

# MXCuBE status at SOLEIL

Martin Savko

[savko@synchrotron-soleil.fr](mailto:savko@synchrotron-soleil.fr)

## 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 µm

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 µm

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

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

Beam size: **20x40 µm**

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 µm**

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
```

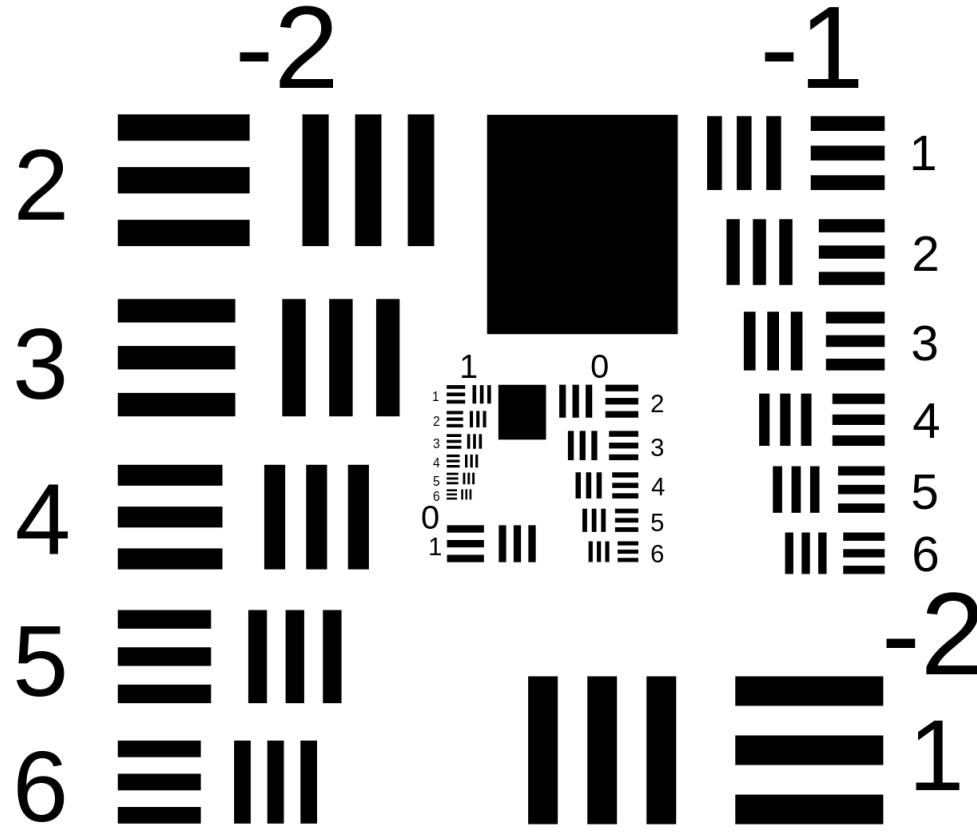
\* executed as a cron job every 4 hours

# Issues

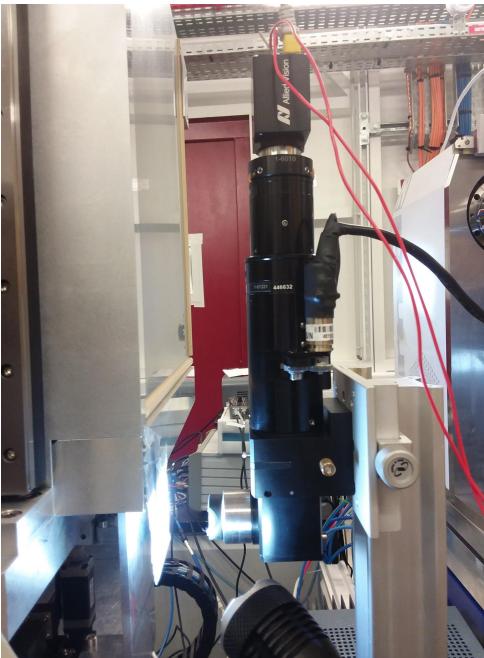
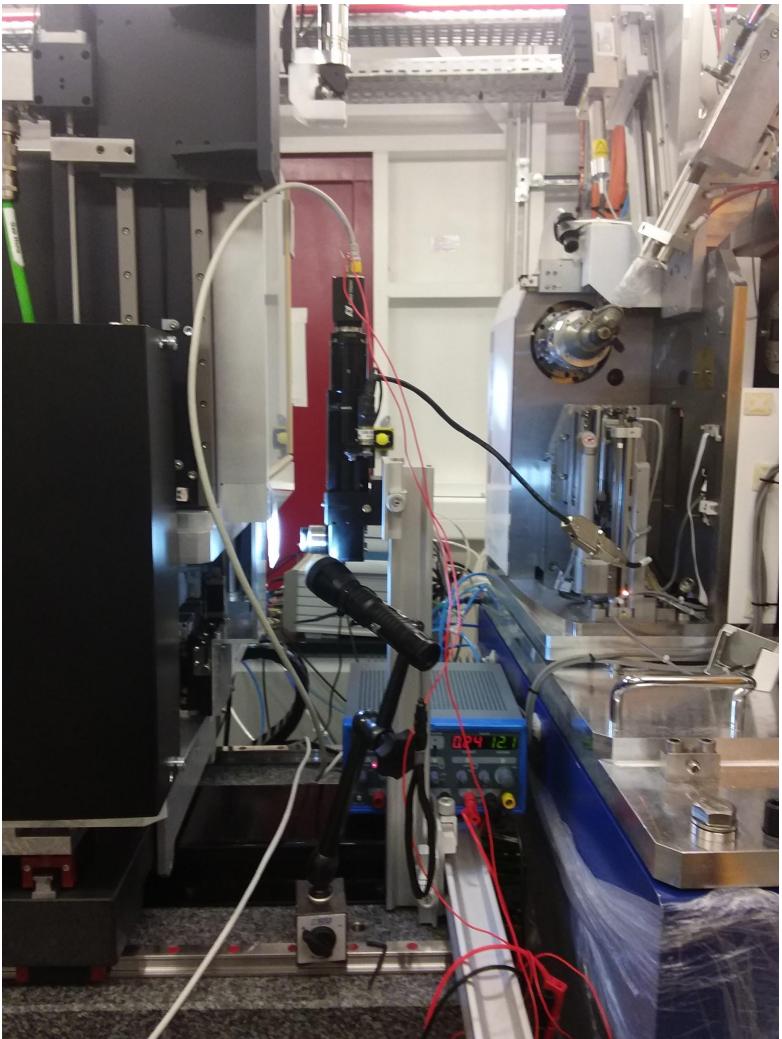
- OAV zoom failure on Proxima 2
  - exchange for a spare and then for a replacement

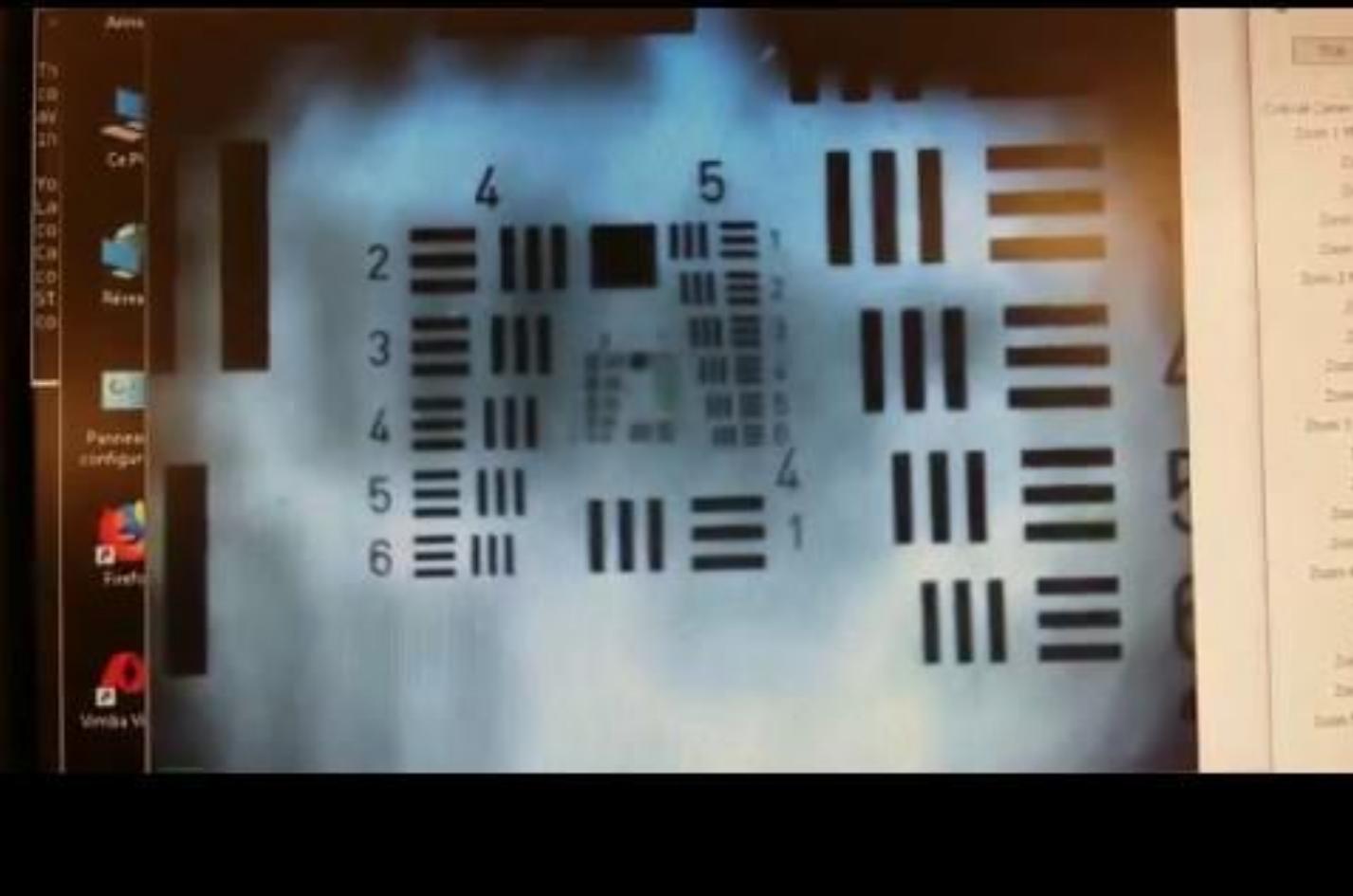
# Issues

- 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



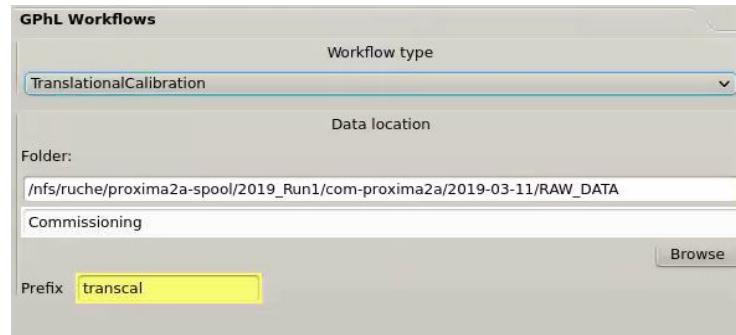


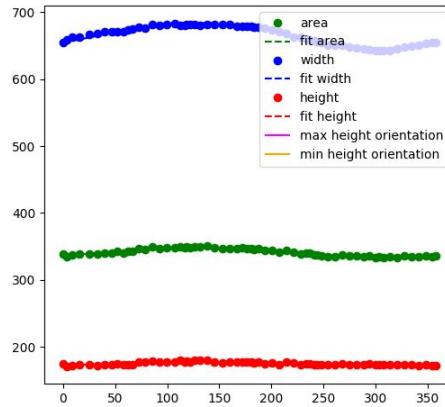
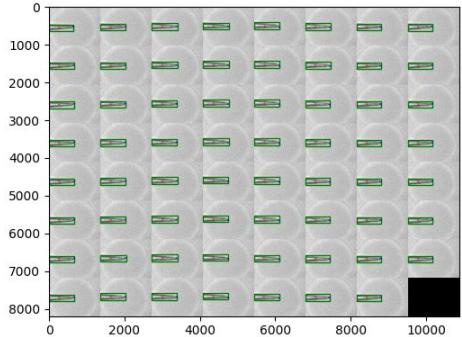
# Issues

- 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 um with kappa closed, ~ 10 um with kappa open (< 5um during SAT)
