



# MXCuBE and Qt4

## Ivars Karpics



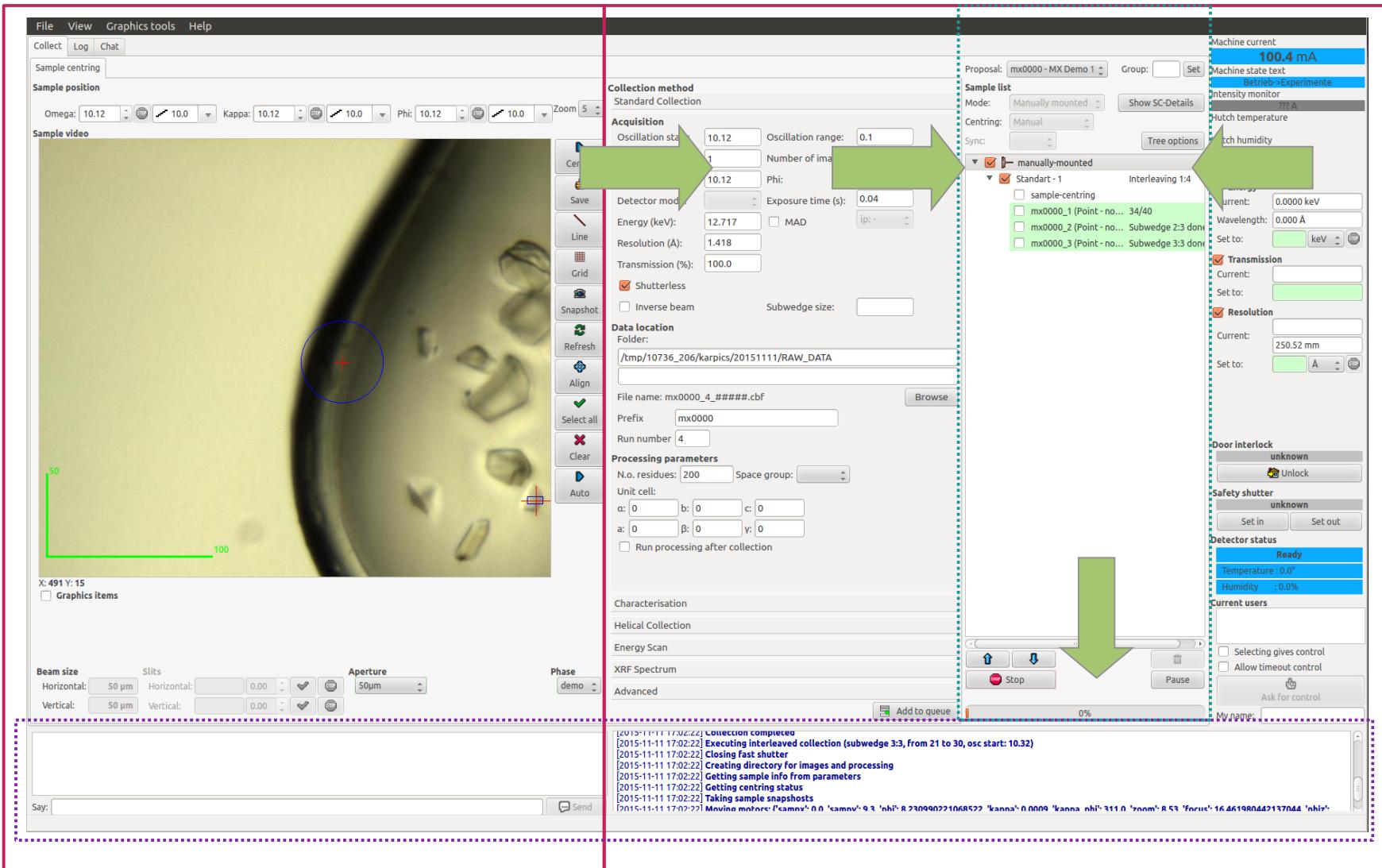
# Content

Current status:

- Available bricks and functions
- Code clean up
- GUI Builder
- GraphicsManger hwobj
- Advanced methods (MeshScan, Xray-centring, etc.)
- Interleave feature

Conclusions and future

# Available bricks (main GUI)



# Available bricks

Proposal: mx0000 - MX Demo 1 Group:

**Sample list**

Mode: Manually mounted  Centring: Manual Sync:

manually-mounted

Sample centring

Sample position

Omega: 10.12  10.0  Kappa: 10.12  10.0  Phi: 10.12  10.0  Zoom 5

Energy Current: 12.7000 keV Wavelength: 0.976 Å Set to:

Transmission Current: 50.32% Set to:

Resolution Current: 2.000 Å 394.80 mm Set to:

Machine current  
**100.3 mA**

Machine state text  
Betrieb->Experimente

Intensity monitor  
??? A

Hutch temperature

Hutch humidity

Door interlock unknown

Safety shutter unknown

Detector status Ready  
Temperature : 0.0°  
Humidity : 0.0%

Current users

Selecting gives control  
 Allow timeout control

My name:

# Available bricks (TaskToolBox)

**Collection method**  
 Standard Collection

**Acquisition**

Oscillation start: 10.12   Oscillation range: 0.1  
 First image: 1   Number of images: 1  
 Kappa: 10.12   Phi: 10.12  
 Detector mode:   Exposure time (s): 0.04  
 Energy (keV): 12.717    MAD   ip: -  
 Resolution (Å): 1.418  
 Transmission (%): 100.0

Shutterless  
 Inverse beam   Subwedge size:

**Data location**  
 Folder: /tmp/10736\_206/karpics/20151111/RAW\_DATA  
  
 File name: mx0000\_1\_#####.cbf     
 Prefix mx0000  
 Run number 1

**Processing parameters**  
 N.o. residues: 200   Space group:   
 Unit cell:  
 a: 0   b: 0   c: 0  
 α: 0   β: 0   γ: 0  
 Run processing after collection

