



MXCuBE status @ ALBA

XALOC Beamline

Jordi Andreu, Control Engineer @ ALBA

MXCuBE meeting, 16th January 2017, Grenoble (ESRF)

Overview

MXCuBE2 @ ALBA

- News
- MXCuBE Integration Strategy
- MXCuBE Current Status
- Next steps
- Project Contribution

News: XAIRA beamline @ ALBA

Microfocus Beamline for Protein Crystallography (XAIRA)

- Phase III beamline.
- **PRINCE2** Project management framework.
- MXCuBE (over Sardana) and ISPyB (LIMS).
- Project at the very beginning stage.
- Foreseen operation in 2020.

Integration of MXCuBE 2 (Qt4) @ ALBA

Xaloc Beamline (BL-13)

- Control system: [SARDANA](#) + [TAURUS](#) + TANGO
- Fully operative beamline...but:
 - Accessibility, current implementation.
 - Missing features (as required by MXCuBE), LIMS, user management.



Integration of MXCuBE 2 @ ALBA

Strategy

- Provide control of individual element through MXCuBE interface: *shutters, CATS, diffractometer, ...*
- Review/revisit current beamline operation procedures: *beam centering, collection methods, ...*
- Design & implement missing features (present in MXCuBE): *data and users management, ...*
- Continuous delivery of MXCuBE features (when possible, standalone applications)
- Take advantage of this situation: improve **reliability** and beamline **robustness**.
- Learning from **experience** (XAIRA design)

