

# MXCuBE status at SOLEIL

Martin Savko

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## Proxima 1

Source: U20 in vacuum undulator

Focussing: KB, CRL

Tunable: 5.5 - 15.5 keV

Flux: 2.0e12 ph/s @ 500mA @ 12.65keV

Beam size: 20x40  $\mu\text{m}$

Area Detector: Eiger X 16M

XRF Detector: Ketek AXAS-M2 H150

OAV Camera: Prosilica GC 1350

Goniometer: SmarGon

Sample Changer: CATS (48 samples)

MXCuBE: Qt4 v 2.3 (CentOS 7)

## Proxima 2

Source: U24 in vacuum undulator

Focussing: KB + horizontal PFM

Tunable: 5.5 - 18.5 keV

Flux: 1.6e12 ph/s @ 500mA @ 12.65keV

Beam size: 5x10  $\mu\text{m}$

Area Detector: Eiger X 9M

XRF Detector: Ketek AXAS-M2 H80

OAV Camera: Prosilica GC 1350

Goniometer: MD2 with MK3

Sample Changer: CATS (144 samples)

MXCuBE: Qt4 v2.3 (Ubuntu 14.04)

## Proxima 1

Source: **U20** in vacuum undulator

Focussing: KB, **CRL**

Tunable: 5.5 - 15.5 keV

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Beam size: **20x40  $\mu\text{m}$**

Area Detector: **Eiger X 16M**

XRF Detector: Ketek AXAS-M2 **H150**

OAV Camera: Prosilica GC 1350

Goniometer: **SmarGon**

Sample Changer: CATS (**48 samples**)

MXCuBE: Qt4 v 2.3 (**CentOS 7**)

## Proxima 2

Source: **U24** in vacuum undulator

Focussing: KB, **horizontal PFM**

Tunable: 5.5 - 18.5 keV

Flux: 1.6e12 ph/s @ 500mA @ 12.65keV

Beam size: **5x10  $\mu\text{m}$**

Area Detector: **Eiger X 9M**

XRF Detector: Ketek AXAS-M2 **H80**

OAV Camera: Prosilica GC 1350

Goniometer: **MD2 with MK3**

Sample Changer: CATS (**144 samples**)

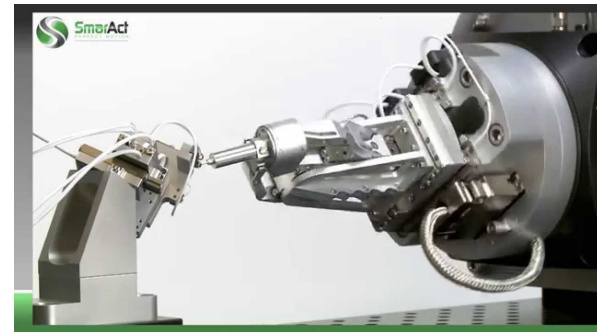
MXCuBE: Qt4 v2.3 (**Ubuntu 14.04**)

# Eiger X on Protein Crystallography Beamlines in SOLEIL

- Firmware version: SIMPLON v. 1.6.4
- User operation
  - Eiger X 9M December 2015 on Proxima 2
  - Eiger X 16M October 2018 on Proxima 1
- bslz4 compression
- Max speeds
  - 133Hz @ 16M
  - 238Hz @ 9M
  - 750Hz @ 4M ROI (stable as of SIMPLON API 1.6.2)

# Multiaxis goniometry

- Smargon goniometer on Proxima 1 (SmarAct)
  - SmarAxis Tango Device Server (C++) developed at SOLEIL

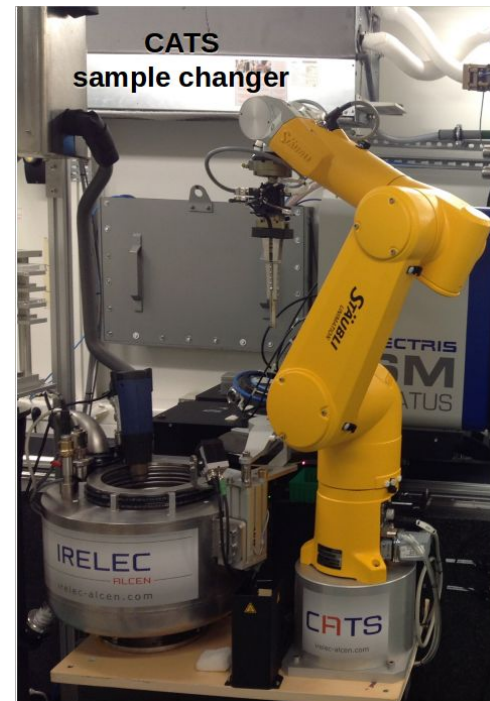


- Minikappa MK3 on Proxima 2 (Arinax)
  - JLIB software accessed through Tango Device server



# Sample changers

- CATS robots on both beamlines. Control via PyCats Tango Device Server
- Mature integration
  - Failure rate below 1 per 1000
  - Exchange time 35 seconds



# Remote access

- NoMachine servers installed on control computers
- Regularly scheduled on both beamlines for both industrial and academic users (5-10%)

# Data handling infrastructure

- 10Gbit network
- Local buffer on the processing server
  - 2.56TB RAM
  - 3TB RAID 6 SAS (to be upgraded by 16TB SSD)
- Medium and long term storage (Active Circle based), NFS access
  - Local cell: 10TB SSD, 20TB SAS
  - Remote cell: 1PB via 10Gbe



# Processing infrastructure

- System dedicated to a single beamline
  - Keeping data close to source
  - Tailor processing power to the detector
  - Minimizing administrative overhead
- Huawei FusionServer RH8100 V3 Rack Server
  - 8 x XEON E7-8890 v3 @ 2.5GHz, 144 cores, 288 threads
  - 2.56 TB RAM (DDR4 1866MHz)
  - 4 x 10GBe
  - 5.76 TFlops
  - spot finding with `dials.find_spots` and Dozor
  - data integration with XDS

\*



```
MAXIMUM_NUMBER_OF JOBS= 10
MAXIMUM_NUMBER_OF PROCESSORS= 32
```

# Performance of the setup

- ~ 1000 MB/sec download speed
  - Using both 10Gbit ports of the DCU
  - ~600 MB/sec with single 10Gbit port
- ~ 114 MB/s is the average data rate
  - Maximum observed data rate ~ 770.57 MB/s
  - In practice no data transfer bottleneck thanks to bitshuffle lz4
- The server has RAM cache of 170 GB
  - ~ 20 min autonomy assuming average data rate in bslz4 compression
- 12.75 is the average observed bslz4 compression ratio
  - x 14.4 per 32bit -- average compressed image size ~3 MB
  - x 10.9 per 16bit -- average compressed image size ~2 MB

# For steady processing

```
# sync; echo 3 > /proc/sys/vm/drop_caches
```

# For steady processing

```
# sync; echo 3 > /proc/sys/vm/drop_caches
```

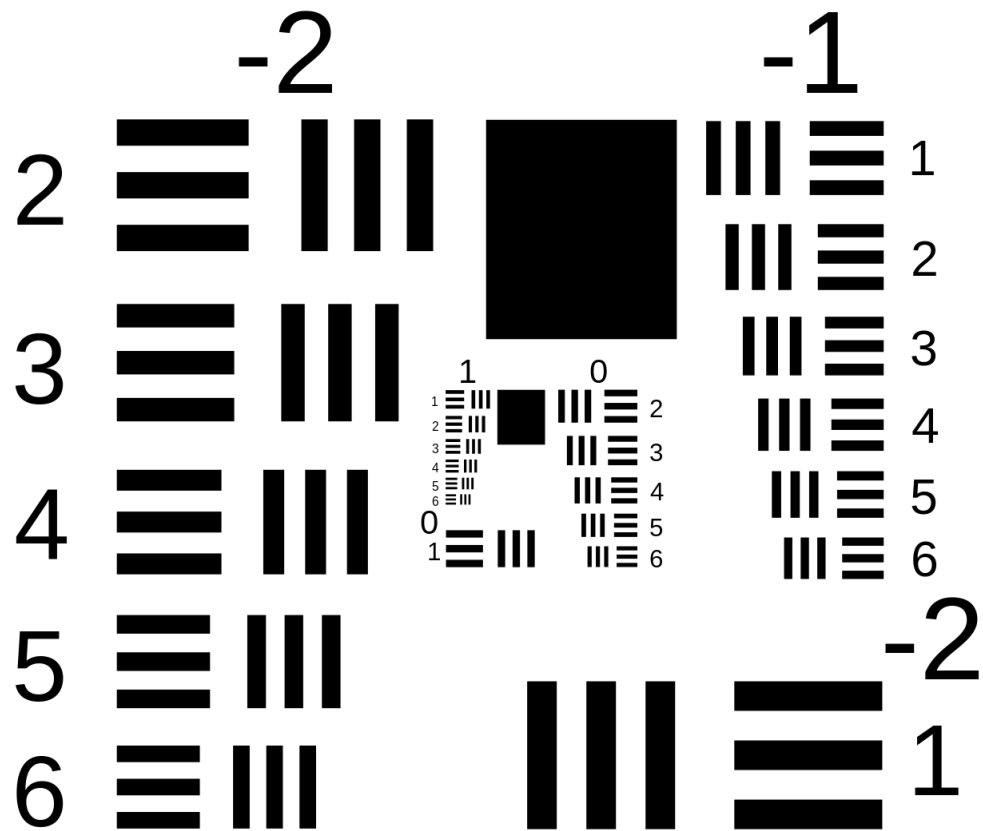
\* executed as a cron job every 4 hours

# Issues

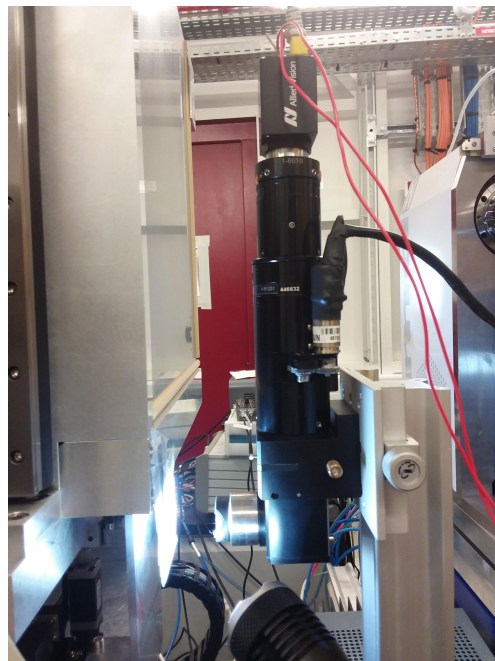
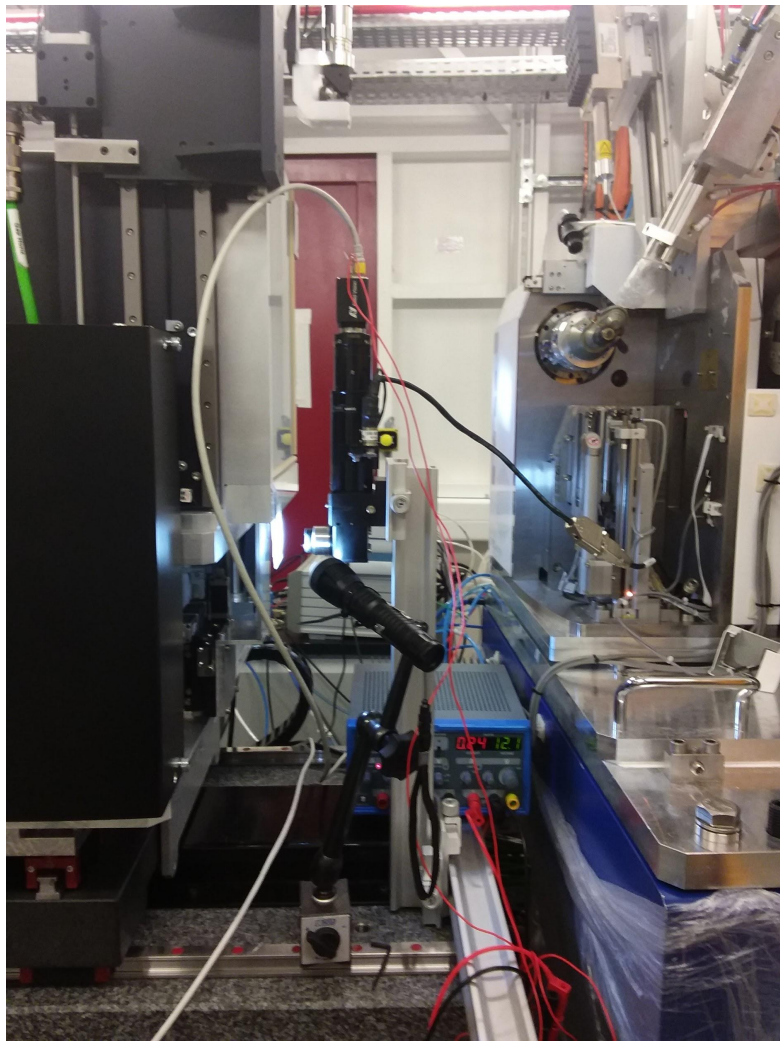
- OAV zoom failure on Proxima 2
  - exchange for a spare and then for a replacement

