# Eiger X at SOLEIL MX beamlines

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**High Data-Rate MX Meeting at DLS** **2019-11-06**

## 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 2A

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

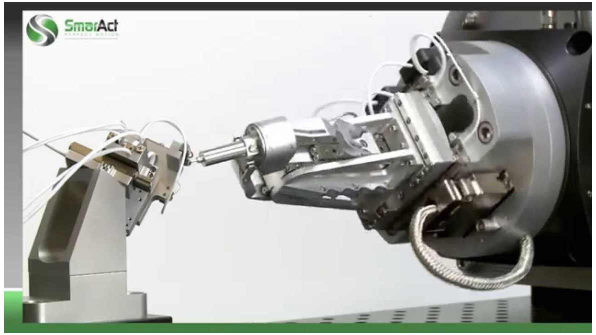
Goniometer: **MD2 with MK3**

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

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

# Multiaxis goniometry

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




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

# Sample changers

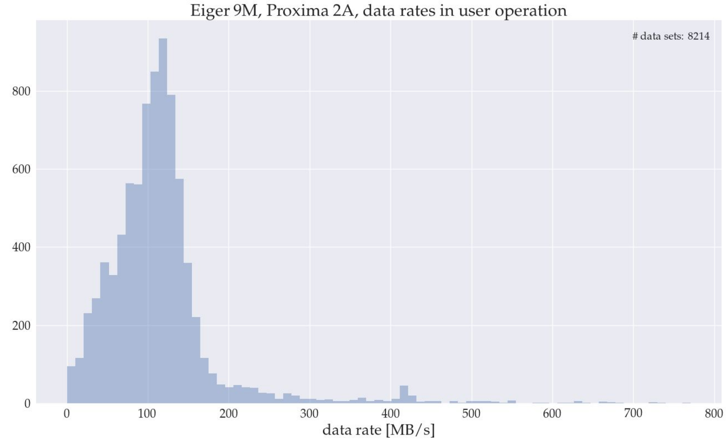
- CATS robots on both beamlines. Control via PyCats Tango Device Server
- Mature integration
    - Failure rate below 1 per 4000
    - Exchange time 35 seconds

# X-ray Area Detectors at SOLEIL’s MX beamlines

- Eiger X 9M (PROXIMA 2A) and 16M (PROXIMA 1)
- Firmware version: SIMPLON v. 1.6.6
- User operation
  - Eiger X 9M December 2015
  - Eiger X 16M October 2018
- bslz4 compression
- Max speeds
  - 750Hz @ 4M ROI
  - 238Hz @ 9M
  - 133Hz @ 16M
- ~10 TB of raw data per day on average
- ~1PB raw data per year, ~100TB with bslz4 compression

# Network and performance of the setup

- 10 GbE network
- ~ 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 t
- 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 (for 9M)
  - x 10.9 per 16bit -- average compressed image size ~2 MB (for 9M)

