

A Light for Science



European Synchrotron Radiation Facility



# MXCuBE 2.0

# Outline

- New features
  - Improved queue system
  - Position history
  - Better integration with LIMS (ISPyB)
  - Improved usability
  - Workflow integration
- Demo
- Design overview

# Overview

*Simple and flexible with possibility to perform complex tasks.*

The screenshot displays the mxCuBE (opid-141) software interface, which is used for controlling X-ray diffraction experiments. The interface is divided into several functional areas:

- Top Bar:** Includes 'File', 'Instrumentation', and 'Help' menus, along with an 'Expert mode' checkbox.
- Left Panel:** Contains a 'Sample list' with checkboxes for various samples (e.g., TRYP-sample1 to TRYP-sample10) and a 'Sample location' tree view.
- Sample Positioning (Center):** Features input fields for 'Omega' (0.35), 'Kappa' (105.97), 'Phi' (0.35), and 'Holder length' (22.073). Below this is a 'Sample video' window showing a live image of the sample with a scale bar (200 μm, 500 μm) and 'Hor' (0.1) and 'Ver' (0.1) movement controls.
- Collection Method (Right):** A 'Discrete' acquisition panel with settings for 'Oscillation range' (0.2), 'Oscillation overlap' (0.0), 'Oscillation start' (0.0), 'Exposure time' (0.1), 'Energy (KeV)', 'Resolution (Å)' (4.3241), and 'Transmission (%)' (100.0).
- Machine Status (Far Right):** Displays real-time data such as 'Machine current' (182.3 mA), 'Flux', 'Energy' (13.28 KeV), and 'Transmission' (100.00%).
- Bottom Panel:** Shows a 'Collect Queue' button and a status bar with collection details and a warning: 'No centred position(s) was selected'. A status bar at the very bottom provides a detailed error message: '[2013-04-05 14:11:17] Collection done [2013-04-05 14:12:08] No centred position(s) was selected [\"sampx\": \"0.067020972752\", \"sampy\": \"0.06482316076294\", \"zph\": \"0.35546875\", \"zoom\": \"0\", \"phi\": \"0.522822222222\", \"psi\": \"22.073\"] (current position) will be used.'

# Enhanced queue

- Generalized tasks
- Pipeline mode with task for user input
- Possibility to modify queue while executing
- Possibility to group tasks (e.g. Collections)

Sample list

Show:

Centring:

Sample location	Status
<input type="checkbox"/> 1:1 - TRYP-sample1	
<input type="checkbox"/> 1:2 - TRYP-sample2	
<input type="checkbox"/> 1:3 - TRYP-sample3	
<input type="checkbox"/> 1:4 - TRYP-sample4	
<input type="checkbox"/> 1:5 - FAE-sample5	
<input type="checkbox"/> 1:6 - FAE-sample6	
<input type="checkbox"/> 1:7 - FAE-sample7	
<input checked="" type="checkbox"/> 1:8 - FAE-sample8	Sample loaded
<input checked="" type="checkbox"/> Discrete - 1	In progress
<input checked="" type="checkbox"/> sample-centring	Waiting for input
<input checked="" type="checkbox"/> FAE-sample8_1	
<input type="checkbox"/> 1:9 - TRYP-sample9	
<input type="checkbox"/> 1:10 - TRYP-sample10	
<input type="checkbox"/> 2:1 -	
<input type="checkbox"/> 2:2 -	
<input type="checkbox"/> 2:3 -	

Sample list







Show:


Centring:


Sample location	Status
<input type="checkbox"/> 1:1 - TRYP-sample1	
<input checked="" type="checkbox"/> 1:2 - TRYP-sample2	
<input type="checkbox"/> 1:3 - TRYP-sample3	
<input type="checkbox"/> 1:4 - TRYP-sample4	
<input type="checkbox"/> 1:5 - FAE-sample5	
<input type="checkbox"/> 1:6 - FAE-sample6	
<input type="checkbox"/> 1:7 - FAE-sample7	
<input checked="" type="checkbox"/> 1:8 - FAE-sample8	Done
<input type="checkbox"/> Discrete - 1	Done
<input type="checkbox"/> sample-centring	Done
<input type="checkbox"/> FAE-sample8_1	Done
<input checked="" type="checkbox"/> Characterisation - 1	
<input checked="" type="checkbox"/> ref-FAE-sample8_1	
<input type="checkbox"/> 1:9 - TRYP-sample9	
<input type="checkbox"/> 1:10 - TRYP-sample10	
<input type="checkbox"/> 2:1 -	
<input type="checkbox"/> 2:2 -	
<input type="checkbox"/> 2:3 -	