# Issues

- OAV zoom failure on Proxima 2
  - exchange for a spare and then for a replacement
  - aligning transfocator optical center and the camera center
  - verifying pixel calibration

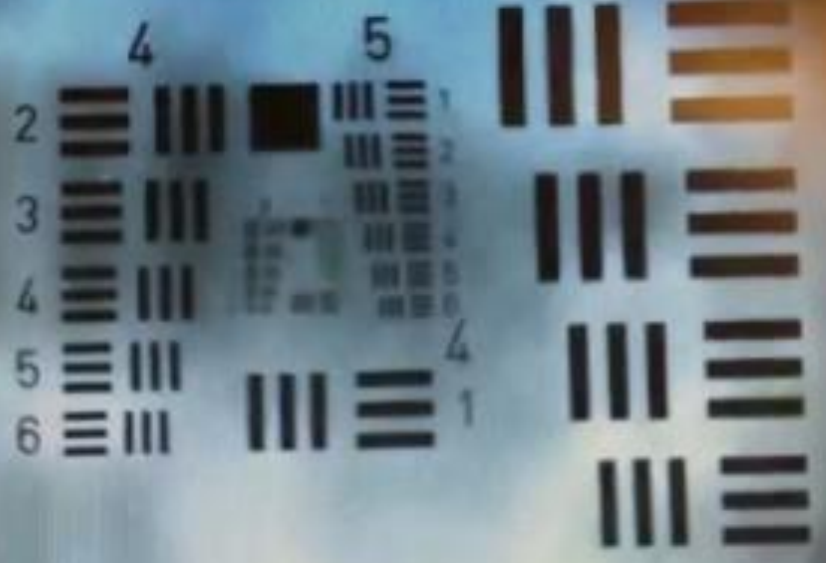


USAF-1951





Windows taskbar with icons for Internet Explorer, Firefox, and Windows Vista.



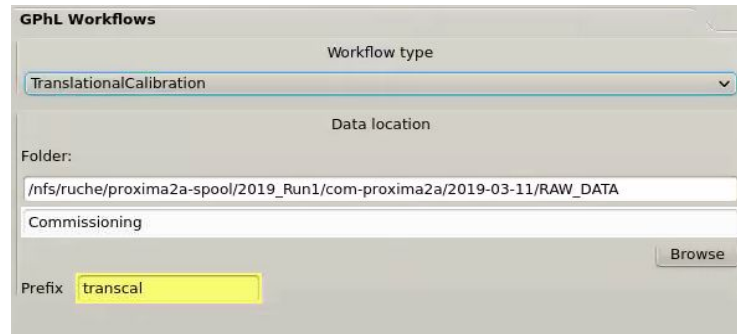
Partial view of a document or book page on the right side of the image.

# Issues

- OAV zoom failure on Proxima 2
  - exchange for a spare and then for a replacement
  - aligning transfocator optical center and the camera center
  - verifying pixel calibration
- Deterioration of sphere of confusion of Omega axis with MK3
  - Discovered during a development session with GPHL in January 2019
  - in vertical from 2.4  $\mu\text{m}$  with kappa closed,  $\sim 10 \mu\text{m}$  with kappa open ( $< 5 \mu\text{m}$  during SAT)
  - horizontal discrepancy of similar magnitude at large kappa

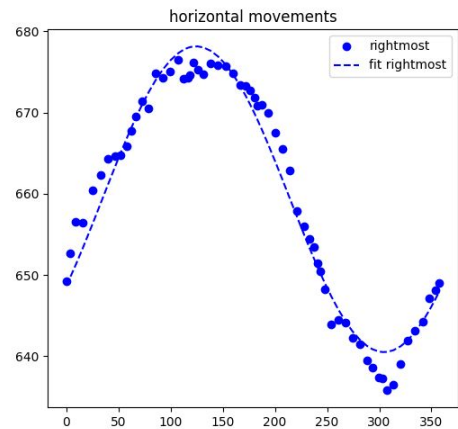
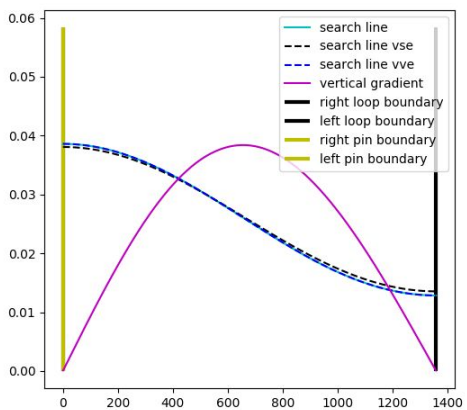
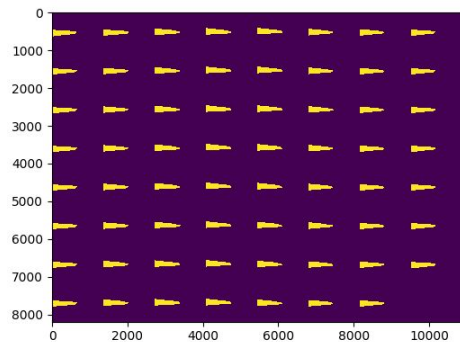
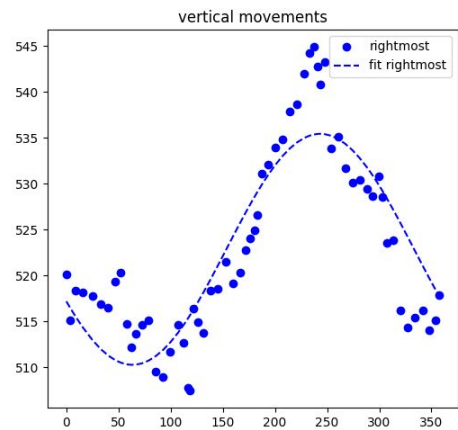
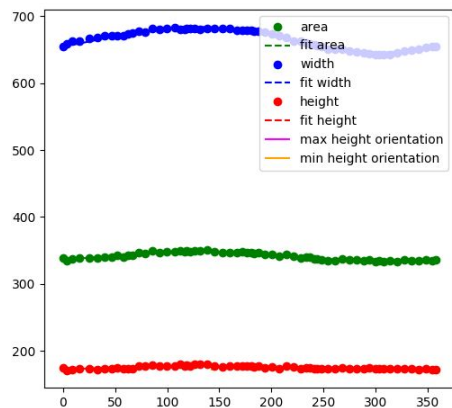
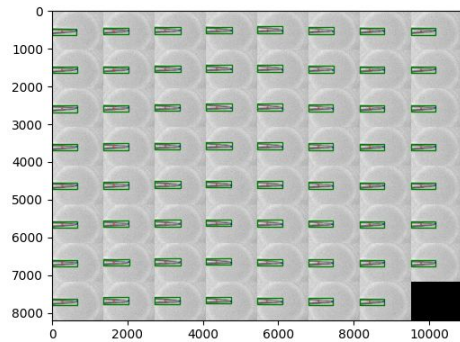
# Issues