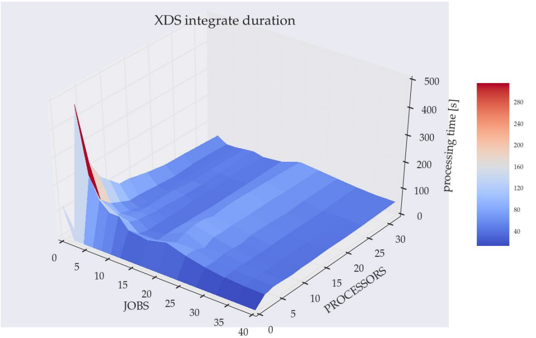


# Processing infrastructure

- Systems 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
```

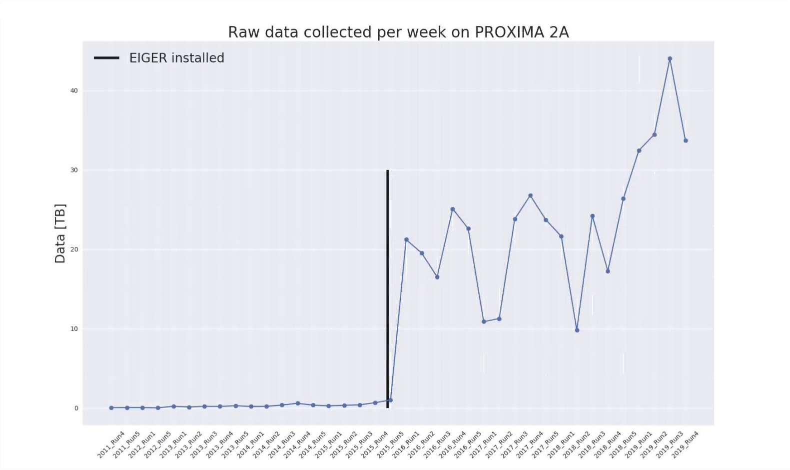



* http://e.huawei.com/en/products/cloud-computing-dc/servers/rh-series/rh8100-v3

# Automated processing of data

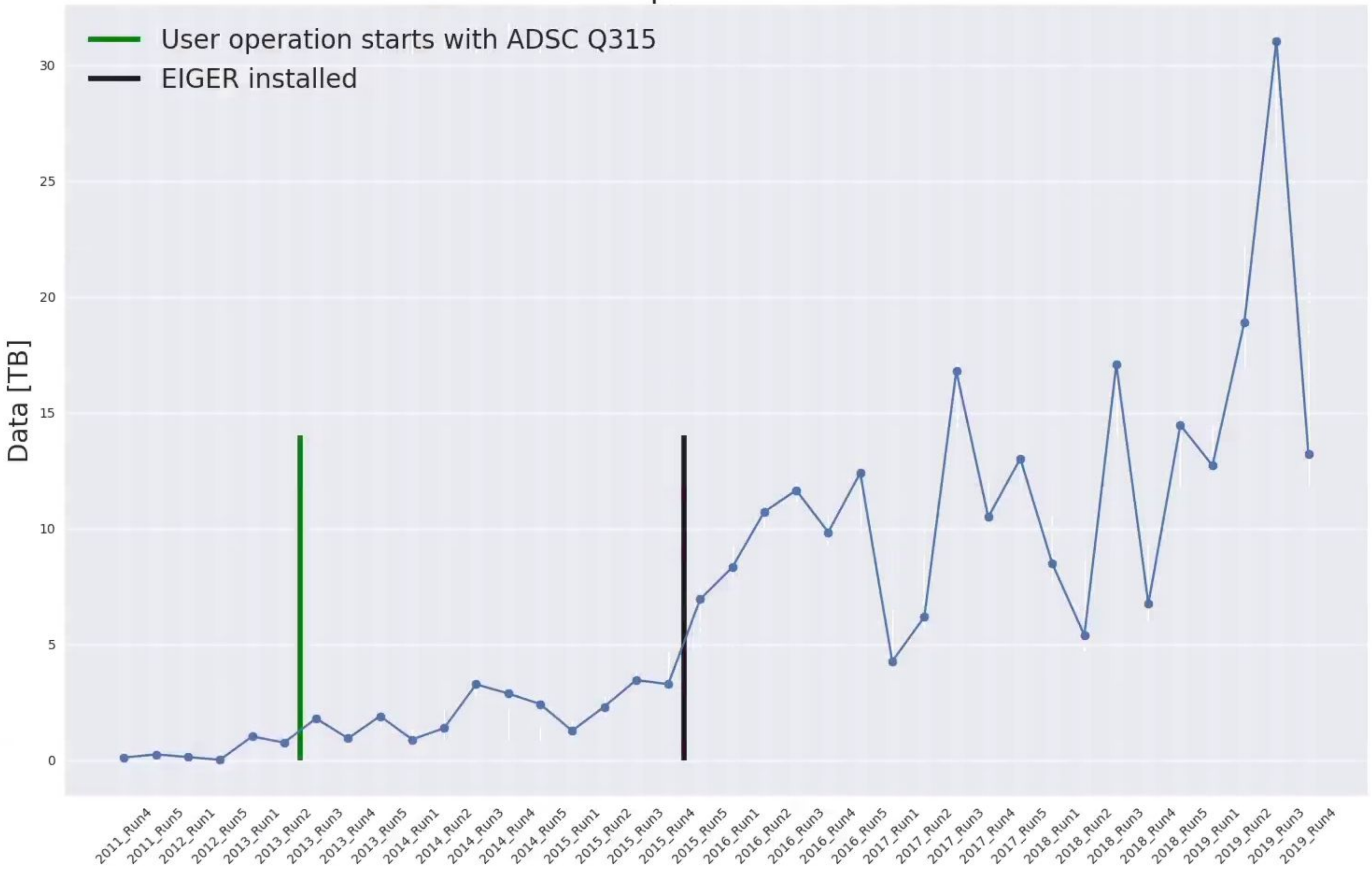
- XDSME data processing for every collect if user logged into ISPyB
  - Stable as of the last three runs
- autoPROC pipeline added over the last run
- Characterization images automatically analyzed
  - dials.find_spots
  - DOZOR
  - xdsme
  - BEST strategy calculation (upon successful integration with xdsme)

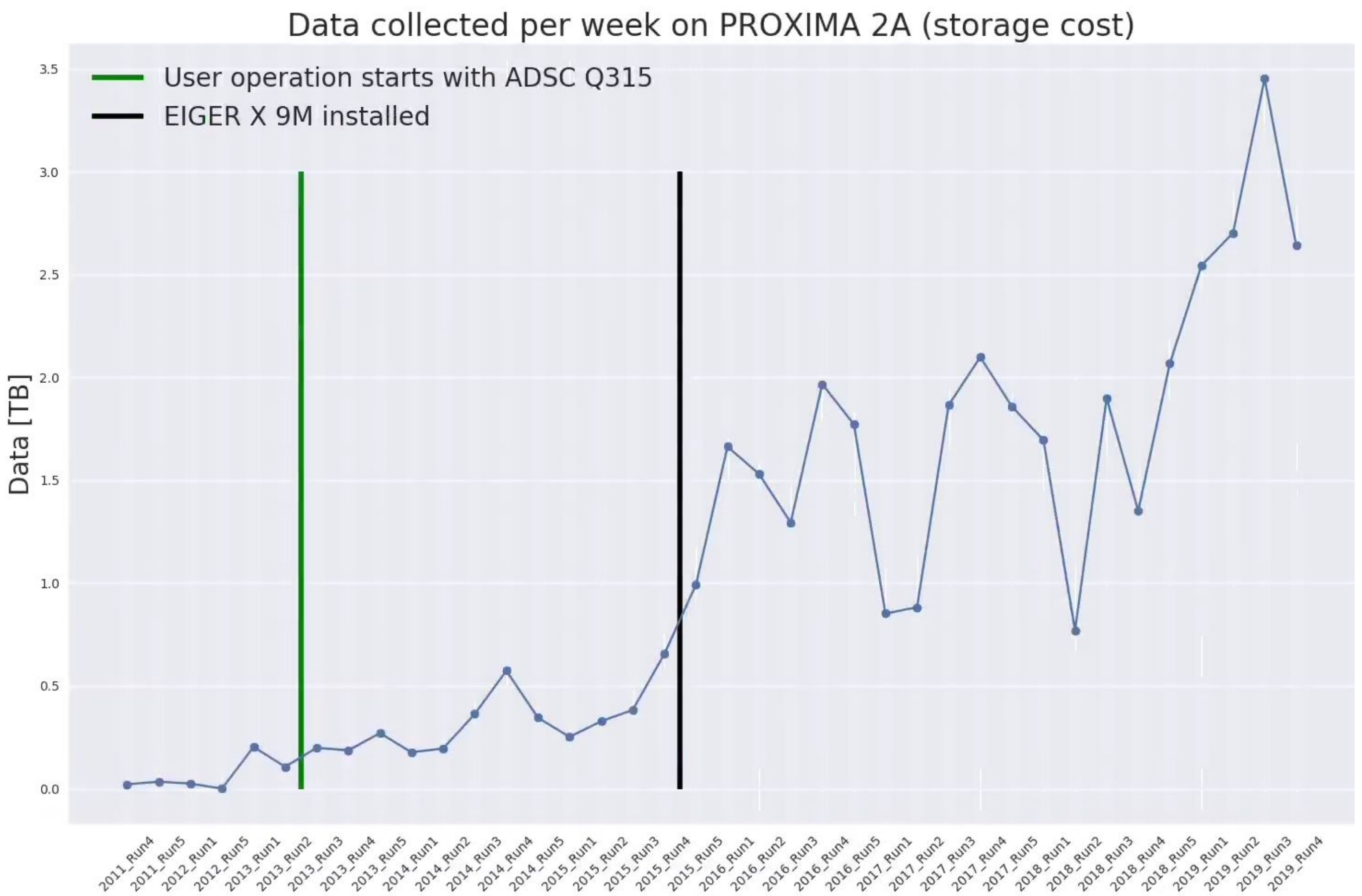
# Data handling infrastructure

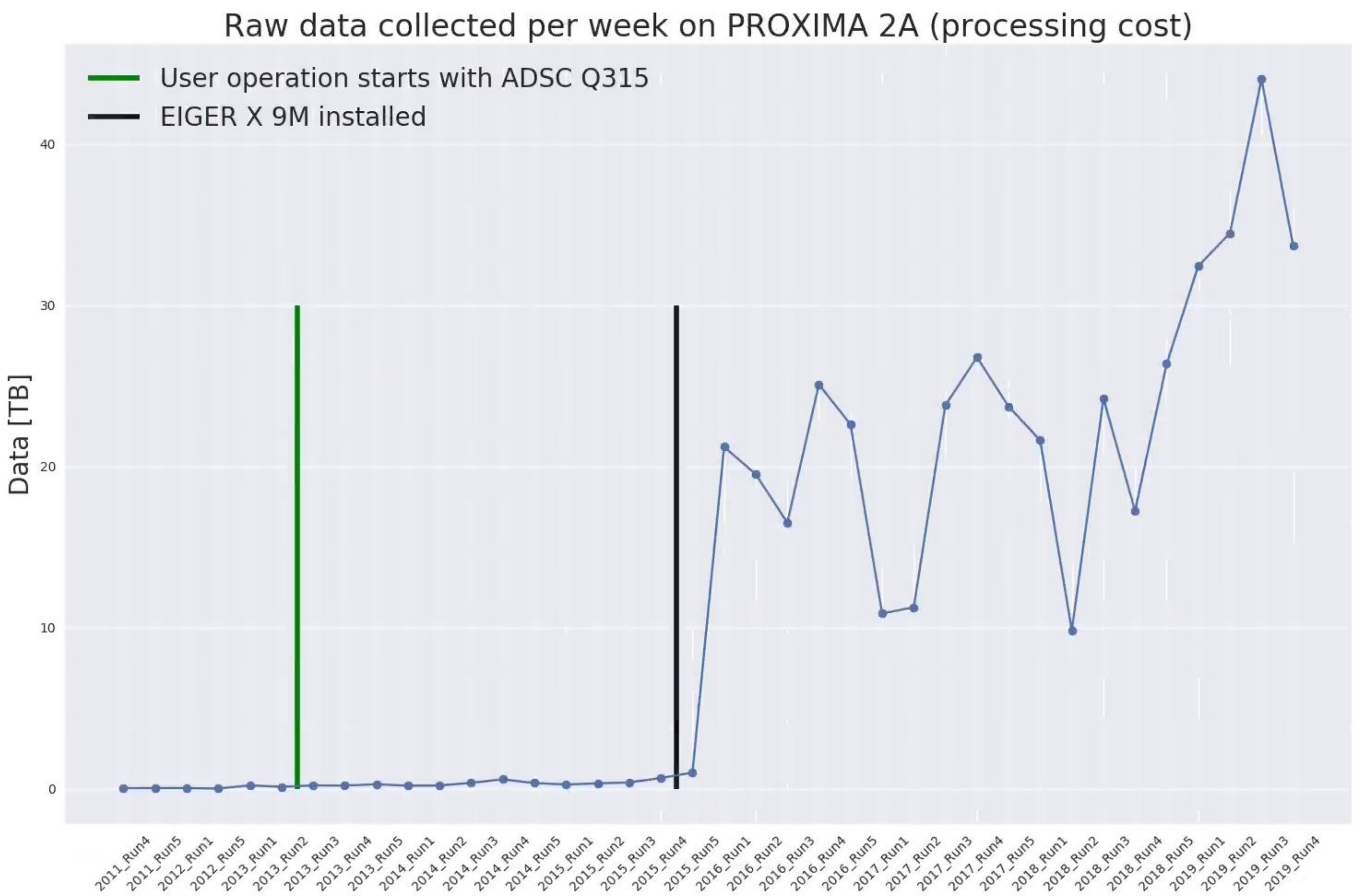



- 10GBe network
- Local buffer on the processing server
  - 2.56TB RAM
  - 3TB RAID 6 SAS + 16TB SSD
  - 256 TB RAID 60 SAS (double that on PX1)
    - Directly attached storage (DELL MD 1400 with PERC H840 SAS external PCI card)