**Helical Collection**

Name	Start point	End point
Line 1	2	1
Line 2	4	3

**Acquisition**

Oscillation start: 10.12   Oscillation range: 0.1  
 First image: 1   Number of images: 1  
 Kappa: 10.12   Phi: 10.12  
 Detector mode:   Exposure time (s): 0.04  
 Energy (keV): 12.717    MAD   ip: -  
 Resolution (Å): 1.418  
 Transmission (%): 100.0

Shutterless  
 Inverse beam   Subwedge size:

**Data location**  
 Folder: /tmp/10736\_206/karpics/20151111/RAW\_DATA  
  
 File name: mx0000\_1\_#####.cbf     
 Prefix mx0000  
 Run number 1

**Characterisation**

**Acquisition**

Number of images: 2 Images   Oscillation range: 1.0  
 Osc start: 10.12   Phi: 10.12  
 Kappa: 10.12   Exposure time (s): 0.04  
 Detector mode:   
 Energy (KeV): 12.717  
 Resolution (Å): 1.418  
 Transmission (%): 100.0

**Data location**  
 Folder: /tmp/10736\_206/karpics/20151111/RAW\_DATA  
  
 File name: ref-mx0000\_1\_#####.cbf     
 Prefix mx0000  
 Run number 1

Characterisation  
 Strategy complexity: Single subwedge  
 Account for radiation damage  
 Optimised SAD

**Crystal**  
 Space group:   
 Vertical crystal dimension (mm):  
 Min: 0.1   Max: 0.1  
 ω at min: 0.0   ω at max: 90

# Available bricks (TaskToolBox)

**Advanced**

Method: MeshScan

**Grid**

Horizontal spacing: 0 Move horizontal:

Vertical spacing: 0 Move vertical:

Name	Beam width ()	Beam height ()	Lines	Images

Draw Remove

**Acquisition**

Oscillation start: 10.12 Oscillation range: 1.0

First image: 1 Number of images: 1

Kappa: 10.12 Phi: 10.12

Detector mode: Exposure time (s): 0.04

Energy (keV): 12.717  MAD

Resolution (Å): 1.418

Transmission (%): 100.0

Shutterless

Inverse beam Subwedge size:

**Data location**  
Folder: /tmp/10736\_206/karpics/20151111/Raw\_DATA  Add to queue

**Energy Scan**

Pb - L3 (82,lead)

H	Li	Be	He																			
Na	Mg	Al	Si	P	S	Cl	Ar															
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr					
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe					
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn					
Fr	Ra	Ac	Fr	Db	Sg	Bh	Hs	Mt	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
									Th	Pa	U	Np	Pu	Am	Em	Bk	Cf	Es	Fm	Md	No	Lr

Edge: L1

**Data location**  
Folder: /tmp/10736\_206/karpics/20151111/Raw\_DATA

File name: mx0000\_1\_#####.raw Browse

Prefix: mx0000  
Run number: 1

**XRF Spectrum**

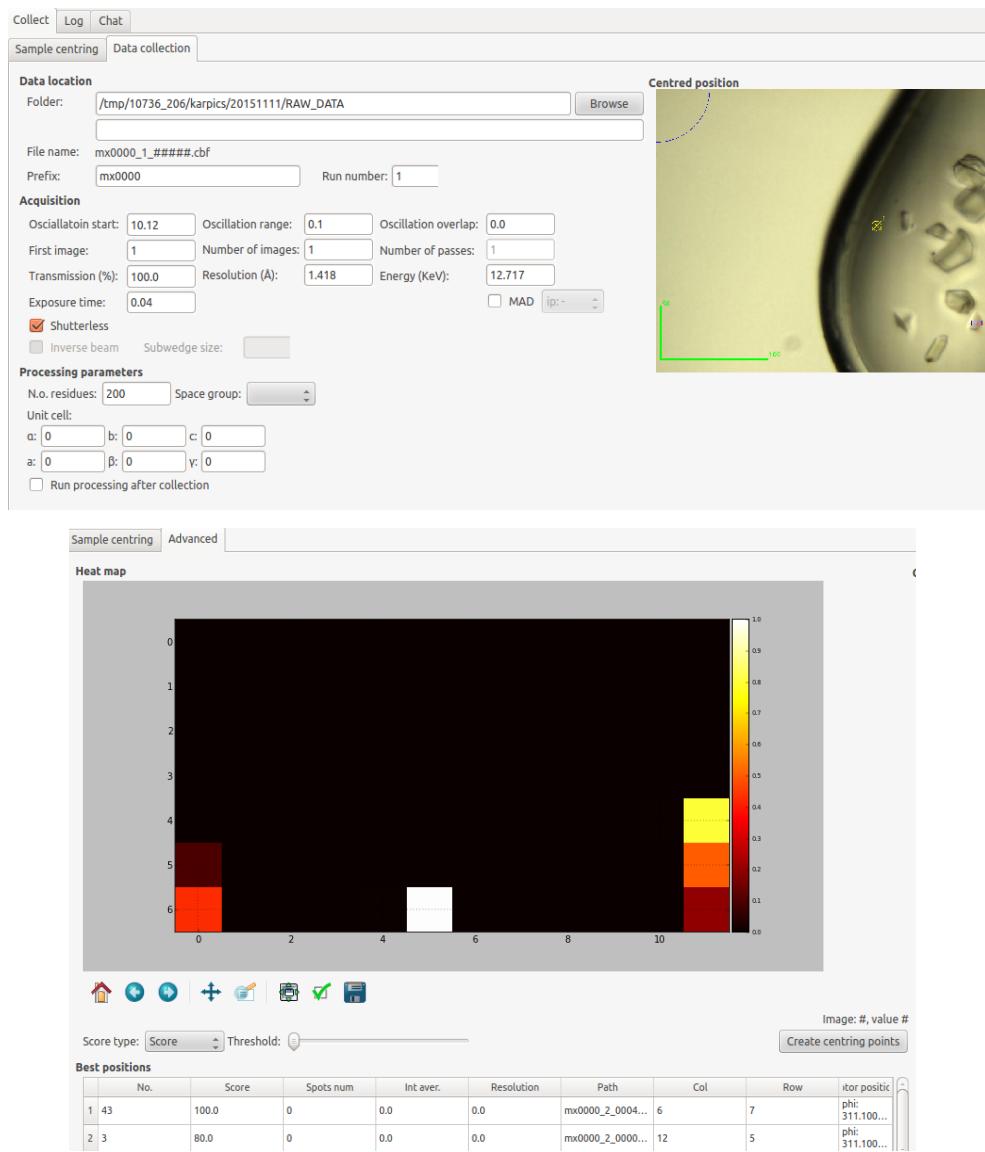
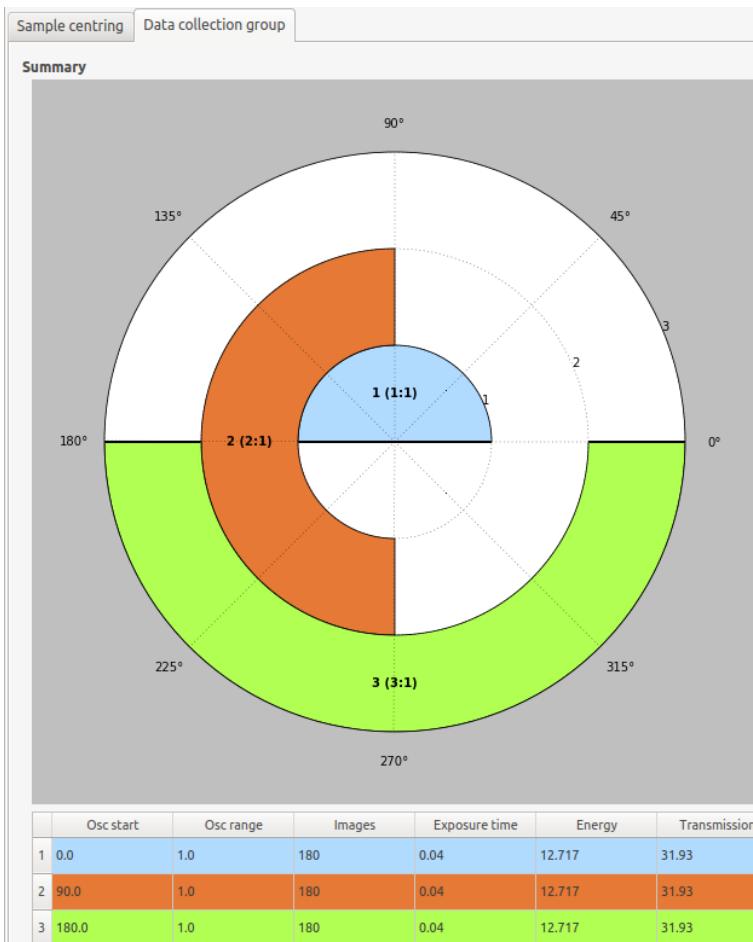
**Data location**  
Folder: /tmp/10736\_206/karpics/20151111/Raw\_DATA