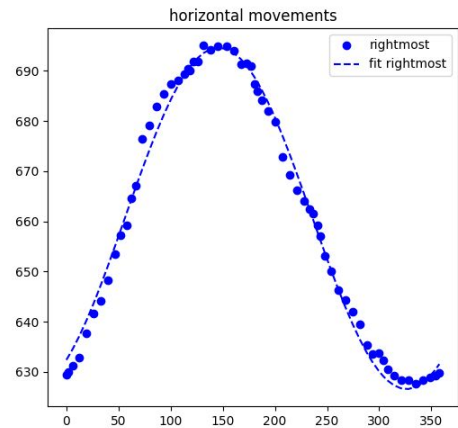
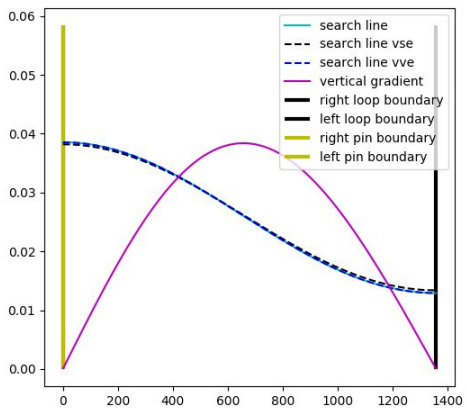
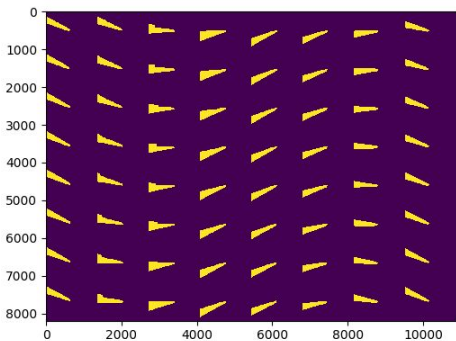
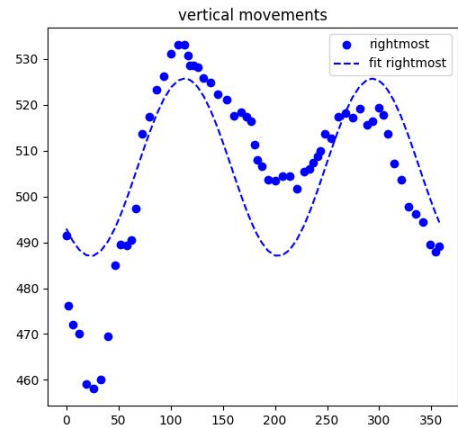
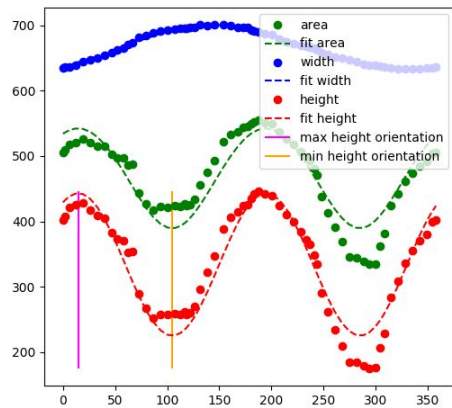
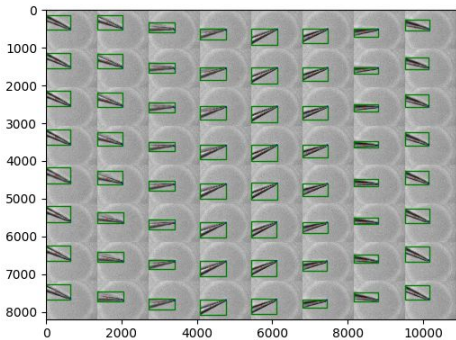
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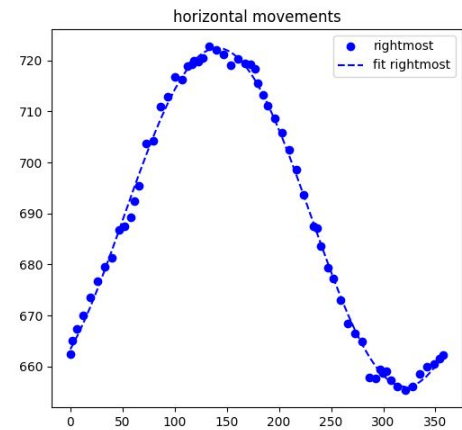
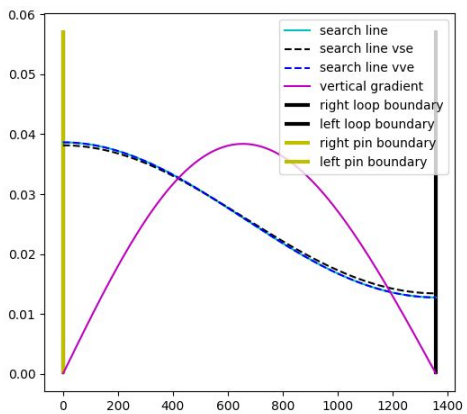
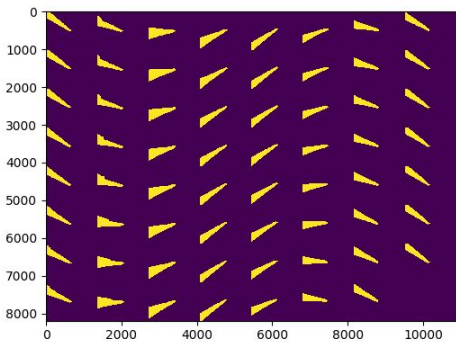
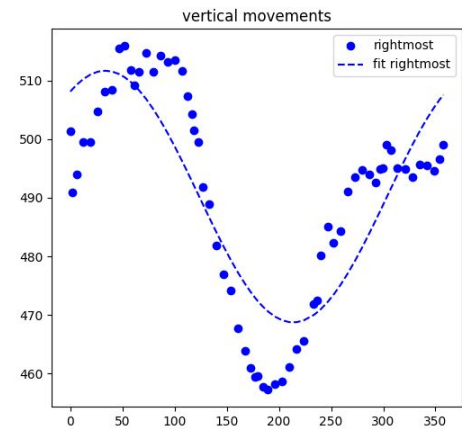
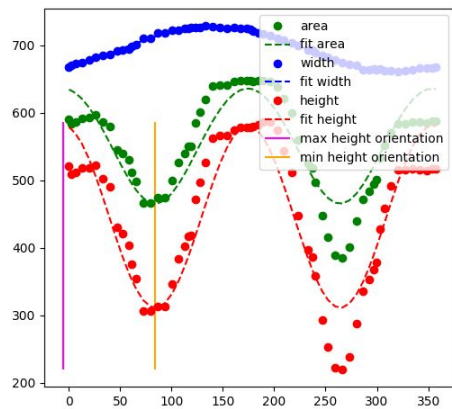
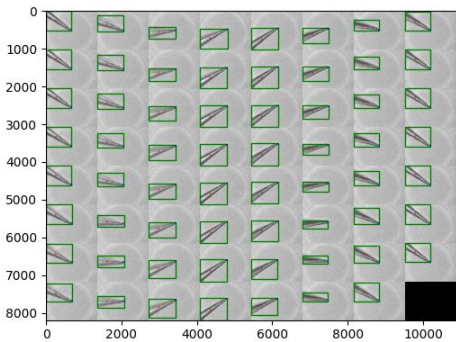


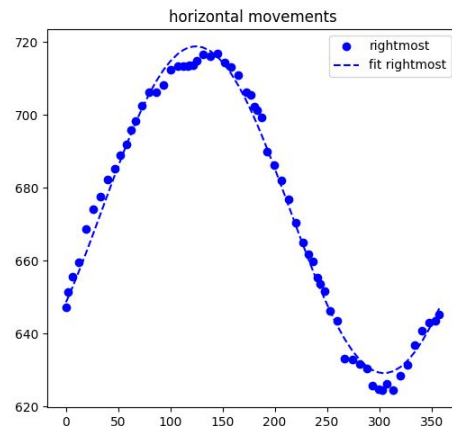
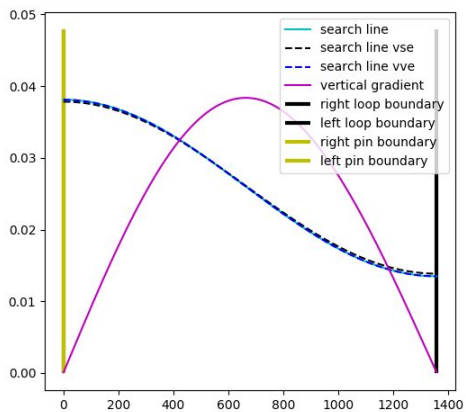
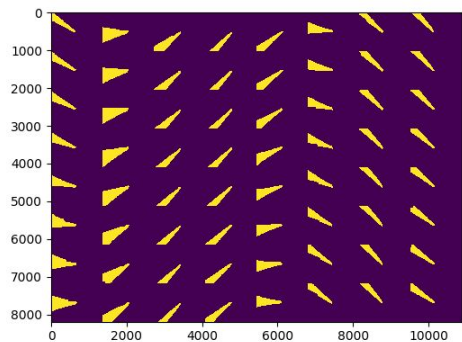
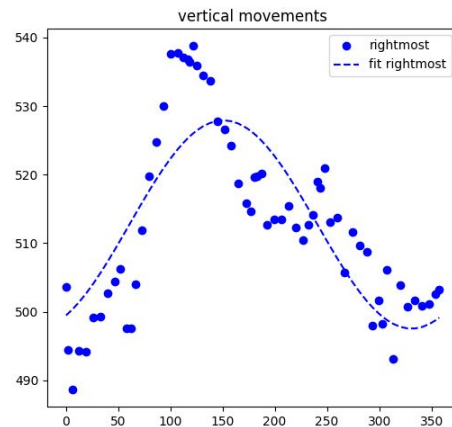
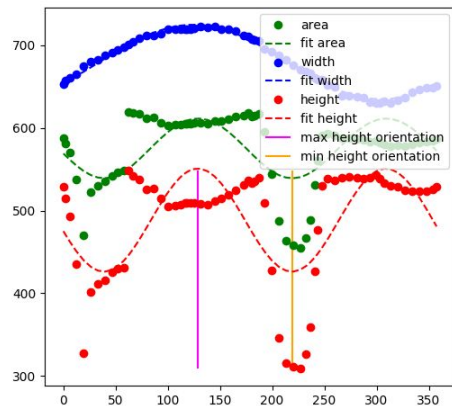
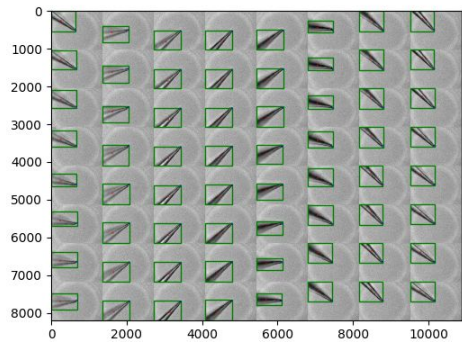
The screenshot shows a software interface titled "GPHL Workflows". It contains several configuration fields:

- Workflow type:** A dropdown menu with "TranslationalCalibration" selected.
- Data location:** A section containing two text input fields:
  - Folder:** "/nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-11/RAW\_DATA"
  - Commissioning:** "Commissioning"
- Prefix:** A text input field containing "transcal", which is highlighted in yellow.
- Browse:** A button located to the right of the Commissioning field.









# Short history of MXCuBE GUI on Proxima 2



User: **mx-com-proxima2a** Group:  Set

Sample list:  
 Mode:    
 Centring:

- 1.1
  - 1.2
  - 1.3
  - 1.4
  - 1.5
  - 1.6
  - 1.7 Centring done
    - Standard - 1
    - cpbs\_26 Collection done
    - Standard - 2
    - cpbs\_27 Collection done
    - Standard - 4
    - cpbs\_28 Collection done
    - Standard - 5
    - cpbs\_29 Collection done
    - Standard - 6
    - cpbs\_30 Collection done
    - Standard - 7
    - cpbs\_31 Collection done
    - Standard - 8
    - cpbs\_32 Collection done
    - Standard - 9
    - cpbs\_33 Collection done
    - Standard - 10
    - cpbs\_34 Collection done
    - Standard - 11
    - cpbs\_35 Collection done
    - Standard - 12
    - cpbs\_36 Collection done
    - Standard - 13
    - cpbs\_37 Collection done
  - 1.8
  - 1.9
  - 1.10
  - 1.11
  - 1.12
  - 1.13
  - 1.14
  - 1.15
  - 1.16
  - 2.1
  - 2.2
  - 2.3
- 

Sample centring | Sample changer

Omega:    45.0

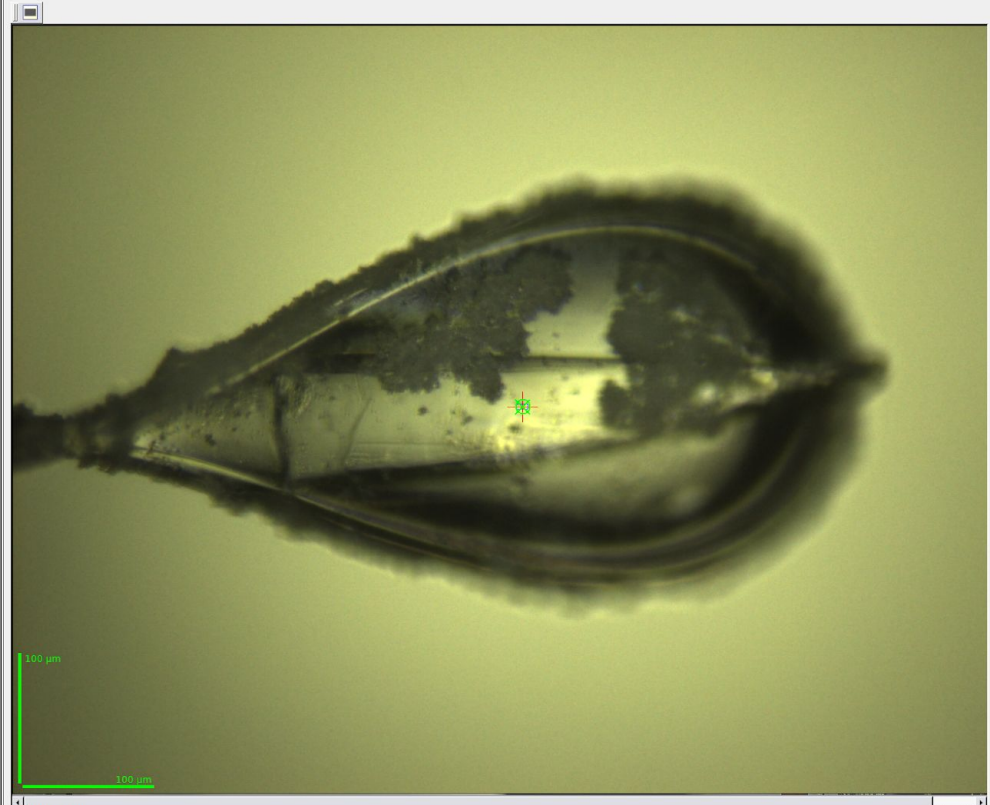
Front Light:

Back Light:

Exposure:

Focus:

zoom:



X: 1303 Y: 656

**Starting collection**

[2018-01-31 03:05:09] Setting energy before collect

[2018-01-31 03:05:13] Setting resolution -- moving the detector.

