



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)

The screenshot displays the main GUI interface, divided into several functional areas:

- Top Left (File View Graphics tools Help):** Contains menu options and a 'Sample centring' section with 'Sample position' controls for Omega, Kappa, and Phi, along with a 'Zoom' control.
- Sample video:** A central video window showing a sample with a red crosshair. Below it is a coordinate system (X: 491 Y: 15) and a 'Graphics items' checkbox.
- Beam size and Slits:** Controls for 'Horizontal' and 'Vertical' beam size (50 µm) and 'Aperture' (50 µm).
- Phase demo:** A dropdown menu currently set to 'demo'.
- Collection method (Standard Collection):** A central panel with 'Acquisition' parameters:
 - Oscillation start: 10.12, Oscillation range: 0.1
 - Number of images: 1, Phi: 10.12
 - Exposure time (s): 0.04
 - Energy (keV): 12.717, Resolution (Å): 1.418, Transmission (%): 100.0
 - Options: Shutterless, Inverse beam, Subwedge size: [empty]
- Data location:** Folder path: /tmp/10736_206/karpics/20151111/RAW_DATA. File name: mx0000_4_#####.cbf. Prefix: mx0000. Run number: 4.
- Processing parameters:** N.o. residues: 200, Space group: [empty]. Unit cell: a: 0, b: 0, c: 0; a₂: 0, b₂: 0, γ: 0. Run processing after collection.
- Characterisation:** Helical Collection, Energy Scan, XRF Spectrum, Advanced.
- Right Panel (Machine status and Sample list):**
 - Machine current: 100.4 mA
 - Machine state text: Betrieb-Experimente
 - Intensity monitor: 777 A
 - Machine temperature: [empty]
 - Machine humidity: [empty]
 - Proposal: mx0000 - MX Demo 1, Group: [empty]
 - Sample list: Manually mounted, Centring: Manual, Sync: [empty]
 - Tree options: manually-mounted, Standard - 1, Interleaving: 1:4
 - Subwedges: mx0000_1 (Point - no... 34/40), mx0000_2 (Point - no... Subwedge 2:3 don...), mx0000_3 (Point - no... Subwedge 3:3 don...)
 - Current: 0.0000 keV, Wavelength: 0.000 Å, Set to: [empty] keV
 - Transmission: Current: [empty], Set to: [empty]
 - Resolution: Current: 250.52 mm, Set to: [empty] Å
 - Door interlock: unknown, Unlock button
 - Safety shutter: unknown, Set in/Set out buttons
 - Detector status: Ready, Temperature: 0.0°, Humidity: 0.0%
 - Current users: [empty]
 - Buttons: Stop, Pause, Add to queue
 - Progress bar: 0%
- Bottom Panel (Log):** A scrollable log window showing system messages:
 - [2015-11-11 17:02:22] Collection completed
 - [2015-11-11 17:02:22] Executing interleaved collection (subwedge 3:3, from 21 to 30, osc start: 10.32)
 - [2015-11-11 17:02:22] Closing fast shutter
 - [2015-11-11 17:02:22] Creating directory for images and processing
 - [2015-11-11 17:02:22] Getting sample info from parameters
 - [2015-11-11 17:02:22] Getting centring status
 - [2015-11-11 17:02:22] Taking sample snapshots
 - [2015-11-11 17:02:22] Moving motors: ('camv': 0.0, 'camv': 0.3, 'nhl': 8.230990221068522, 'kappa': 0.0009, 'kappa_nhl': 311.0, 'zoom': 8.53, 'focus': 16.461980442137044, 'nhl': ...)

Available bricks

Proposal: Group:

Sample list

Mode:

Centring:

Sync:

manually-mounted

Energy

Current:

Wavelength:

Set to:

Transmission

Current:

Set to:

Resolution

Current:

Set to:

Sample centring

Sample position

Omega: Kappa: Phi: Zoom

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 Browse
Prefix: mx0000
Run number: 1

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

Helical Collection

Line

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

Create Remove

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 Browse
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 Browse
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


 


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

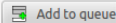
Transmission (%): 100.0

Shutterless

Inverse beam Subwedge size: 

Data location

Folder: /tmp/10736_206/karpics/20151111/RAW_DATA




Energy Scan

H																	He				
Li	Be	Pb - L3 (82,lead)														B	C	N	O	F	Ne
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	Rf	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	Cm	Bk	Cf	Es	Fm	Md	No	Lr								