- Medium and long term storage (Active Circle based), NFS access
  - Local cell: 10TB SSD, 20TB SAS
  - Remote cell: 1PB via 10Gbe

Data collected per run on PROXIMA 2A




Data collected per week on PROXIMA 2A (storage cost)
User operation starts with ADSC Q315
EIGER X 9M installed
Data [TB]
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
2011_Run4
2011_Run5
2012_Run1
2012_Run5
2013_Run1
2013_Run2
2013_Run3
2013_Run4
2013_Run5
2014_Run1
2014_Run2
2014_Run3
2014_Run4
2014_Run5
2015_Run1
2015_Run2
2015_Run3
2015_Run4
2015_Run5
2016_Run1
2016_Run2
2016_Run3
2016_Run4
2016_Run5
2017_Run1
2017_Run2
2017_Run3
2017_Run4
2017_Run5
2018_Run1
2018_Run2
2018_Run3
2018_Run4
2018_Run5
2019_Run1
2019_Run2
2019_Run3
2019_Run4


Raw data collected per week on PROXIMA 2A (processing cost)
User operation starts with ADSC Q315
EIGER X 9M installed
Data [TB]
0
10
20
30
40
2011_Run4
2011_Run5
2012_Run1
2012_Run5
2013_Run1
2013_Run2
2013_Run3
2013_Run4
2013_Run5
2014_Run1