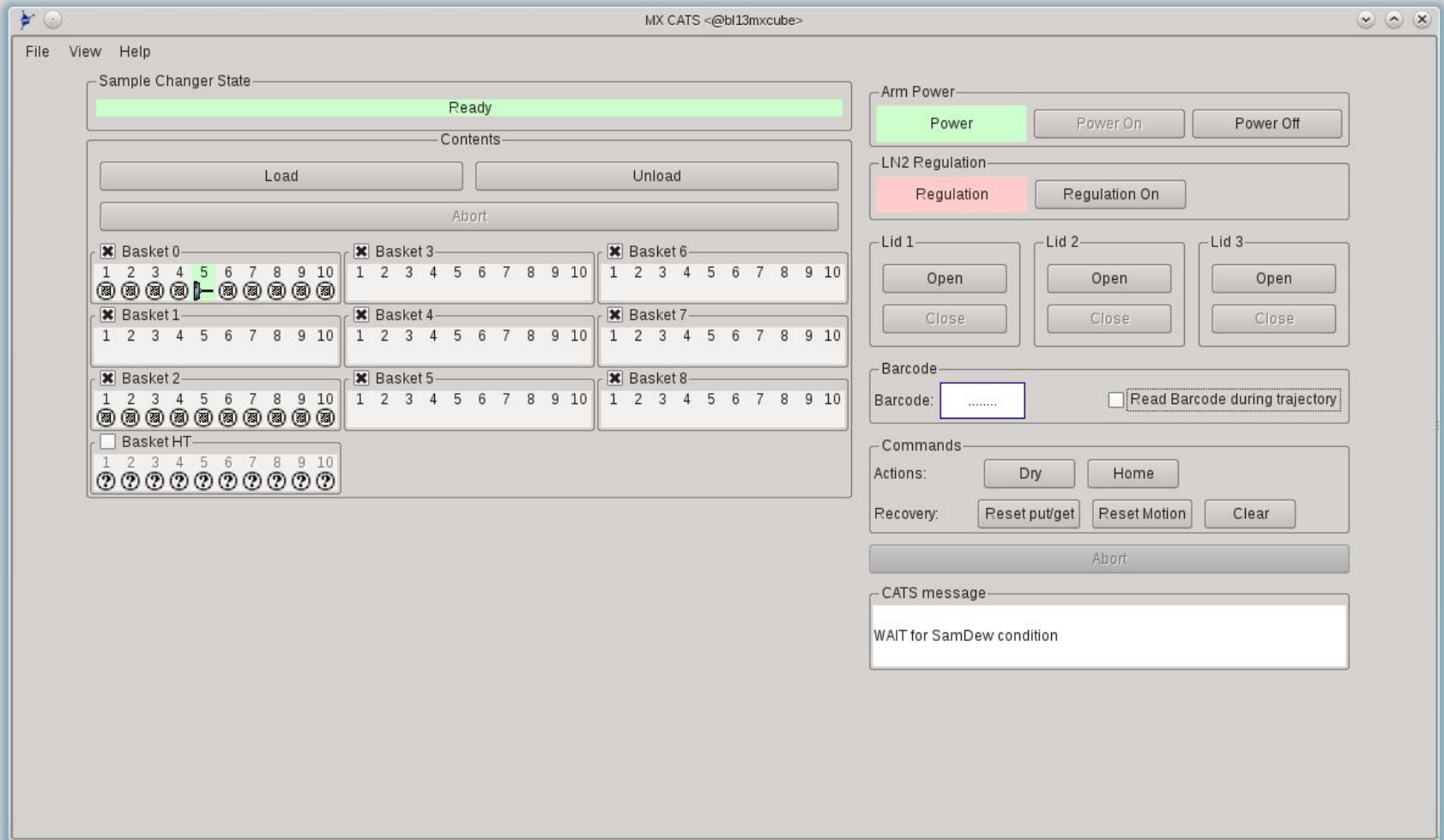
Integration of MXCuBE 2 @ ALBA

Current Status

- Qt4 version (master branch).
- Bixente Rey visits.
- MXCuBE interface for all individual beamline elements.
- Two new **Tango DS** required for XALOC:
Diffraction Manager
Beamline Supervisor
- **mxCATS** as standalone application.