[2018-01-31 03:05:13] Capillary beamstop in the beam path, starting to collect.

[2018-01-31 03:05:15] Moving the detector -- done.

[2018-01-31 03:05:15] Setting resolution -- done.

[2018-01-31 03:05:15] Capillary beamstop in the beam path, starting to collect.

[2018-01-31 03:05:26] Collection completed

[2018-01-31 03:07:20] CATS: Power On

[2018-01-31 03:08:22] Manual centring used, waiting for user to center sample

[2018-01-31 03:09:30] Centring saved

[2018-01-31 03:10:16] Manual centring used, waiting for user to center sample

[2018-01-31 03:10:53] Centring saved

Collection method

Standard Collection

**mxima2a-spool/2018\_Run1/2018-01-30/com-proxima2a/RAW\_DATA**

/Commissioning/CPBS

Characterisation

Helical Collection

Energy Scan

Advanced

Soleil machine current

**450.9 mA**

Hybrid filling

Lifetime: 13.23 h

Undul. HU: 640:

Energy

Current:

Move to:  keV

Detector distance

Current:

Move to:  mm

Transmission

Current:

Set to:

Aperture

Diameter:

Phase:

Position:

Scintillator:

Guillotine

Frontend shutter

Safety shutter

Fast shutter

LN2 Regulation

Optical hutch Experimental hutch

Current users

Selecting gives control

Allow timeout control

My name: proxima2a-5

# MXCuBE Qt4 mid 2018

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) Collect
  - Standard - 2
    - test\_26\_2 (Point 1) Collect
- 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 0.98011159619,
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 focus: -0.11

backlight: 25 frontlight: 5 zoom: 5

X: 907 Y: 602  
Point 1 (kappa: 0.00 phi: 0.00) selected

Standard Collection Sample: 1:7

Acquisition

Oscillation start: 181.94 Osc. range per frame: 0.1  
 Number of images: 3600 Total osc. range: 360.0  
 First image: 1  
 Exposure time (s): 0.025 Detector mode: Full range  
 Kappa: 0.0005 Phi: 0  
 Energy (keV): 12.65 MAD: 0  
 Resolution (Å): 2  
 Transmission (%): 50  
 Shutterless

Data location

Folder: /nfs/ruche/proxima2a-spool/2018\_Run1/2013-06-11/000/RAW\_DATA  
 /Commissioning/test12  
 Browse

File name: test\_26\_3\_####.hs  
 Prefix: test\_26  
 Run number: 3

Processing

N.o. residues: 200 Space group: [ ]  
 Unit cell:  
 a: 0 b: 0 c: 0  
 a: 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: 1AS

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. ready Opt. ready

# MXCuBE Qt4 mid 2018

ISPyB proposal  
 Logout Group:  Set

Sample tree

Mode: Sample changer Show SC-details

Sample:  ISPyB

Centring: Manual 3-click

Filter:  No Filter

- 1:7
  - Advanced - 1
    - idtest000\_1 (Mesh 1: 58 x 72)
      - 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
  - 2:10
  - 2:11

Display history view

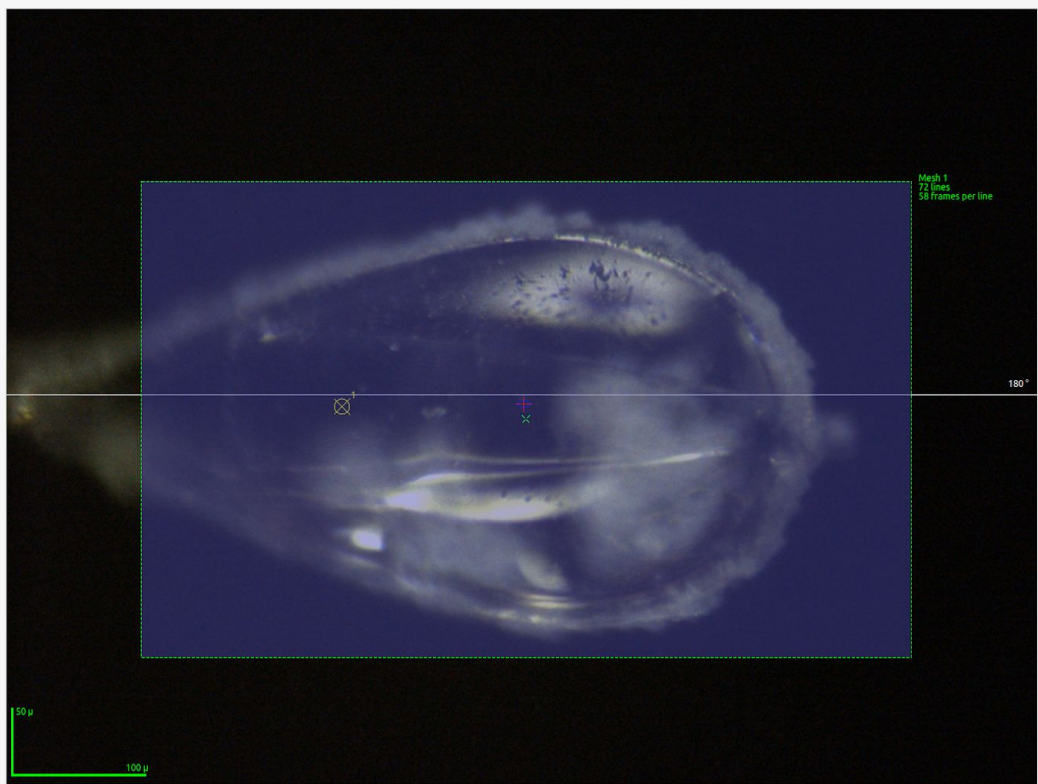
collect Queue

Pause

Sample centring

omega: 180.06 k: 10.0 phi: 0.00 horizontal: -1.18 vertical: -0.13

backlight: 0 frontlight: 5 zoom: 5 focus: -0.11



X: 933 Y: 634

Graphics Items

Centering Point: 1 (kappa: 0.00 phi: 0.00) created

Standard Collection idtest000\_1 (Mesh 1: 58 x 72)

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

Advanced

Method: MeshScan

Grid

Horizontal spacing (μm) 10.00 Move horizontal:

Vertical spacing (μm) 5.00 Move vertical:

Adjust size

Snapshot

Name	Lines	Frames per line
Mesh 1	72	58

Refresh

Visual align

Select all

Clear all

Auto

Display overlay:   Overlay color

Acquisition

Oscillation start: 180.06 Osc. range per frame: 0.01

Number of images: 4176 Total osc. range per line: 0.58

First image: 1

Exposure time (s): 0.025 Detector mode: 0

Kappa: 0 Phi: 0

Energy (keV): 12.65  MAD

Resolution (Å): 2

Transmission (%): 65.8

Shutterless

Data location

Folder:

File name: idtes000\_1\_####.h5

Prefix:

Run number:

Soleil Machine Current

**451.7 mA**

Hybrid filling

Lifetime: 13.32 h

Undul. HU\_640:

Energy

Current:

Wavelength: 0.980 Å

Set to:

Transmission

Current:

Set to:

Resolution

Current:

Set to:

Diameter:

Phase:

Position:

Scintillator:

Safety shutter

Exp.  Opt.

**Sample tree**

Mode: **Sample changer** Show SC-details

Sample: ISPyB

Centring: **Manual 3-click**

Filter: No filter

- Puck 1
- Puck 2
- Puck 3
- Puck 4
- Puck 5
- Puck 6
- Puck 7
- Puck 8
- Puck 9

Queue history

Collect Queue

Pause

Standard Collection Sample: manually-mounted

**Acquisition**

Oscillation start: 360 Osc. range per frame: 0.1

Number of images: 1800 Total osc. range: 0

First image: 1 Full range

Exposure time (s): 0.025 Detector mode: 0

Kappa: 0.0009 Phi: 0.0028

Energy (keV): 12.6531 MAD ip:

Resolution (Å): 2.658

Transmission (%): 12.745

Shutterless

Data location Folder: /nfs/data/testQt4/2018-06-21/local-user/RAW\_DATA

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

Advanced

Collect Now Add to queue

# MXCuBE Qt4 October 2018

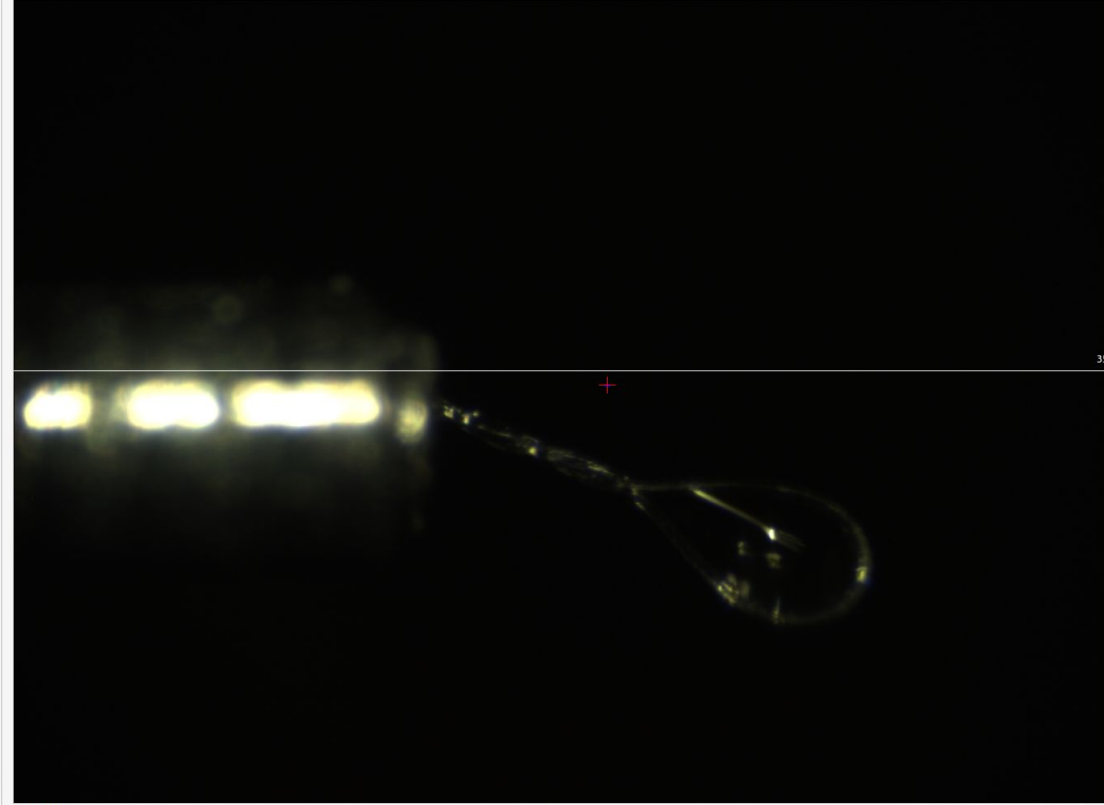
Sample centring

Omega stage

Omega: 360.00 10.0 Kappa: 0.00 SampX: 0.000 SampY: 0.000

X: -0.423 Y: -1.027 Z: -0.050 Phi: 0.00 Focus: 0.000 Vertical: 0.000

Sample video



X: 662 Y: 265

Graphics items

Light control

Front: 15 Back: 0

Phase

Transfer

Aperture

100µ BEAM

Centre Save Line Grid Focus Snapshot Refresh Align Select all Clear all Auto

**FrontEnd** open Open Close

**Safety shutter** open Open Close

Machine current: **449.8 mA**

Machine state: Thu Jun 21 17:38, Shift Lignes filling: Hybrid

Beam usable

Hutch temperature: 21.8 °C

Flux

Remeasure flux!