# Position / Shape History

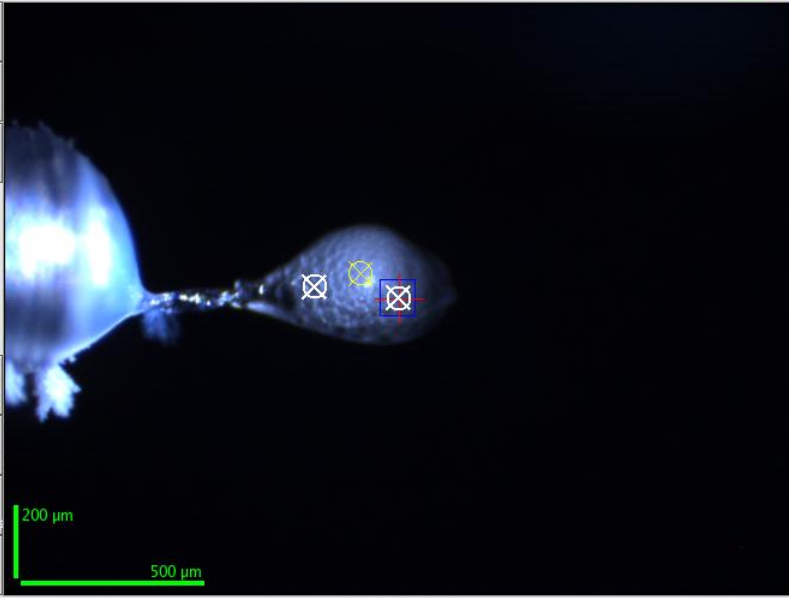
Sample video


Light: 0.21   Focus: -0.3  0.001  Front light: 2.0  Zoom: 1 


Centre 


Save 


Snapshot 



Centre beam 







Quick realign 


fake powders  200  $\mu\text{m}$


Anneal  500  $\mu\text{m}$


Sample is centred!

