Implementing New Methods in MXCuBE

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Outline

- Purpose of a Graphical User Interfaces
- Native MXCuBE experimental methods
- Motivation for extended catalog of methods
- Implementing a method
  - Choosing between a native method and an external workflow
  - Third option
  - Is there a right way ?
- Beyond MX
  - Alignment of beamline components
  - Beam characterisation
  - 3D sample characterisation (Optical and X-ray tomography)

Purpose of a graphical user interface

- Streamlining use of a beamline
- Exploring sample
- Defining experiment
- Presenting results

Native methods of MXCuBE

- Scan
  - position, orientation and a rotation axis
  - scan_range, scan_start_angle, angle_per_frame, transmission, photon_energy, resolution
- Characterisation
  - axes, wedge_range, scan_start_angles, angle_per_frame …
  - collect followed by inspection or automated analysis
- Helical scan
  - scan parameters + translation vector
- Fluorescence spectrum
  - photon_energy, count_time
- Energy scan
  - element, edge, scan_range, sampling rate

Native methods

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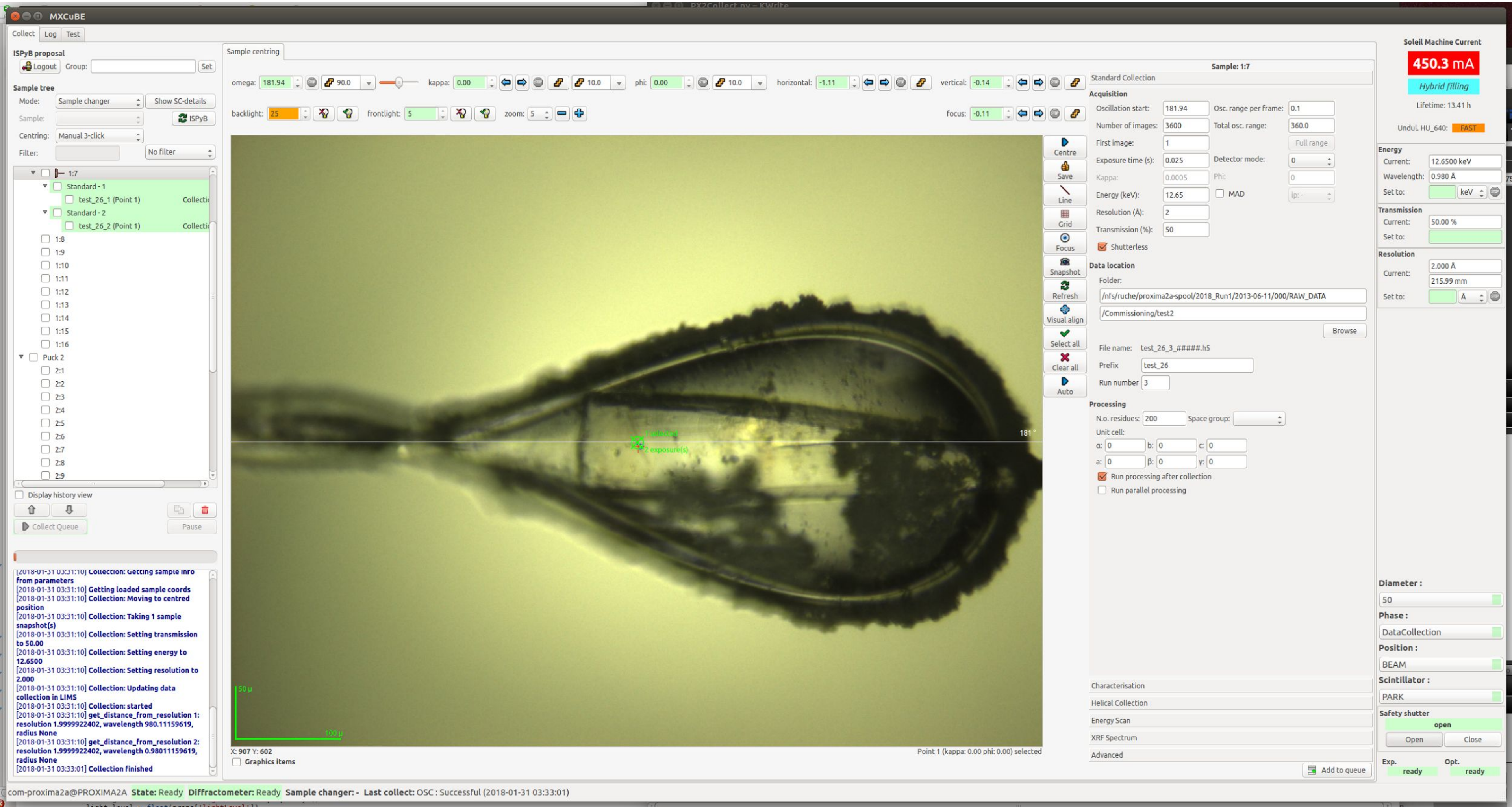
- Energy scan
  - element, edge, scan_range, sampling rate
- Optical alignment
  - 3+orientations manual or automated(circular model)