Cryostream In place

sample temperature: 100.0 K

Sample changer

Low level alarm, refill ON

Storage disc space

**DataCollection**

[2018-06-22 10:00:17] Diffractometer: Current phase changed to Transfer

[2018-06-22 10:03:26] Diffractometer: Current phase changed to DataCollection

[2018-06-22 10:07:28] Diffractometer: Current phase changed to Transfer

[2018-06-22 10:10:39] Diffractometer: Current phase changed to DataCollection

[2018-06-22 10:23:10] Diffractometer: Current phase changed to Transfer

[2018-06-22 10:26:39] Diffractometer: Current phase changed to DataCollection

[2018-06-22 10:43:50] Diffractometer: Current phase changed to Transfer

[2018-06-22 10:46:14] Diffractometer: Current phase changed to DataCollection

[2018-06-22 11:01:23] Diffractometer: Current phase changed to Transfer

[2018-06-22 11:04:38] Diffractometer: Current phase changed to DataCollection

[2018-06-22 11:14:18] Diffractometer: Current phase changed to Transfer

[2018-06-22 11:14:18] Diffractometer: Current phase changed to DataCollection

[2018-06-22 11:22:01] Diffractometer: Current phase changed to Transfer

[2018-06-22 11:26:26] Diffractometer: Current phase changed to DataCollection

[2018-06-22 11:30:50] Diffractometer: Current phase changed to Transfer

[2018-06-22 11:32:13] Diffractometer: Current phase changed to DataCollection

[2018-06-22 11:41:44] Diffractometer: Current phase changed to Transfer

[2018-06-22 11:44:14] Diffractometer: Current phase changed to DataCollection

[2018-06-22 11:53:01] Diffractometer: Current phase changed to Transfer

Say: Send

# MXCuBE Qt4 now (march 2019)

Sample centring

Wavelength: 270.00 nm, K $\alpha$ : 0.00, Focus: 360.00 mm

Front: 0, Back: 10

Centre, Save, Line, Grid, Snapshot, Select all, Clear all, Beam, Auto, Anneal, Excite

Phase: Transfer



X: 77 Y: 41

Graphics items

Sample manually-mounted

ISPyB proposal: Code: mx, Password: [redacted], Login

Sample tree: Mode: Sample changer, Sample: [redacted], Centring: Manual n-clicks, n-clicks: 3, step: 120.0, Filter: No Filter

Request: 0, Range per frame: 0.1, Oscillation start: 1800, Total range: 0, Number of images: 1, First image: 1, Exposure time (s): 0.025, Detector mode: 9M, Kappa: 0.0012, Phi: 360, Energy (keV): 12.65, Resolution (Å): 6.776, Transmission (%): 20, Shutterless: [checked]

Data location: Folder: /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA, File name: prefix\_1\_#####.h5, Prefix: prefix, Run number: 1

Processing: N.o. residues: 200, Space group: [redacted], Unit cell: a: 0, b: 0, c: 0,  $\alpha$ : 0,  $\beta$ : 0,  $\gamma$ : 0, Run processing after collection: [checked], Run Dozor: [unchecked]

Characterisation, Helical Collection, Energy Scan, XRF Spectrum, GPHL Workflows, Advanced, Collect Now, Add to queue

[2019-03-08 16:19:25] Data collection is enabled

FrontEnd: disabled, Safety shutter: disabled, Machine current: 0, Machine state: None, Hutch temperature: 21.7 C, Flux: [redacted], Remeasure flux: [redacted], Cryostream: In place, temperature: 230.0 K, Sample changer: Low level alarm! refill OFF, Storage disc space: [redacted]

Resolution: Current: 6.776 Å, Set to: [redacted] Å, Transmission: Current: [redacted], Set to: [redacted], Energy: Current: 12.6500 keV, Wavelength: 0.980 Å, Set to: [redacted] keV

# **Improving ergonomomy of the interface**

# making number of clicks and centring step easily visible and configurable

Sample centring

wt: 270.00    10.0    k: 0.00    qv: 360.00    Focus: -0.137    Zoom: 1

Front: 0    Back: 10

Centre Save Line Grid Snapshot Select all Clear all Beam Auto Anneal Excite

Phase Transfer

X: 77 Y: 41

Graphics items

Standard Collection

Sample manually-mounted

ISPyB proposal

Code: mx    Password:    Login

Sample tree

Mode: Sample changer    Show SC-details

Sample:    SPyB

Centring: Manual n-clicks    n-clicks: 3    step: 120.0

Filter:    No filter

- Puck 1
  - 1:1
  - 1:2
  - 1:3
  - 1:4
  - 1:5
  - 1:6
  - 1:7
  - 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

Queue history

Collect Queue

Pause

FrontEnd disabled    Safety shutter disabled

Open Close    Open Close

Machine current: 0

Machine state: None

Hutch temperature: 21.7 C

Flux:    Remeasure flux:    Cryostream: In place temperature: 230.0 K

Sample changer: Low level alarm! refill OFF

Storage disc space:    Add to queue

[2019-03-08 16:19:25] Data collection is enabled

Resolution: 6.776 Å    Set to:    A    [X]


Current: 800.00 mm

Transmission:    Set to:    [X]

Energy: 12.6500 keV    Wavelength: 0.980 Å    Set to:    keV    [X]

# making number of clicks and centring step easily visible and configurable


ISPyB proposal

20100023  Logout Group:  Set


**Sample tree**

Mode:

Sample:

Centring:   ISPyB

Filter:

 manually-mounted

- Standard - 1
  - Manual centring (... Skipped)
  - mx20100023\_1 (... Collecting)



# annealing dialog

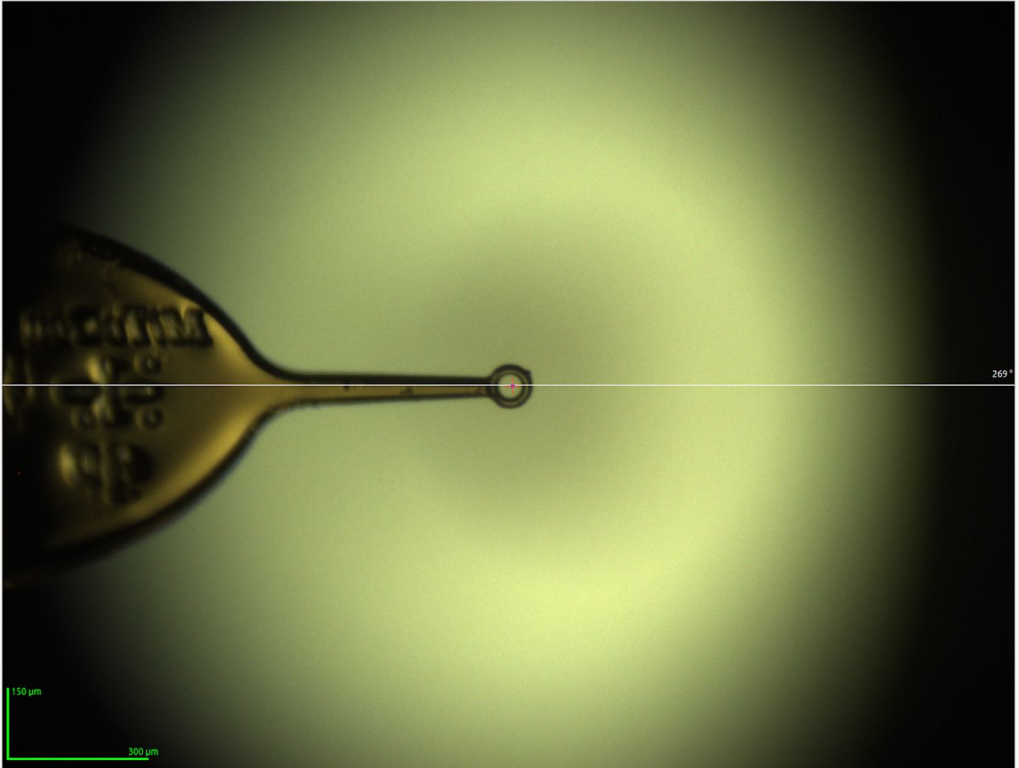
Sample centring

wt: 270.00    k: 0.00    Focus: -0.137    Zoom: 1

Front: 0    Back: 10

Centre   Save   Line   Grid   Snapshot   Select all   Clear all   Beam   Auto   **Anneal**   Exit

Phase: Transfer



X: 77 Y: 41

Graphics items

Standard Collection    Sample manually-mounted

Code: mx    Password:    Login

Acquisition

Oscillation start: 0    Range per frame: 0.1

Number of images: 1800    Total range: 0

First image: 1    Full range

Exposure time (s): 0.025    Detector mode: 9M

Kappa: 0.0012    Phi: 360

Energy (keV): 12.65    MAD

Resolution (Å): 6.776    lp:   

Transmission (%): 20

Shutterless

Data location

Folder: /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA

File name: prefix\_1\_#####.h5    Browse

Prefix: prefix

Run number: 1

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 Dozor

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

GPH Workflows

Advanced

[2019-03-08 16:19:25] Data collection is enabled

ISPyB proposal

Code: mx    Password:    Login

Sample tree

Mode: Sample changer

Sample:    Show SC-details

Centring: Manual n-clicks    n-clicks: 3    step: 120.0

Filter:    No Filter

- Puck 1
  - 1:1
  - 1:2
  - 1:3
  - 1:4
  - 1:5
  - 1:6
  - 1:7
  - 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

Queue history

FrontEnd: disabled    Safety shutter: disabled

Open    Close    Open    Close

Machine current: 0

Machine state: None

Hutch temperature: 21.7 C

Flux:   

Remeasure flux:   

Cryostream: In place    temperature: 230.0 K

Sample changer: Low level alarm    refill OFF

Storage disc space:   

Resolution

Current: 6.776 Å

800.00 mm

Set to:    A   

Transmission

Current:   

Set to:   