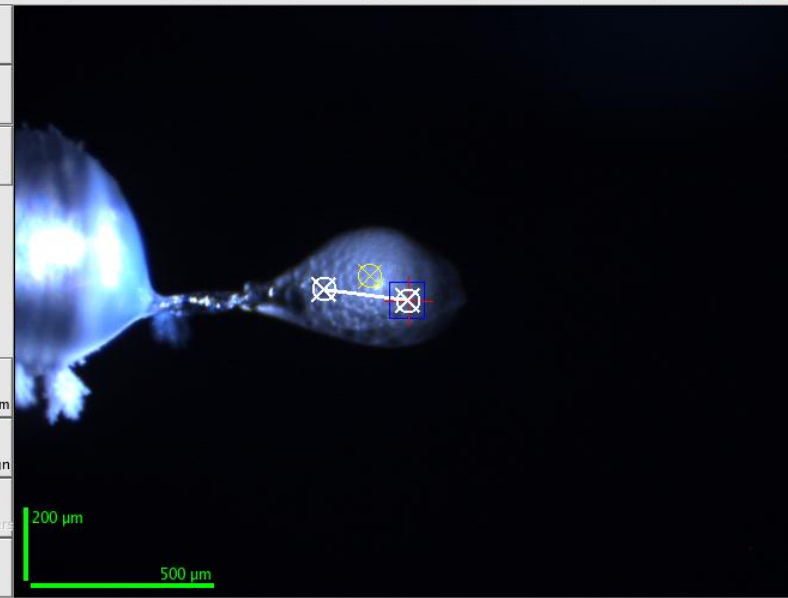
Sample video


Light: 0.21   Focus: -0.3  0.001  Front light: 2.0  Zoom: 1 


Centre 


Save 


Snapshot 



Centre beam 

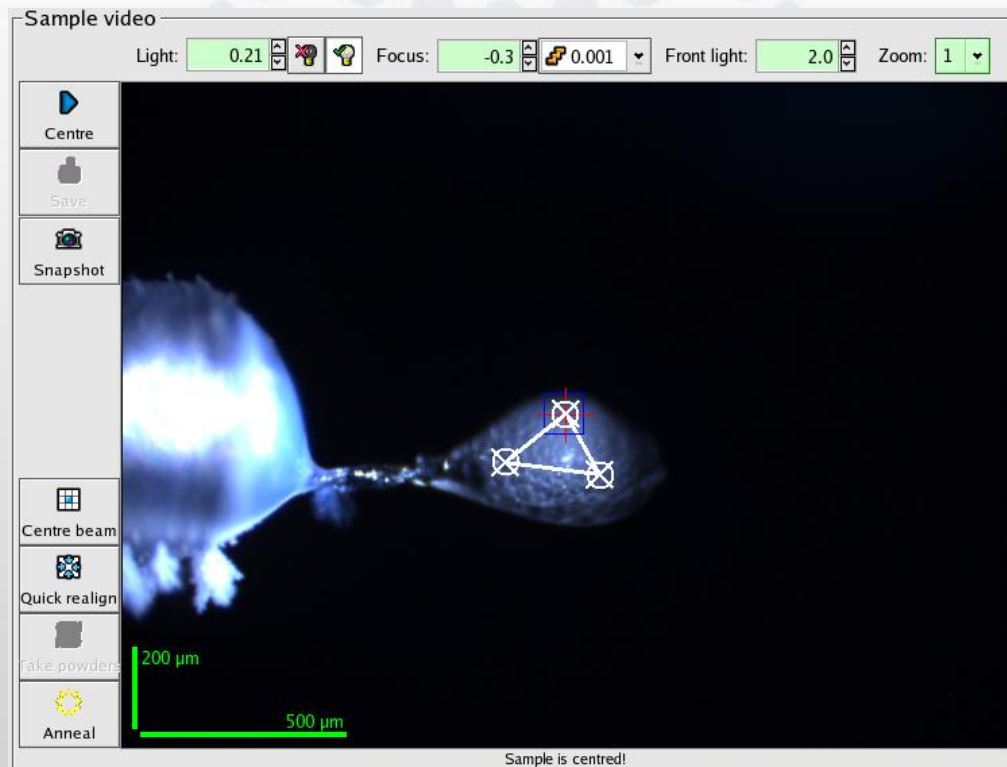
Quick realign 

fake powders  200  $\mu\text{m}$

Anneal  500  $\mu\text{m}$

Sample is centred!

# Several lines



# Better integration with LIMS (ISPyB)

The screenshot displays the ISIS software interface with several key components highlighted in red boxes:

- Sample list (left):** A tree view showing sample locations such as '1.1 - TRYP-sample1' through '1.10 - TRYP-sample10'. Item '1.2 - TRYP-sample2' is selected.
- Sample centring (top center):** A panel for adjusting sample position with parameters: Omega: 0.35, Kappa: 105.97, Phi: 0.35, Holder length: 22.073.
- Data location (middle right):** A panel for specifying file paths, showing 'Folder: /data/14eh1/inhouse/opic141/20130405/RAW\_DATA' and 'File name: TRYP-sample2\_1\_%04d.img'.


Other visible interface elements include 'Sample position' controls, 'Sample video' window, 'Collection method' settings, and a status bar at the bottom with a log of collection events.



# Better integration with LIMS (ISPyB)

Sample list

Show:

Centring:  

Sample location	Status
<input type="checkbox"/> 1:1 - TRYP-sample1	
<input type="checkbox"/> 1:2 - TRYP-sample2	
<input type="checkbox"/> 1:3 - TRYP-sample3	
<input type="checkbox"/> 1:4 - TRYP-sample4	
<input type="checkbox"/> 1:5 - FAE-sample5	
<input type="checkbox"/> 1:6 - FAE-sample6	
<input type="checkbox"/> 1:7 - FAE-sample7	
<input checked="" type="checkbox"/> 1:8 - FAE-sample8	Done
<input type="checkbox"/> Discrete - 1	Done
<input type="checkbox"/> sample-centring	Done
<input type="checkbox"/> FAE-sample8_1	Done
<input checked="" type="checkbox"/> Characterisation - 1	
<input checked="" type="checkbox"/> ref-FAE-sample8_1	
<input type="checkbox"/> 1:9 - TRYP-sample9	
<input type="checkbox"/> 1:10 - TRYP-sample10	
<input type="checkbox"/> 2:1 -	
<input type="checkbox"/> 2:2 -	
<input type="checkbox"/> 2:3 -	

Data location

Folder:

File name:

Prefix

Run number

Processing

Process and analyse data    N.o. residues:

Anomalous                      Space group:

Unit cell:  
a:  b:  c:   $\alpha$ :   $\beta$ :   $\gamma$ :