  - horizontal discrepancy of similar magnitude at large kappa

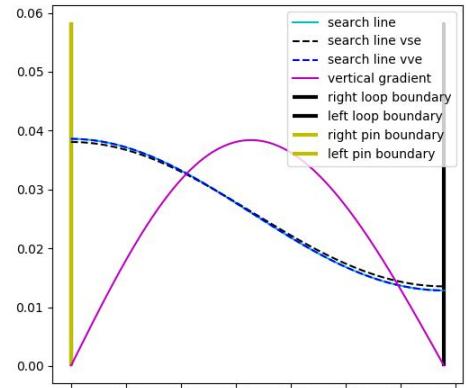
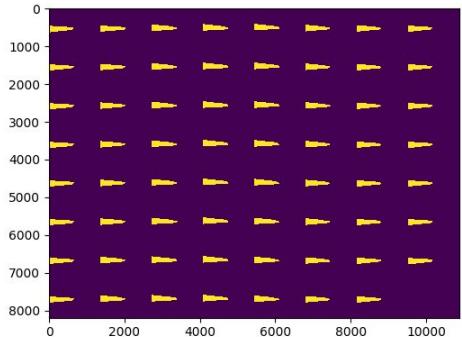
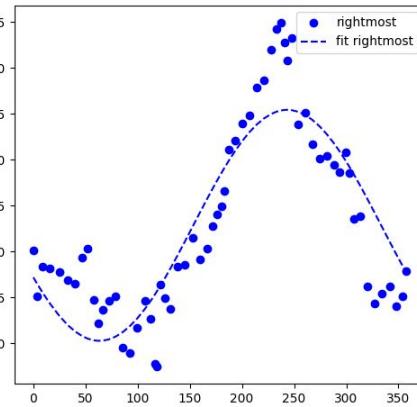
# Issues

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  - aligning transfocator optical center and the camera center
  - verifying pixel calibration
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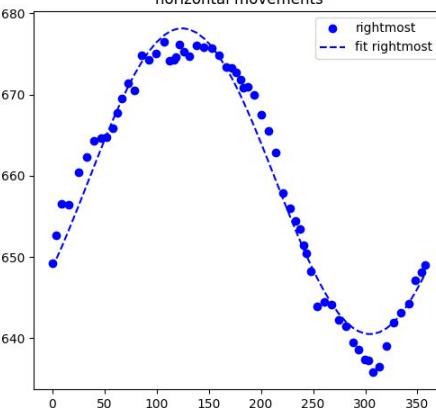


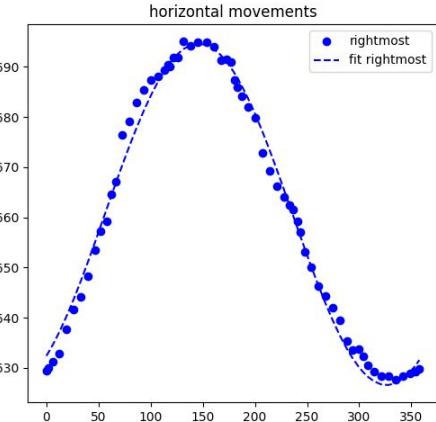
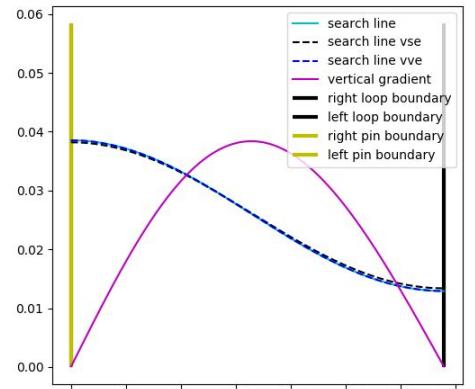
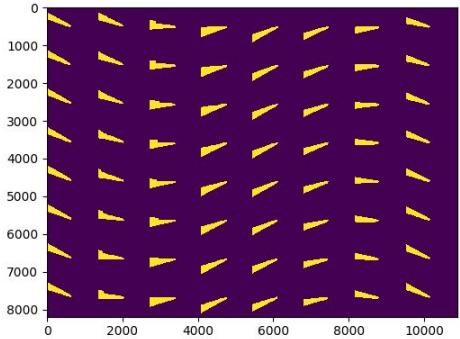
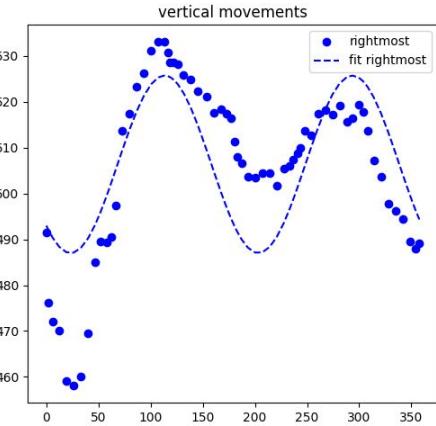
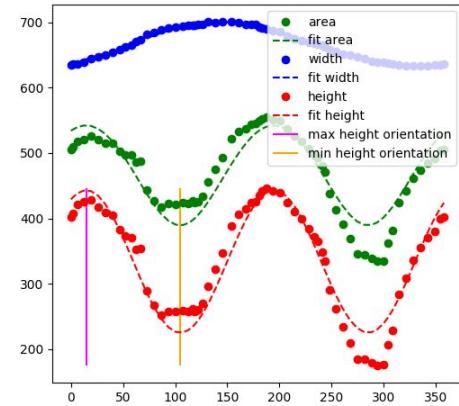
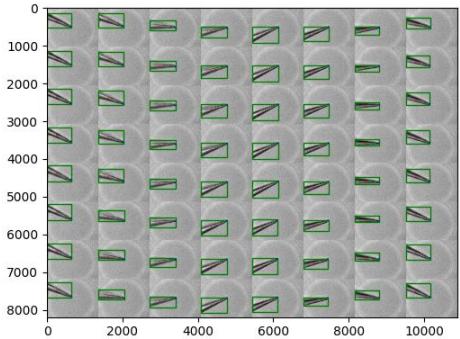


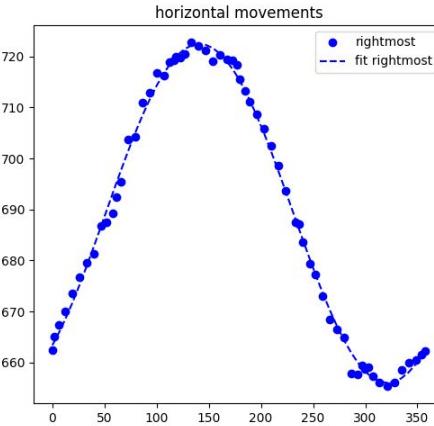
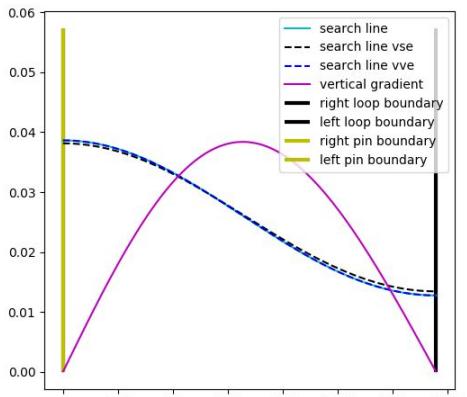
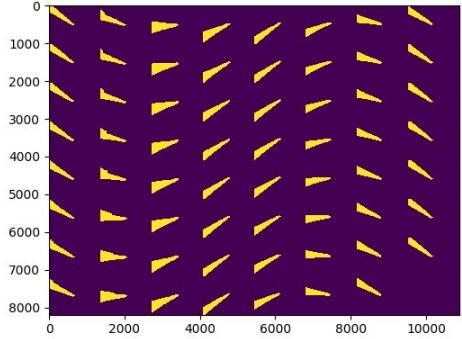
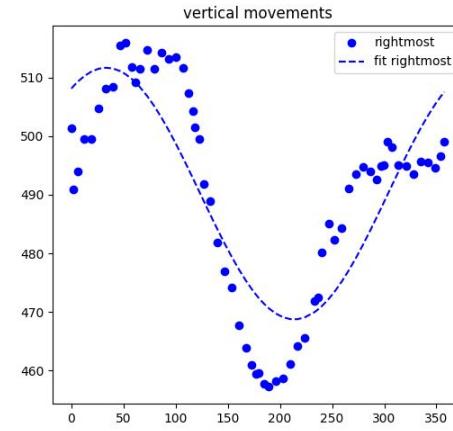
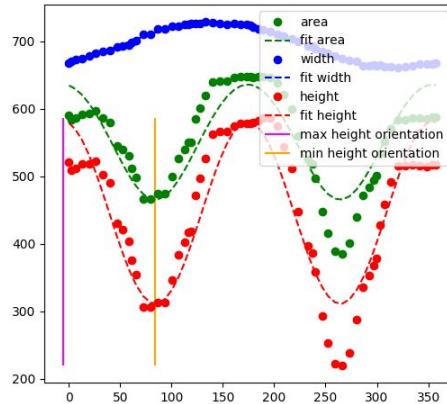
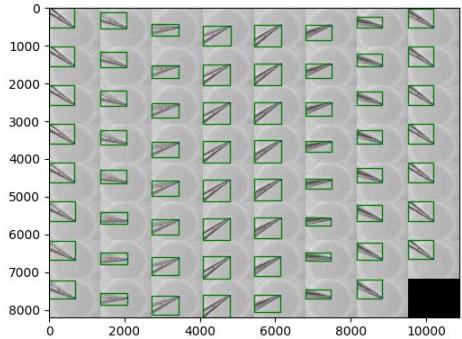
vertical movements

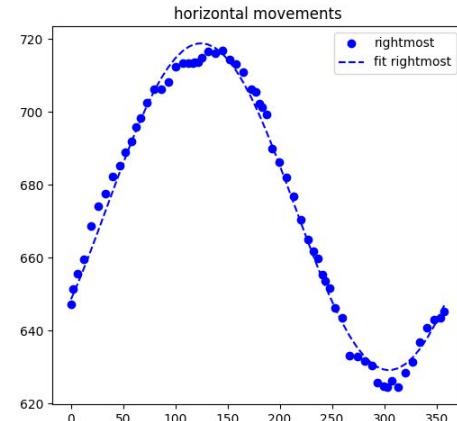
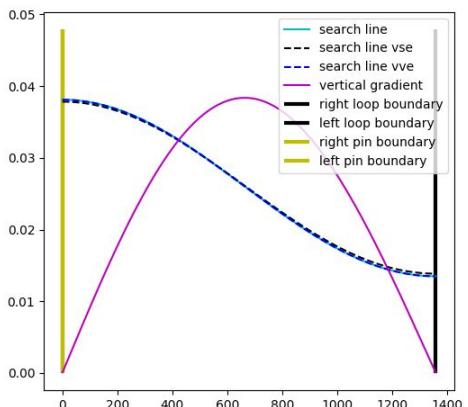
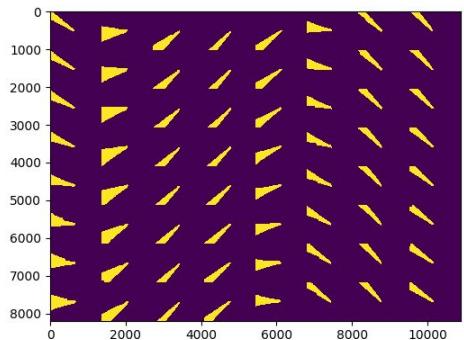
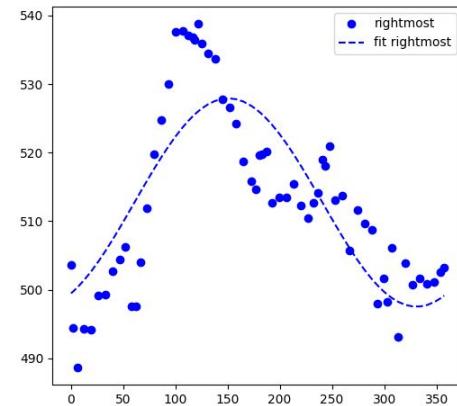
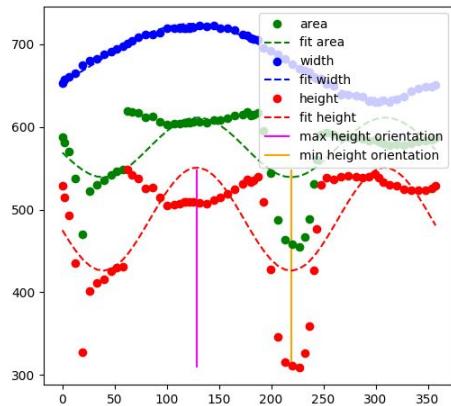