Energy

Current: 12.6500 keV

Wavelength: 0.980 Å

Set to:    keV

# annealing dialog

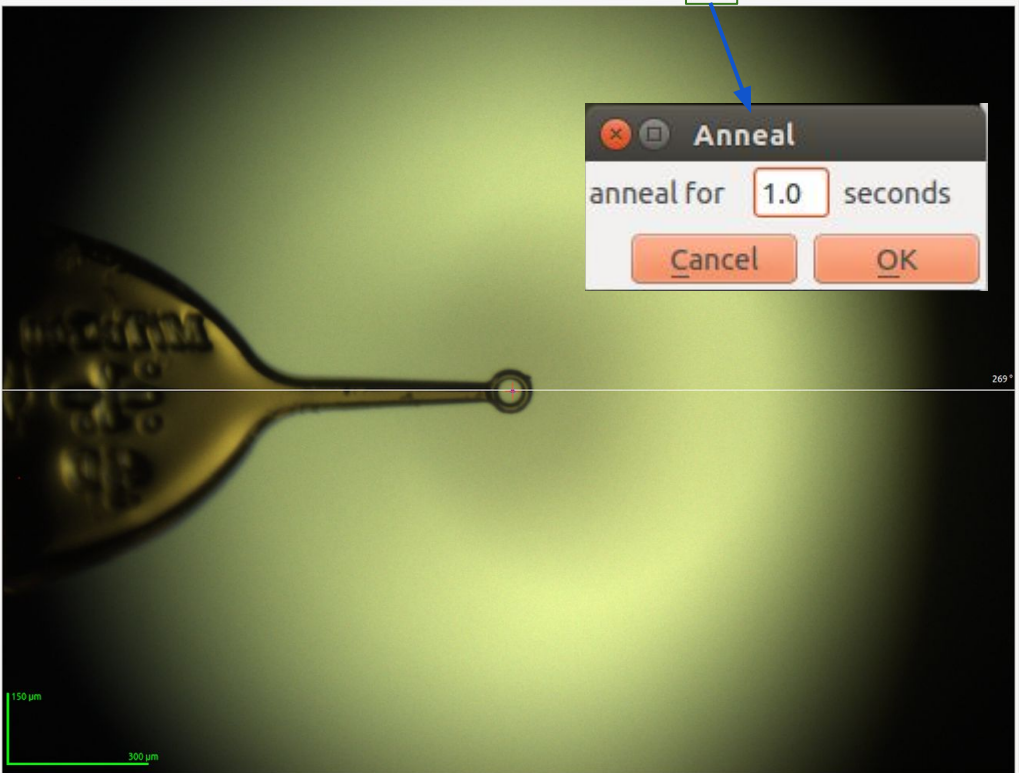
Sample centring

wt: 270.00    k: 0.00    Focus: -0.137    Zoom: 1

Front: 0    Back: 10

Centre Save Line Grid Snapshot Select all Clear all Beam Auto Anneal Excenter

Phase Transfer



X: 77 Y: 41

Graphics items

Anneal

anneal for 1.0 seconds

Cancel OK

Standard Collection

Sample manually-mounted

Acquisition

Oscillation start: 0 Range per frame: 0.1

Number of images: 1800 Total range: 0

First image: 1

Exposure time (s): 0.025 Detector mode: 9M

Kappa: 0.0012 Phi: 360

Energy (keV): 12.65 MAD

Resolution (Å): 6.776

Transmission (%): 20

Shutterless

Data location

Folder: /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA

File name: prefix\_1\_#####.h5

Prefix: prefix

Run number: 1

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 Dozor

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

GPHL Workflows

Advanced

[2019-03-08 16:19:25] Data collection is enabled

ISPyB proposal

Code: mx Password: Login

Sample tree

Mode: Sample changer

Sample: -

Centring: Manual n-clicks

n-clicks: 3 step: 120.0

Filter: No Filter

- Puck 1
  - 1:1
  - 1:2
  - 1:3
  - 1:4
  - 1:5
  - 1:6
  - 1:7
  - 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

Queue history

FrontEnd disabled Safety shutter disabled

Open Close Open Close

Machine current: 0

Machine state: None

Hutch temperature: 21.7 C

Flux: 800.00 mm

Remeasure flux

Cryostream: In place temperature: 230.0 K

Sample changer: Low level alarm refill OFF

Storage disc space

Resolution

Current: 6.776 Å

Set to: 800.00 mm

Transmission

Current: -

Set to: -

Energy

Current: 12.6500 keV

Wavelength: 0.980 Å

Set to: - keV

# Simplifying x-ray centring

Sample centring

wt: 270.00    10.0    k: 0.00    Focus: -0.137    Zoom: 1

Front: 0    Back: 10    Centre    Save    Line    Grid    Snapshot    Select all    Clear all    Beam    Auto    Anneal    **Excenter**    Phase    Transfer

X: 77 Y: 41

Graphics items

Standard Collection    Sample: manually-mounted

Acquisition

Oscillation start: 0    Range per frame: 0.1

Number of images: 1800    Total range: 0

First image: 1    Full range

Exposure time (s): 0.025    Detector mode: 9M

Kappa: 0.0012    Phi: 360

Energy (keV): 12.65    MAD

Resolution (Å): 6.776    lp: -

Transmission (%): 20

Shutterless

Data location

Folder: /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA

File name: prefix\_1\_#####.h5    Browse

Prefix: prefix

Run number: 1

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 Dozor

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

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Advanced

[2019-03-08 16:19:25] Data collection is enabled

ISPyB proposal

Code: mx    Password:    Login

Sample tree

Mode: Sample changer

Sample:    Show SC-details

Centring: Manual n-clicks    n-clicks: 3    step: 120.0

Filter:    No Filter

- Puck 1
  - 1:1
  - 1:2
  - 1:3
  - 1:4
  - 1:5
  - 1:6
  - 1:7
  - 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

Queue history

FrontEnd: disabled    Safety shutter: disabled

Open    Close    Open    Close

Machine current: 0

Machine state: None

Hutch temperature: 21.7 C

Flux

Remeasure flux

Cryostream: In place    temperature: 230.0 K

Sample changer: Low level alarm    refill OFF

Storage disc space

Resolution

Current: 6.776 Å

8000.00 mm

Set to:    A   

Transmission

Current:   

Set to:   

Energy

Current: 12.6500 keV

Wavelength: 0.980 Å

Set to:    keV

# Simplifying x-ray centring

Sample centring

wt: 270.00    k: 0.00    Focus: -0.137    Zoom: 1

Front: 0    Back: 10

Centre   Save   Line   Grid   Snapshot   Select all   Clear all   Beam   Auto   Anneal   Excenter

Phase   Transfer

X: 77 Y: 41

Graphics items

**Excenter**

scan length  mm

Standard Collection    Sample manually-mounted

Code: mx    Password:    Login

Acquisition

Oscillation start: 0    Range per frame: 0.1

Number of images: 1800    Total range: 0

First image: 1    Full range

Exposure time (s): 0.025    Detector mode: 9M

Kappa: 0.0012    Phi: 360

Energy (keV): 12.65    MAD

Resolution (Å): 6.776    lp:   

Transmission (%): 20

Shutterless

Data location

Folder: /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA

File name: prefix\_1\_#####.h5    Browse

Prefix: prefix

Run number: 1

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 Dozor

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

GPH Workflows

Advanced

[2019-03-08 16:19:25] Data collection is enabled

ISPyB proposal

Code: mx    Password:    Login

Sample tree

Mode: Sample changer

Sample:    Show SC-details

Centring: Manual n-clicks    n-clicks: 3    step: 120.0

Filter:    No Filter

- Puck 1
  - 1:1
  - 1:2
  - 1:3
  - 1:4
  - 1:5
  - 1:6
  - 1:7
  - 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

Queue history

FrontEnd: disabled    Safety shutter: disabled

Machine current: 0

Machine state: None

Hutch temperature: 21.7 C

Flux:   

Remeasure flux:   

Cryostream: In place    temperature: 230.0 K

Sample changer: Low level alarm    refill OFF

Storage disc space:

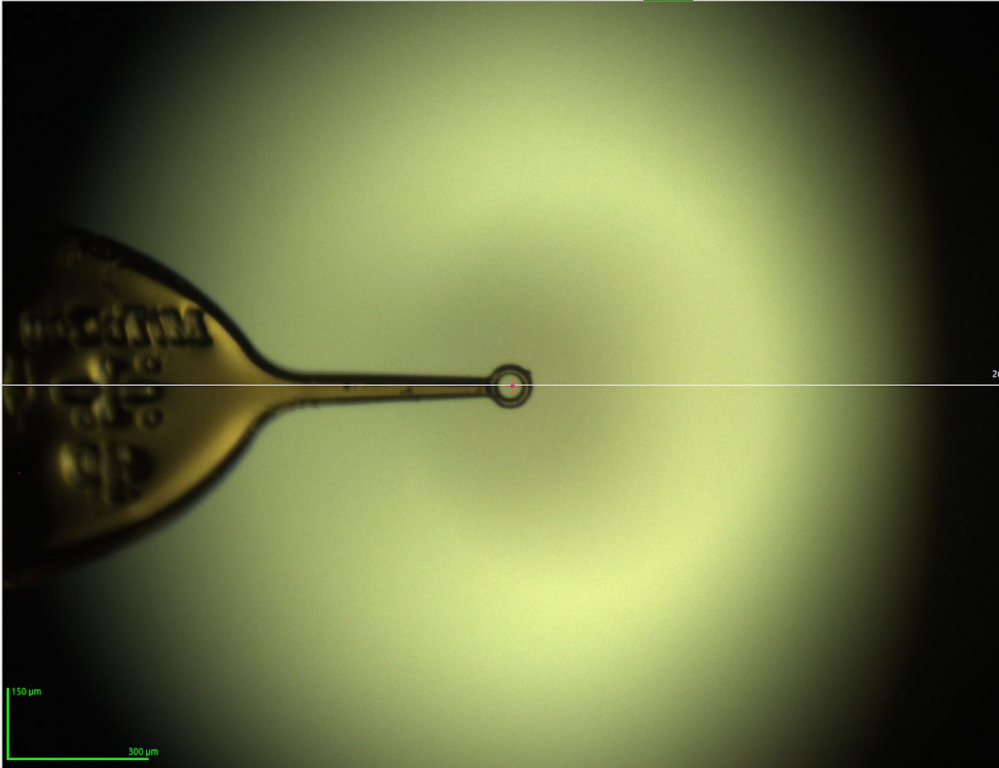
Sample centring

wt: 270.00    k: 0.00    q: 360.00    Focus: -0.137    Zoom: 1

Front: 0    Back: 10

Centre Save Line Grid Snapshot Select all Clear all Beam Auto Anneal Excenter

Phase Transfer



X: 77 Y: 41

Graphics items

Standard Collection    Sample manually-mounted

Code: mx    Password:    Login

Acquisition

Oscillation start: 0    Range per frame: 0.1

Number of images: 1800    Total range: 0

First image: 1    Full range

Exposure time (s): 0.025    Detector mode: 9M

Kappa: 0.0012    Phi: 360

Energy (keV): 12.65    MAD

Resolution (Å): 6.776    lp:   

Transmission (%): 20

Shutterless

Data location

Folder: /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA

File name: prefix\_1\_#####.h5    Browse

Prefix: prefix

Run number: 1

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 Dozor

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

GPH Workflows

Advanced

ISPyB proposal

Code: mx    Password:    Login

Sample tree

Mode: Sample changer    Show SC-details

Sample:    ISPyB

Centring: Manual n-clicks    n-clicks: 3    step: 120.0

Filter:    No Filter

- Puck 1
  - 1:1
  - 1:2
  - 1:3
  - 1:4
  - 1:5
  - 1:6
  - 1:7
  - 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

Queue history

FrontEnd: disabled    Safety shutter: disabled

Resolution

Current: 6.776 Å

800.00 mm

Set to:    A   

Transmission

Current:   

Set to:   

Energy

Current: 12.6500 keV

Wavelength: 0.980 Å

Set to:    keV   

Machine current: 0

Machine state: None

Hutch temperature: 21.7 C

Flux:   

Remeasure flux:   

Cryostream: In place    temperature: 230.0 K

Sample changer: Low level alarm    refill OFF

Storage disc space:   

- State: - Diffractometer: Ready    Sample changer: -    Last collect: -

# Automated optical centring with pin/stem/loop segmentation in all orientations

Sample centring:     Focus:  Zoom:

Acquisition: Oscillation start:  Range per frame:  Number of images:  Total range:  First image:  Full range:  Exposure time (s):  Detector mode:

Sample tree: Mode:  Sample:  Centring:

ISPyB proposal: Code:  Password:

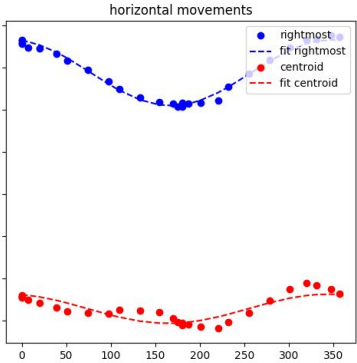
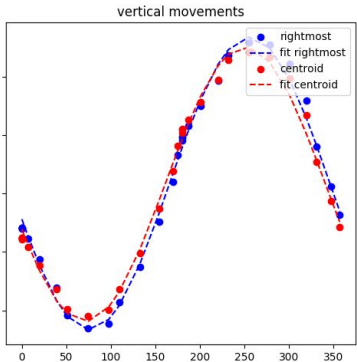
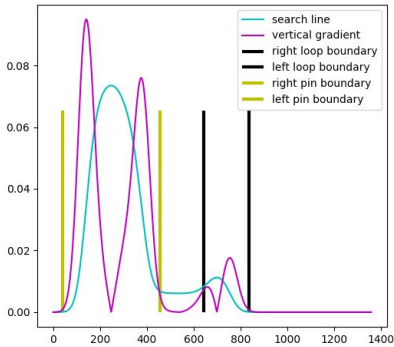
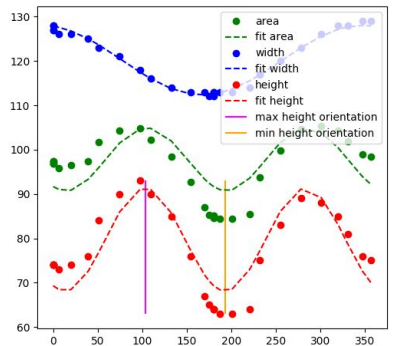
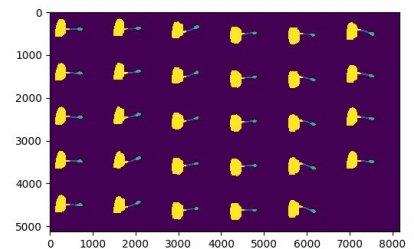
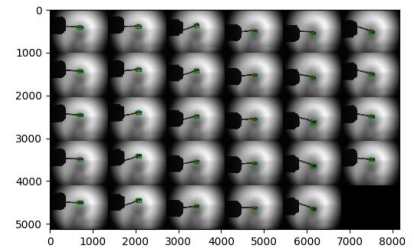
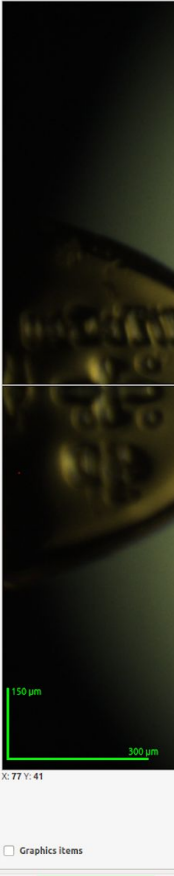
ISPyB:

Show SC-details:  n-clicks:  step:  No Filter:

Front:  Back:  Centre Save Line Grid Snapshot Select all Clear all Beam Auto Anneal Exciter

Phase:

/nfs/data/Martin/Research/radiation\_damage/2018-07-28/puck0027/7/7\_z1a



Machine current:

Machine state:

Hutch temperature:

Flux:

Remeasure flux:

Cryostream:

Sample changer:

Storage disc space:

Pause:

# Rapid beam realignment - steering small beam to the center of the camera (optical center of the OAV)

GUI controls for the diffraction experiment. The main window shows a camera image of a small beam spot on a sample. The beam spot is centered in the camera's field of view. The image is labeled with a scale of 150  $\mu\text{m}$  and 300  $\mu\text{m}$ . The camera coordinates are X: 77 Y: 41. A green arrow points to the 'Beam' button in the top toolbar.

Front: 0 Back: 10 Centre Save Line Grid Snapshot Select all Clear all **Beam** Auto Anneal Excite

Phase Transfer

X: 77 Y: 41

Graphics items

Standard Collection configuration panel. The sample is manually-mounted. Acquisition parameters include 1800 images over a range of 0 to 0.1, with an exposure time of 0.025 s. The energy is 12.65 keV and the resolution is 6.776 Å. The data location is /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA. The file name is prefix\_1\_#####.h5. Processing parameters include 200 residues and a space group. The Run Dozor checkbox is unchecked.

Standard Collection Sample: manually-mounted

Code: mx Password: Login

Acquisition

Oscillation start: 0 Range per frame: 0.1

Number of images: 1800 Total range: 0

First image: 1 Full range

Exposure time (s): 0.025 Detector mode: 9M

Kappa: 0.0012 Phi: 360

Energy (keV): 12.65 MAD

Resolution (Å): 6.776

Transmission (%): 20

Shutterless

Data location

Folder: /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA

File name: prefix\_1\_#####.h5 Browse

Prefix: prefix

Run number: 1

Processing

N.o. residues: 200 Space group:

Unit cell:

a: 0 b: 0 c: 0

$\alpha$ : 0  $\beta$ : 0  $\gamma$ : 0

Run processing after collection

Run Dozor

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

GPH Workflows

Advanced

[2019-03-08 16:19:25] Data collection is enabled

ISPyB proposal and sample tree configuration. The sample tree shows a list of Puck 1 and Puck 2 samples. The n-clicks are set to 3 and the step is 120.0. The machine current is 0, and the machine state is None. The flux is 21.7 C. The cryostream is in place at 230.0 K. The storage disc space is available.

ISPyB proposal Code: mx Password: Login

Sample tree

Mode: Sample changer Show SC-details

Sample: ISPyB

Centring: Manual n-clicks n-clicks: 3 step: 120.0

Filter: No filter

Puck 1

- 1:1
- 1:2
- 1:3
- 1:4
- 1:5
- 1:6
- 1:7
- 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

Queue history

FrontEnd disabled Safety shutter disabled

Open Close Open Close

Machine current: 0

Machine state: None

Hutch temperature: 21.7 C

Flux: 21.7 C

Remeasure flux

Cryostream: In place temperature: 230.0 K

Sample changer: Low level alarm refill OFF

Storage disc space

# Getting rid of what is not necessary

ISPyB proposal

Logout Group: [ ] Set

Sample tree

Mode: Sample changer Show SC-details

Sample: [ ] ISPyB

Centring: Manual 3-click

Filter: [ ] No Filter

- 1:7
  - Advanced - 1
    - idtest000\_1 (Mesh 1: 58 x 72)
    - 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
    - 2:10
    - 2:11

Display history view

collect Queue

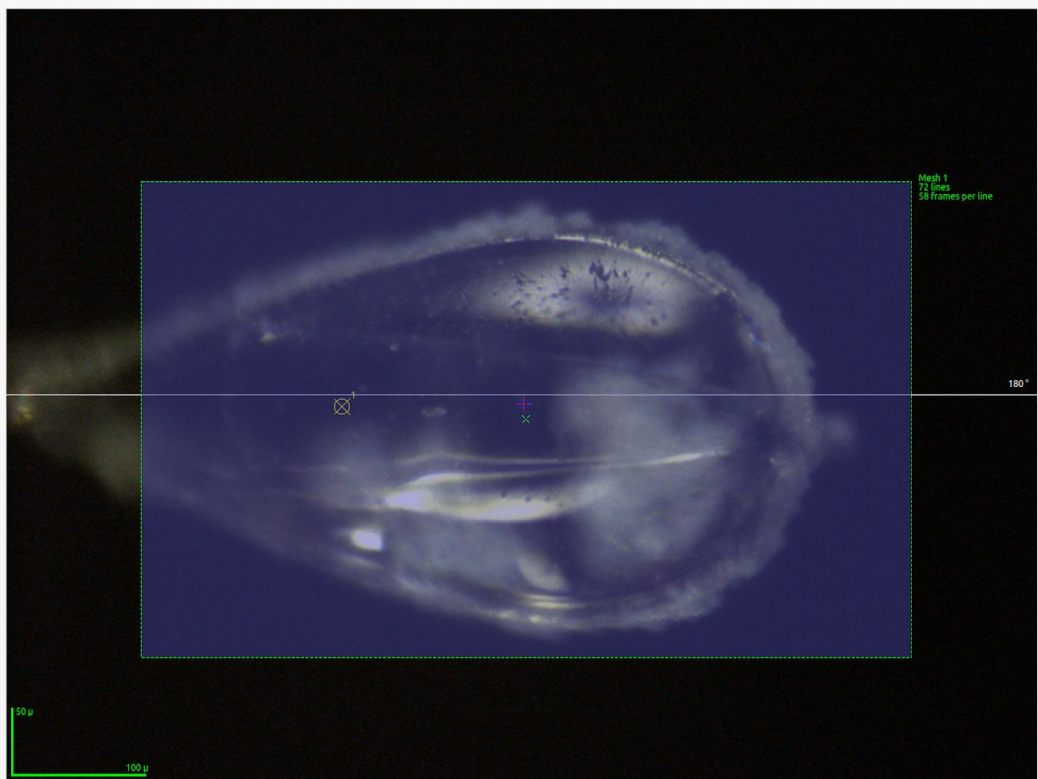
Pause

```

[2018-01-31 03:50:33] Diffractometer: Current phase
changed to DataCollection
[2018-01-31 03:50:33] Diffractometer: Current phase
changed to DataCollection
[2018-01-31 03:50:33] Data collection is enabled
[2018-01-31 03:50:38] update buttons (ready)
[2018-01-31 03:51:01] ISPyB proposal: idtest000 - operator
on IDTESTst1
[2018-01-31 03:52:03] DataCollectionQueueEntry_init_
  
```

omega: 180.06 k: 10.0 phi: 0.00 horizontal: -1.18 vertical: -0.13

backlight: 0 frontlight: 5 zoom: 5 focus: -0.11



Standard Collection idtest000\_1 (Mesh 1: 58 x 72)

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

Advanced

Method: MeshScan

Grid

Horizontal spacing (μm) 10.00 Move horizontal: [ ] [ ]

Vertical spacing (μm) 5.00 Move vertical: [ ] [ ]

Adjust size

Snapshot

Name	Lines	Frames per line
Mesh 1	72	58

Refresh

Visual align

Select all

Clear all

Auto

Display overlay: [ ] [ ] Overlay color [ ]

Draw Move to grid center Remove

Acquisition

Oscillation start: 180.06 Osc. range per frame: 0.01

Number of images: 4176 Total osc. range per line: 0.58

First image: 1 Fill range [ ]

Exposure time (s): 0.025 Detector mode: 0

Kappa: 0 Phi: 0

Energy (keV): 12.65 MAD [ ] [ ]

Resolution (Å): 2

Transmission (%): 65.8

Shutterless

Data location

Folder: [ ]

File name: idtes000\_1\_####.h5

Prefix: idtest000

Run number: 1

Browse

Add to queue

Soleil Machine Current

451.7 mA

Hybrid filling

Lifetime: 13.32 h

Undul. HU\_640: [ ]

Energy

Current: 12.6500 keV

Wavelength: 0.980 Å

Set to: [ ] keV

Transmission

Current: [ ]

Set to: [ ]

Resolution

Current: 2.000 Å

215.99 mm

Set to: [ ] Å

Diameter:

100

Phase:

DataCollection [ ]

Position:

BEAM [ ]

Scintillator:

PARK [ ]

Safety shutter

open

Open Close

Exp. ready Opt. ready



# Getting rid of what is not necessary

Sample centring

Control panel for the diffractometer. At the top, there are various status indicators: **wt: 270.00**, **κ: 0.00**, **Focus: -0.137**, and **Zoom: 1**. Below these are icons for **Centre**, **Save**, **Line**, **Grid**, **Snapshot**, **Select all**, **Clear all**, **Beam**, **Auto**, **Anneal**, and **Exciter**. The main display shows a phase image of a sample, with a green crosshair indicating the center. The image is labeled with **269°** and **150 μm** (vertical scale) and **300 μm** (horizontal scale). The bottom left corner shows coordinates **X: 77 Y: 41** and a **Graphics items** checkbox.