PDB:  Upload  Use code

# Better integration with LIMS (ISPyB)

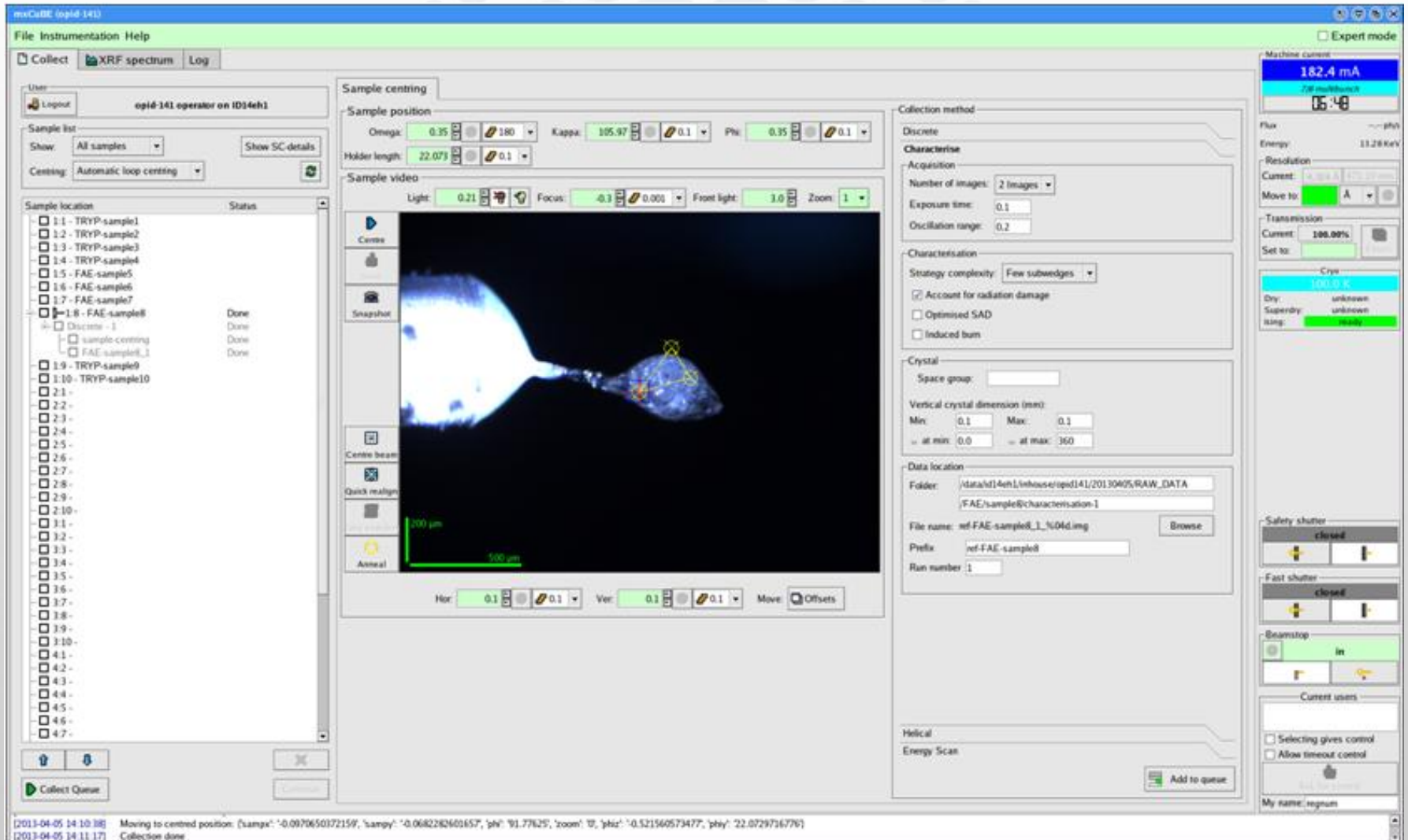
## Sample

Name: sample2  
 Data matrix:  
 Holder length 22.0  
 Basket location 1  
 Sample location 2

## Crystal:

Protein acronym TRY  
 Space group P212121  
 Monomers in assymmetric unit:  
 Amino acid resiuiues per monomer:  
 DNA nucleotides per monomer:  
 RNA nucleotides per monomer:  
 Unit cell:  
 a: 54.1 b: 58.2 c: 66.6  $\alpha$ : 90.0  $\beta$ : 90.0  $\gamma$ : 90.0

# Improved usability with perspectives



The screenshot displays the mxCuBE (opid 141) software interface, which is used for controlling the X-ray diffraction experiment. The interface is divided into several functional areas:

- File Instrumentation Help:** The top menu bar.
- Collect XRF spectrum Log:** Buttons for data collection and logging.
- User:** Shows the current user as 'opid 141 operator on ID14eh1'.
- Sample list:** A list of samples (1.1-4.7) with checkboxes and status indicators (e.g., 'Done').
- Sample centring:** Controls for sample position, including Omega (0.35), Kappa (105.97), Phi (0.35), and Holder length (22.073).
- Sample video:** A central video window showing a perspective view of the sample with a scale bar (200 µm, 500 µm) and controls for Light (0.21), Focus (-0.3), Foot light (1.0), and Zoom (1).
- Collection method:** Settings for discrete collection, including acquisition parameters like Number of images (2), Exposure time (0.1), and Oscillation range (0.2).
- Characterisation:** Settings for strategy complexity (Few subwedges) and options for radiation damage, SAD, and induced burn.
- Crystal:** Settings for space group and vertical crystal dimension (mm).
- Data location:** Fields for folder path, file name, prefix, and run number.
- Machine control:** A vertical panel on the right showing machine status (182.4 mA, 05:48), Flux, Energy (11.28 KeV), Resolution, Current, Transmission (100.00%), Cryo (100.0 K), and Safety shutter status (closed).
- Fast shutter:** Status indicator (closed).
- Beamstop:** Status indicator (in).
- Current users:** A list of users and their control status.
- Helical Energy Scan:** A section at the bottom right with an 'Add to queue' button.

