



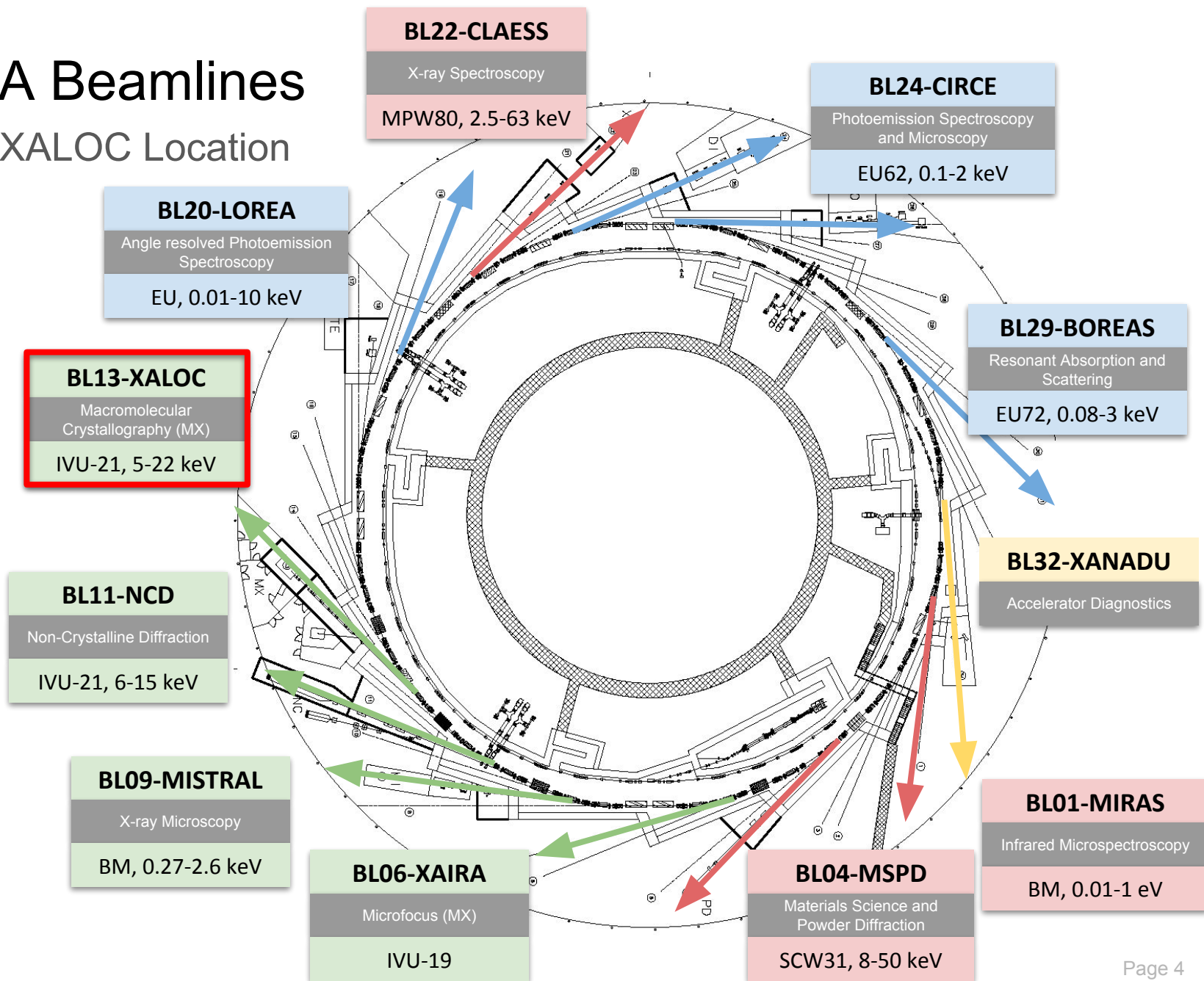
MXCuBE 2 @ ALBA status report

Jordi Andreu,
On behalf of the controls group

MXCuBE meeting, 11 September 2018,
Elettra (Trieste)

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 + Tango7.

OS platform: Linux (openSuSE 11.1/12.1)

Remote connection: NX Enterprise (No Machine)

Integration of MXCuBE 2 (Qt4) @ ALBA

A looong way...