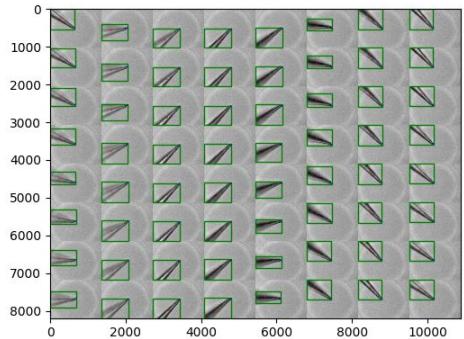


horizontal movements









# Short history of MXCuBE GUI on Proxima 2

File Beamline script Checks Admin Help

Collect XRF spectrum Log Chat (1)

User: mx-com-proxima2a Group: Set Logout

Sample list Mode: Sample changer Hide SC-details Centring: Manual Sync ISPBY

Sample centring Sample changer

Omega 0.00 45.0 Front Light 5 Back Light 15 Exposure 0.050 Focus 0.110 zoom 5

**MXCuBE Qt3 mid 2018**

Collection method Standard Collection

Soleil machine current 450.9 mA Hybrid filling Lifetime: 13.23 h Undul. HU\_640:

Energy 12.650 keV Current: 0.980 Å Move to: keV

Detector distance 4.286 Å Current: 499.94 mm Move to: mm

Transmission Current: 100.00% Set to:

Aperture cpbs Diameter: 50 Phase: Transfer

Position : Scintillator: BEAM PARK

Guillotine insert extract insert

Frontend shutter open

Safety shutter open

Fast shutter out LN2 Regulation ON

Optical hatch Experimental hatch ready ready

Characterisation Helical Collection

Energy Scan Advanced

Add to queue

Collect Queue Pause

2018-01-31 03:04:07] 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 -- done.  