2014_Run2
2014_Run3
2014_Run4
2014_Run5
2015_Run1
2015_Run2
2015_Run3
2015_Run4
2015_Run5
2016_Run1
2016_Run2
2016_Run3
2016_Run4
2016_Run5
2017_Run1
2017_Run2
2017_Run3
2017_Run4
2017_Run5
2018_Run1
2018_Run2
2018_Run3
2018_Run4
2018_Run5
2019_Run1
2019_Run2
2019_Run3
2019_Run4

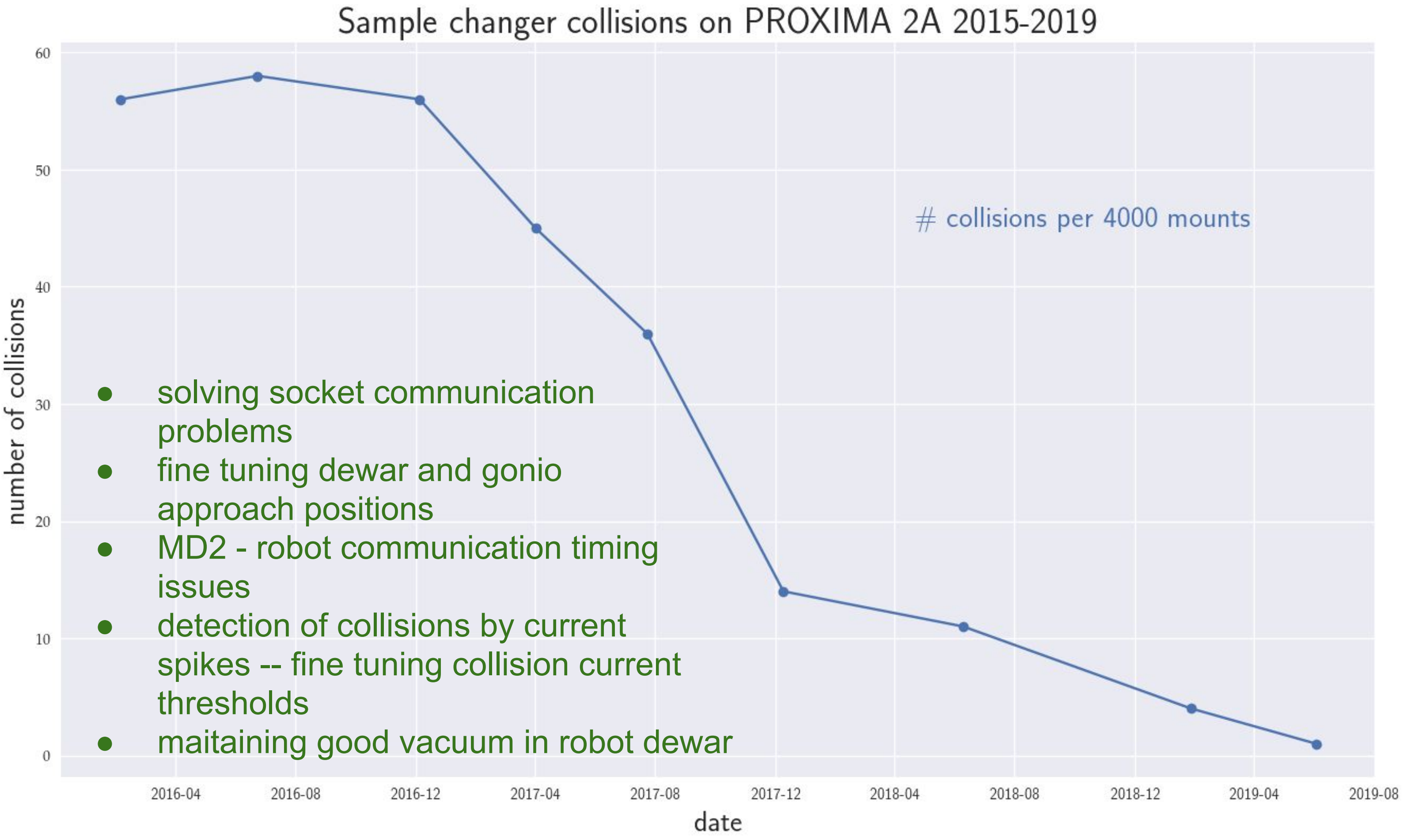
# Handling On Axis Viewer

- 1024x1360 pixels
- run @20Hz
- using Vimba
- redis in-memory database used to distribute images to unlimited number of clients
- 5TB data per day

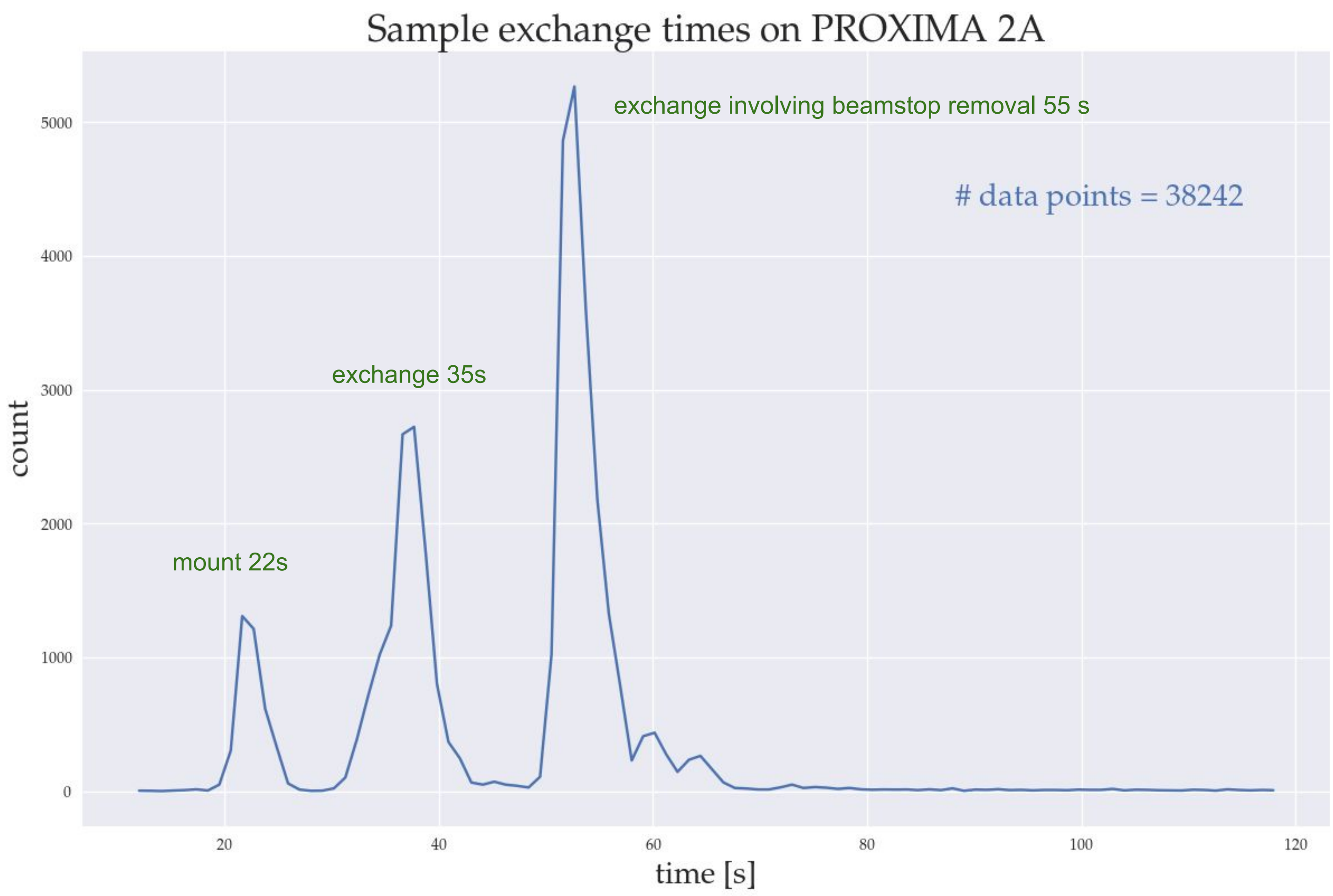
# Addressing bottlenecks

- sample changer reliability
- sample alignment robustness
  - better model of the sample and its environment
  - making x-ray centring non-intrusive and fast to allow to make it the default part of characterization
- sample supply
  - user scheduling

Increasing robot reliability over time



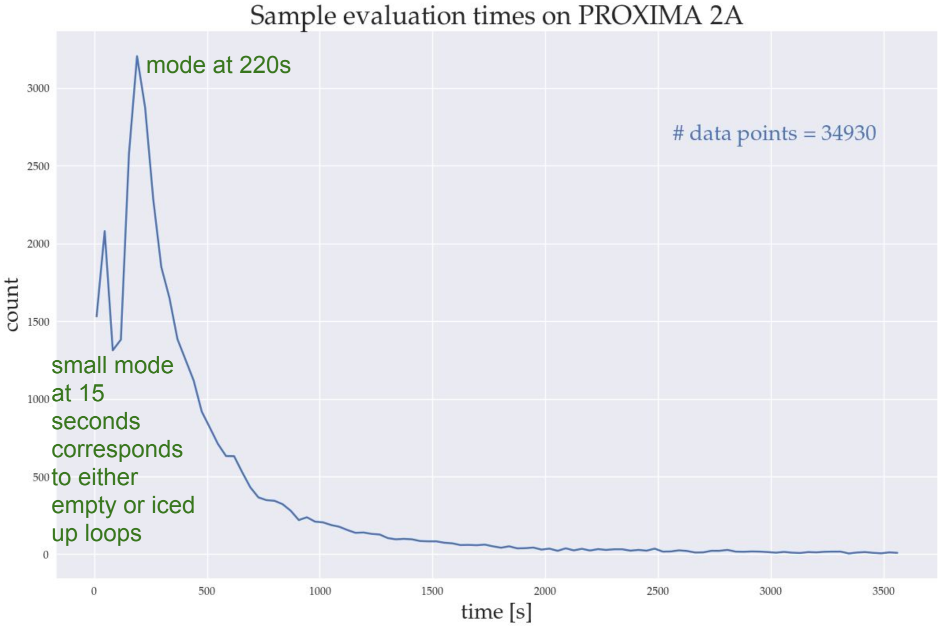

- solving socket communication problems
- fine tuning dewar and gonio approach positions