File name: mx0000\_1\_#####.raw Browse

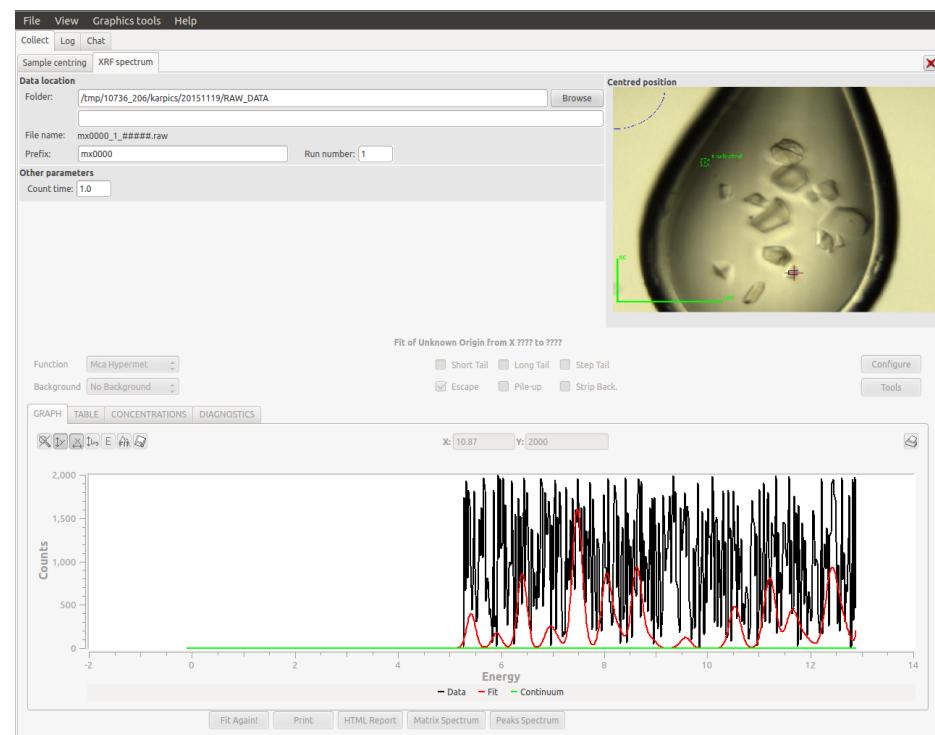
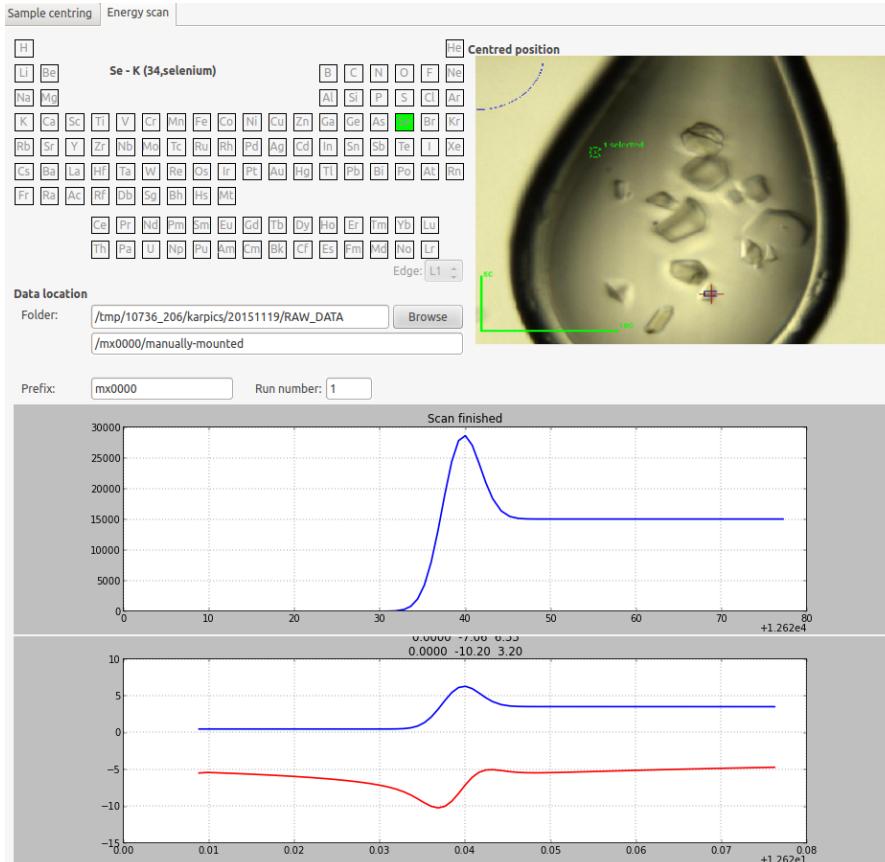
Prefix: mx0000  
Run number: 1