[2018-01-31 03:05:13] 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 03:07:22] Manual centring used, waiting for user to center sample  
[2018-01-31 03:09:30] Centring saved  
[2018-01-31 03:10:18] Manual centring used, waiting for user to center sample  
[2018-01-31 03:10:53] Centring saved

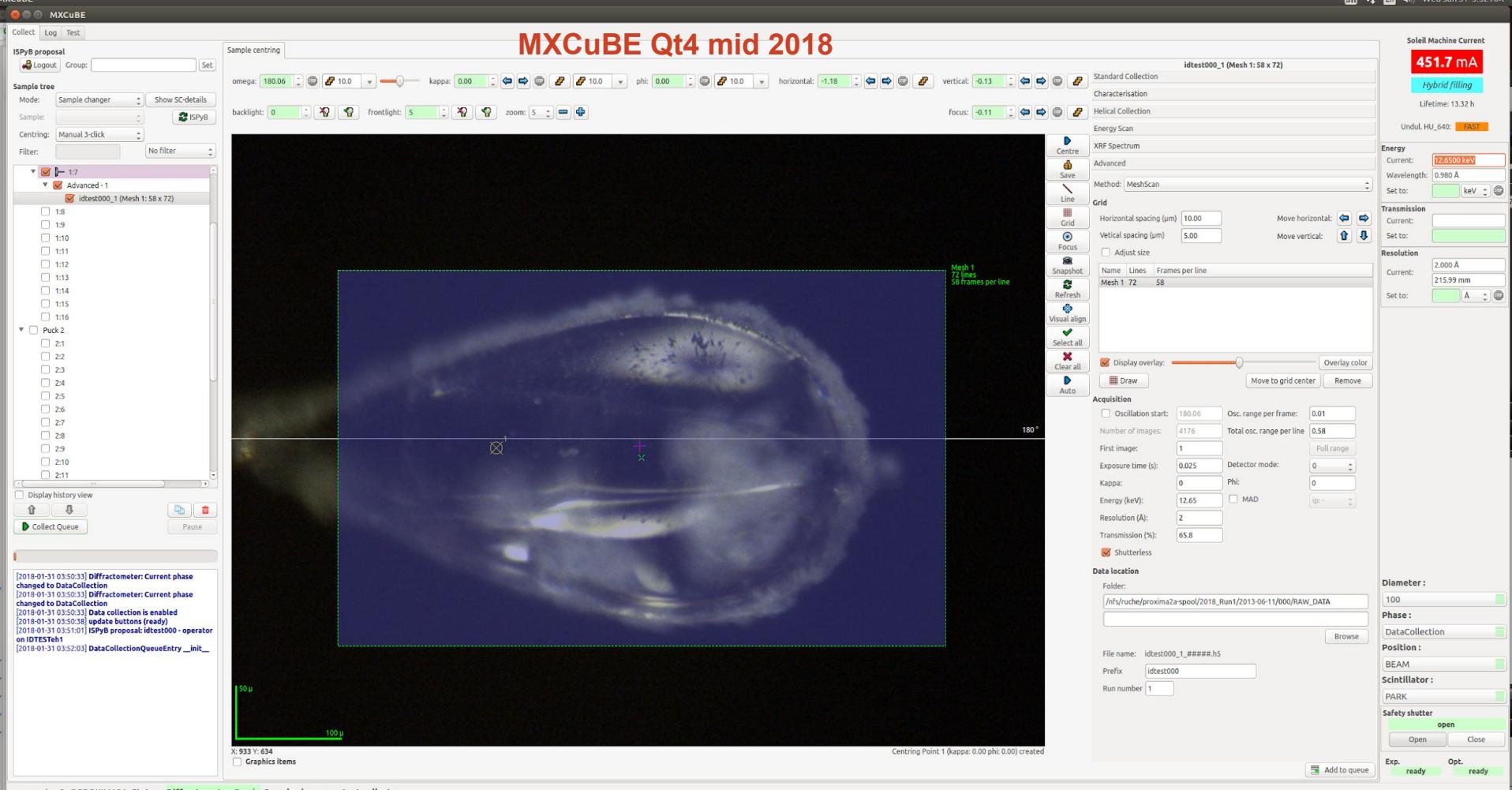
100 µm 100 µm

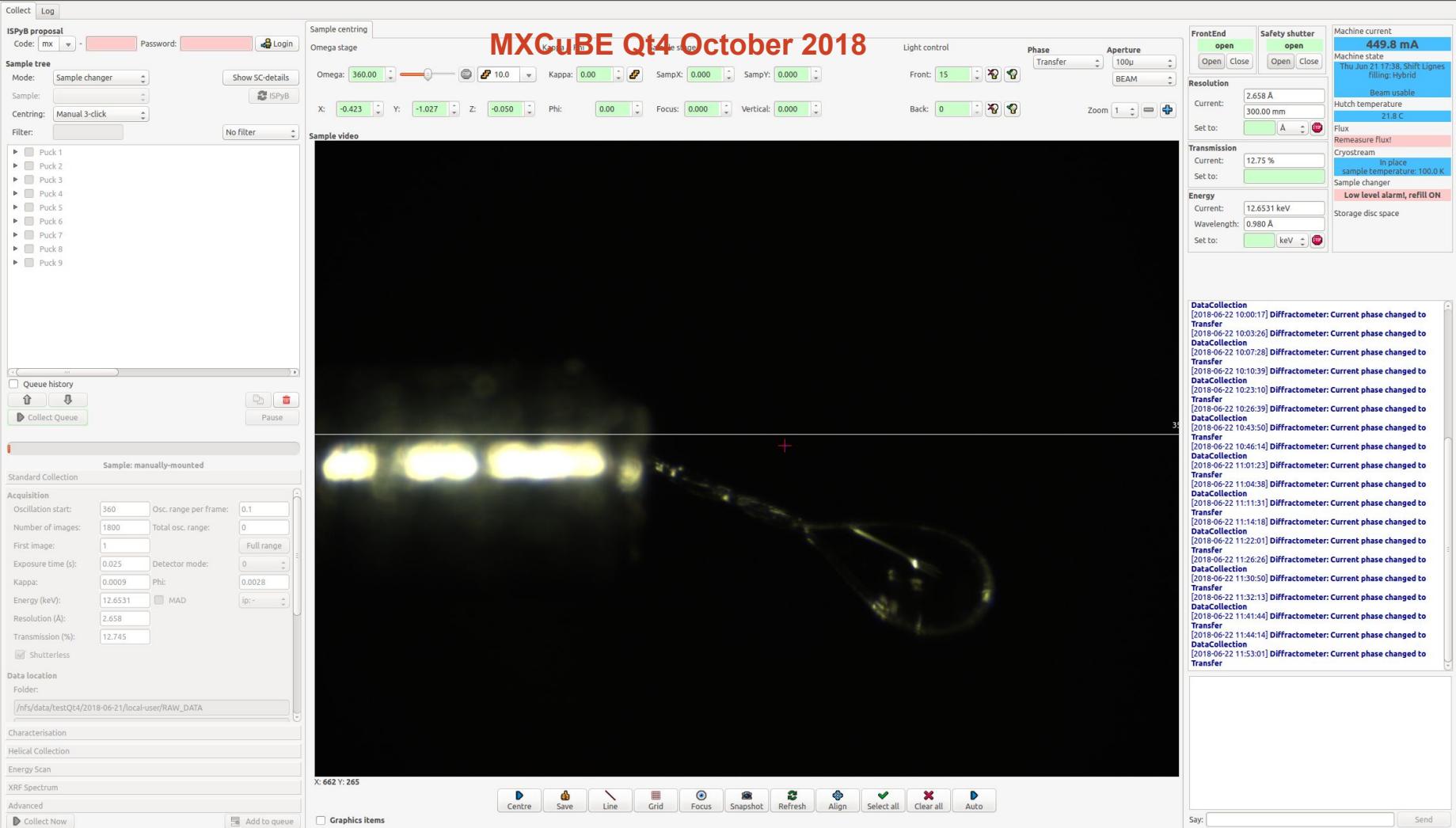
X: 1303 Y: 656

Centre Snapshot BeamPosition ApertureAlign Add Center Point

Selecting gives control Allow timeout control My name: proxima2a-5

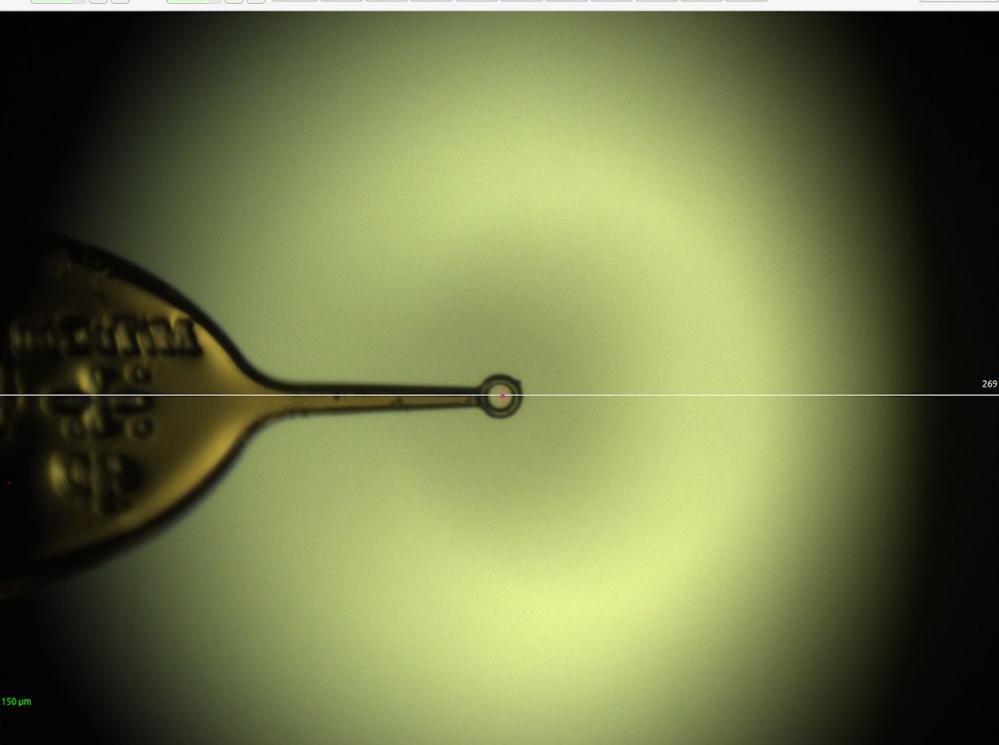






Sample centring

# MXCuBE Qt4 now (march 2019)



Front: 0 Back: 10

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

wc: 270.00 K: 0.00 φc: 360.00 Focus: 1.00 Aperture: 2.00

Phase Transfer

150 μm  
300 μm

X: 77 Y: 41

Graphics items

Sample: manually-mounted

Acquisition

Oscillation start: 0 Range per frame: 0.1

Number of images: 1800 Total range: 0

First image: 1 Full range: 9M

Exposure time (s): 0.025 Detector mode: 360

Kappa: 0.0012 Phi: 6.776

Energy (keV): 12.65 MAD

Resolution (Å): 6.776

Transmission (%): 20

Shutterless

Data location

Folder: /nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RRAW\_DATA

File name: prefix\_t\_#####.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

GPhi 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:

- 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 Safety shutter Machine current  
 disabled disabled 0  
 Open Close Open Close  
 Resolution Current: 6.776 Å Machine state None  
 Set to:  Å Hutch temperature 21.7 °C  
 Flux Remeasure flux!  