Edge: L1

Data location

Folder: /tmp/10736_206/karpics/20151111/RAW_DATA

File name: mx0000_1_#####.raw 


Prefix: mx0000

Run number: 1

XRF Spectrum

Data location

Folder: /tmp/10736_206/karpics/20151111/RAW_DATA

File name: mx0000_1_#####.raw 

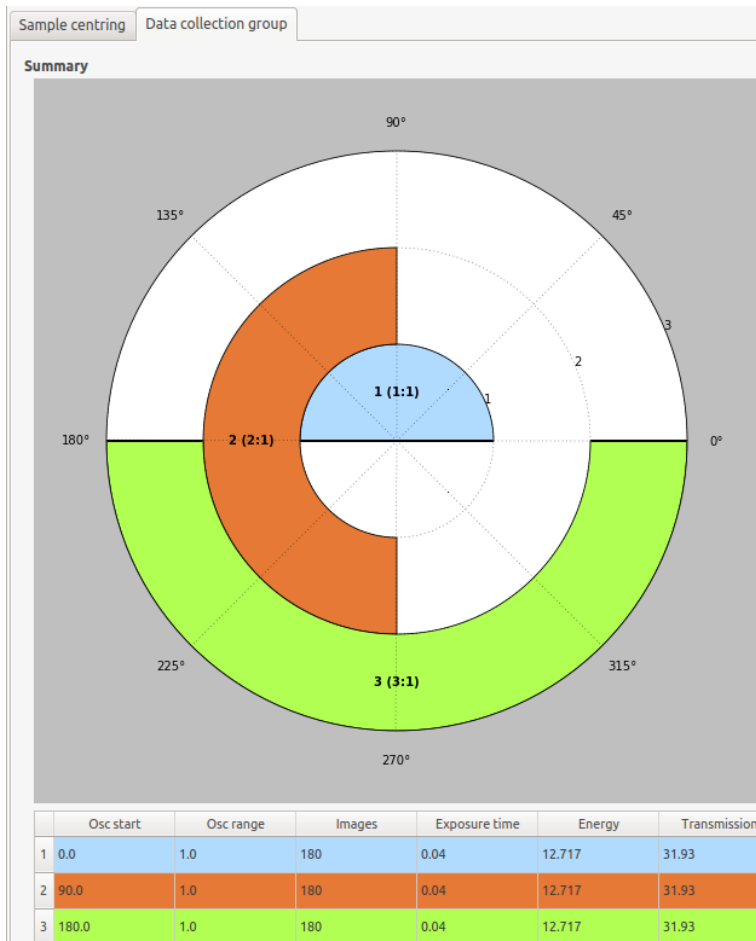
Prefix: mx0000

Run number: 1

Parameters

Count time (sec.): 1

Available bricks (Parameters/Results)



Collect | Log | Chat

Sample centring | Data collection

Data location

Folder: /tmp/10736_206/karpics/20151111/RAW_DATA

File name: mx0000_1_#####.cbf

Prefix: mx0000 Run number: 1

Acquisition

Oscillation start: 10.12 Oscillation range: 0.1 Oscillation overlap: 0.0

First image: 1 Number of images: 1 Number of passes: 1

Transmission (%): 100.0 Resolution (Å): 1.418 Energy (KeV): 12.717

Exposure time: 0.04 MAD ip: -

Shutterless Inverse beam Subwedge size:

Processing parameters

N.o. residues: 200 Space group:

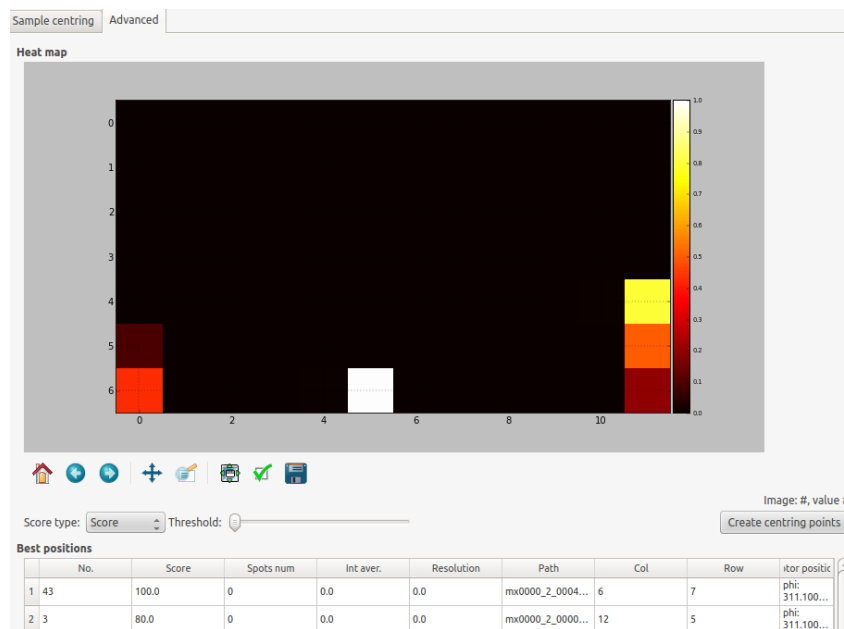
Unit cell:

a: 0 b: 0 c: 0

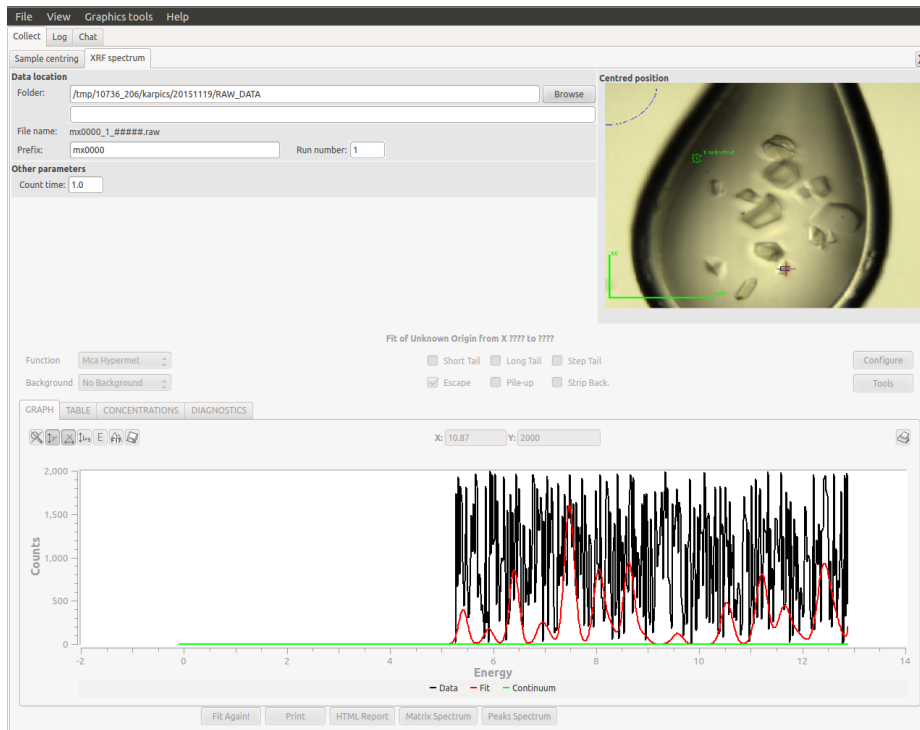
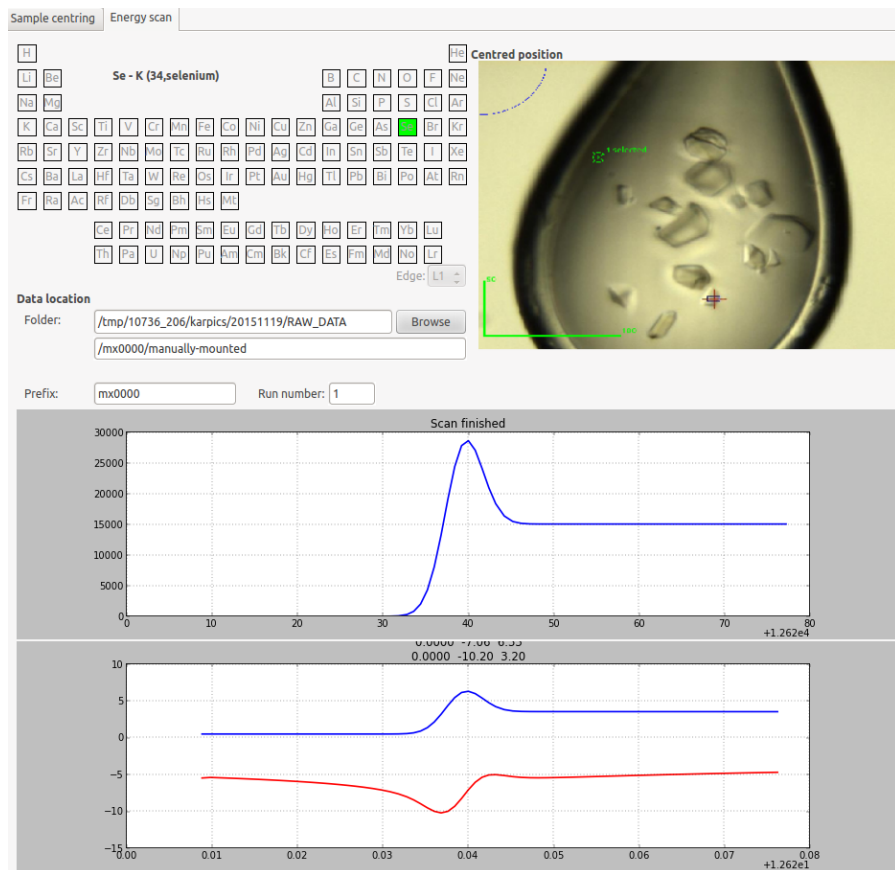
α: 0 β: 0 γ: 0

Run processing after collection

Centred position



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.

