

MXCuBE 3 - General Layout and Sample Centring

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Outline



- Review of MXCuBE 3
- Proposed layout for the web interface
- Demo video and current status
- Next steps

Backend

- Python **Flask** microwebframework:
 - web server made simple
 - extensions (database, login, ...)
 - easily adaptable to your needs while scalable
 - big community
- http request **API**: rest like (but probably not fully rest)
 - an url for each function
 - Simple to add new features without changing existing ones
- Flask **socketio** for sending HO messages
 - server-client bi-directional communication, websocket based
- Reuse the existing Hardware Repository

Http requests

- API for the calls from client to server (*GET, PUT, POST...*)
- Decoupling the server and the client
- Should be easy to understand by the client
 - ➔ (<http://example.com/mybeamline/mymotors/omega/move/45>)
- Url routings for sample centring/video: already working

Sample Centring API

PUT /mxcube/api/v0.1/samplecentring/centring/start3click

Start 3 click centring procedure

Args:

None

Return:

'True' if command issued successfully, otherwise 'False'

Note:

This does not mean if the centring is successful or not

PUT /mxcube/api/v0.1/samplecentring/centring/startauto

Start automatic (lucid) centring procedure

Args:

None

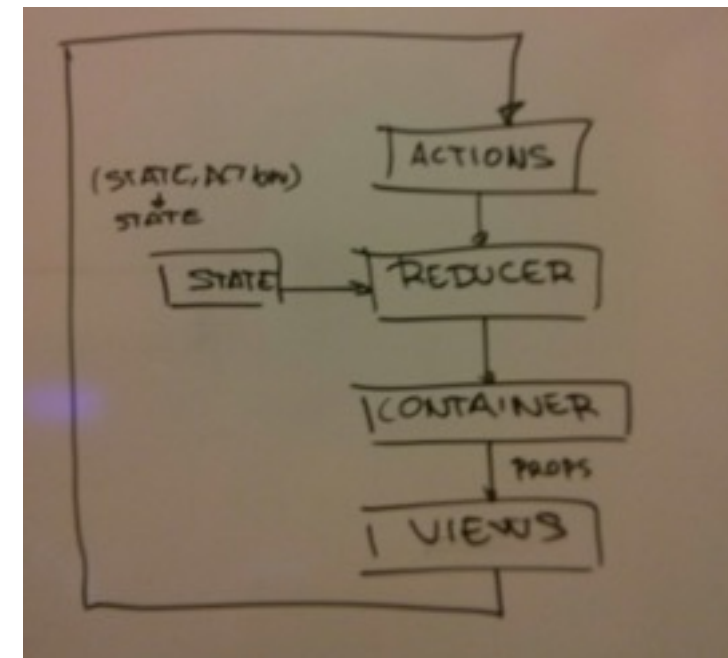
Return:

'True' if command issued successfully, otherwise 'False'

```
@mxcube.route("/mxcube/api/v0.1/samplecentring/centring/start3click", methods=['PUT'])
def centre3click():
    """
    Start 3 click centring procedure
    Args: None
    Return: 'True' if command issued successfully, otherwise 'False'. Note that this
           does not mean\
           if the centring is successful or not
    """
    logging.getLogger('HWR.MX3').info('[Centring] 3click method requested')
    try:
        currentCentringProcedure = mxcube.diffractometer.start3ClickCentring()
        return "True" #this only means the call was successful
    except:
        return "False"
```

Frontend

- **Javascript/React** library (Facebook)
- Only for the user interface (the view in MVC)
- Virtual html DOM kept as internal state
 - Different components programmed independently
- Reusing existing code when the layout changes
- **Redux** application architecture/pattern
 - Predictable state container for JavaScript apps ...
 - ➔ the way to go if you use React
 - Unidirectional data flow
 - Changes on the internal state in a single place