Bessy (June 2015)



DESY (June 2016)



Diamond (February 2017)

ALBA (December 2015)

ESRF (February 2017)

Trieste (September 2018)



Integration of MXCuBE 2 @ ALBA

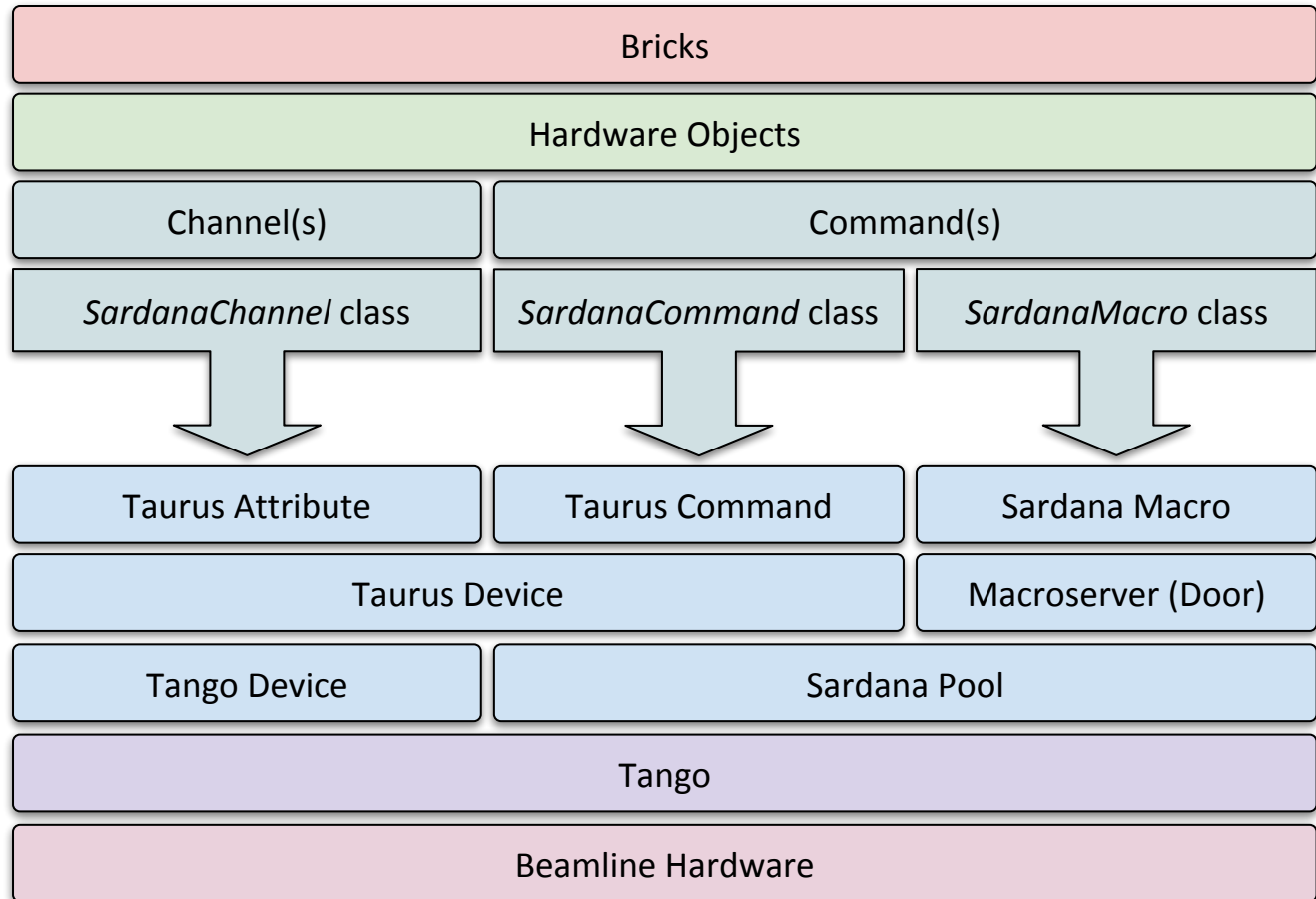
Implementation

1. Add support to SARDANA/TAURUS.
2. Operate Beamline Phases (Tango DS)
3. Implement HwObjs & Bricks