Sample list
Mode: Sample changer
Centring: ISPyB (selected), CRIMS
Sync: [Tree options]

Sample list
Mode: Plate
Centring: Manual
Sync: [Tree options]

- Row A
- Row B
 - B1:1
 - B1:2
 - B1:3 (selected) **Centring done!**
 - B2:1
 - B2:2
 - B2:3

Sample centring Sample changer one

Unknown
Unknown [Reset]
Sample changer can load/unload
Minidiff motors can move
Switch to Sample Transfer mode

Current basket
Position: 0 [Scan]

Current sample
New mounted sample
Position: 10
Holder length: 22 mm

Contents
Reset sample changer contents
Double-click loads the sample
Scan selected baskets

- Basket 0
1 2 3 4 5 6 7 8 9 10
- Basket 1
1 2 3 4 5 6 7 8 9 10
- Basket 2
1 2 3 4 5 6 7 8 9 10
- Basket 3
1 2 3 4 5 6 7 8 9 10

Sample centring Sample changer two

Plate barcode: TTP3000807 [Search]

	1	2	3	4	5	6	7	8	9	10	11	12		
A														
B														x
C														
D														x
E														
F														
G														
H														

Current location: Col: 0 Row: 1 X: 0.50 Y: 0.75

Element	Label	Login	Row	Col	Comment
▼ TTP3000807	IQ_3_flat_uv				
	D2A2 ...	toto	mlaursen	C	8

Move to crystal Use crystal repositioning [Abort]

GUI builder

The screenshot displays the GUI builder interface. The top window, titled "GUI Preview: mxCuBE - MXCuBE Qt4", shows a complex control panel with various tabs and settings. The "Sample position" tab is active, showing a grid of buttons for "C", "K", "P", and "Z". Other tabs include "Collection method", "Sample list", "Acquisition", "Characterisation", "Helical Collection", "Energy Scan", "XRF Spectrum", and "Advanced". The "Acquisition" section includes "Oscillation start", "First image:", "Kappa:", "Detector mode:", "Energy (keV):", "Resolution (Å):", and "Characterisation". The "Sample list" section includes "Mode:", "Centring:", and "Sync:". The "Energy" section includes "Energy Current:", "Wavelength:", and "Set to:". The "Transmission" section includes "Current:" and "Set to:". The "Resolution" section includes "Current:" and "Set to:". The "Door interlock" section includes "unknown" and "Unlock". The "Safety shutter" section includes "unknown", "Set in", and "Set out". The "Detector status" section includes "Ready", "Temperature: 0.0%", and "Humidity: 0.0%". The "Current users" section includes "Selecting gives control" and "Allow timeout control".

The "Properties" window is open, showing a table of properties and values:

Properties	Values
1 alignment	none
2 color	Color... reset
3 fixedheight	-1
4 fixedwidth	-1
5 frameshape	default
6 hsizepolicy	default
7 icon	
8 label	Sample video
9 margin	0
10 shadowstyle	default
11 spacing	0
12 vsizepolicy	default

The bottom window, titled "Connection Editor", shows a table of connections between windows and objects:

Windows	Objects	Signals	Windows	Objects	Slots
mxCuBE	chat_brick	enableExpertMode	mxCuBE		
mxCuBE	log_view_brick	isHidden	mxCuBE		
mxCuBE	parameters_tab	isShown	mxCuBE		
mxCuBE	proposal_brick	quit	mxCuBE		
mxCuBE	sample_changer_brick		mxCuBE		
mxCuBE	tab0		mxCuBE		

The "Established connections" table is also visible:

Emitter windc	Emitter objec	Signal	Receiver wind	Receiver objec	Slot
mxCuBE	tab0	notebookP...	mxCuBE	log_view_b...	tabSelected
mxCuBE	task_tollbo...	getTreeBrick	mxCuBE	tree_brick	get_tree_brick
mxCuBE	proposal_b...	loggedIn	mxCuBE	tree_brick	logged_in
mxCuBE	proposal_b...	loggedIn	mxCuBE	task_tollbo...	logged_in
mxCuBE	proposal_b...	sessionSele...	mxCuBE	task_tollbo...	set_session

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 formatting 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    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)
```