- MD2 - robot communication timing issues
- detection of collisions by current spikes -- fine tuning collision current thresholds
- maitaining good vacuum in robot dewar


Sample exchange times on PROXIMA 2A
exchange involving beamstop removal 55 s
# data points = 38242
exchange 35s
mount 22s
count
time [s]
0
1000
2000
3000
4000
5000
20
40
60
80
100
120

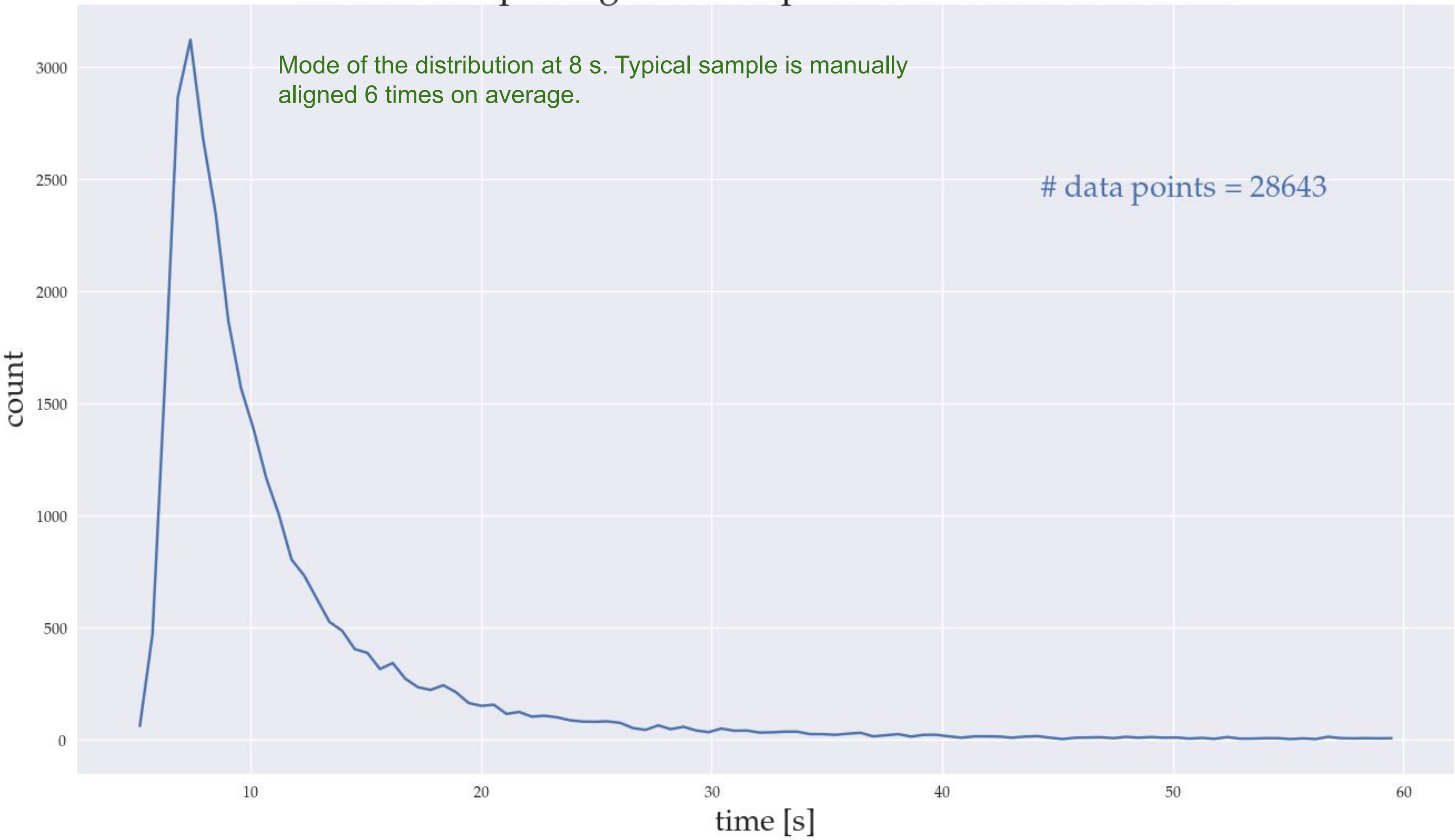
# Sample evaluation times on PROXIMA 2A

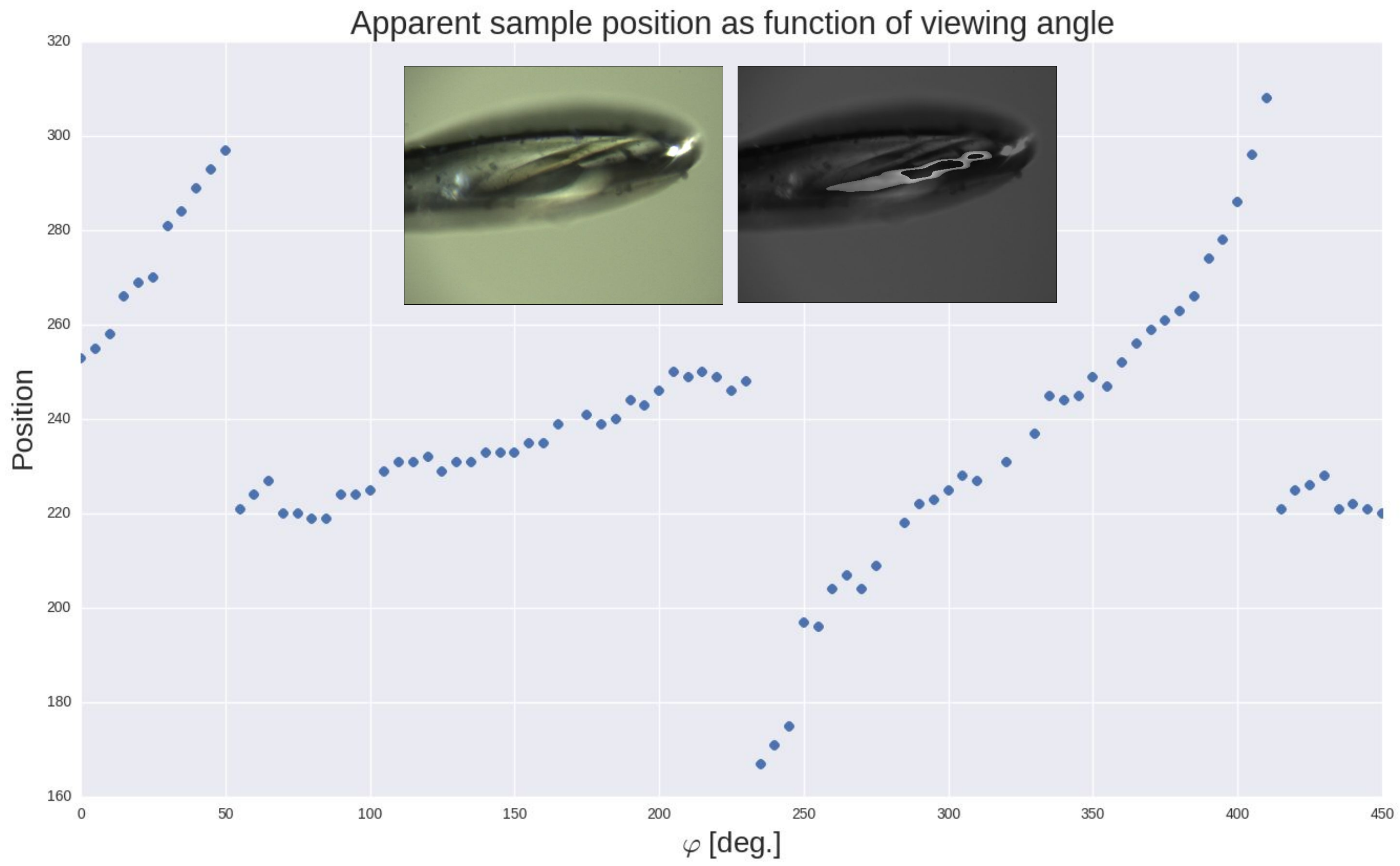
# Beamline throughput

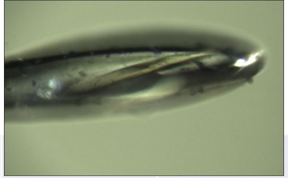
- PROXIMA 2A now passes ~10000 samples per year
- The raw throughput (given current technology) is at least 5 times higher

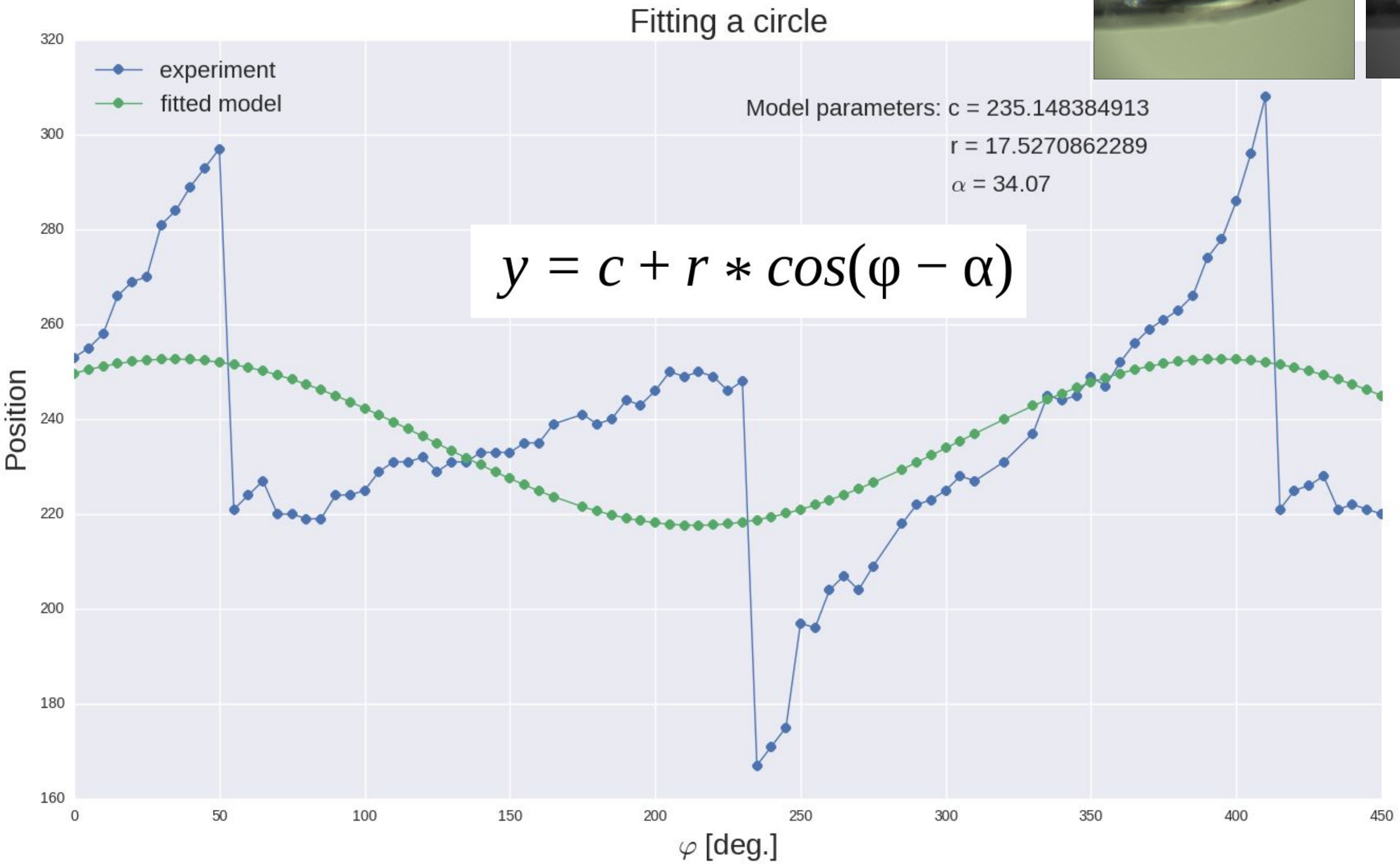


# Manual sample alignment elapsed time on PROXIMA 2A




Apparent sample position as function of viewing angle
Position
φ [deg.]
320
300
280
260
240
220
200
180
160
0
50
100
150
200
250
300
350
400
450





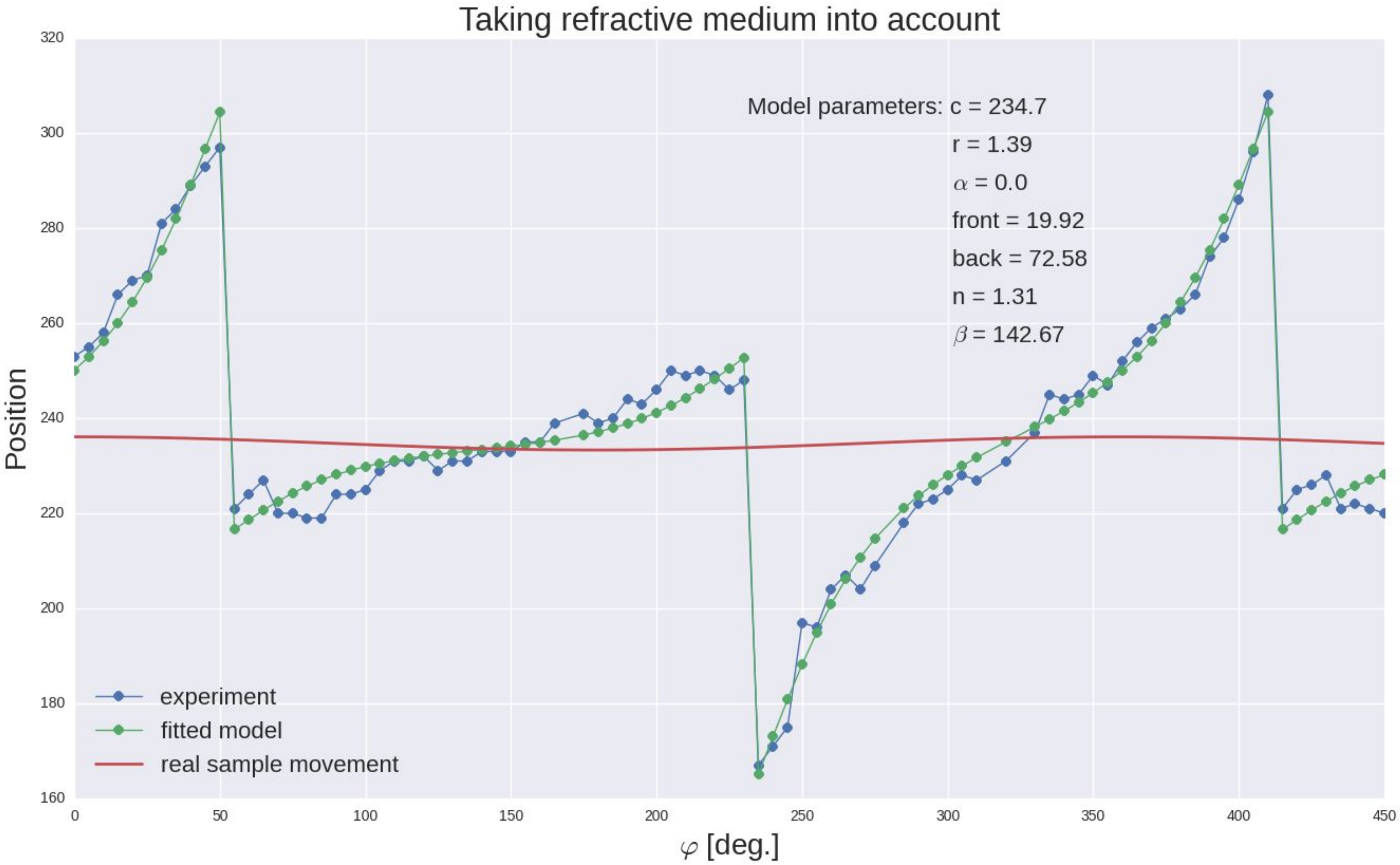
Fitting a circle
experiment