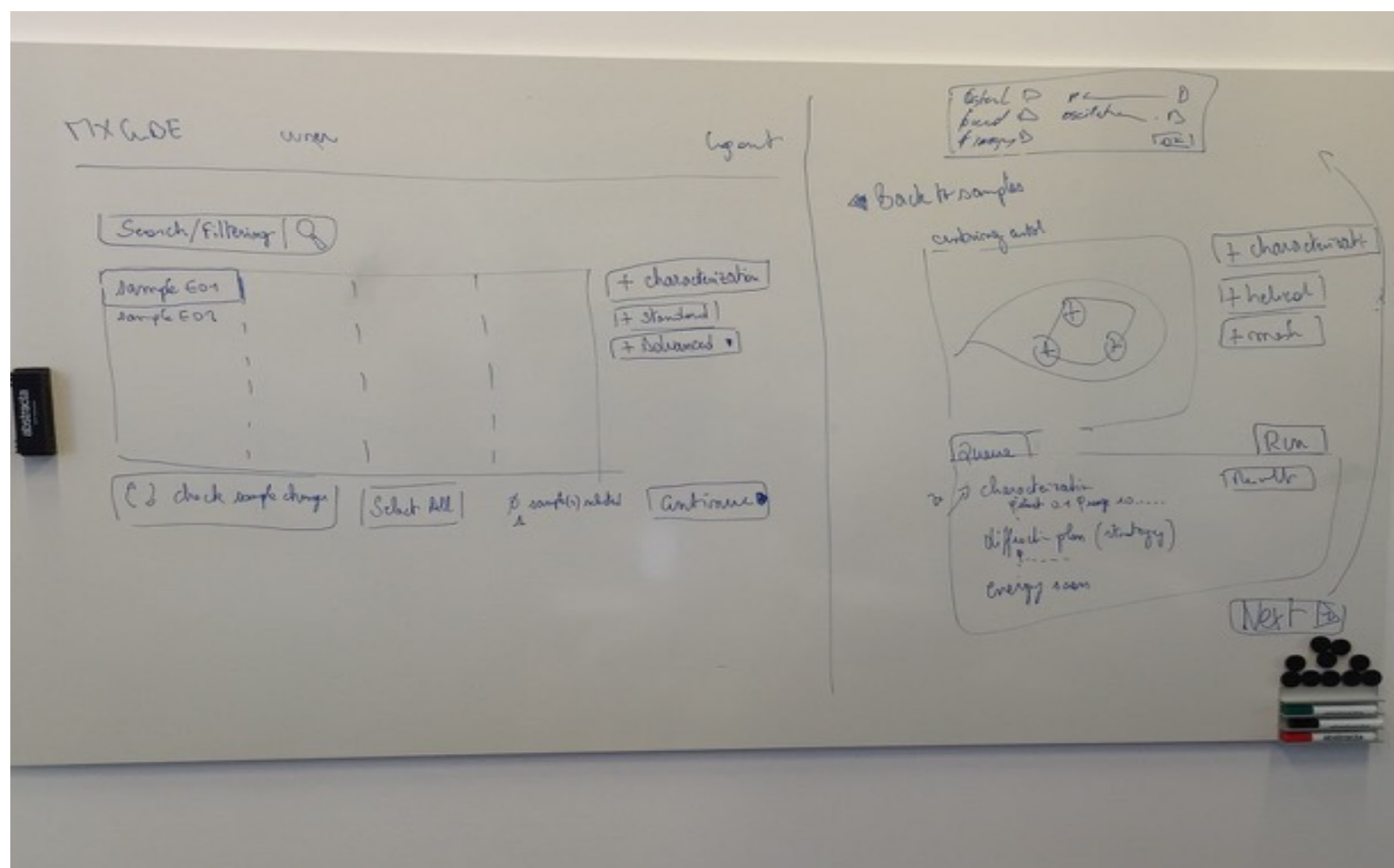


Redux architecture

Layout

- Before going to *react* a main objective was identified
 - Improve the user experience !!!
- And for that it is useful to
 - Have a clean interface
 - Use modern web technologies
 - Learn current usage and feedback
- And finally... a big question arises:
 - Is this really possible?