At the bottom of the window, a status bar shows the following information:

```

[2013-04-05 14:10:38] Moving to centred position: {sample: '-0.0970650172159', 'sarep': '-0.0682282601657', 'phi': '91.77625', 'zoom': '0', 'kpsi': '-0.521560573477', 'psi': '22.0729716776'}
[2013-04-05 14:11:17] Collection done
  
```

# Detailed view

Sample centring
Characterisation
X

Reference images

**Acquisition parameters**

Data location

Folder:

File name: ref-FAE-sample8\_1\_%04d.img Browse

Prefix:  Run number:

---

Acquisition

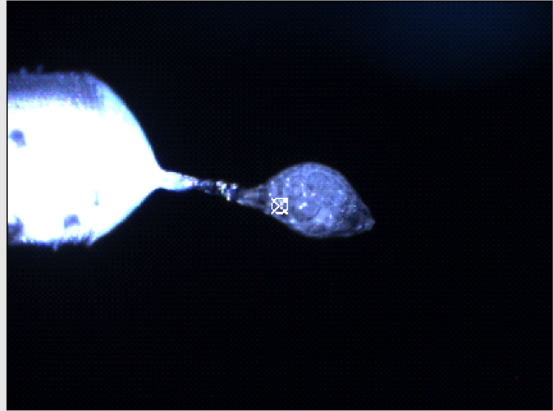
Oscillation start:  Oscillation range:  Oscillation overlap:

First image:  Number of images:  Number of passes:

Transmission (%):  Resolution (Å):  Energy (KeV):

Exposure time:   MAD

Centred position



Characterisation type

**Routine-DC**

Use min dose  Dose limit MGy:

Use min time  Total time limit (s):

Account for radiation damage

---

SAD

Radiation damage

Optimization parameters

Aimed  $I/\sigma$  at highest resolution:  Strategy complexity:

Aimed completeness:   Use permitted rotation range:

Maximum resolution:   $\omega$ -start:

Aimed multiplicity:   $\omega$ -end:

Calculate low resolution pass strategy

Radiation damage model

$\beta$  Å<sup>2</sup>/MGy:

$\gamma$  1/MGy:

Sensitivity:

Crystal

Space group:

Vertical crystal dimension (mm):

Min:  Max:

$\omega$  at min:   $\omega$  at max:

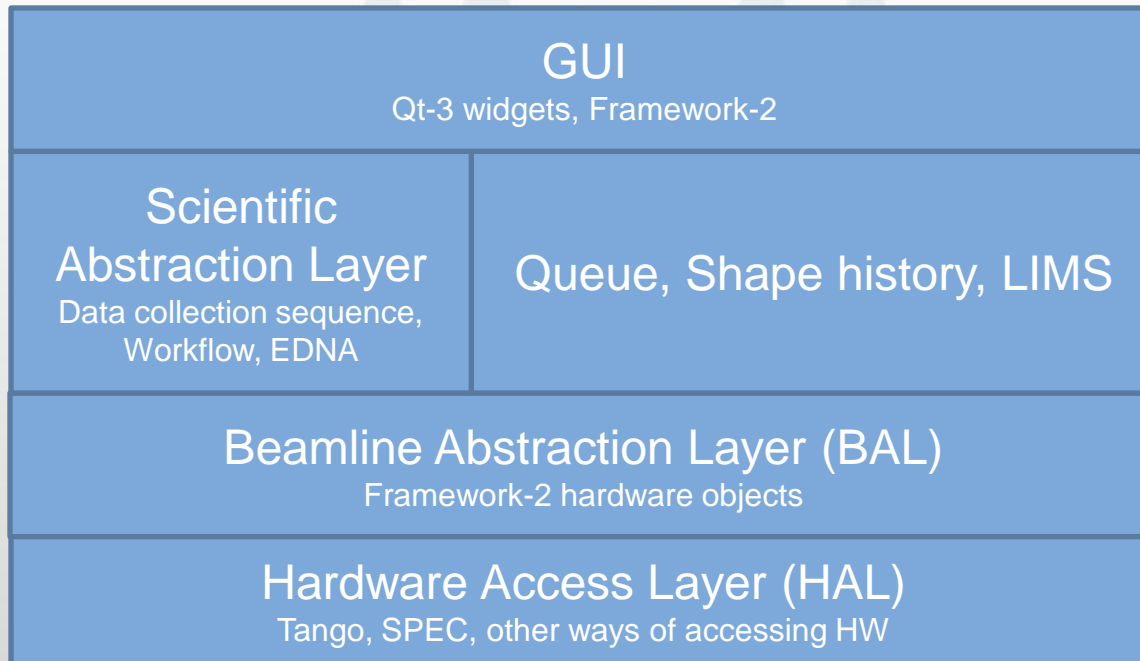
# Workflows

- Using the enhanced queuing system
- Predefined widgets
- XML-RPC

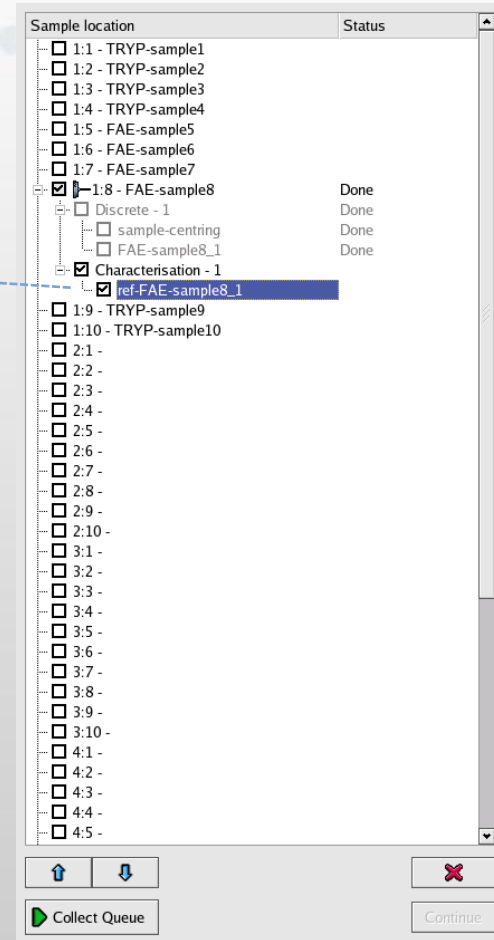
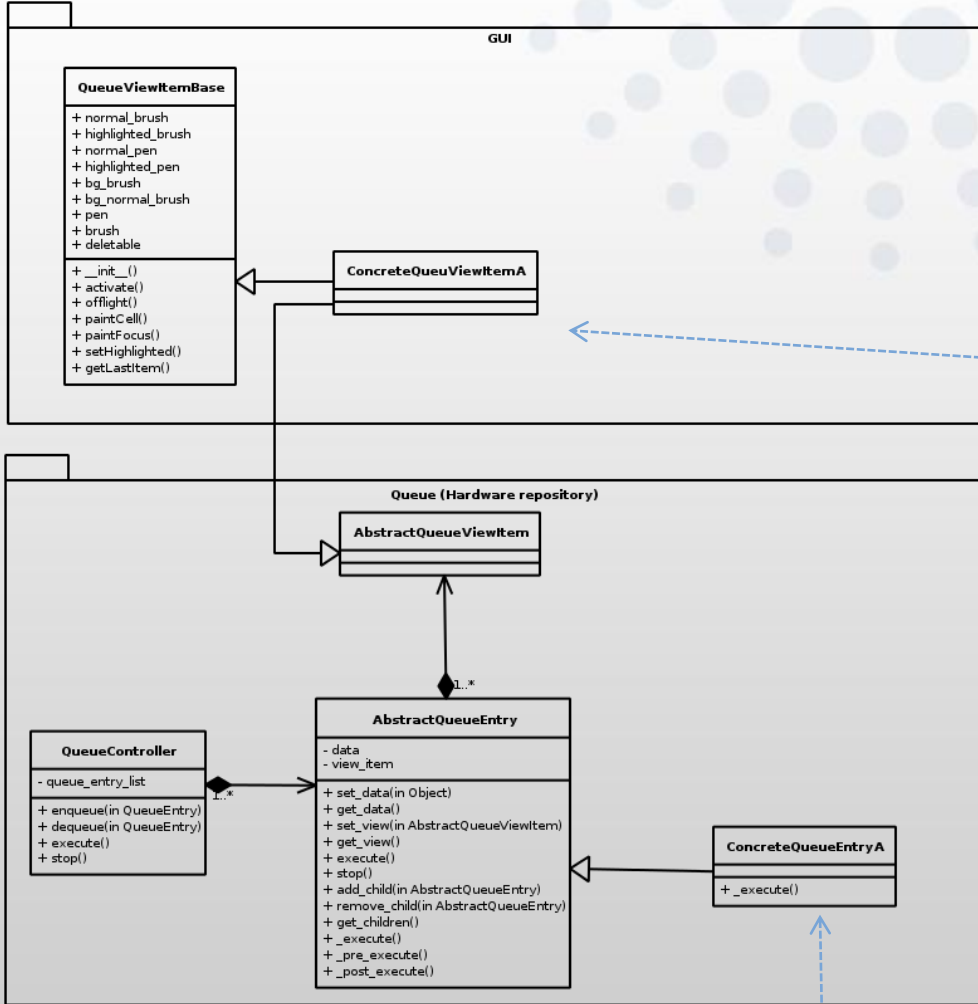
A decorative graphic consisting of numerous light blue circles of varying sizes, arranged in a roughly circular pattern around the central text.