**Parameters**  
Count time (sec.): 1

# Available bricks (Parameters/Results)



# Available bricks (TaskToolBox)



# Available bricks (Sample changer, Plate manipulator)

1. Possibility to configure two sample changers.
2. Information about plate from CRIMS.
3. Qt4\_SampleChanger brick.
4. Qt4\_PlateBrick to navigate in cell or move to crystal position.

The screenshot displays two panels of a graphical user interface for managing sample changers and plates.

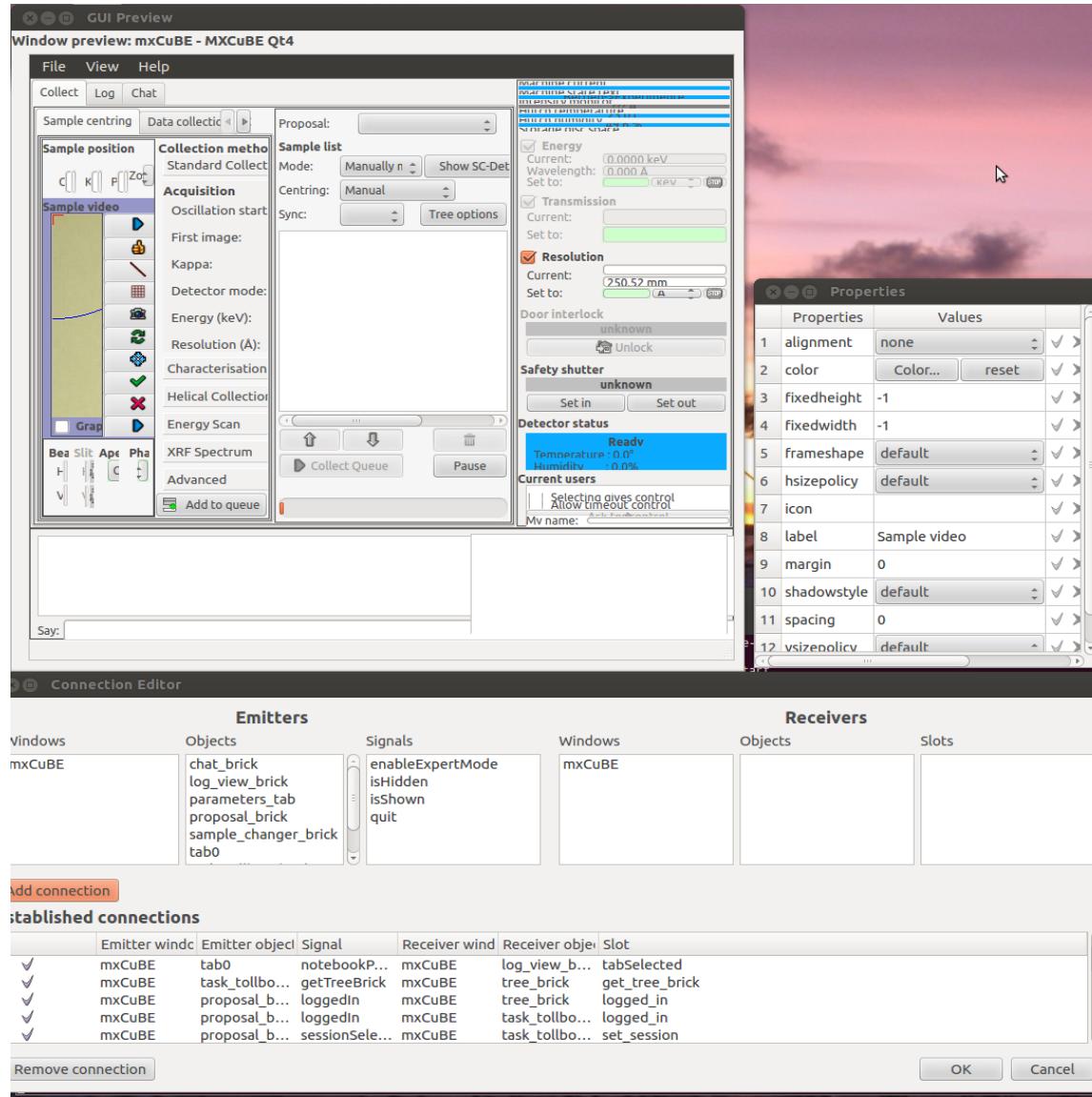
**Sample list Panel:**

- Mode: Sample changer
- Centring: ISPyB (highlighted with a red box)
- Sync: CRIMS