 Transmission Current: Cryostream In place  
 Set to:  Temperature: 290.0 K  
 Energy Current: 12.6500 keV Sample changer Low level alarm! refill Off  
 Wavelength: 0.980 Å Set to:  keV Storage disc space

# **Improving ergonomy of the interface**

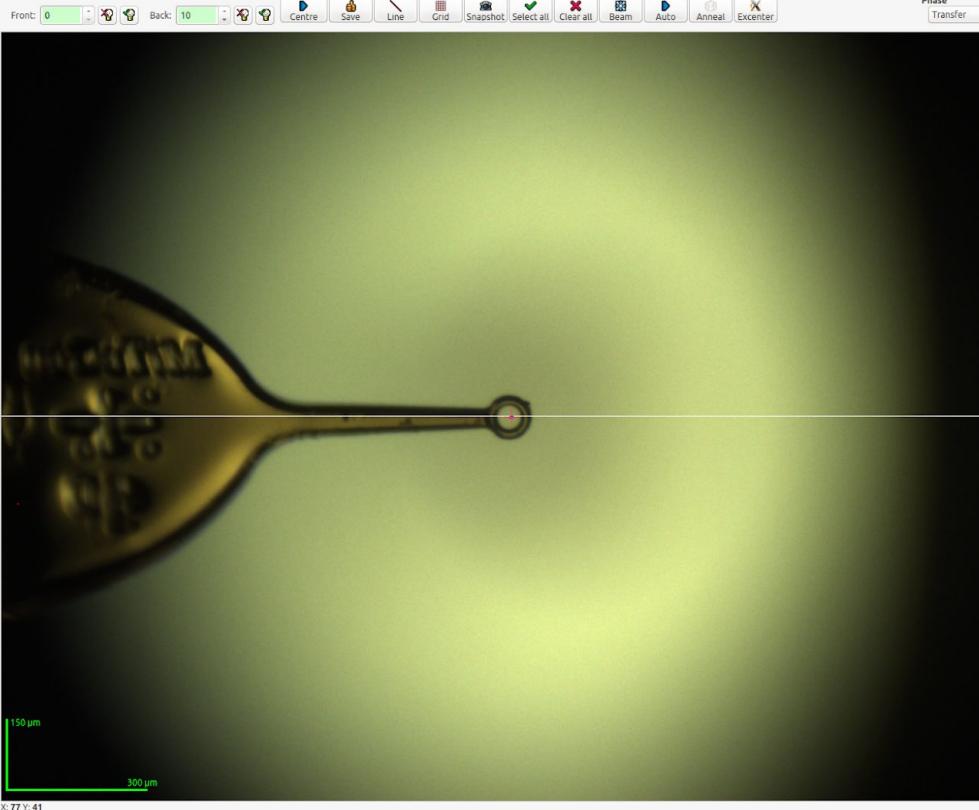
# making number of clicks and centring step easily visible and configurable

Sample centring

w: 270.00  10.0  K: 0.00  qc: 360.00  Focus: -0.137  Zoom: 1

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

Phase  Transfer



269

150 µm  300 µm

X: 77 Y: 41

Graphics items

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

Standard Collection

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<sup>-1</sup>  
Transmission (%): 20  
 Shutterless

Data location

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

File name: prefix\_t\_#####.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

GPhi Workflows

Advanced

Collect Now  Add to queue

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

ISPyB proposal

Code: mx  Password:  Login

Sample tree

Mode: Sample changer  Show SC-details

Sample:

Centring: Manual n-clicks

n-clicks: 3 step: 120.0  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 Safety shutter

disabled disabled

Open Close Open Close

Machine current 0

Machine state None

Hutch temperature 21.7 °C

Flux

Remeasure flux!

Cryostream In place

Temperature: 290.0 K

Sample changer Low level alarm! refill Off

Storage disc space

Resolution 6.776 Å

Current: 800.0 mm Set to:

Transmission

Current: Set to:

Energy

Current: 12.6500 keV Wavelength: 0.980 Å Set to:

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

ISPyB proposal  
20100023      Logout Group: Set

**Sample tree**

Mode: Manually mounted      Show SC-details

Sample:      ISPyB

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

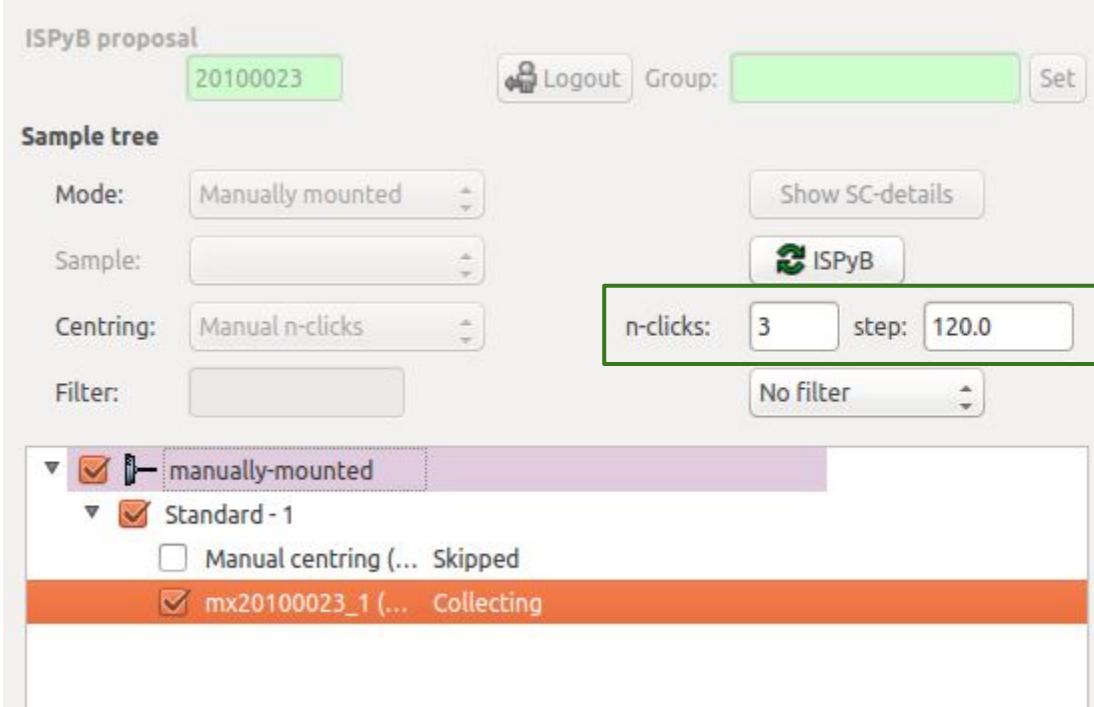
Filter: No filter

▼   manually-mounted

▼  Standard - 1

Manual centring (... Skipped)

mx20100023\_1 (... Collecting)



Sample centring

# annealing dialog

annealing dialog

Front: 0 Back: 10

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

w: 270.00 K: 0.00 phi: 360.00 Focus: -0.137 Zoom: 1

Phase Transfer

Sample: manually-mounted

Standard Collection

Acquisition

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

Data location

Folder: /nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/Raw\_DATA

File name: prefix\_t\_#####.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

GPhi Workflows

Advanced

Collect Now Add to queue

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

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

Collect Queue  Pause

FrontEnd Safety shutter

disabled disabled

Open Close Open Close

Machine current 0

Machine state None

Hutch temperature 21.7 °C

Flux

Remeasure flux!