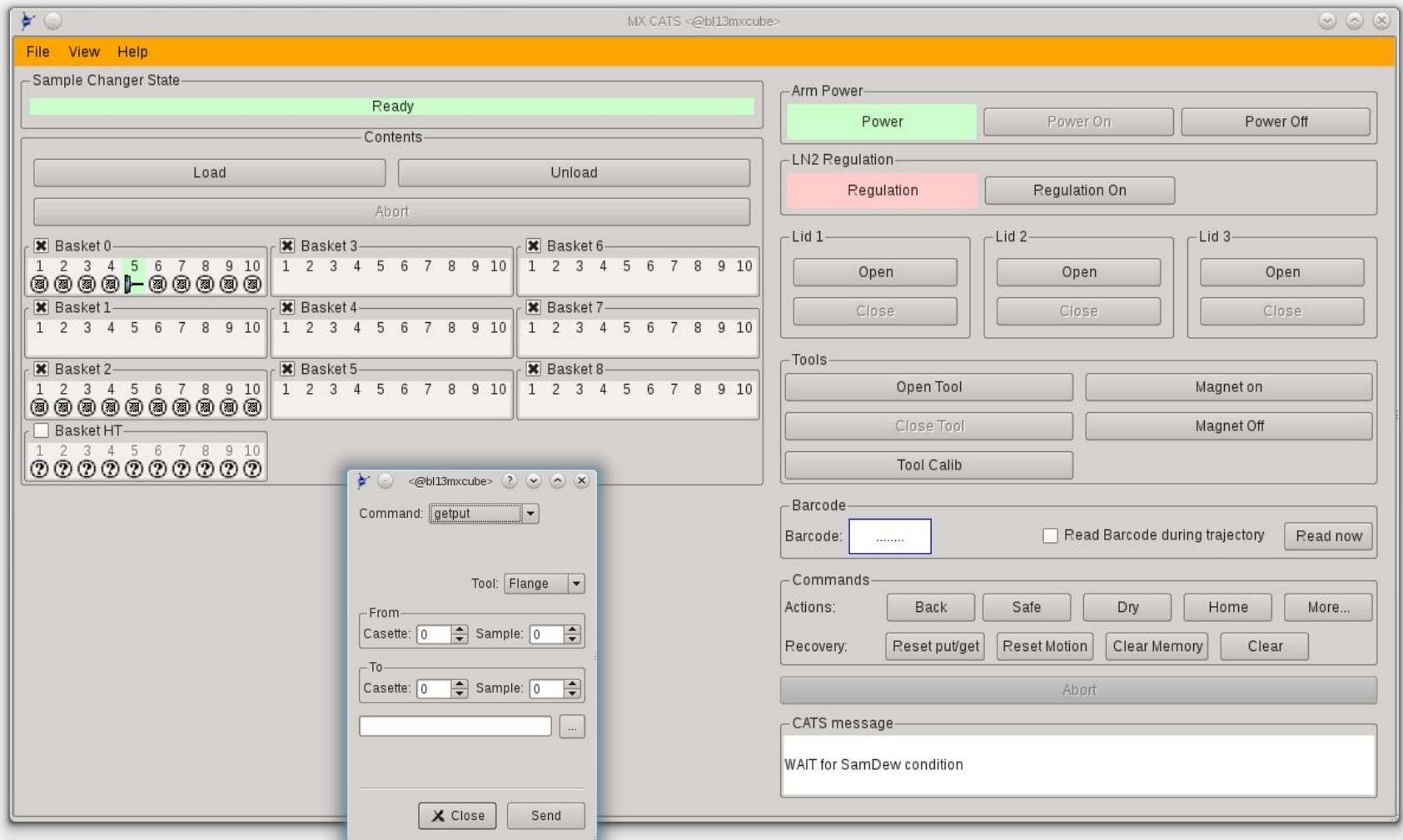
Integration of MXCuBE 2 @ ALBA

mxCats: standalone application



Integration of MXCuBE 2 @ ALBA

mxCats: expert mode



Integration of MXCuBE 2 @ ALBA

<https://github.com/mxcube/mxcube>

PR#148: Changes related with SampleChanger.

- Allow to derive it for a CatsSimpleBrick (a simplify version of the latter).
- Add a "Select" sample on "singleclick"

PR#147: Test environment / Qt4_CatsMaintenance / ALBA specific Bricks.

- Create of a module MXCuBE_Test_Environment.py to test HardwareObjects or Bricks
- Add a Qt4_CatsMaintenance.py brick (converted from original qt3)
- Add a number of ALBA specific Bricks *shutters, Lights, etc...)
- Add a convenience QLed widget.

Integration of MXCuBE 2 @ ALBA

<https://github.com/mxcube/HardwareObjects>

PR#168: XMLRPCServer and other ALBA Changes

- Minor changes on XMLRPCServer.py.
- Adding extra optional "shifts" parame for load, unload commands in CATS.
- Add extra commands in CatsMaint.py.
- Get limits for position from SardanaChannel minval, maxval.
- Add a series of ALBA Specific Hardware Objects.

PR#171: LimaVideo and SampleChanger code

- Generic Sample change and Cats90.
- Qt4_LimaVideo (dual library-tango server support).

waiting

Integration of MXCuBE 2 @ ALBA

<https://github.com/mxcube/HardwareRepository>

PR#12 : `Sardana.py` - finding `minval`, `maxval` depending on Taurus version.

- Get limits for `SardanaChannel`. Make condition depending on Taurus version.

Integration of MXCuBE 2 @ ALBA

<https://github.com/mxcube/BlissFramework>

PR#14: Small Qt4_widget_colors changes /
Qt4_LightControlBrick.

- All colors in Qt4_widget_colors are now instances QColor
- New color_to_hexa() function added in Qt4_widget_colors (to be used in calls of type setStyleSheet())
- New Qt4_LightControlBrick() (converted from Qt3)

Integration of MXCuBE 2 @ ALBA

Next steps

- Implement basic collection methods.
- Design data & user management schemes.

Acknowledgements

The team(s)

XALOC staff

- Roeland Boer
- Jordi Juanhuix
- Fernando Gil
- Barbara Machado
- Xavi Carpena

Controls

- Guifre Cuni
- Jordi Andreu

Externals

- Bixente Rey (TXO)

**Thank you for
your attention**

Integration of MXCuBE 2 (Qt4) @ ALBA

Evolution of MXCuBE implementation @ ALBA



Bessy (June 2015)



ALBA (December 2015)



DESY (June 2016)



ESRF (February 2017)

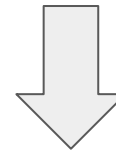
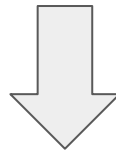
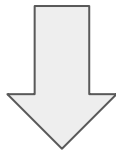
Integration of MXCuBE 2 @ ALBA