```
self._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 high 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        |
+-----+-----+-----+-----+
```

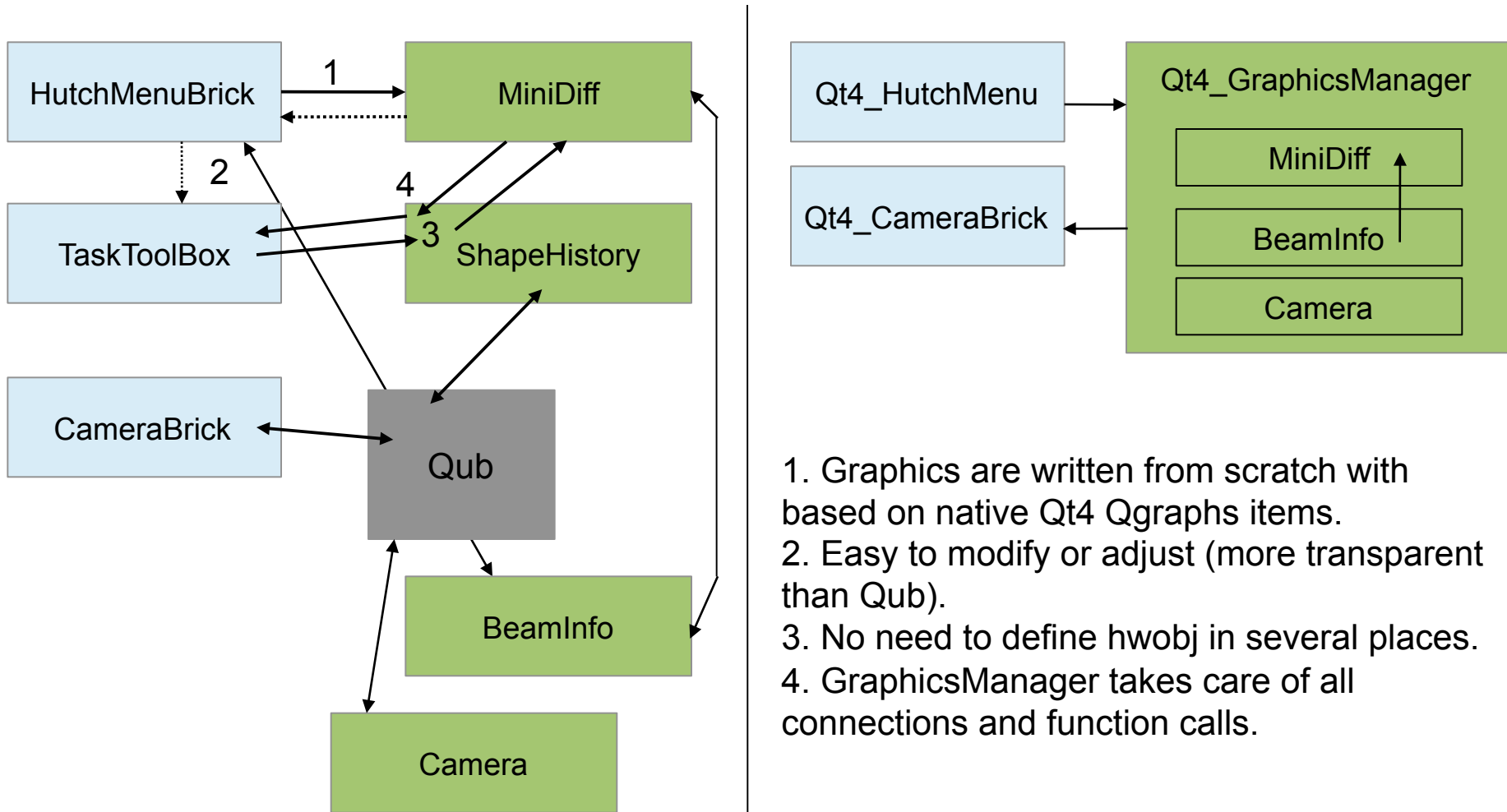
```
mxuser@mxVirtual:~$ radon cc mxcubeGit/Bricks/Qt4_*.py -a -nc
mxcubeGit/Bricks/Qt4_ProposalBrick2.py
  M 696:4 Qt4_ProposalBrick2.select_proposal - C
  M 618:4 Qt4_ProposalBrick2.propertyChanged - C
  M 801:4 Qt4_ProposalBrick2.select_todays_proposal - C
mxcubeGit/Bricks/Qt4_SampleChangerBrick3.py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

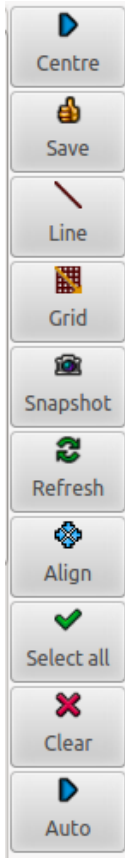
Example: creating a new centring position with 3 clicks