fitted model
Model parameters: c = 235.148384913
r = 17.5270862289
$\alpha$ = 34.07
$y = c + r * cos(\varphi - \alpha)$
Position
$\varphi$ [deg.]
320
300
280
260
240
220
200
180
160
0
50
100
150
200
250
300
350
400
450

# Slab model

$$i = arcsin(sin(\frac{\varphi}{n})) - \beta$$

$$y_{corr} = y - \frac{front * sin(\varphi - i)}{cos(i)}$$

$$y_{corr} = y - \frac{back * sin(-\varphi - i)}{cos(i)}$$



Taking refractive medium into account
Model parameters: c = 234.7
r = 1.39
$\alpha$ = 0.0
front = 19.92
back = 72.58
n = 1.31
$\beta$ = 142.67
experiment
fitted model
real sample movement
Position
$\varphi$ [deg.]
320
300
280
260
240
220
200
180
160
0
50
100
150
200
250
300
350
400
450

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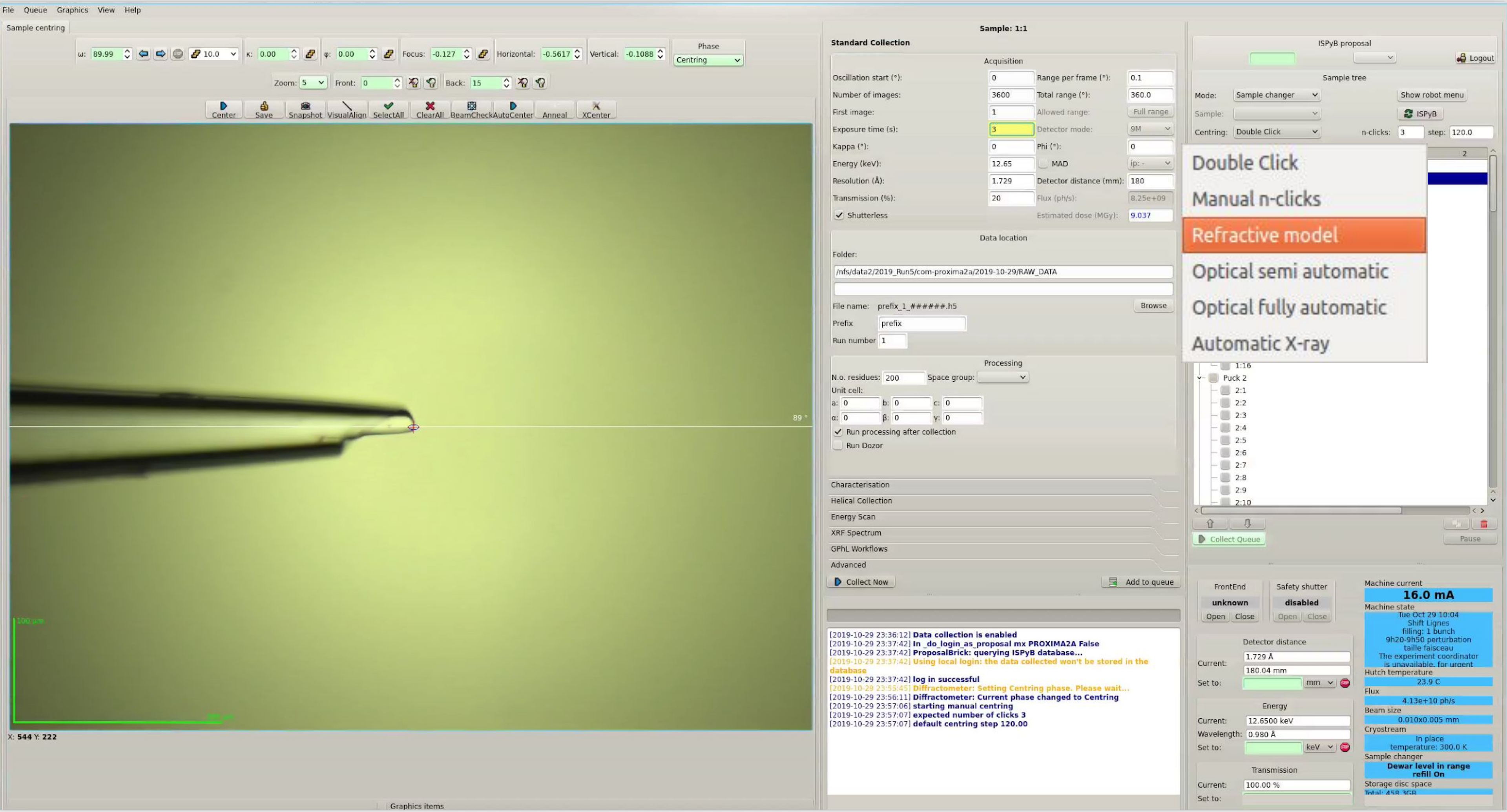
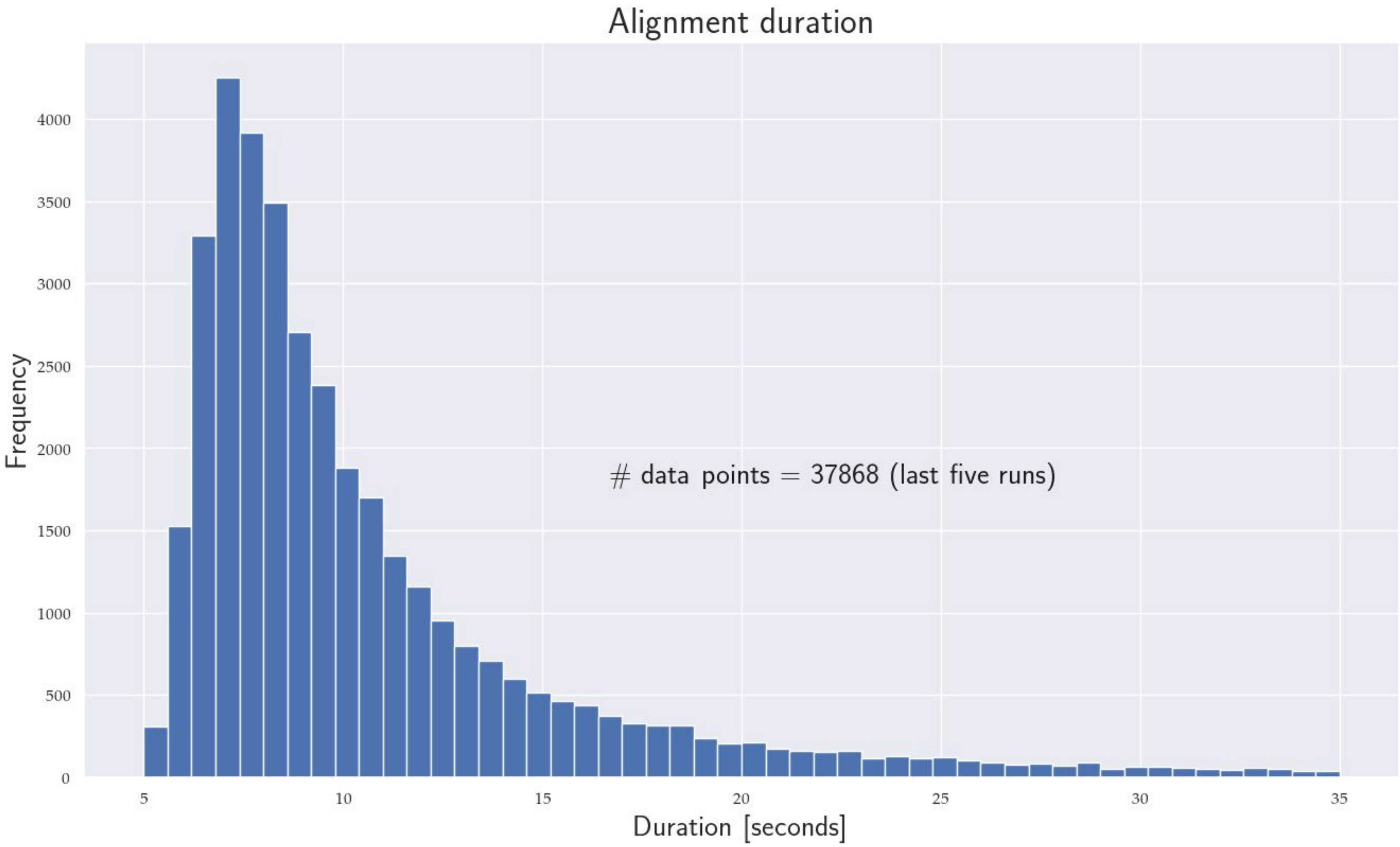
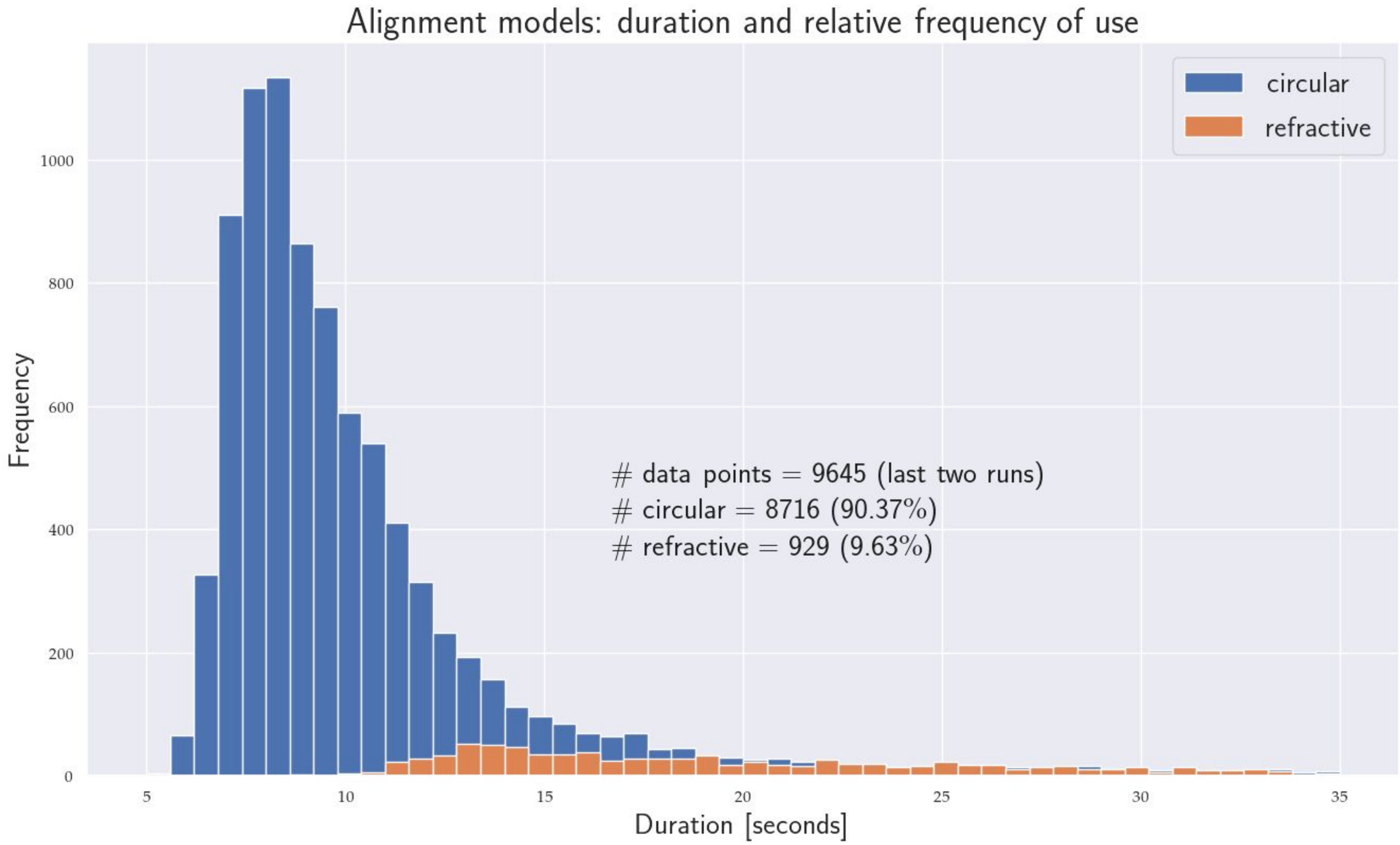
- sample supply
  - user scheduling


File Queue Graphics View Help
Sample centring
ω: 89.99
10.0
κ: 0.00
φ: 0.00