Current status

- Under development for XALOC Beamline (BL13) @ ALBA.
- Basic operations available (centering, autofocus, etc...)
- Early stage on the Qt4 implementation (*Qt3->Qt4 overhead*).
- *Limited access* for development due to beamline in fully operation.

we were:

Developing on branch 2.1	Qt3 Graphical Interface	EDNA @ workstation
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we are:

Developing on branch 2.2 (stable)	Qt4 Graphical Interface	EDNA @ cluster
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Integration of MXCuBE 2 @ ALBA

New implementations

HardwareObjects: PR #168 (**XMLRPCServer and other ALBA Changes (New objects, Cats evolution, SardanaMotor)**)

- Adding extra optional "shifts" parameter for some of the CATS commands allow to specify "shifts" in load, unload commands in CATS.
- Add extra commands in CatsMaint Add some more commands to CatsMaint.py.
- Update SardanaMotor.py. Get limits for position from SardanaChannel minval, maxval.
- ALBA Hardware Objects. Add a series of ALBA Specific Hardware Objects.

Integration of MXCuBE 2 @ ALBA

XALOC: Current status



The screenshot shows the MXCuBE control software interface. On the left, there is a 'Sample video' window displaying a live image of a sample with a scale bar indicating 100 μm and 200 μm. Below the video are controls for 'Beam size' (Horizontal: 10 μm, Vertical: 10 μm) and 'Slits' (Horizontal: 0.00, Vertical: 0.00). The main area contains a 'Standard Collection' configuration panel with fields for 'Oscillation start', 'Exposure time (s)', 'Kappa', 'Energy (keV)', 'Resolution (Å)', and 'Transmission (%)'. There are also checkboxes for 'Shutterless' and 'Inverse beam'. To the right, a 'Sample list' panel shows 'Mode: Manually mounted' and 'Centring: Manual'. The top right corner displays 'Machine current: 0.1 mA', 'Machine status: ON', and 'TopUp Remaining: 720.1 s'. At the bottom right, there are buttons for 'Collect Queue', 'Pause', and 'Set in/Set out'. A status bar at the bottom left shows error messages: '[2016-06-16 09:52:59] Could not load beamline setup check configuration 1.' and '[2016-06-16 09:52:59] Could not load beamline setup check configuration 1.'

Qt4 Graphical Interface

General: Camera in Qt4 (PR # 74 to branch 2.2)

- Modifications to the **Qt4_LimaVideo.py** HwObj to provide support for Basler cameras *via* **LiMA** library.
- Supported pixel types:
 - *YUV 422 packed* (Color)
 - *Y8* (Black and White)
- The implementation is **QUB** independent.
- Depends on **OpenCV** library python interface.
- Easily extensible to other pixel formats.

CONFIGURATION:

```
<device class="Qt4_LimaVideo" >
  <type>basler</type>
  <address>84.89.227.72 </address>
  <encoding>yuv422p</encoding>
  <gain>0.3</gain>
  <exposure>0.01</exposure>
  <interval>30</interval>
</device>
```

Qt4 Graphical Interface

ALBA Specific: Xaloc Hardware Objects (PR # 73 to branch 2.2)

- The parent class of (ALBA specific) **XalocMinidiff** HwObj has been changed from **MiniDiff** to **GenericDiffractometer** class.
- Hutch menu brick works fine: Centering routines, focus (sardana macro), snapshot, etc...
- ...**BUT** we still using the old centering routines module.

- **Overhead:** We had the need to adapt some HardwareObjects which were already running for Qt3 version: MachineInfo, SafetyShutter, Beamstop, etc...