Layout - first sketch



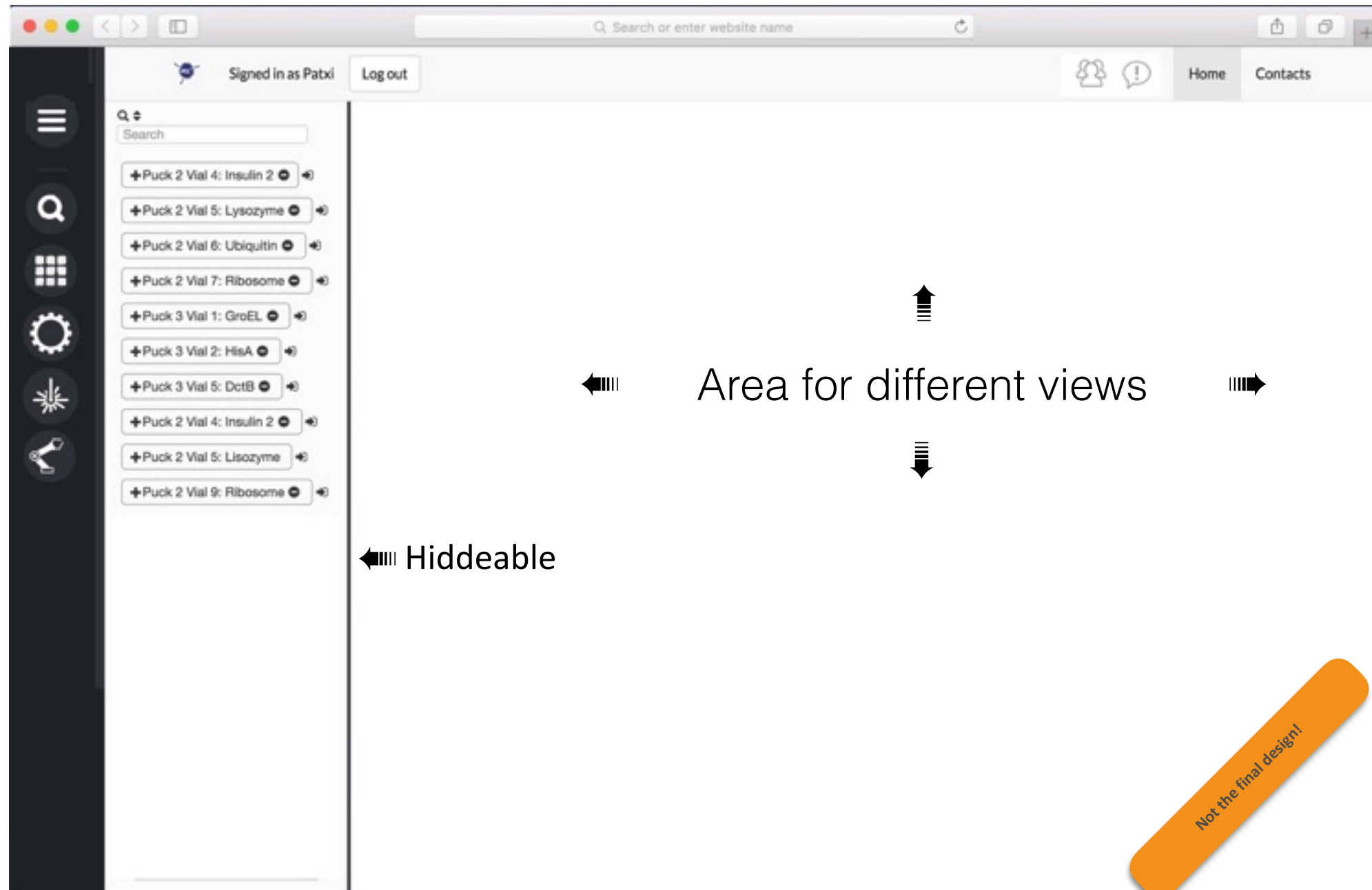
MAXIV-ESRF Sep. 2015

- Experiment configuration in a batch like mode
 - All available samples
- Experiment management for each sample
 - centring mechanism
 - should also be automatic and transparent for the user

Transitions between views to be defined

Layout - first real design

- Common parts



Not the final design!

Layout - first real design

- Sample Grid

The screenshot displays a web-based interface for managing a sample grid. At the top, there is a search bar and navigation links for 'Home' and 'Contacts'. The user is signed in as 'Pabx'. A sidebar on the left contains various icons for navigation and control. The main area features a grid of sample cards, each with a unique identifier, a sample name, and a status indicator. A 'Filter' section is located above the grid, and a 'Check sample changer contents' button is positioned above the first row. A dropdown menu is open on the right side of the grid, showing options like 'Manual', 'Automatic', and 'Something else here'. At the bottom of the grid, there is an 'Add +' button and a 'Run', 'Pause', 'Stop' control panel.

Sample ID	Sample Name	Status
f01 (A-TIM)	HA1234567	4:4
hfd01 (A-TIM)	HA1234567	4:1
testsd1 (A-TIM)	HA1234567	6:1
testpuck6 (A-TIM)	HA1234567	3:1
d01 (A3155)	HA1234567	4:2
d02 (A3155)	HA1234567	4:3
xtal1 (cp)	HA1234567	2:1
xtal2 (cp)	HA1234567	2:2
xtal2 (cp)	HA1234567	2:2
xtal5 (cp)	HA1234567	2:6
xtal6 (cp)	HA1234567	2:6
xtal3 (cp)	HA1234567	2:3
xtal4 (cp)	HA1234567	2:4
xtal4 (cp)	HA1234567	2:4
d01 (FAE)	HA1234567	4:6
Dimple1 (LysoTetra)	HA1234567	10:1
xtal7 (cp)	HA1234567	2:7
xtal8 (cp)	HA1234567	2:8
xtal8 (cp)	HA1234567	2:8
dimple2 (THAU)	HA1234567	24:1
dimple1 (tryp)	HA1234567	1:1
dimple2 (THAU)	HA1234567	24:1
dimple1 (tryp)	HA1234567	1:1
dimple1 (tryp)	HA1234567	1:1

Not the final design!