Cryostream In place

Temperature: 290.0 K

Sample changer Low level alarm! refill Off

Storage disc space

Resolution 6.776 Å

Current: 800.0 mm Set to:  Å

Transmission

Current: Set to:

Energy

Current: 12.6500 keV Wavelength: 0.980 Å Set to:  keV

Graphics items

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

Sample centring

# annealing dialog

The screenshot shows the CCP4g software interface. At the top, there's a toolbar with various icons for sample centring, including 'Centre', 'Save', 'Line', 'Grid', 'Snapshot', 'Select all', 'Clear all', 'Beam', 'Auto', 'Anneal', and 'Excenter'. A green arrow points from the 'Anneal' icon in the toolbar to a modal dialog window titled 'Anneal' in the center. The dialog contains the text 'anneal for 1.0 seconds' with 'Cancel' and 'OK' buttons. Below the dialog is a grayscale image of a biological specimen, likely a virus, with a scale bar at the bottom left indicating 150 μm and 300 μm. The status bar at the bottom left shows 'X: 77 Y: 41'. On the right side of the screen, there's a detailed control panel for 'Standard Collection' with sections for 'Acquisition' (Oscillation start, Number of images, First image, Exposure time, Kappa, Energy, Resolution, Transmission), 'Data location' (Folder, File name, Prefix, Run number), 'Processing' (N.o. residues, Space group, Unit cell, Run processing after collection, Run Dozor), 'Characterisation' (Helical Collection, Energy Scan, XRF Spectrum, QPhi Workflows), 'Advanced' (Collect Now, Add to queue), and a log message '[2019-03-08 16:19:25] Data collection is enabled'. To the far right, there's a 'Machine current' section with values 0 and 21.7 °C, and a 'Machine state' section with 'None' and 'In place'. The top right corner also shows an 'ISPyB proposal' section with fields for 'Code: mx', 'Password:', and 'Login'.

Standard Collection

Sample: manually-mounted

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

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

Anneal

anneal for 1.0 seconds

Cancel OK

150 μm 300 μm

X: 77 Y: 41

Graphics items

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

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

Transmission (%): 20

Shutterless

Data location

Folder: /nfs/rutherford/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/Raw\_Data

File name: prefix\_t\_#####.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

QPhi Workflows

Advanced

Collect Now Add to queue

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

FrontEnd Safety shutter

disabled disabled

Open Close Open Close

Resolution

Current: 6.776 Å Set to: [ ] Å

800.00 mm

Flux

Hutch temperature: 21.7 °C

Remeasure flux!

Cryostream

Current: In place Set to: [ ]

Temperature: 290.0 K

Sample changer

Low level alarm! refill Off

Storage disc space

Machine current: 0

Machine state: None

Machine current: 21.7 °C

Machine state: In place

Machine current: 290.0 K

Machine state: Low level alarm! refill Off

Machine current: 0

Machine state: None

Machine current: 21.7 °C

Machine state: In place

Machine current: 290.0 K

Machine state: Low level alarm! refill Off

Machine current: 0

Machine state: None

Machine current: 21.7 °C

Machine state: In place

Machine current: 290.0 K

Machine state: Low level alarm! refill Off

Machine current: 0

Machine state: None

Machine current: 21.7 °C

Machine state: In place

Machine current: 290.0 K

Machine state: Low level alarm! refill Off

Sample centring

# Simplifying x-ray centring

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

Phase Transfer

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: [redacted]

Standard Collection

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: /nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RRAW\_DATA

File name: prefix\_t\_#####.h5 Prefix: prefix Run number: 1

Browse

Processing

N.o. residues: 200 Space group: P1  
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

QPhi Workflows

Advanced

Collect Now Add to queue

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

FrontEnd Safety shutter

Machine current 0

Machine state None

Hutch temperature 21.7 °C

Flux Remeasure flux!

Cryostream In place Temperature: 290.0 K

Sample changer Low level alarm! refill Off

Storage disc space

Resolution Current: 6.776 Å Set to: 6.776 Å 800.0 mm

Transmission Current: Set to:

Energy Current: 12.6500 keV Wavelength: 0.980 Å Set to:

Graphics items

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

Sample centring

# Simplifying x-ray centring

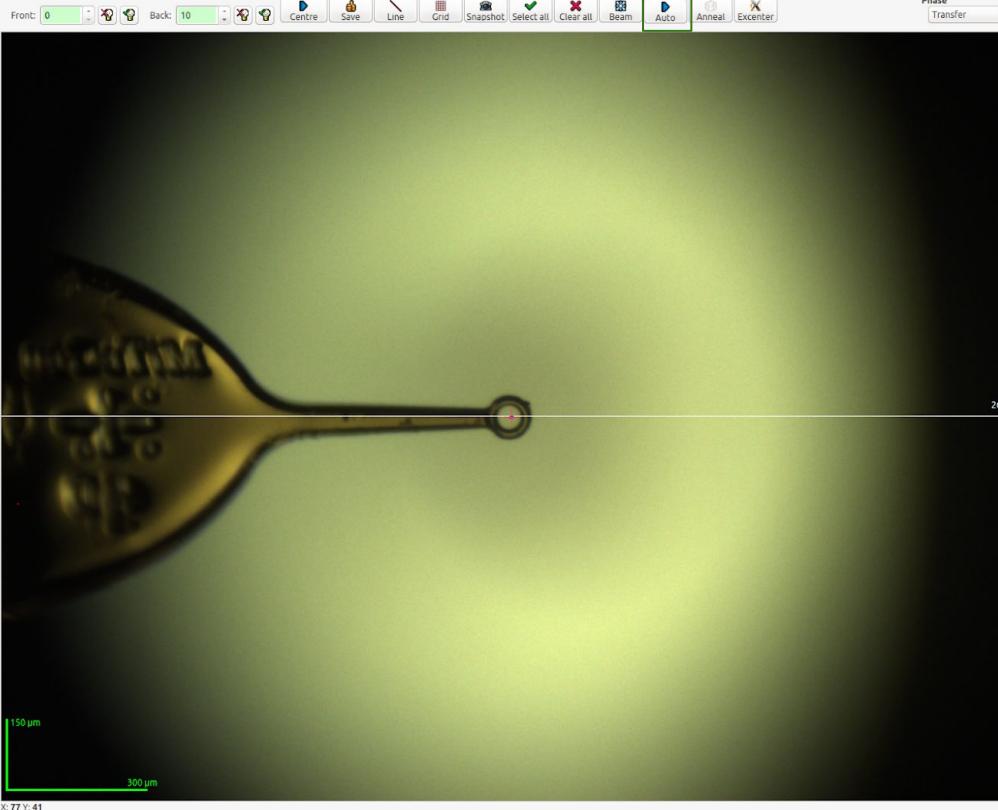
The screenshot shows a beamline control interface with several panels:

- Top Left:** Beamline controls (Front: 0, Back: 10, Centre, Save, Line, Grid, Snapshot, Select all, Clear all, Beam, Auto, Anneal) and a zoom tool.
- Top Center:** Phase selection (Phase Transfer).
- Top Right:** ISPyB proposal (Code: mx), Sample tree (Mode: Sample changer, Sample: Puck 1, Centring: Manual n-clicks, Filter: 3), and a login button.
- Middle Left:** A preview image of a sample with a scale bar (150 µm and 300 µm) and coordinates (X: 77 Y: 41). A green arrow points from the "Excenter" button in the top bar down to the "Excenter" dialog window.
- Middle Center:** The "Excenter" dialog window with "scan length" set to 0.1 mm, "Cancel" and "OK" buttons.
- Right Side:** Acquisition parameters (Oscillation start: 0, Range per frame: 0.1, Number of images: 1800, Total range: 0, Full range: 9M, 360, 1p), Data location (Folder: /nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RRAW\_DATA, File name: prefix\_t\_#####.h5, Prefix: prefix, Run number: 1), Processing (N.o. residues: 200, Space group: P1, 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, QPhi Workflows), Advanced (Collect Now, Add to queue), and a message [2019-03-08 16:19:25] Data collection is enabled.
- Bottom Right:** Machine status (FrontEnd disabled, Safety shutter disabled, Resolution: 6.776 Å, Current: 800.0 mm, Set to: 6.776 Å, Hutch temperature: 21.7 °C, Flux, Remeasure flux!, Cryostream, Current: In place, Set to: In place, Sample changer, Low level alarm! refill Off, Storage disc space), and a "Machine current" panel showing 0.