EDNA plugins

Strategy & Fast autoproc plugins

- **EDNA Strategy: EDPluginControlInterfaceToMXCuBEv1_3**
 - Already in production (Tango EDNA server).
 - Running on workstation (8 cores) Intel(R) Xeon(R) CPU E31275 @ 3.40GHz.
- **EDNA Fast Autoproc plugin: EDPluginControlAutoprocV1_0**
 - Testing @ Cluster (direct batch queue).
 - Running on a HPC node (16 cores) Intel(R) Xeon(R) CPU E5-2650 v2 @ 2.60GHz

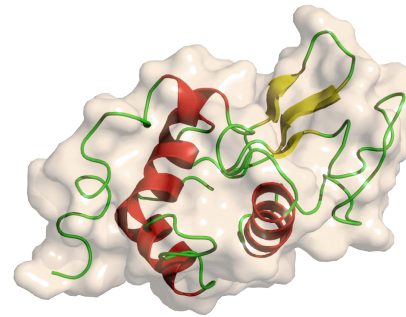
EDNA performance

Strategy & Fast autoproc plugins

- Lysozyme (1800 images set)

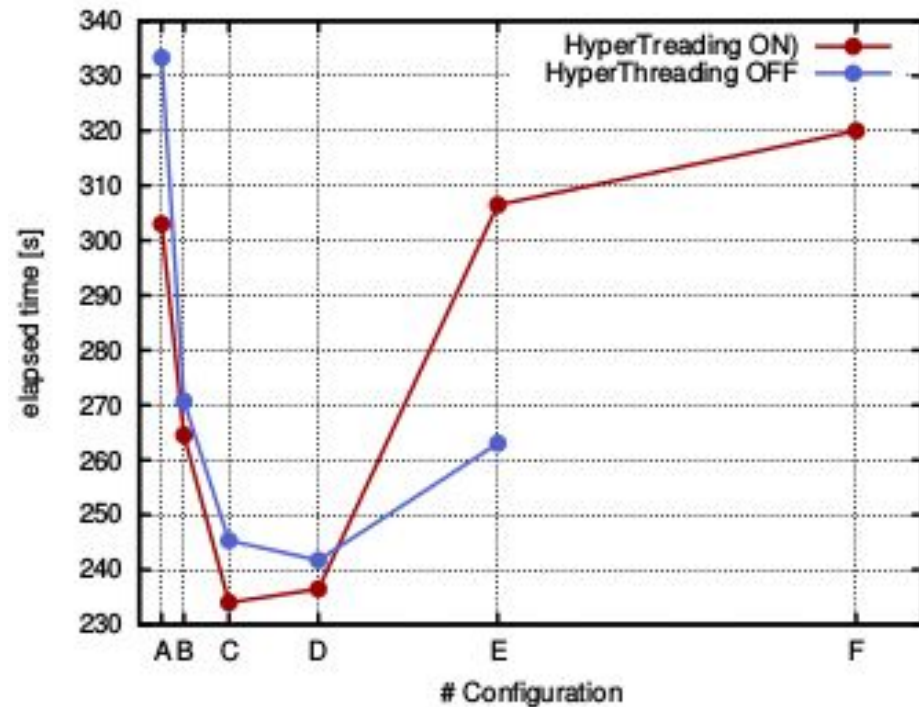
Cluster geometry for XDS

http://xds.mpimf-heidelberg.mpg.de/html_doc/xds_parameters.html



config	# procs	# jobs
A	1	32
B	2	16
C	4	8
D	8	4
E	16	2
F	32	1

JOBS: independent subprocesses
PROCS: parallel OpenMP