Layout - first real design

- Sample Video

Signed in as Patxi | Log out

Search or enter website name

Home | Contacts

Search

→ Puck 2 Vial 4: Insulin 2
Spacegroup I 21 3 Unit Cell a=b≠c≠78.04
α=β≠γ=90
Comments: High resolution data is needed
Crystallization condition:
Cryoprotectant:
Sample Centring
Characterisation
Standard Collection
Helical Scan

→ Puck 2 Vial 5: Lysozyme
Sample Centring
Characterisation
Standard Collection

→ Puck 2 Vial 6: Ubiquitin
Sample Centring
Characterisation
Standard Collection

→ Puck 2 Vial 7: Ribosome
Sample Centring
Characterisation
Standard Collection

→ Puck 3 Vial 1: GroEL
Sample Centring
Characterisation
Standard Collection

→ Puck 3 Vial 2: HisA
→ Puck 3 Vial 5: DctB
→ Puck 2 Vial 4: Insulin 2
→ Puck 2 Vial 5: Lysozyme
Sample Centring
Characterisation
Standard Collection

Run | Pause | Stop

Current Setup
Beam Energy: 12.6 keV / Lambda: 0.98 Å Size: 50 µm
Detector Distance: 500 mm / Resolution: 2.3 Å
MiniKappa Omega: 1.55 Kappa: 0.00 Phi: 90.0

Experimental Setup
Data storage: /data/data1/visit/oms20090101/20140101/RAW_DATA/ sample/cryst1
Prefix: test Run number: 1
Energy: 12.6 keV / Lambda: 0.98 Å
Resolution: 1.5 Å / Detector distance: 350 mm
Beamsize(µm): 10 30 50 75 120
Exposure time: 30 ms Transmission: 20.2 %
Oscillation: 0.2 Start: 70.00 Kappa: 0 Phi: 90

Characterization | Grid Scan

Number of Images: 1 2 4 90 degree apart
 Radiation Damage Anomalous Signal
 Element Analysis