Advanced methods

- Mesh scan (grid, raster, area mapper…)
  - Usually a rectangular region -- vertical and horizontal dimensions, horizontal and vertical pitch
  - photon_energy, transmission (flux), resolution
  - analysis, interpretation ...
- X-ray centring
  - series of mesh scans
  - analysis
- Burn strategy
  - determining rate of radiation damage in a sample
  - radiation damage induced phasing
  - ...


MXCuBE
Collect
Log
Test
ISPyB proposal
Logout
Group:
Set
Sample tree
Mode:
Sample changer
Show SC-details
Sample:
ISPyB
Centring:
Manual 3-click
Filter:
No filter
1:7
Standard - 1
test_26_1 (Point 1)
Standard - 2
test_26_2 (Point 1)
1:8
1:9
1:10
1:11
1:12
1:13
1:14
1:15
1:16
Puck 2
2:1
2:2
2:3
2:4
2:5
2:6
2:7
2:8
2:9
Display history view
Collect Queue
Pause
[2018-01-31 03:31:10] Collection: Getting sample info from parameters
[2018-01-31 03:31:10] Getting loaded sample coords
[2018-01-31 03:31:10] Collection: Moving to centred position
[2018-01-31 03:31:10] Collection: Taking 1 sample snapshot(s)
[2018-01-31 03:31:10] Collection: Setting transmission to 50.00
[2018-01-31 03:31:10] Collection: Setting energy to 12.6500
[2018-01-31 03:31:10] Collection: Setting resolution to 2.000
[2018-01-31 03:31:10] Collection: Updating data collection in LIMS
[2018-01-31 03:31:10] Collection: started
[2018-01-31 03:31:10] get_distance_from_resolution 1: resolution 1.9999922402, wavelength 980.11159619, radius None
[2018-01-31 03:31:10] get_distance_from_resolution 2: resolution 1.9999922402, wavelength 0.98011159619, radius None
[2018-01-31 03:33:01] Collection finished
Sample centring
omega: 181.94
90.0
kappa: 0.00
10.0
phi: 0.00
10.0
horizontal: -1.11
vertical: -0.14
backlight: 25
frontlight: 5
zoom: 5
focus: -0.11
Centre
Save
Line
Grid
Focus
Snapshot
Refresh
Visual align
Select all
Clear all
Auto
181°
50 µ
100 µ
X: 907 Y: 602
Graphics items
Point 1 (kappa: 0.00 phi: 0.00) selected
Sample: 1:7
Standard Collection
Acquisition
Oscillation start: 181.94
Osc. range per frame: 0.1
Number of images: 3600
Total osc. range: 360.0
First image: 1
Full range
Exposure time (s): 0.025
Detector mode: 0
Kappa: 0.0005
Phi: 0
Energy (keV): 12.65
MAD
Resolution (Å): 2
Transmission (%): 50
Shutterless
Data location
Folder:
/nfs/ruche/proxima2a-spool/2018_Run1/2013-06-11/000/RAW_DATA
/Commissioning/test2
Browse
File name: test_26_3_#####.h5
Prefix test_26
Run number 3
Processing
N.o. residues: 200
Space group:
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0
Run processing after collection
Run parallel processing
Characterisation
Helical Collection
Energy Scan
XRF Spectrum
Advanced
Add to queue
Soleil Machine Current
450.3 mA
Hybrid filling
Lifetime: 13.41 h
Undul. HU_640: FAST
Energy
Current: 12.6500 keV
Wavelength: 0.980 Å
Set to: keV
Transmission
Current: 50.00 %
Set to:
Resolution
Current: 2.000 Å
215.99 mm
Set to: Å
Diameter :
50
Phase :
DataCollection
Position :
BEAM
Scintillator :
PARK
Safety shutter
open
Open
Close
Exp.
Opt.
ready
ready
com-proxima2a@PROXIMA2A State: Ready Diffractometer: Ready Sample changer: - Last collect: OSC : Successful (2018-01-31 03:33:01)

Atom of an execution

- Scan (helical)
  - Any diffraction experiment currently supported by MXCuBE can be mapped to a series of helical scans
  - Translation vector set to zero for standard and characterisation, non-zero for helical, x-ray centring and mesh collection
- If queuing is available, any current experiment outline can be reformulated as a series of scans

Experiment finality

What is the question we are asking ?