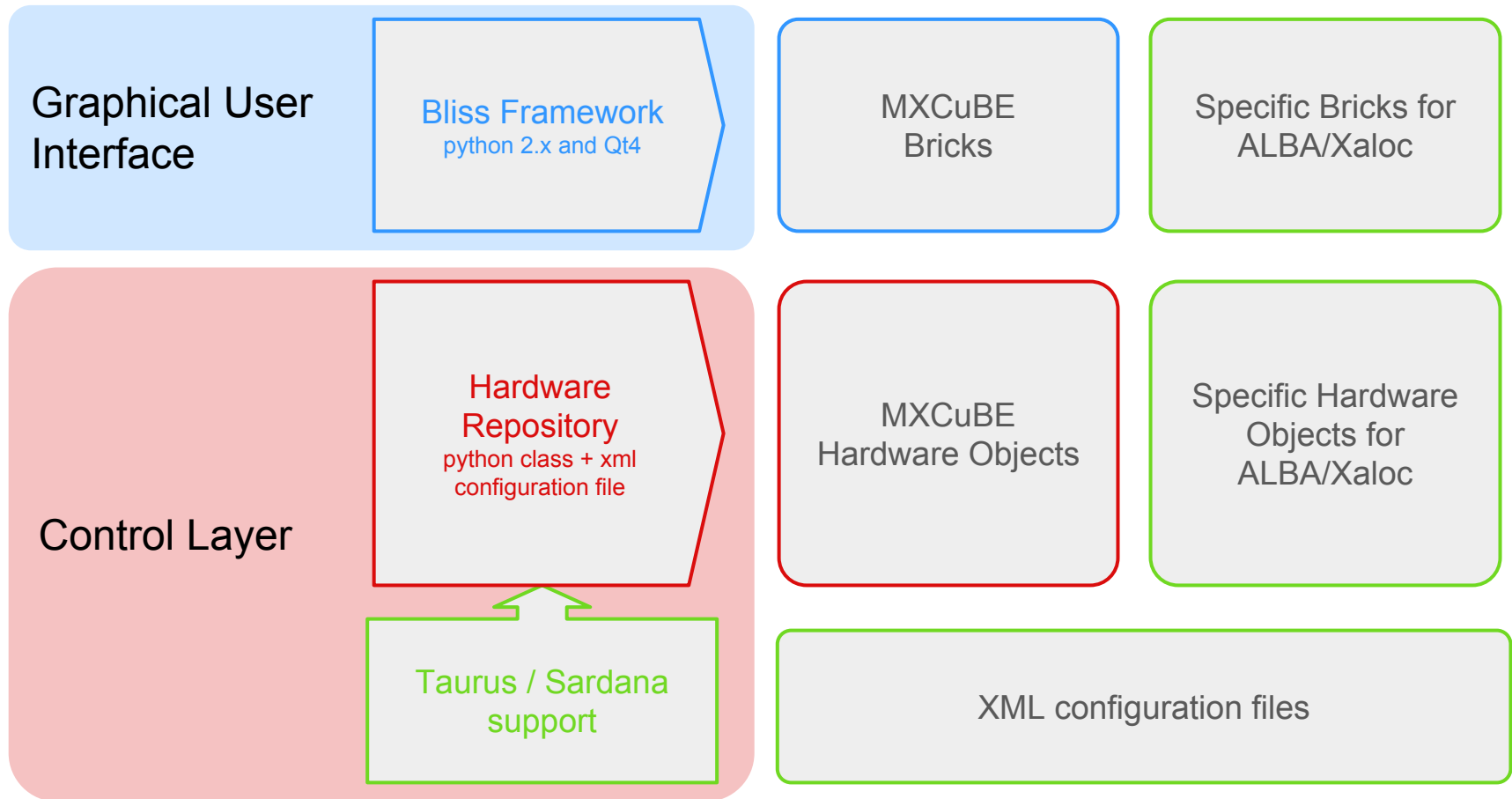


MXCuBE 2 @ ALBA

Based on SARDANA & TAURUS Control System

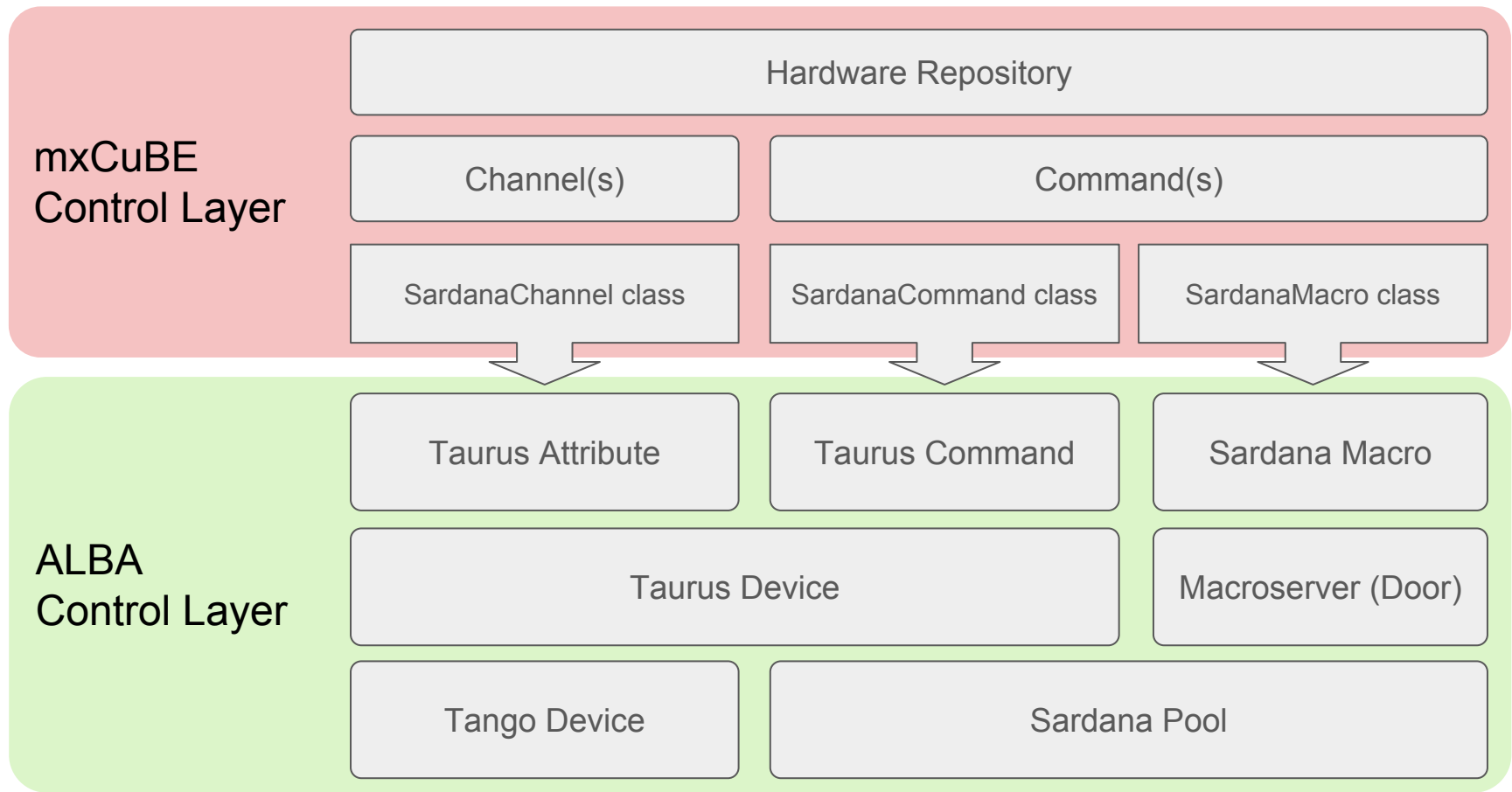
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Over Sardana Control layer



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Sardana Support for Hardware Repository (V. Rey)



*Implemented by V. Rey in *CommandContainer.py* and *Sardana.py* files from Hardware Repository (ALBA branch @ github)

Integration of MXCuBE 2 @ ALBA

Sardana Support for Hardware Repository

Hardware Object configuration (Sardana Layer):

```
<object class="SardanaXfeSpectrum">
  <doorname>door/mxcube/1</doorname>
  <command type="sardana" name="configure">senv ActiveMntGrp mg_fluodet</command>
  <command type="sardana" name="acquire">ct %s</command>
  <channel type="sardana" taurusname="fluodet_timer" name="spectro">spectrum</channel>
</object>
```

macro name

taurus device name

attribute name

Integration of MXCuBE 2 @ ALBA

Sardana Support for Hardware Repository

Sardana Motor:

Position and State (channels) and Stop (command) are defined by default...

```
<device class="SardanaMotor">  
  <username>Omega Z</username>  
  <taurusname>omegaz</taurusname>  
</device>
```

...even they can specified in the configuration file:

```
<device class="SardanaMotor">  
  <username>Omega Z</username>  
  <taurusname>omegaz</taurusname>  
  <channel type="sardana" polling="events" name="position">Position</channel>  
  <channel type="sardana" polling="events" name="state">State</channel>  
  <command type="sardana" name="stop">Stop</command>  
</device>
```