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

Sample centring

Front: 0 Back: 10



wc: 270.00 ϕ: 10.0 K: 0.00 φ: 360.00 Focus: -0.137 Zoom: 1

Centre Save Line Grid Snapshot Select all Clear all Beam Auto Phase Transfer

150 μm 300 μm X: 77 Y: 41

Graphics items

Sample: manually-mounted

Standard Collection

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<sup>-1</sup>  
Transmission (%): 20  
 Shutterless

Data location

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

File name: prefix\_t\_#####.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

GPhi Workflows

Advanced

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

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  Safety shutter

Machine current: 0 Machine state: None

Hutch temperature: 21.7 °C

Resolution: 6.776 Å Current: 800.0 mm

Set to:  Å

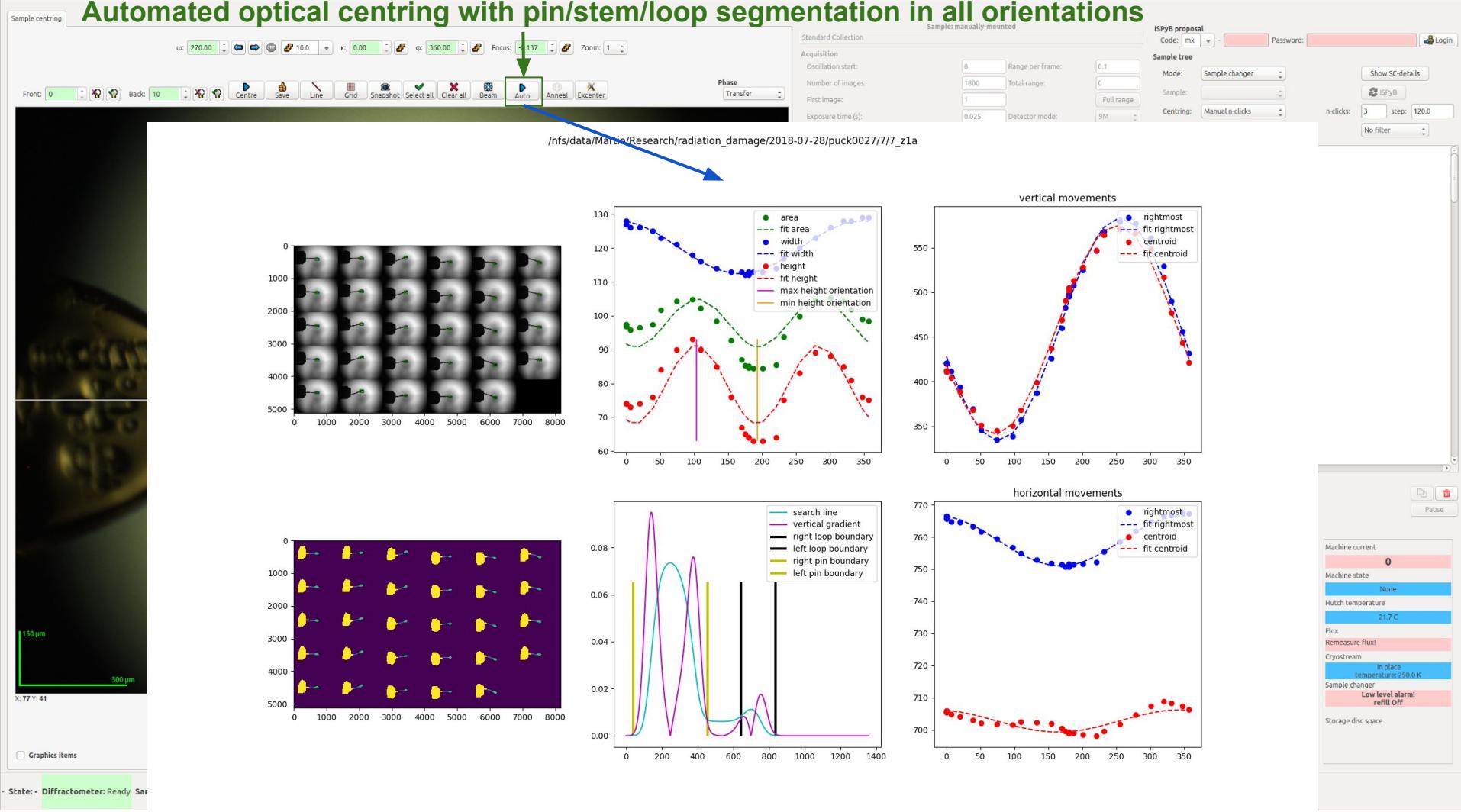
Flux: Remeasure flux!

Cryostream: In place Temperature: 290.0 K

Sample changer: Low level alarm! refill Off

Storage disc space:

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



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

Sample: manuall-mounted

ISPyB proposal  
Code:  Password:  Login

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

Focus: -0.137 Zoom: 1

269

150 μm 300 μm X: 77 Y: 41

Graphics items

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

Standard Collection

Acquisition

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

Data location

Folder: /nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RAW\_DATA  
File name: prefix\_t\_#####.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

GPhi Workflows

Advanced

Collect Now Add to queue

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

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 Safety shutter Machine current  
disabled disabled 0  
Open Close Open Close  
Machine state None  
Hutch temperature 21.7 °C  
Resolution 6.776 Å  
Current: 800.0 mm  
Set to:

Transmission

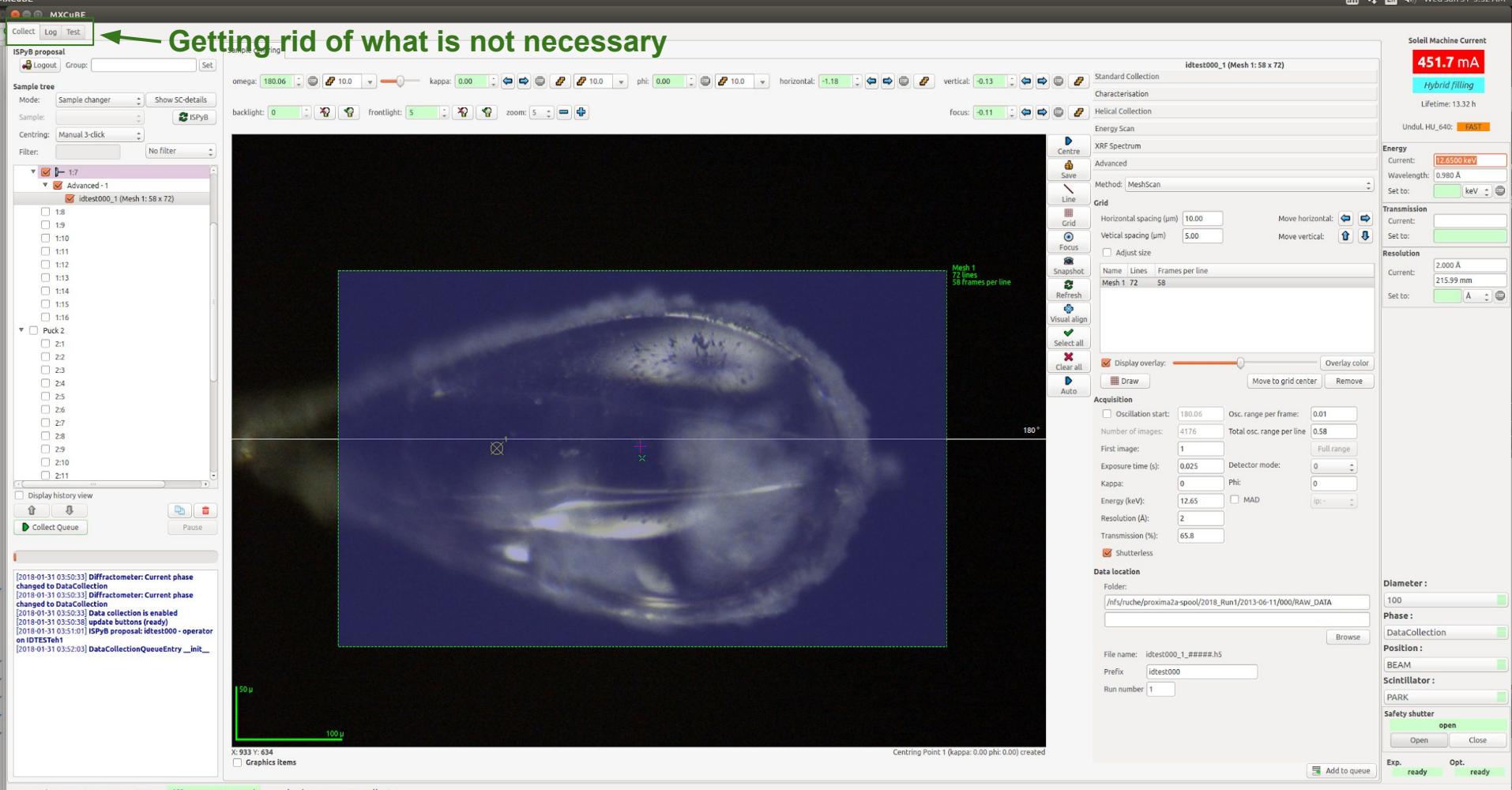
Current:

Cryostream In place  
Temperature: 290.0 K

Storage disc space

Energy

Current: 12.6500 keV  
Wavelength: 0.980 Å  
Set to:



com-proxima2a@PROXIMA2A State: - Diffractometer: Ready Sample changer: - Last collect: -

**← Getting rid of what is not necessary**

Sample centring

Standard Collection

Acquisition

Sample: manually-mounted

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

Phase Transfer

Oscillation start: 0 Range per frame: 0.1

Number of images: 1800 Total range: 0

First image: 1 Full range 9M

Exposure time (s): 0.025 Detector mode: 360

Kappa: 0.0012 Phi: 6.776

Energy (keV): 12.65 MAD

Resolution (Å): 6.776

Transmission (%): 20

Shutterless

Data location

Folder: /nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RRAW\_DATA

File name: prefix\_t\_#####.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

GPhi Workflows

Advanced

Collect Now Add to queue

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

FrontEnd Safety shutter

Machine current 0

Machine state None

Hutch temperature 21.7 °C

Resolution 6.776 Å

Current: 800.0 mm

Set to:

Flux

Remeasure flux!