Integration of MXCuBE 2 @ ALBA

Sardana Support for BlissFramework

BlissFramework
Hardware Repository



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

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

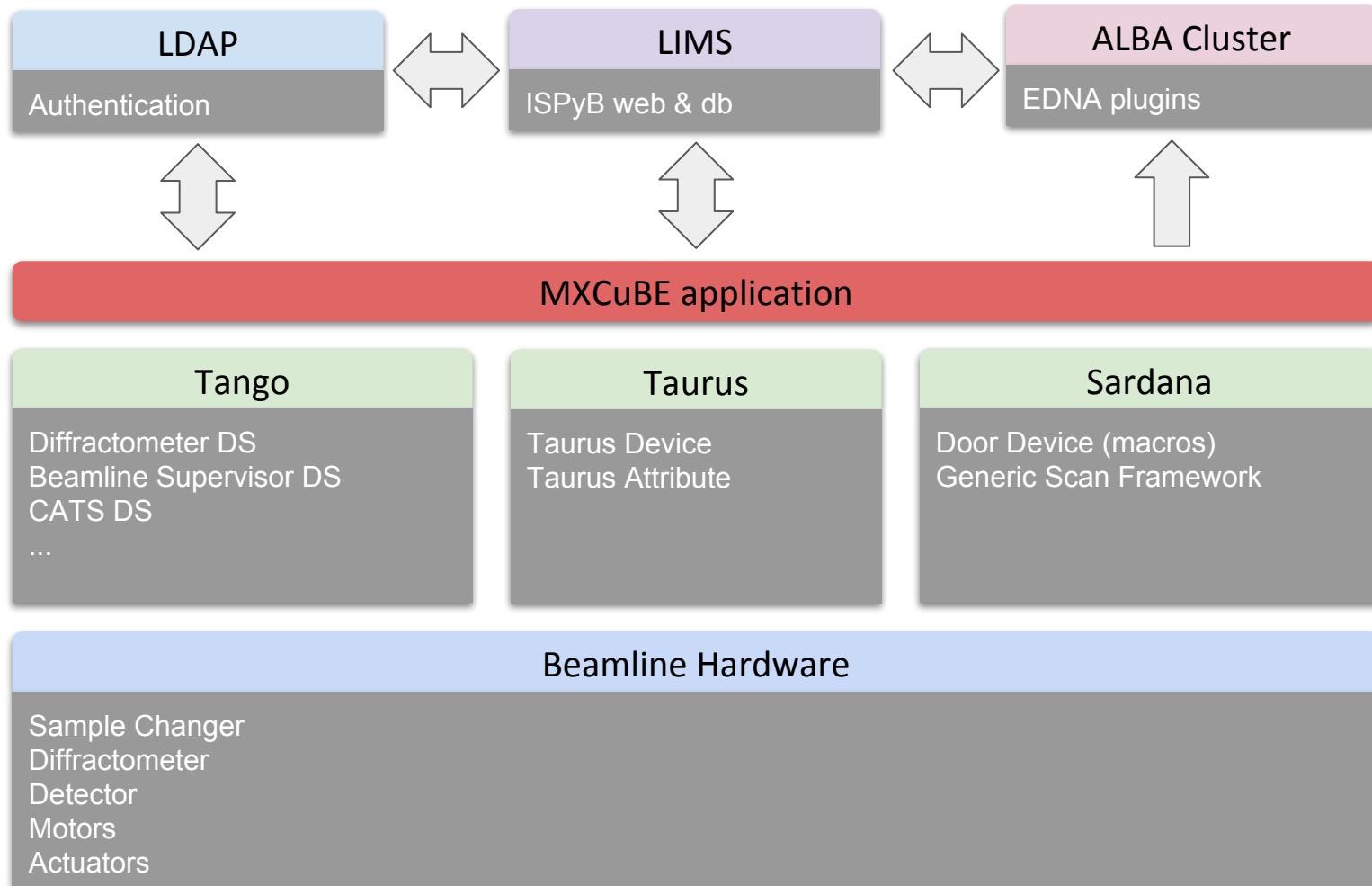
DetDistanceSafe
DetCoverOpen
CryoPosition
FastShutterCollectPosition