**Sample centring Panel:**

- Sample centring tab is active.
- Sample changer one tab is active.
- Plate barcode: TTP3000807
- Search button.
- Current basket: Position 0, Scan button.
- Current sample: No mounted sample, Position 10, Holder length 22 mm.
- Contents section:
  - Reset sample changer contents button.
  - Double-click loads the sample checkbox, Scan selected baskets button.
  - Basket 0: Positions 1-10.
  - Basket 1: Positions 1-10.
  - Basket 2: Positions 1-10.
  - Basket 3: Positions 1-10.
- Current location: Col: 0 Row: 1 X: 0.50 Y: 0.75.
- Element: TTP3000807
- Label: IQ\_3\_flat\_uv
- Login: D2A2 ...
- Row: C
- Col: 8
- Comment: mlaursen
- Move to crystal button, Use crystal repositioning checkbox, Abort button.

# GUI builder



# Code clean up

- All main bricks and widgets transformed to Qt4\_.
- New layout manager for BlissFramework GUI.
- Qt4 branch merged in master branch and deleted after the merge.
- Improved code formating based on PEP 0008, regular check with pylint.
- New style Qt4 signal/slots between Bricks and widgets.
- Qt4 Designer used to create most of the widgets.

```
qt.QObject.connect(self._list_box, qt.SIGNAL(\n    "selectionChanged()"), self.list_box_selection_changed)
```

```
prefix_ledit = self._data_path_widget.\n    data_path_widget_layout.child('prefix_ledit')\nrun_number_ledit = self._data_path_widget.\n    data_path_widget_layout.child('run_number_ledit')
```

```
self.connect(prefix_ledit, qt.SIGNAL("textChanged\\n\n    (const QString &)"), self._prefix_ledit_change)
```

```
self.connect(run_number_ledit,\n    qt.SIGNAL("textChanged(const QString &)"),\n    self._run_number_ledit_change)
```

```
self.connect(self._data_path_widget,\n    qt.PYSIGNAL("path_template_changed"),\n    self.handle_path_conflict)
```

```
self._lines_listwidget.itemSelectionChanged.connect(\n    self.lines_listwidget_selection_changed)\n\nself._data_path_widget.data_path_layout.prefix_ledit.textChanged.\n    connect(self._prefix_ledit_change)\nself._data_path_widget.data_path_layout.run_number_ledit.\n    textChanged.connect(self._run_number_ledit_change)\nself._data_path_widget.pathTemplateChangedSignal.connect(\n    self.handle_path_conflict)
```



# How to improve code

1. pylint for code formatting and style.

2. radon to compute.

- Cyclomatic Complexity (A – F from low - simple block to very high - error-prone, unstable block)

- Maintainability Index score (A – C from very hight to Extremely low).

```
Global evaluation
-----
Your code has been rated at 8.54/10

Raw metrics
-----
+-----+-----+-----+-----+
| type | number | %   | previous | difference |
+=====+=====+=====+=====+
| code | 653   | 68.59 | NC      | NC        |
+-----+-----+-----+-----+
| docstring | 171   | 17.96 | NC      | NC        |
+-----+-----+-----+-----+
| comment | 37    | 3.89  | NC      | NC        |
+-----+-----+-----+-----+
| empty   | 91    | 9.56  | NC      | NC        |
+-----+-----+-----+-----+
```

