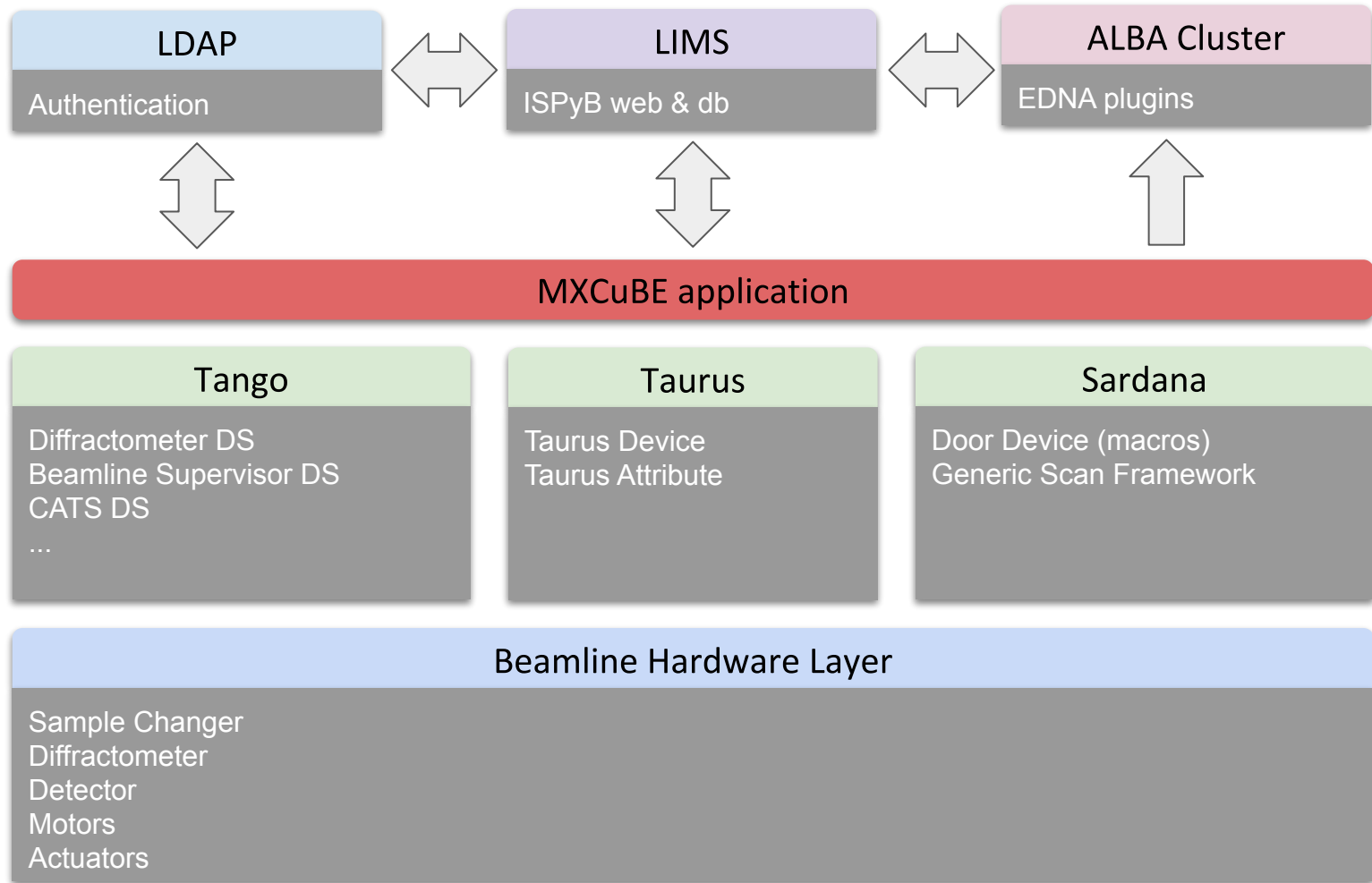
- Change OS:
 - OpenSuSE 11/12 -- > Debian9 (adapt scripts)
 - Native Debian packages (no more Bliss Packages , rpm).
 - New CI pipelines: from push to deployment.
 - New deployment tools: SALT.
 - Replace hardware by new machines..
- Upgrade Tango7/Tango8 → Tango9 (Debian packages).
- Upgrade Taurus3 → Taurus4. Supports PyQt4/PyQt5 and Py2/Py3.
- Upgrade Sardana Py2 → Sardana Py3 (no longer support to Py2 version).

Ongoing projects @ XALOC:

- Integrate new OAV system (BZoom, Arinax).
- MXCuBE/ISPyB user experience improvements.
- Improve post-processing cluster access/performance.

Integration of MXCuBE 2 @ BL13-XALOC

Architecture



MXCuBE 2 @ BL13-XALOC

General controls system migration

	pcbl1307* (Control host)	tbl13 (Tango DataBase)	ibl1303 (Arinax Server)	ibl1304 (Tango DS)
Debian 9	x	x	x	x
Tango 9	client	x	x	x
Taurus 4	x**	-	-	x
Sardana Py2	client	-	-	x

*QuadCore Intel(R) Xeon(R) W-2123 CPU @ 3.60GHz, 32Gb.

**Taurus 3 in a pyenv for old GUIs.

+ Python 3

Acknowledgements

The people

**Thank you for
your attention**

BL13-XALOC

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Fernando Gil
Barbara Machado
Xavi Carpena

Controls

Guifre Cuni
Jordi Andreu

IT Systems

Sergi Puso
Ramon Escriba

MIS

Daniel Salvat
Daniel Sanchez

Phases for MXCuBE 2 @ ALBA

Diffractionmeter TANGO DS

Diffractionmeter TANGO DS

*Control the diffractionmeter
and sample environment
for safety operations.*

*Any access to the
equipment is done
through this DS (when
available).*

Goniometer

omega
omegax
omegay
omegaz
centx
centy
kappa

Aperture

aperx
aperz

Fixed Beamstop

bstopx
bstopz

Moveable Beamstop

bsx
bsy
bsz

Detector table

diftabx
diftabz

DUSP

yagy
yagz

PLC signals

Sample on magnet, ...