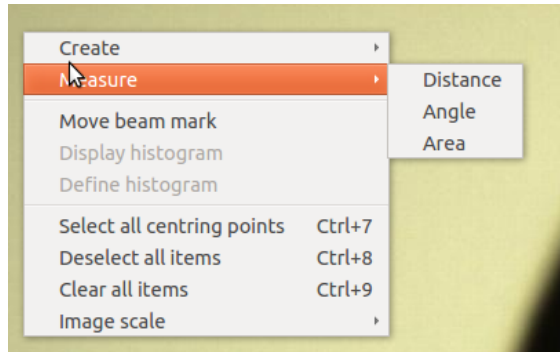
Graphics

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

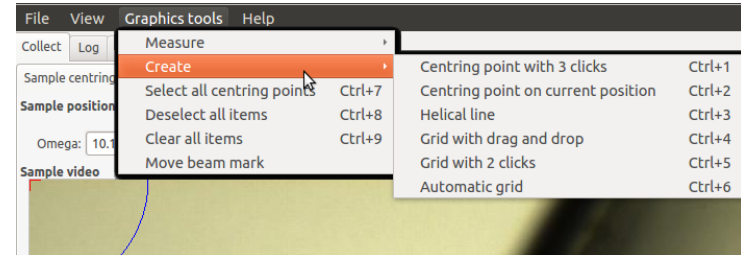
1. HutchMenu



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

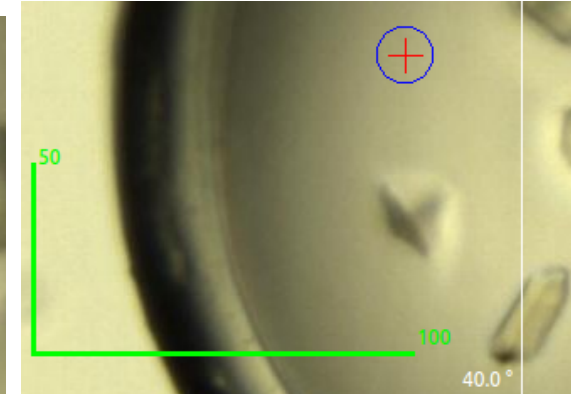
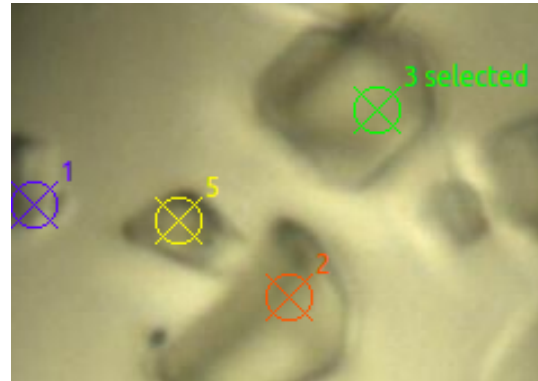
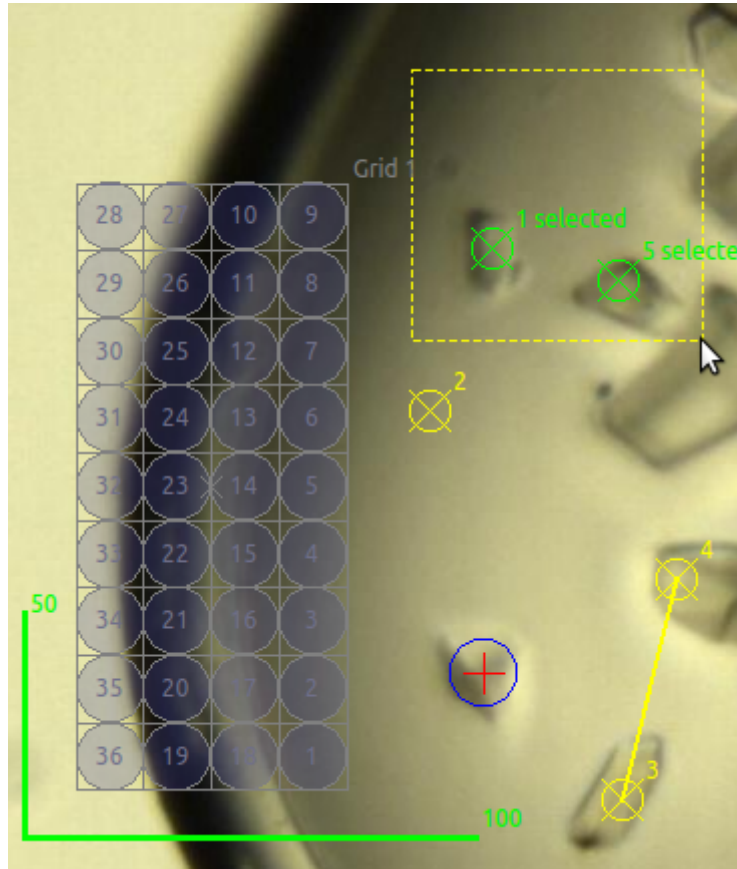
Ctrl+3 - Create helical line

...

Esc - cancel command

Graphics

1. Basic graphics items available.
2. Qt4_GraphicsManagerBrick to add, remove and customize items.



X: 579 Y: 588

Graphics items

All shapes

Display Points Lines Grids

Display all

Hide all

Clear all

No.	Type	Visible	Selected	Used for collection
1	Point 1	True	True	False
2	Point 2	True	True	False
3	Line 1	True	True	True
4	Grid 1	True	True	0

Selected:

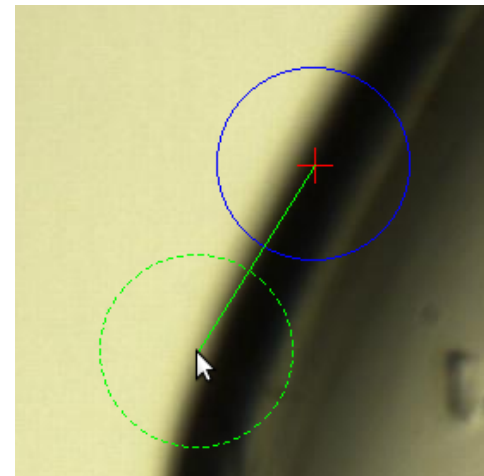
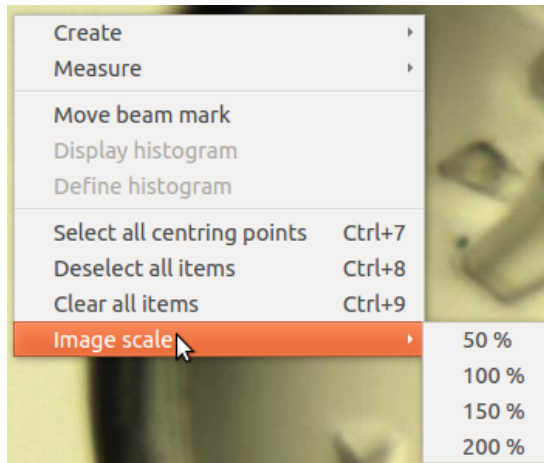
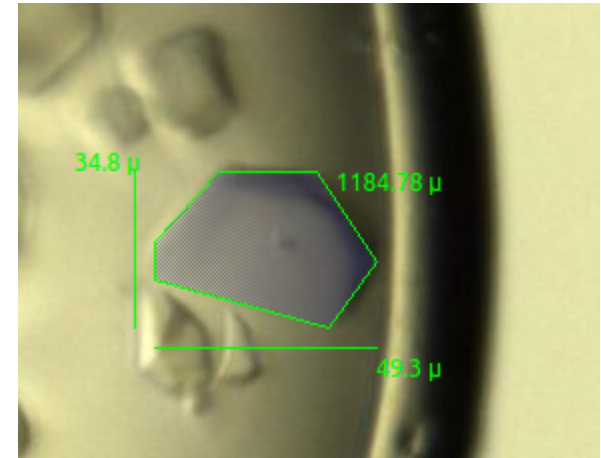
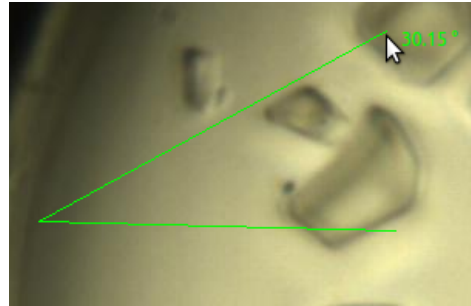
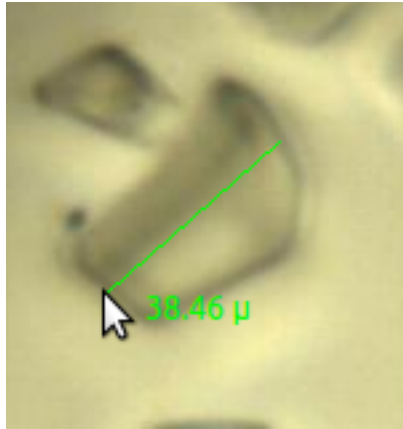
Points

Lines

Grids

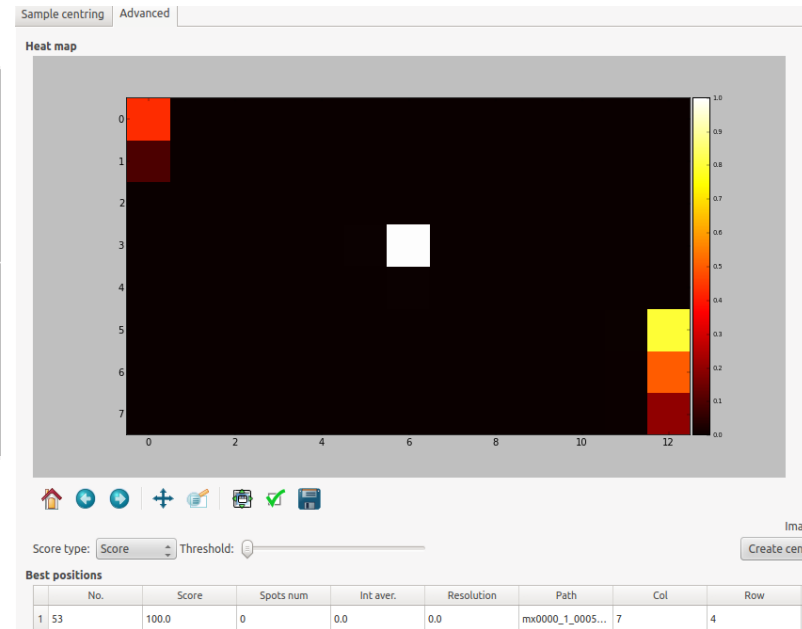
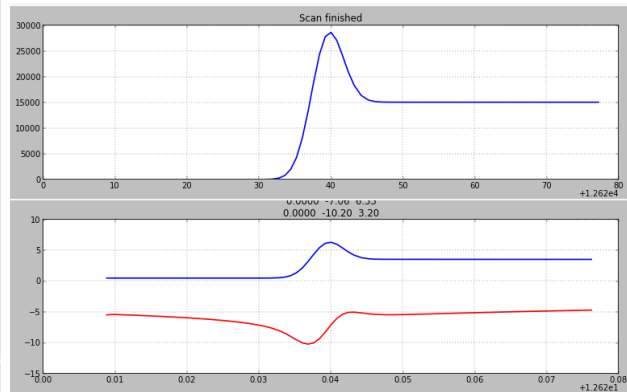
Graphics manager brick