Actions

GoBeamViewPhase
GoSampleViewPhase
GoTransferPhase
GoCollectPhase

Integration of MXCuBE 2 @ BL13-XALOC

Architecture



MXCuBE 2 @ BL13-XALOC

MXCuBE app snapshot

The screenshot displays the MXCuBE 2 control software interface. The main window is titled "<@bl13mxcube>". The interface includes a menu bar (File, Queue, View, Graphics, Help) and a toolbar with buttons for Collect, Log, Chat, and Test. The left sidebar shows the "Sample tree" with a list of pucks (Puck 1 to Puck 3) and a "Sample" dropdown. The central area features a "Sample centring" section with "Omega" and "Front" controls, and a "Sample video" window showing a live image of a sample. The right sidebar contains "Standard collection" parameters such as "Oscillation start", "Exposure time", "Energy", and "Resolution". The bottom-right corner displays "Machine info" including "Machine current: 151.2 mA" and "Machine status: ON". A large red watermark "Under Commissioning" is overlaid across the center of the interface. The status bar at the bottom indicates "State: Diffractometer: Not ready" and "Sample changer: Ready".

MXCuBE 2 @ BL13-XALOC

ISPyB portal snapshot

The screenshot displays the ISPyB portal interface. At the top, there's a navigation bar with links like Home, Lab-contacts, Shipment, Samples, Prepare experiment, Data collection, Feedback, References, and Help. The main content area shows session details for a selected session (Proposal: mx2018012551, Start Date: 27-08-2018, BeamLine: MX-XALOC). Below this, there are sections for Session Information (Local Contact, Comments), Session Statistics (Nb Collect: 1, Nb Test: 1, Nb Energy Scan: 0, Nb XRF Spectra: 0), and Reports (General report, Searching report). The main table lists data collections with columns for Exp. Type, Image Prefix, Run#, Parameters, Results, Image Thumbnail, Crystal snapshot, Graph, and Comments. Two rows are visible: 'OSC' and 'Characterization', each with associated images and graphs. A large red watermark 'Under Commissioning' is overlaid diagonally across the page.

Exp. Type	Image Prefix	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Comments
OSC	sample	1	Nb images: 600 Exp. time: 0.326 s Phi range: 0.25 ° Flux: 3.49926068856E9 Detector resolution: 1.7 Å Transmission: 69.49 Wavelength: 0.979 Å Total expo time: 60 s	EDNA_proc autoPROC Space Group: P 63 Completeness: 100%				
Characterization	ref-sample	1	Nb images: 10 Exp. time: 0.10 s Phi range: 0.25 ° Flux: 3.49926068856E9 ph/sec Detector resolution: 1.79 Å Transmission: 100.00 Wavelength: 0.979 Å Total expo time: 1 s	Indexing Strategy Space Group: P3 Unit Cell: a, b, c: 102.14, 102.14, 59.13 α β γ: 90.00, 90.00, 120.00 Mosaicity: 0.40 ° Detector Resolution: 2.00 Å				

MXCuBE 2 @ BL13-XALOC

MXCuBE development and features

- Development on Qt4/master branch (merging, PRs pending).
- Systems and MIS actively involved.
- Bixente Rey (TXO Solutions).

Done

Optical Centring procedures.
Standard Data Collection.
LDAP authentication.
EDNA postprocessing.
ISPyB database.
Remote Access.

ToDo

Migration to Debian9.
Integrate to Sardana Scan Framework
(trigger by position)

- Energy Scan.
- Helical Data Collection.
- Mesh Data Collection.

X-ray Centring.

MXCuBE 2 @ BL13-XALOC

EDNA / ISPyB developments and features

- Development on master branch (PRs submitted).
- Optimize cluster performance (ongoing work).

Done

ToDo

EDPluginControlInterfaceToMXCuBEv1_3
EDPluginControlAutoPROCV1_0
EDPluginControlEDNAprocv1_0

EDPluginControlDozorv1_1

ISPyB status on thursday morning session (by Daniel Salvat from MIS).

Acknowledgements

The people

**Thank you for
your attention**

BL13-XALOC

Roeland Boer
Fernando Gil
Barbara Machado
Xavi Carpena

Controls

Guifre Cuni
Jordi Andreu

IT Systems

Sergi Puso
Ramon Escriba

MIS

Daniel Salvat
(Alfonso Burgos)
Daniel Sanchez

Externals

Bixente Rey