BL parameters

Pinlength, ...

Actions

GoBeamViewPhase
GoSampleViewPhase
GoTransferPhase
GoCollectPhase

Phases for MXCuBE 2 @ ALBA

Beamline Supervisor TANGO DS

Beamline Supervisor TANGO DS

Coordinate the beamline elements for safety phase transitions.

Prepare the beamline elements according to the phase description.

Instruments

diffractometer
sample changer
shutters
cryostream

PLC signals

DetDistanceSafe
DetCoverOpen
CryoPosition
FastShutterCollectPosition

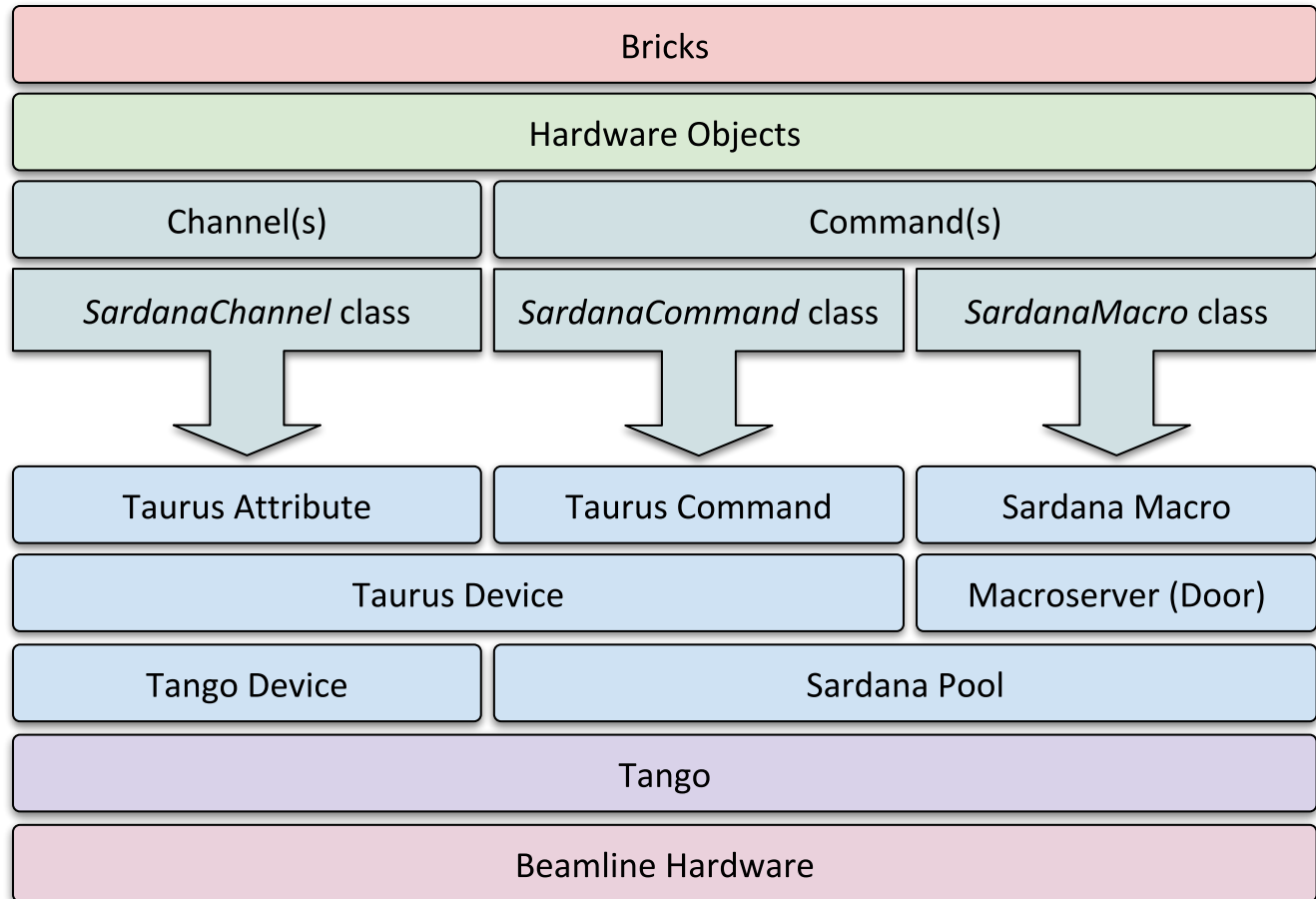
Actions

GoBeamViewPhase
GoSampleViewPhase
GoTransferPhase
GoCollectPhase

Integration of MXCuBE 2 @ ALBA

Sardana Support for BlissFramework

BlissFramework
Hardware Repository



*Implemented by V. Rey in *CommandContainer.py* and *Sardana.py* files.

ALBA Cluster

Infrastructure

- 11 nodes CPU - 1 node GPU.
- CPUs: Intel(R) Xeon(R) CPU E5-2650 v2 @ 2.60GHz.
- GPU: NVIDIA Tesla P100 16GB.
- 2,4 Tflops of computing capacity.
- 216 CPU cores with 1408 GB RAM.
- 1 Gbps and 10 Gbps Ethernet connections.
- Mpi 3.0.
- 40TB distributed scratch space in 2 nodes.

- Linux as operating system.
- Slurm for High Performance Computing.
- BeeGFS for scratch space.