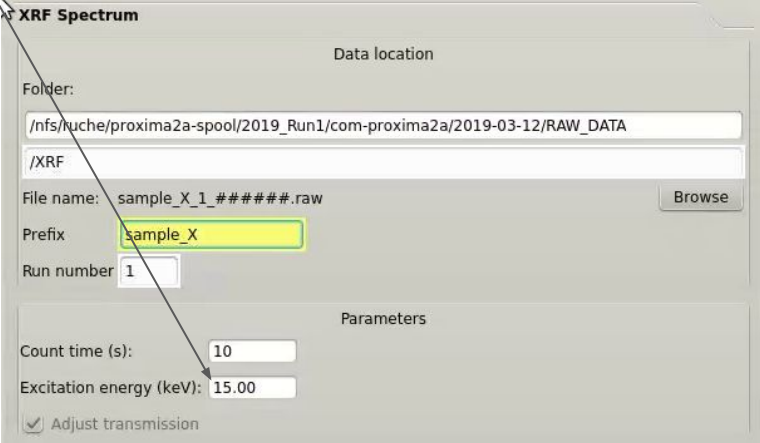
Configuration and data location settings. **Standard Collection** is selected. **Acquisition** parameters include: **Oscillation start:** 0, **Range per frame:** 0.1, **Number of images:** 1800, **Total range:** 0, **First image:** 1, **Exposure time (s):** 0.025, **Detector mode:** 9M, **Kappa:** 0.0012, **Phi:** 360, **Energy (keV):** 12.65, **Resolution (Å):** 6.776, **Transmission (%):** 20, and **Shutterless** is checked. **Data location** settings include: **Folder:** /ifs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA, **File name:** prefix\_1\_#####.h5, **Prefix:** prefix, **Run number:** 1, **N.o. residues:** 200, **Unit cell:** a: 0, b: 0, c: 0, α: 0, β: 0, γ: 0. **Processing** options include **Run processing after collection** (checked) and **Run Dozor** (unchecked). **Characterisation** and **Helical Collection** are disabled. **Energy Scan**, **XRF Spectrum**, and **Advanced** are also disabled. **Collect Now** and **Add to queue** buttons are present. A status message at the bottom reads: **[2019-03-08 16:19:25] Data collection is enabled**.

System status and monitoring. **ISPyB proposal** Code: mx, Password: [redacted]. **Sample tree** shows **Puck 1** (1-16) and **Puck 2** (2:1-2:7). **Queue history** and **Collect Queue** buttons are visible. **Machine current:** 0. **Machine state:** None. **Hutch temperature:** 21.7 C. **Flux:** 800.00 mm. **Remeasure flux:** [redacted]. **Cryostream:** In place, temperature: 230.0 K. **Sample changer:** Low level alarm, refill OFF. **Storage disc space:** [redacted]. **FrontEnd** and **Safety shutter** are both disabled. **Resolution:** Current: 6.776 Å, Set to: 800.00 mm. **Transmission:** Current: [redacted], Set to: [redacted]. **Energy:** Current: 12.6500 keV, Wavelength: 0.980 Å, Set to: [redacted] keV.

- State: - **Diffractometer: Ready** Sample changer: - Last collect: -

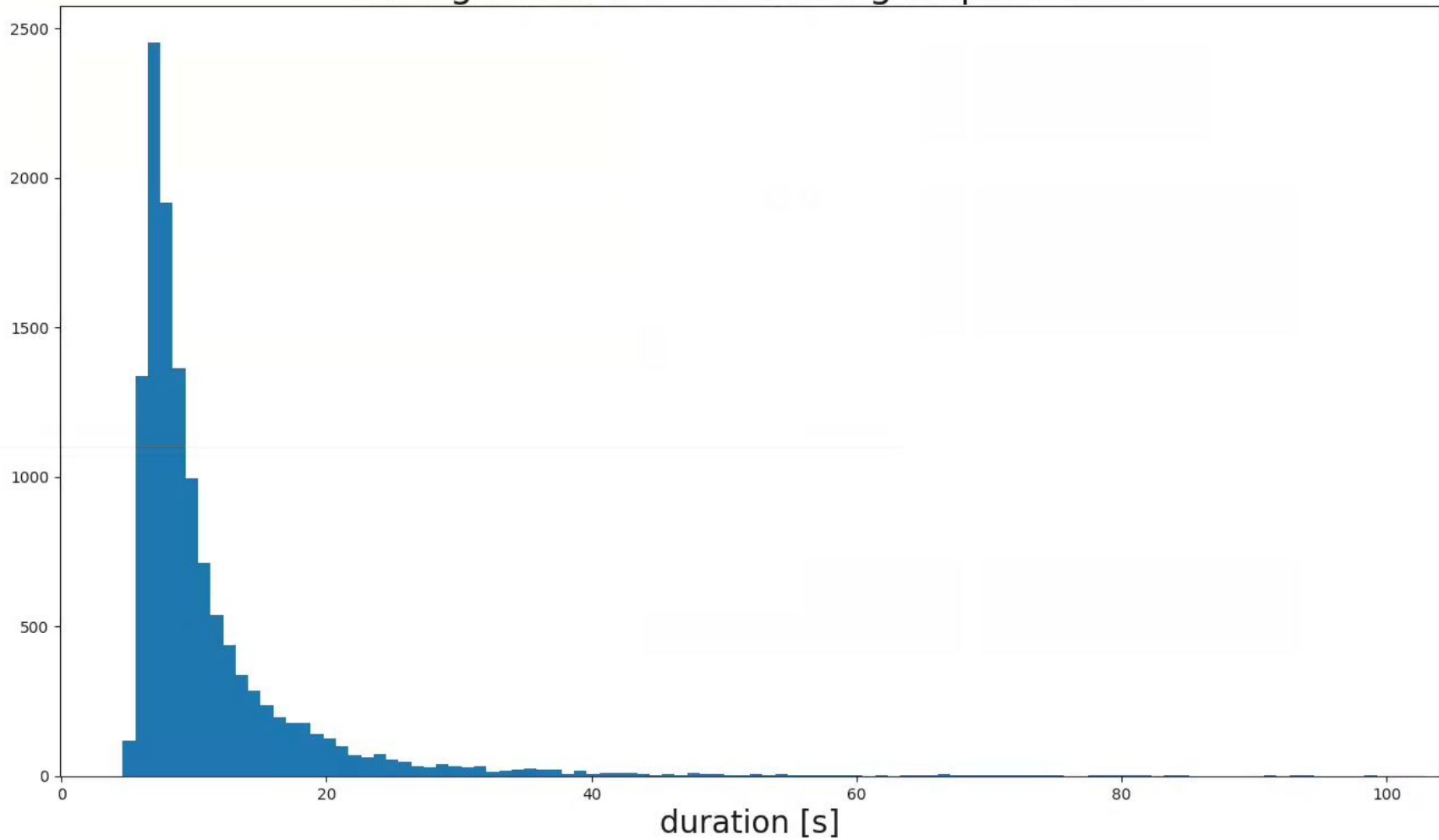
# Other developments

- Shutterless Energy Scan
  - faster acquisition while not losing accuracy
  - [https://github.com/MartinSavko/chooch\\_python\\_translation](https://github.com/MartinSavko/chooch_python_translation)
    - translating mucal.c and chooch.c into python
- Adding excitation energy parameter for XRF
  - Useful information when performing the fit
  - Automated fit of the most common scatterers
- Learning from users about centring
  - database of 15k centring for last couple of runs



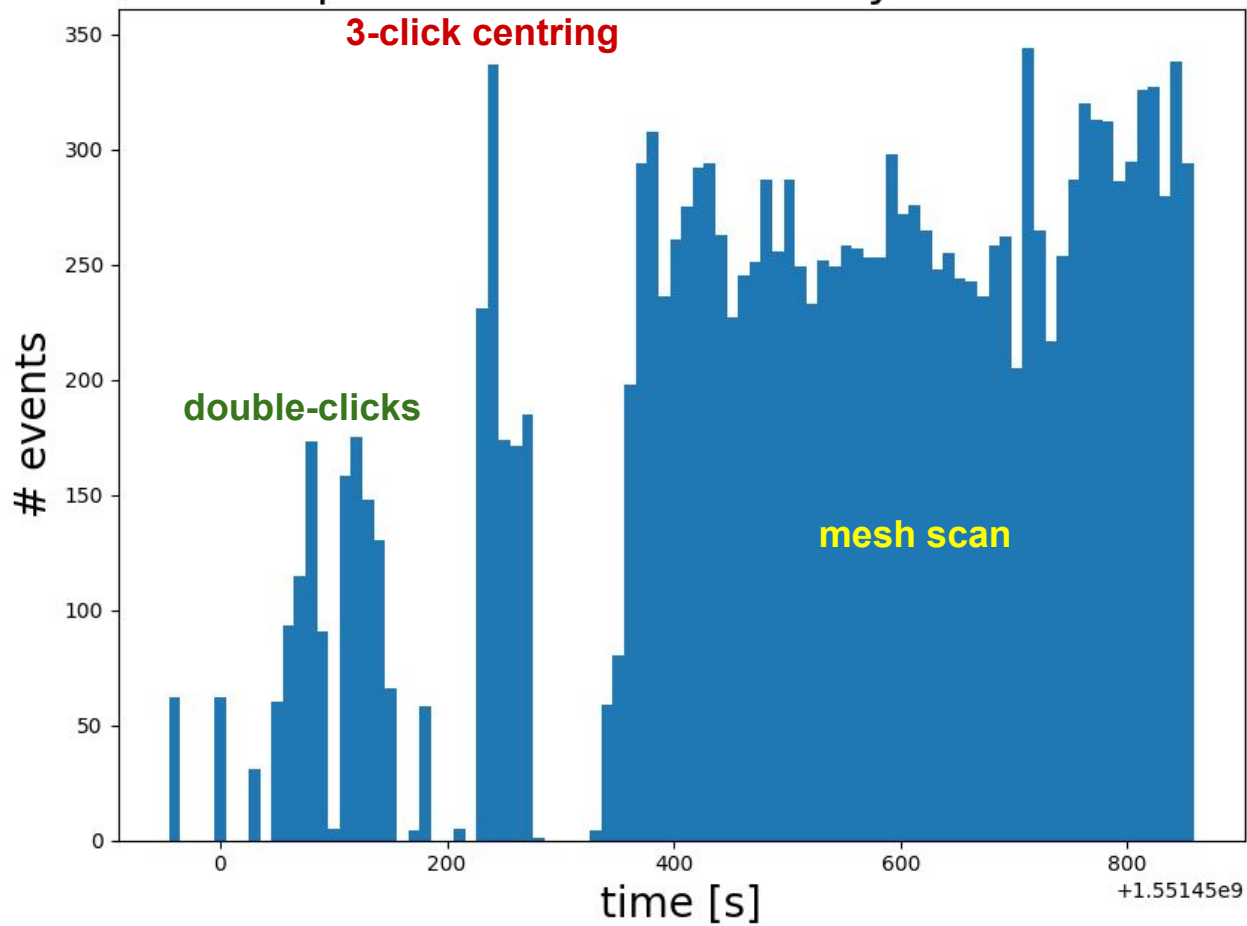
The screenshot shows the 'XRF Spectrum' software interface. It is divided into two main sections: 'Data location' and 'Parameters'. In the 'Data location' section, the 'Folder' is set to '/nfs/luce/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-12/RAW\_DATA' and the 'File name' is 'sample\_X\_1\_#####.raw'. The 'Prefix' field is highlighted in yellow and contains 'sample\_X'. The 'Run number' is set to '1'. In the 'Parameters' section, the 'Count time (s)' is '10' and the 'Excitation energy (keV)' is '15.00'. There is a checked checkbox for 'Adjust transmission'.

# Histogram of n-click centring elapsed time





# Exporter events handled by MXCuBE



# Wrap up

- Improving smoothness ergonomics of the GUI
  - tango with events (with exception of sample changer)
  - exporter events for MD2
- resolved problem with MD2 stutter
  - problems stabilising Omega axis at the end of movements
  - executing `startSimultaneousMoveMotors()` as opposed to writing to an attribute
- stripped down non essential components
  - start-up time 15 seconds (down from about 55 second at the beginning of the campaign)
- focus on ergonomy
  - three column design
- making the useful features obvious
  - x-ray centring, n-click centring options, automated alignment

MXCuBE is embodiment of Experimenter's dream of performing a perfect experiment

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