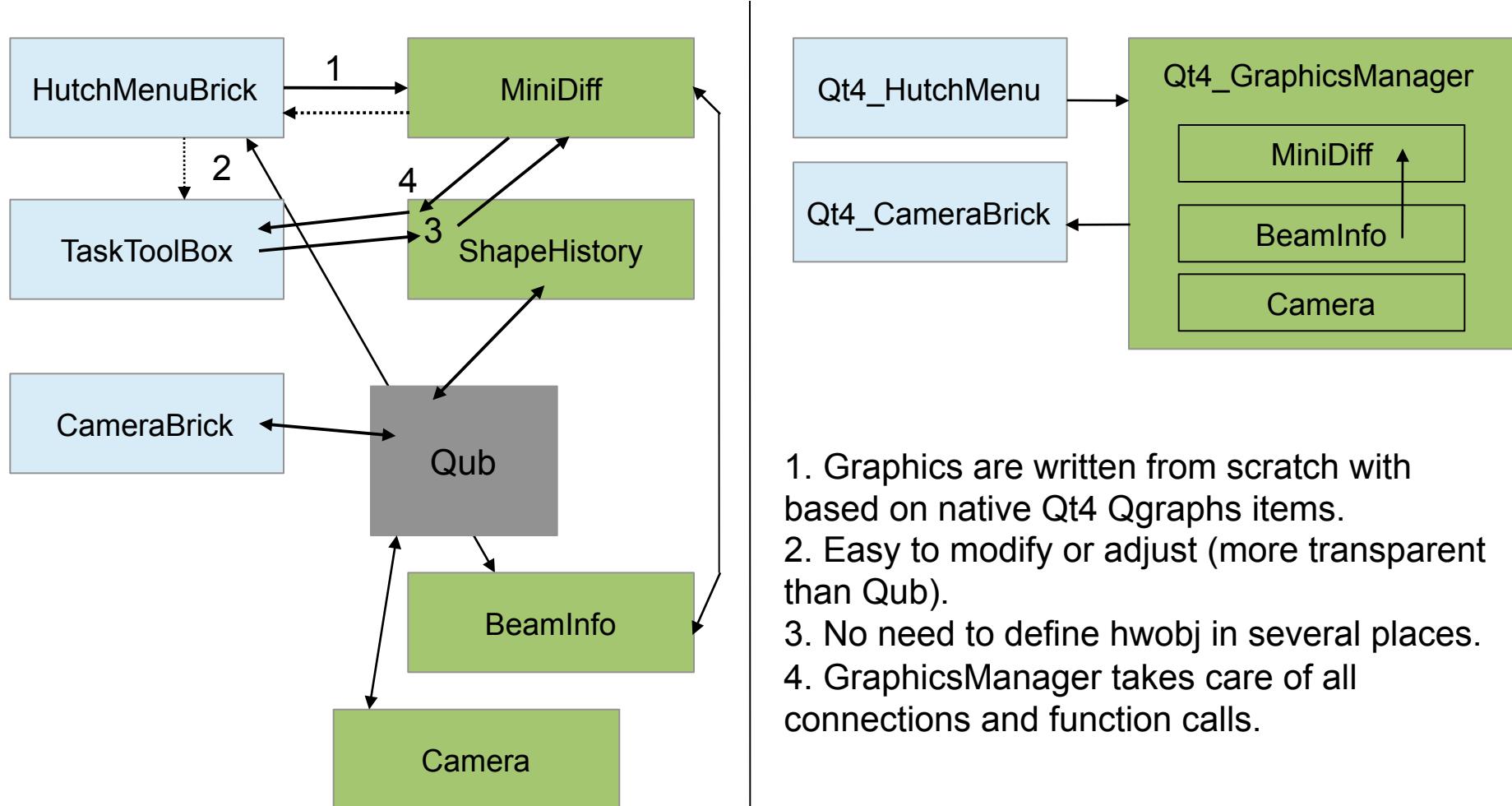
```
mxuser@mxVirtual:~$ radon cc mxcubeGit/Bricks/Qt4_*.py -a -nc
mxcubeGit/Bricks/Qt4_ProposalBrick2.py
    M 696:4 Qt4_ProposalBrick2.select_proposal - C
    M 618:4 Qt4_ProposalBrick2.propertyChanged - C
    M 801:4 Qt4_ProposalBrick2.select_todays_proposal - C
mxcubeGit/Bricks/Qt4_SampleChangerBrick3.py
    M 819:4 Qt4_SampleChangerBrick3.propertyChanged - C
    M 1055:4 Qt4_SampleChangerBrick3.infoChanged - C
mxcubeGit/Bricks/Qt4_TreeBrick.py
    M 190:4 Qt4_TreeBrick.propertyChanged - C
    M 383:4 Qt4_TreeBrick.refresh_sample_list - C

7 blocks (classes, functions, methods) analyzed.
Average complexity: C (13.2857142857)
```

```
mxuser@mxVirtual:~$ radon mi mxcubeQt4/Bricks/Qt4_*.py -s
mxcubeQt4/Bricks/Qt4_AdvancedBrick.py - A (79.42)
mxcubeQt4/Bricks/Qt4_BeamSizeBrick.py - A (73.53)
mxcubeQt4/Bricks/Qt4_CharParametersBrick.py - A (76.33)
mxcubeQt4/Bricks/Qt4_DCGBrick.py - A (100.00)
mxcubeQt4/Bricks/Qt4_DCParametersBrick.py - A (72.85)
mxcubeQt4/Bricks/Qt4_DetectorStatusBrick.py - A (72.28)
mxcubeQt4/Bricks/Qt4_DoorInterlockBrick.py - A (72.98)
mxcubeQt4/Bricks/Qt4_EnergyScanParametersBrick.py - A (89.50)
mxcubeQt4/Bricks/Qt4_GraphicsManagerBrick.py - A (50.43)
```

# GraphicsManager hwobj

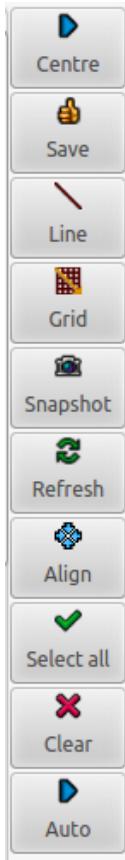
Example: creating a new centring position with 3 clicks



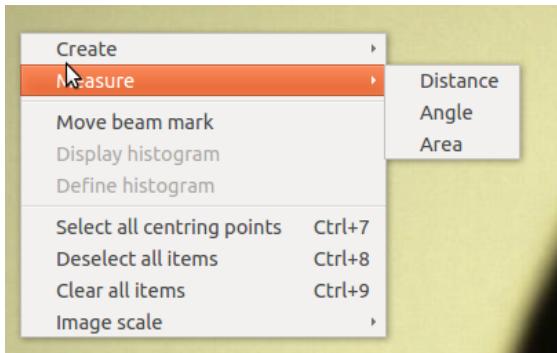
# Graphics

- Main functions accessible via different controls.
- Easy way to customize the look.

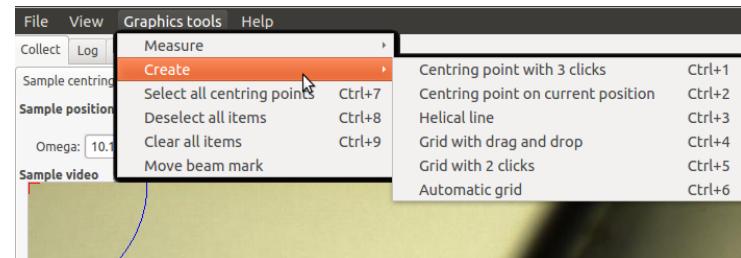
## 1. HutchMenu



## 2. Popup menu (right click on the view)



## 3. Toplevel menu bar



## 4. Drag and drop toolbar



## 5. Shortcuts:

Ctrl+1 - Create centring point with 3 click

Ctrl+2 - Create centring point on current position

Ctrl+3 - Create helical line

...