# Demo

# Architecture - overview



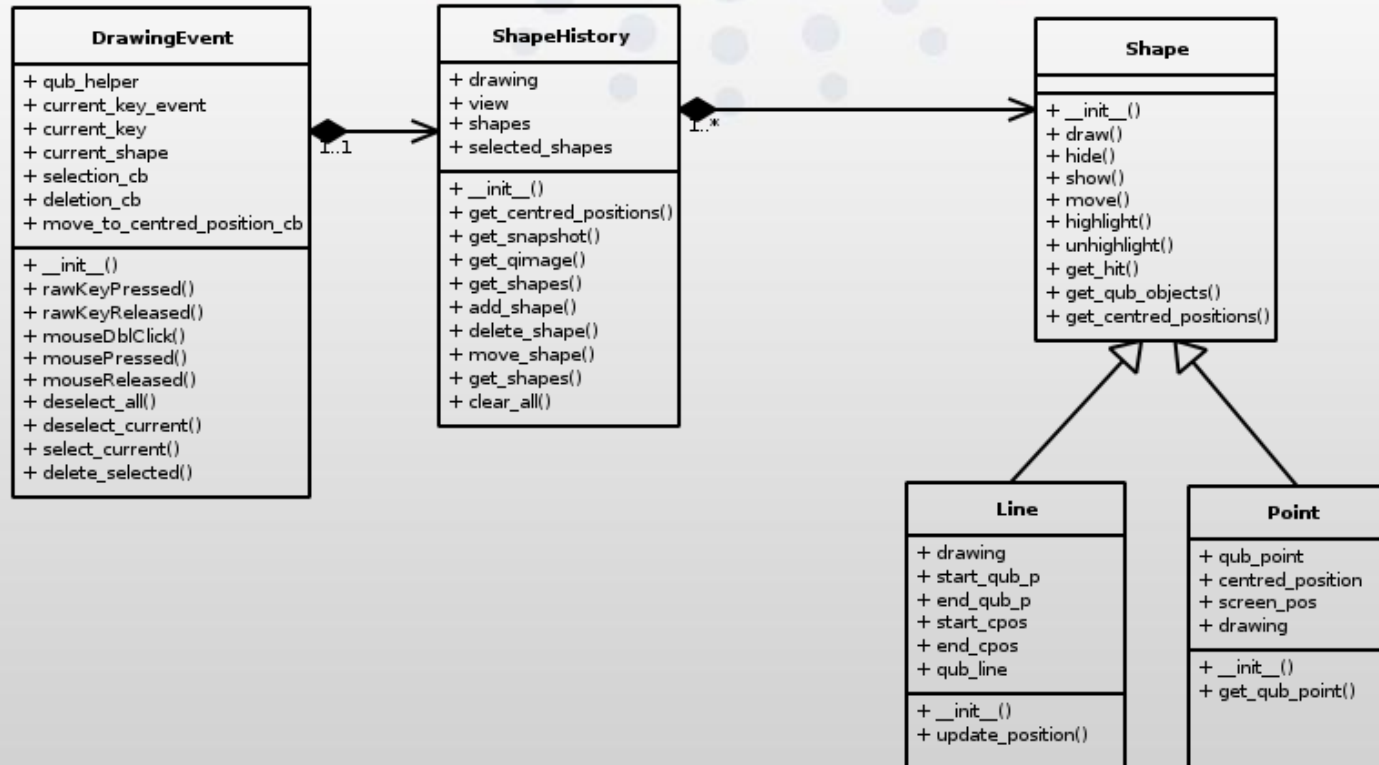
# Generalized tasks



Implementation of the task e.g. data collection sequence.