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



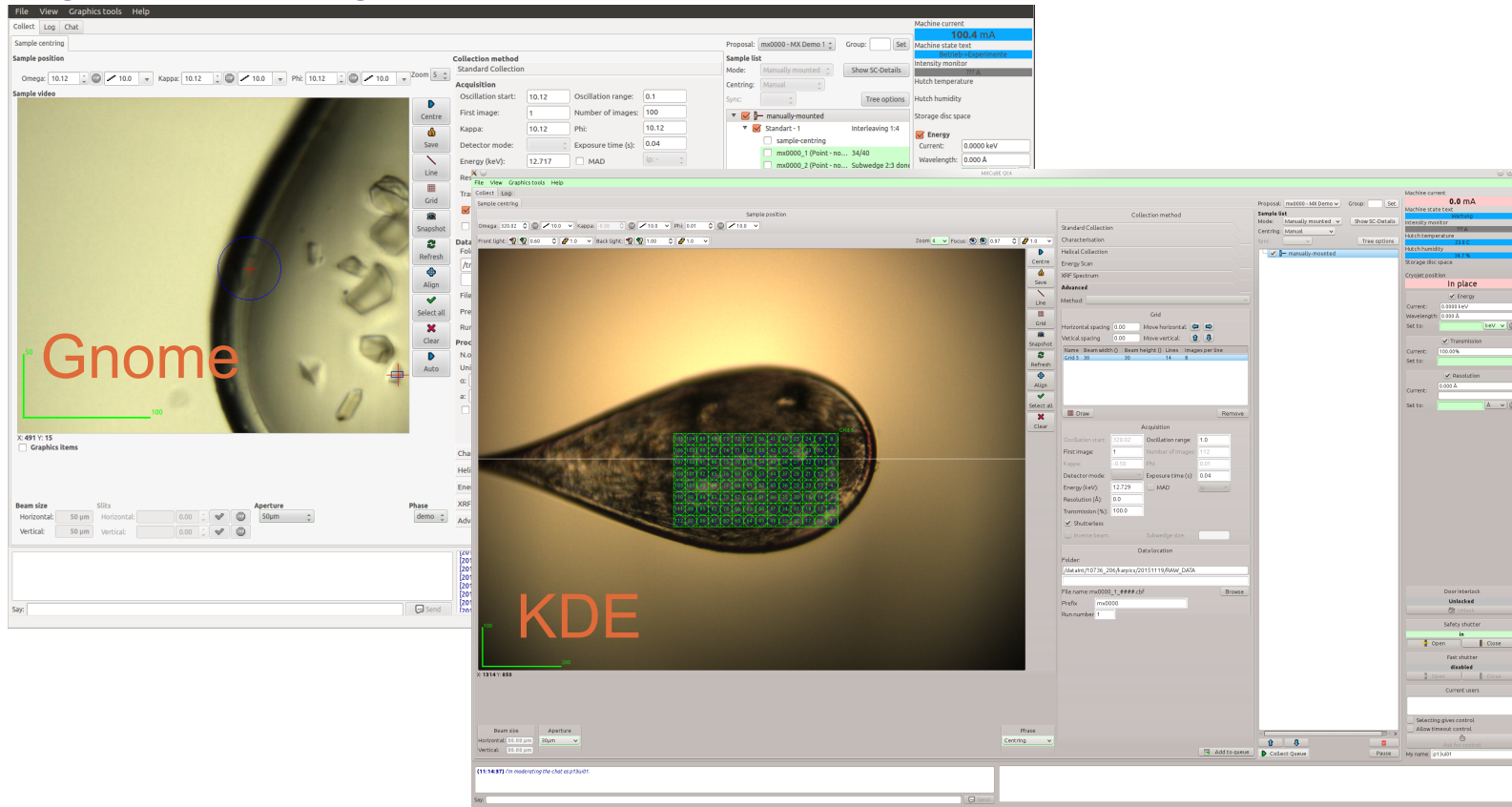
Embedded matplotlib in MXCuBE

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 synch with git (lesson learned with 2 reps).
5. Bug reports and feedback are welcome!

Thank you for your attention