Is experiment best characterised by it ? Analysis should be an inherent part of a definition of a method.

Experiment is really defined by the analysis.

New features for characterisation method

- Fine sliced wedges instead of single images
- Combining x-ray centring with characterisation
    - Helical scan orthogonal to the rotational axis during wedge measurement
- Strategy + Sample shape determination + Alignment (offsets)

List of available methods

- Scan, Characterisation, Helical Scan, X-ray centring, Mesh, SSX, MAD, Burn, Interleaved, Energy scan, Tomography, XRF spectrum, N-click optical alignment, Sample optical segmentation, Detector pixel health analysis

Hierarchy of available methods

- Experiment
  - Xray
    - Diffraction
      - Scan,
        - Characterisation, Burn, MAD, Interleaved, detector pixel health analysis
      - Helical Scan
        - Helical, X-ray centring, Mesh, SSX
    - Fluorescence
      - Energy scan, XRF spectrum
    - Absorption
      - Tomography
    - Intensity
      - Flux measurement, Slits alignment, Monochromator tuning
  - Optical
    - N-click centring, Sample segmentation

Implementing a method

- Declare necessary equipment and methods and procedures for a class of experiments
  - inherit from AbstractCollect -- diffraction based experiments (Scan, Characterisation, Helical, Interleaved experiments)
  - Can be used for Energy scan, fluorescence spectrum and optical alignment as well ?
- queue_entry
  - pre_execute, execute, post_execute
- data_model
- input widget
  - Parameter specification, queue insertion
- Make Collect object aware of it.

```
Class AbstractCollect(device):
    ...
    @abc.abstractmethod
    def data_collection_hook(self):
        """
        Descript. :
        """
        pass

Class PX2Collect(AbstractCollect):
     ...
     def data_collection_hook(self):
         if experiment_type == 'OSC':
             name_pattern = template[:-8]

             os = omega_scan(name_pattern,
                             directory,
                             photon_energy=energy,
                             transmission=transmission,
                             resolution=resolution,
                             simulation=True)
             os.execute()
```

Supported methods

1. `from omega_scan import omega_scan`
2. `from inverse_scan import inverse_scan`
3. `from reference_images import reference_images`
4. `from helical_scan import helical_scan`
5. `from fluorescence_spectrum import fluorescence_spectrum`
6. `from energy_scan import energy_scan`
7. `from xray_centring import xray_centring`
8. `from raster_scan import raster_scan`
9. `from nested_helical_acquisition import nested_helical_acquisition`
10. `from tomography import tomography`
11. `from film import film`

Beyond MX experiment control in MXCuBE

- Using MXCuBE framework as a GUI for beamline characterisation and optimisation
    - alignment of slits, apertures and collimators
    - undulator tuning curves
    - monochromator alignment
    - precise beam shape and flux determination
    - determination of beam center on the detector (function of focussing mode, energy, distance)
    - detector pixels health verification
- https://github.com/MartinSavko/experimental_methods

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Additional methods

1. `from omega_scan import beamcenter_calibration`
2. `from monochromator_scan import monochromator_scan`
3. `from fast_shutter_scan import fast_shutter_scan`
4. `from monochromator_pitch_scan import monochromator_pitch_scan`

Advantages

- Possible to test from command line (evaluation of GUI overhead in execution)
- Easier debugging
- Command line interface for every method
- Complexity encapsulation
- Full control of the execution at the inner most level of the procedure
- Full awareness of the finality and any parameter of the experiment at any time

Drawbacks

- At the moment the connections to lower level objects are recreated
- Many methdods in AbstractCollect are left unused

More is more

- Sharing experiment protocols via catalog of methods native to MXCuBE
  - Benefiting from shared knowledge
- Sharing analysis protocols as well (ideally inherent to the method definition)
  - Even more useful
- Society of experimental methods flowering in MXCuBE ecosystem
  - Many levels of complexity -- from slit scans to multisweep interleaved experiments

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