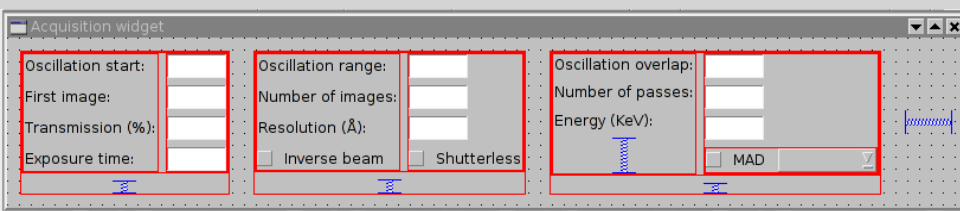
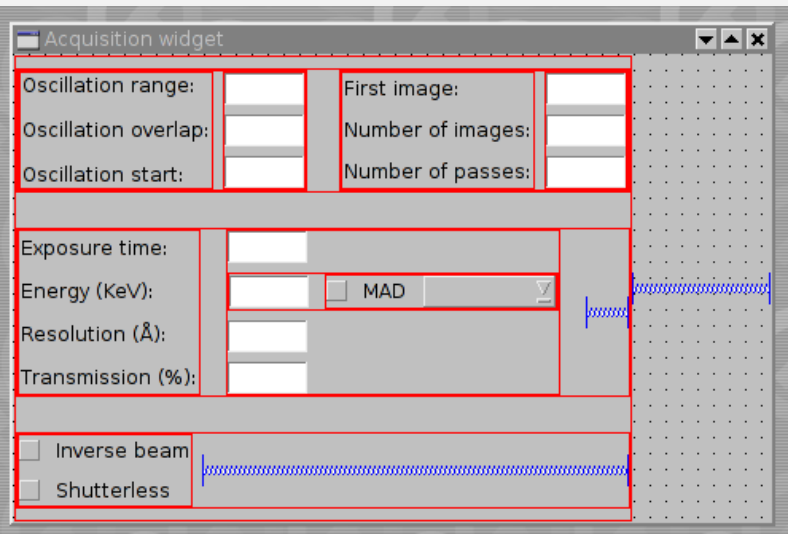


# Shape history



# Good practices

- Possibility to use GUI designer
- Model and model binder



```

self._acquisition_mib = DataModelInputBinder(self._acquisition_parameters)
self._path_template_mib = DataModelInputBinder(self._path_template)

#
# Layout
#
h_layout = qt.QHBoxLayout(self)

if layout:
    self.acq_widget_layout = layout(self)
else:
    self.acq_widget_layout = AcquisitionWidgetHorizontalLayout(self)

h_layout.addWidget(self.acq_widget_layout)

#
# Logic
#
self._acquisition_mib.bind_value_update('osc_start',
                                         self.acq_widget_layout.osc_start_ledit,
                                         float,
                                         qt.QDoubleValidator(0, 1000, 2, self))

self._acquisition_mib.bind_value_update('first_image',
                                         self.acq_widget_layout.first_image_ledit,
                                         int,
                                         qt.QIntValidator(1, 1000, self))

self._acquisition_mib.bind_value_update('exp_time',
                                         self.acq_widget_layout.exp_time_ledit,
                                         float,
                                         qt.QDoubleValidator(0.001, 6000, 3, self))

self._acquisition_mib.bind_value_update('osc_range',
                                         self.acq_widget_layout.osc_range_ledit,
                                         float,
                                         qt.QDoubleValidator(0.001, 1000, 2, self))
    
```

```

self._acquisition_mib = DataModelInputBinder(self._acquisition_parameters)
self._path_template_mib = DataModelInputBinder(self._path_template)

#
# Layout
#
h_layout = qt.QHBoxLayout(self)

if layout:
    self.acq_widget_layout = layout(self)
else:
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h_layout.addWidget(self.acq_widget_layout)

#
# Logic
#
self._acquisition_mib.bind_value_update('osc_start',
                                         self.acq_widget_layout.osc_start_ledit,
                                         float,
                                         qt.QDoubleValidator(0, 1000, 2, self))

self._acquisition_mib.bind_value_update('first_image',
                                         self.acq_widget_layout.first_image_ledit,
                                         int,
                                         qt.QIntValidator(1, 1000, self))

self._acquisition_mib.bind_value_update('exp_time',
                                         self.acq_widget_layout.exp_time_ledit,
                                         float,
                                         qt.QDoubleValidator(0.001, 6000, 3, self))

self._acquisition_mib.bind_value_update('osc_range',
                                         self.acq_widget_layout.osc_range_ledit,
                                         float,
                                         qt.QDoubleValidator(0.001, 1000, 2, self))
  
```

A decorative graphic consisting of numerous light blue circles of varying sizes, scattered across the upper half of the slide, creating a soft, abstract pattern.

# Questions