Esc - cancel command

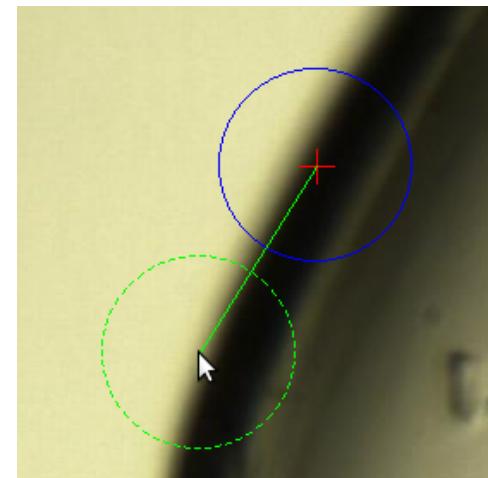
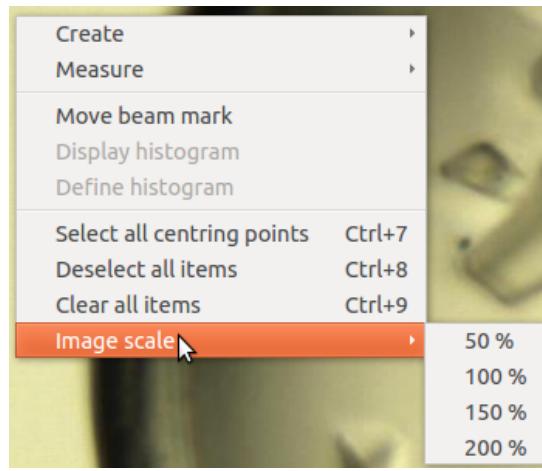
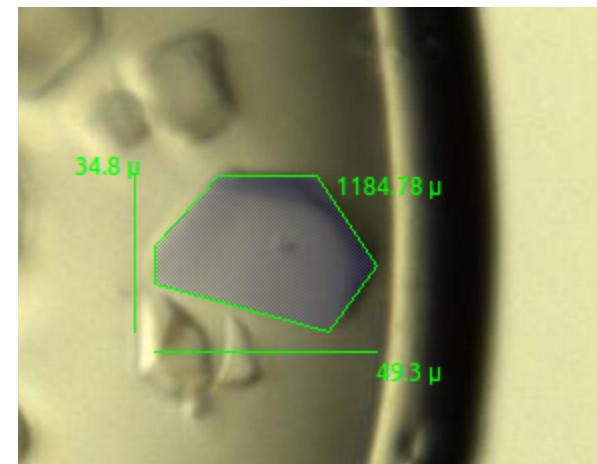
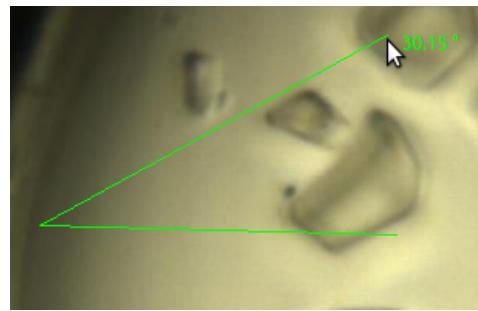
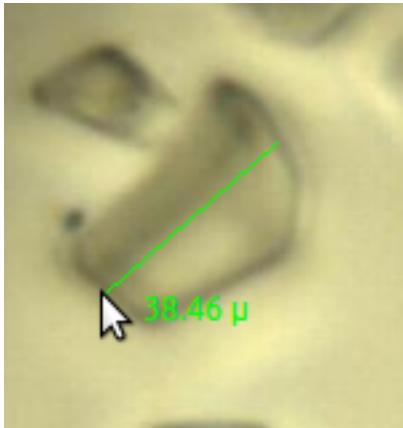
# Graphics

1. Basic graphics items available.
2. Qt4\_GraphicsManagerBrick to add, remove and customize items.



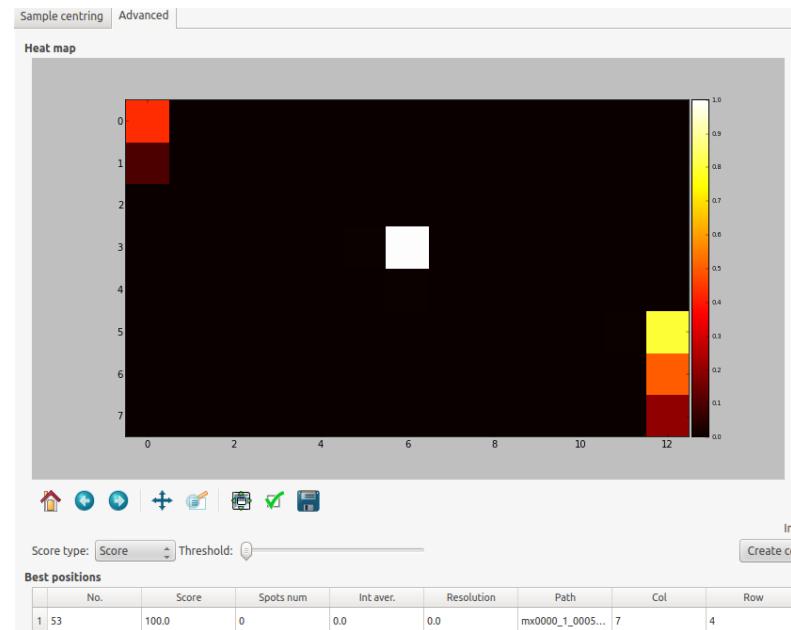
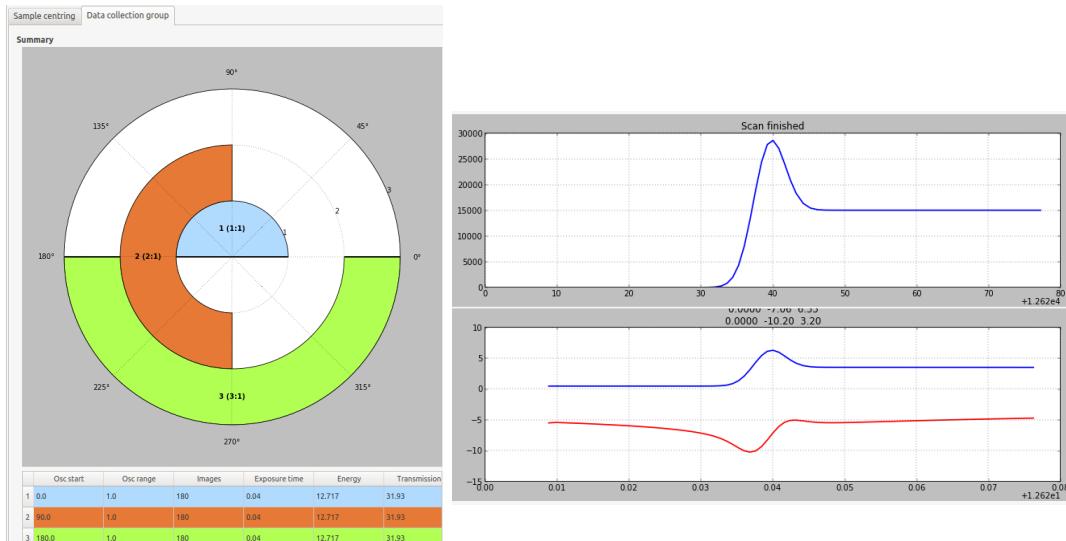
# Graphics manager brick