Cryostream In place

Temperature: 290.0 K

Sample changer Low level alarm! refill Off

Storage disc space

Graphics items

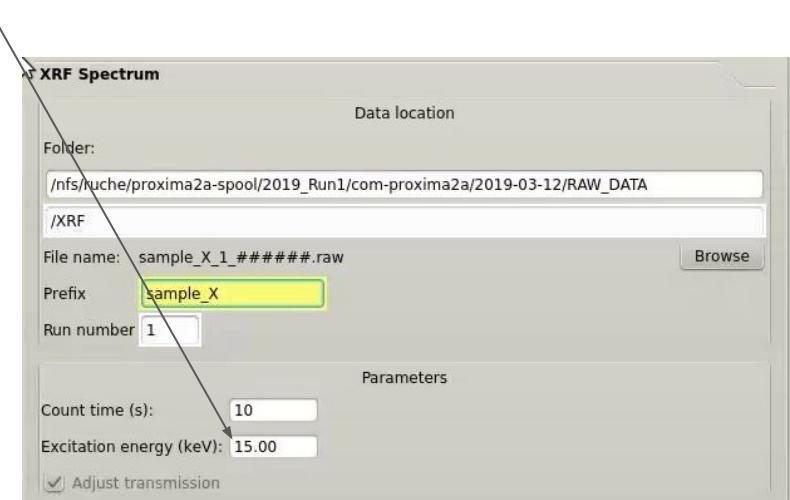
150 µm 300 µm

X: 77 Y: 41

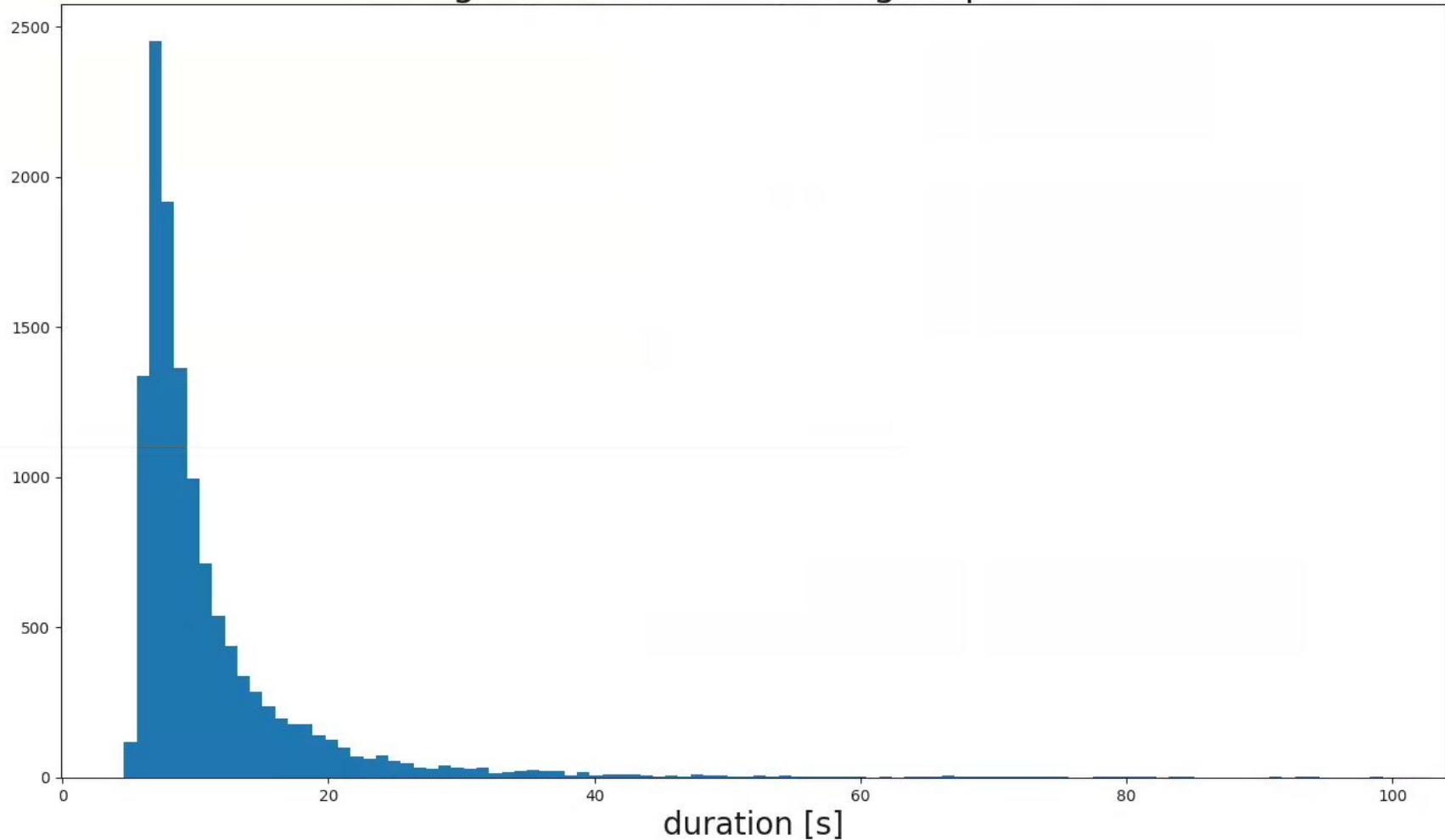
- State: - Diffractometer: Ready Sample changer: - Last collect: -

# 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 miscal.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



# Histogram of n-click centring elapsed time



Sample centring

Phase Transfer

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

wc: 270.00 ϕ: 10.0 K: 0.00 φ: 360.00 Focus: -0.137 Zoom: 1

269

15 μm 300 μm X: 77 Y: 41

Graphics items

Sample: manually-mounted

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

Standard Collection

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: /nfs/ruche/proxima2a-spool/2019\_Run1/com-proxima2a/2019-03-08/RRAW\_DATA

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

Prefix: prefix

Run number: 1

Processing

N.o. residues: 200 Space group: a: 0 b: 0 c: 0  
a: 0 b: 0 c: 0 x: 0 y: 0 z: 0  
Run processing after collection  
Run Dozor

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

GPhi Workflows

Advanced

Collect Now Add to queue

[2019-03-08 14:19:25] Data collection is enabled

Single most popular button  
Thanks, Ivars!

FrontEnd Safety shutter

Machine current 0 Machine state None

Hutch temperature 21.7 °C

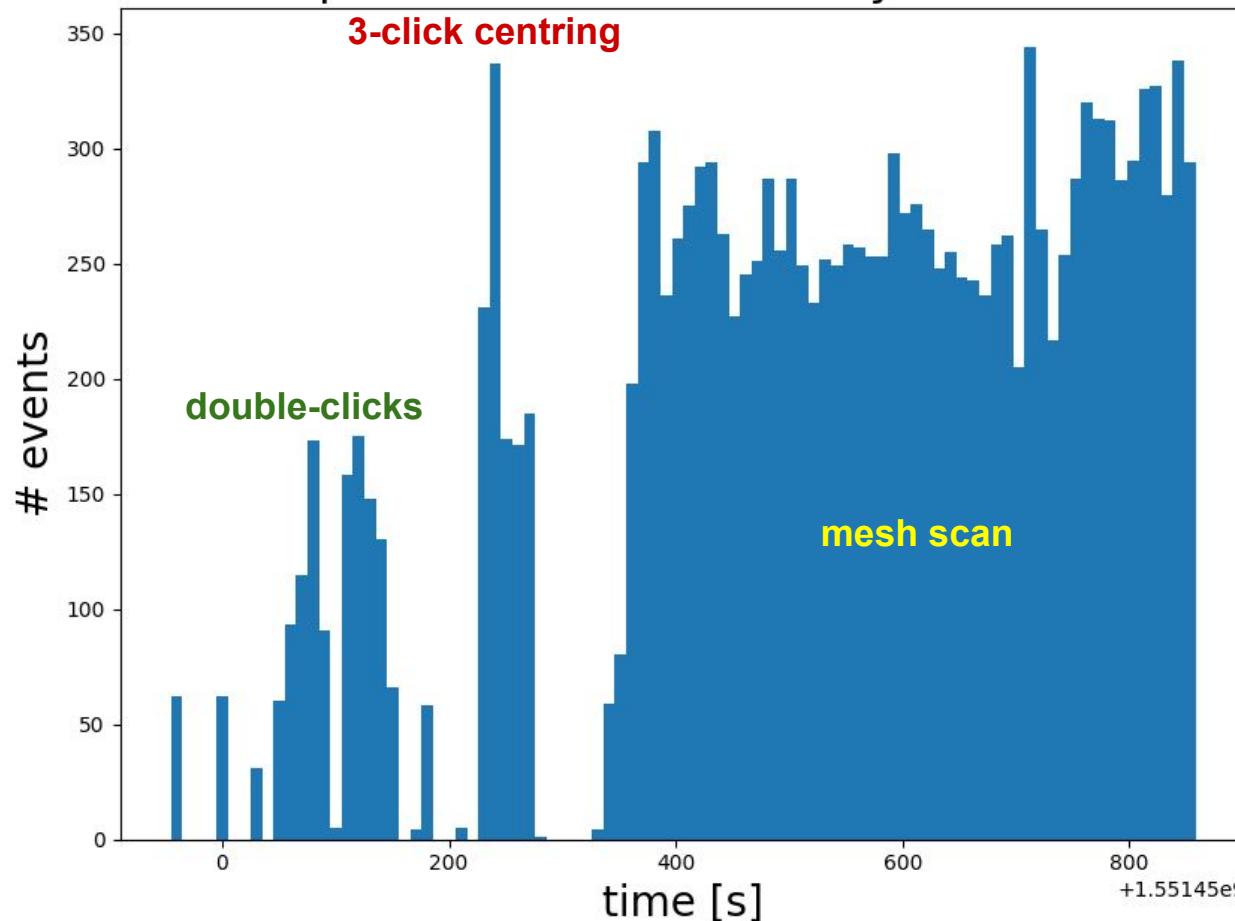
Flux Remeasure flux!

Cryostream In place Temperature: 290.0 K

Sample changer Low level alarm! refill Off

Storage disc space

# 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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