Standard | Helical | Raster

1 Start Image 900 Number of Images
 Shutterless

Energy Scan | XRF

Ni Element
 AnOption

Points
pos1 S C D
pos2 S C D
pos3 S C D

Lines
line1 S C D
line2 S C D
New Add

Grids
Grid1: 5x10 S C D
Grid2: 20x20 S C D
New Add

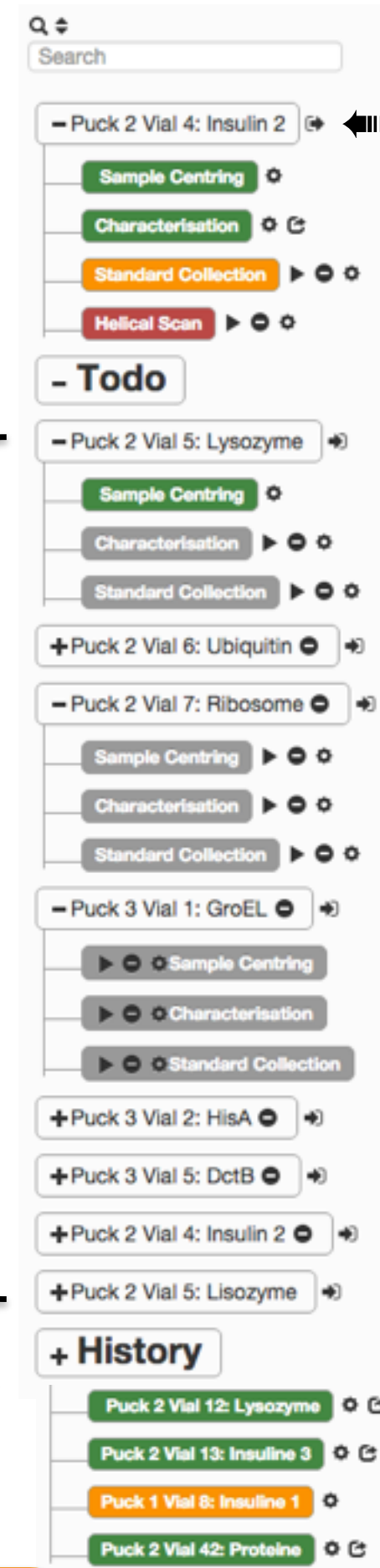
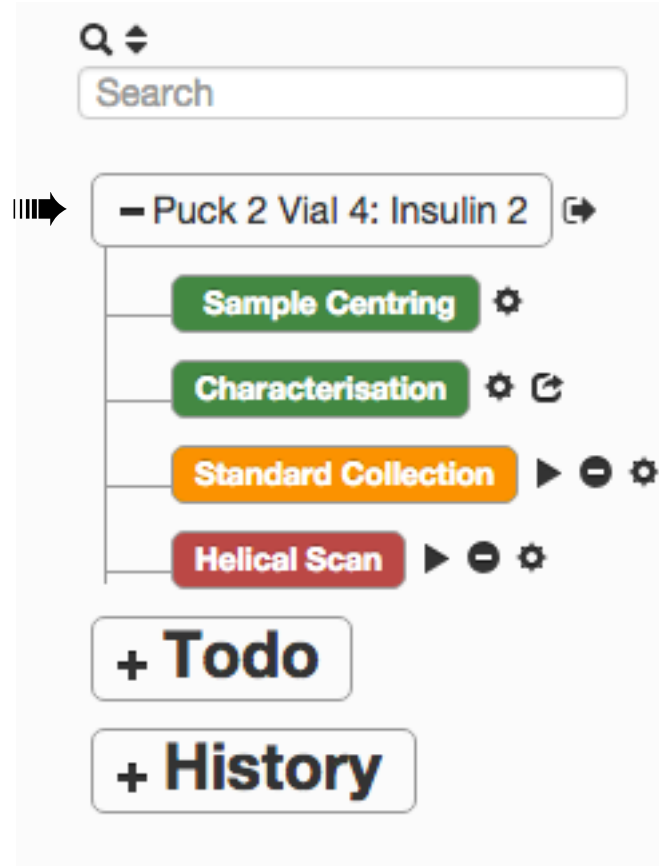
100 µm
100 µm

Not the final design!

Layout - Queue

- Queue:
 - Current sample always on top
 - Todo and History (collapsable)
 - Drag&Drop, search, reorder, skip ...

Current sample



Current sample

Not the final design!

MXCuBE 3 - demo

- Sample Centring and video

The screenshot displays a web browser window with the address bar showing `192.168.56.101:8081`. The main content area is titled "Sample Centring" and features a video feed of a sample. A blue circle highlights a specific feature on the sample. In the bottom-left corner of the video, the text "Zoom 1" is visible. To the right of the video, there is a panel labeled "Panel content". Below the video is a "Controls" section with various icons for file operations, navigation, and zooming. At the bottom, there are input fields for "Kappa" (kappa), "Omega" (omega), and "Phi" (Phi).

Current Status

- Working on core packages - Jan16 milestone ([Antonio's talk](#))
 - Diffractometer controlled: code reused in *any* layout
 - Setting up development environment/workflow ([Matias' talk](#))
 - Web interface layout designed (at least until further discussion)
 - Mockups + real environment
- Github => 138 commits | 25 pull requests | 38 issues

<https://github.com/mxcube/mxcube3>

The screenshot shows a GitHub project dashboard with two milestones. At the top, it indicates '2 Open' and '0 Closed' items, along with a 'Sort' dropdown. The first milestone is for 'January 2016', due by January 15, 2016, and last updated about 17 hours ago. It shows a progress bar that is 44% complete (green), with 10 open and 8 closed items. The description states: 'All core packages should be running, mxcube3 will be used at Biomax for commissioning the diffractometer (not all the features will be used but the ones related to the udiff)'. The second milestone is for 'June 2016', due by June 21, 2016, and last updated about 18 hours ago. It shows a progress bar that is 0% complete (grey), with 4 open and 0 closed items. The description states: 'By this date we should be able to do an experiment at BioMAX'. Both milestones have 'Edit', 'Close', and 'Delete' options.

Next steps

- Real testing
 - Maxlab 911 mx beamline to be closed...
 - MaxIV laboraty setup: MD2? + virtual beamline
 - ESRF beamlines (Matias)

- Work towards Jan16 milestone
 - HO integration in the server (http requests)
 - Frozen design: gimp => web
 - Implementation of the queue
 - Sample Grid

MXCuBE3 People

Main developers:

MAX IV: M. Eguirraun, A. Milan-Otero, J. Nan, F. Bolmsten

ESRF: M. Guijarro

Supported by:

MXCuBE collaboration

MAX IV MX and KITS teams

ESRF BCU team

Thanks for your attention!