- Measurement tools, image scaling, beam mark move, rotation axis



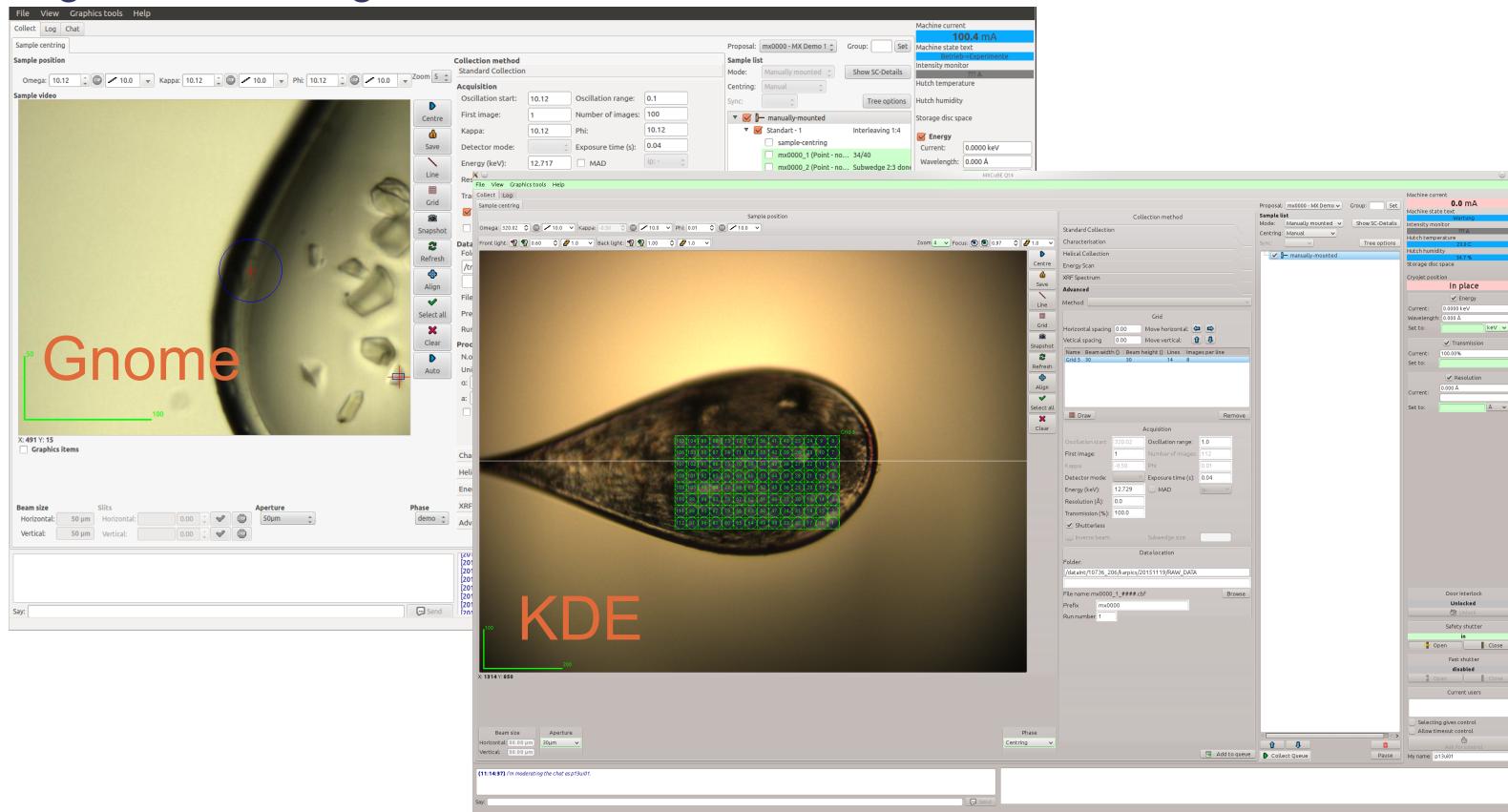
# Embedded matplotlib in MXCuBE

1. Well know tool for plotting scientific data.
2. No extra dependencies.
3. Zoom, navigation, image save and other build-in functions.
4. Curves, 2d maps, polar charts and 3D maps.
5. Qt4\_matplot\_widget.py in progress and will substitute pymca plots.



# Dependencies

1. ubuntu 12, 14, (15), macos,
2. python and PyQt4 comes with ubuntu
3. sudo apt-get install python-gevent, python-louie, python-suds, python-numpy, python-scipy, python-matplotlib, pymca
5. get code from git and run



# Conclusion

1. Qt4 version allows easy to implement new features and advanced methods like interleaved collections, mesh scans, x-ray centring and others.
2. Qt4 is well documented and supported.
3. Reduced list of dependencies comparing Qt3 version.
4. Integrated matplotlib for scientific data plotting.

## Future:

1. Full migration to Qt4 has been started.
2. No more new features to Qt3 bricks.
3. Qt4 version as a desktop version and possibly web version for remote access.
4. Running code from and sync with git (lesson learned with 2 reps).
5. Bug reports and feedback are welcome!

**Thank you for your attention**