Focus: -0.127
Horizontal: -0.5617
Vertical: -0.1088
Phase
Centring
Zoom: 5
Front: 0
Back: 15
Center
Save
Snapshot
VisualAlign
SelectAll
ClearAll
BeamCheck
AutoCenter
Anneal
XCenter
89 °
X: 544 Y: 222
Graphics items
Sample: 1:1
Standard Collection
Acquisition
Oscillation start (°): 0
Range per frame (°): 0.1
Number of images: 3600
Total range (°): 360.0
First image: 1
Allowed range:
Full range
Exposure time (s): 3
Detector mode: 9M
Kappa (°): 0
Phi (°): 0
Energy (keV): 12.65
MAD
Resolution (Å): 1.729
Detector distance (mm): 180
Transmission (%): 20
Flux (ph/s): 8.25e+09
Shutterless
Estimated dose (MGy): 9.037
Data location
Folder:
/nfs/data2/2019_Run5/com-proxima2a/2019-10-29/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
GPhL Workflows
Advanced
Collect Now
Add to queue
[2019-10-29 23:36:12] Data collection is enabled
[2019-10-29 23:37:42] In _do_login_as_proposal mx PROXIMA2A False
[2019-10-29 23:37:42] ProposalBrick: querying ISPyB database...
[2019-10-29 23:37:42] Using local login: the data collected won't be stored in the database
[2019-10-29 23:37:42] log in successful
[2019-10-29 23:55:45] Diffractometer: Setting Centring phase. Please wait...
[2019-10-29 23:56:11] Diffractometer: Current phase changed to Centring
[2019-10-29 23:57:06] starting manual centring
[2019-10-29 23:57:07] expected number of clicks 3
[2019-10-29 23:57:07] default centring step 120.00
ISPyB proposal
Logout
Sample tree
Mode: Sample changer
Show robot menu
Sample:
ISPyB
Centring: Double Click
n-clicks: 3
step: 120.0
Double Click
Manual n-clicks
Refractive model
Optical semi automatic
Optical fully automatic
Automatic X-ray
1:16
Puck 2
2:1
2:2
2:3
2:4
2:5
2:6
2:7
2:8
2:9
2:10
Collect Queue
Pause
FrontEnd
unknown
Open Close
Safety shutter
disabled
Open Close
Machine current
16.0 mA
Machine state
Tue Oct 29 10:04
Shift Lignes
filling: 1 bunch
9h20-9h50 perturbation
taille faisceau
The experiment coordinator
is unavailable. for urgent
Hutch temperature
23.9 C
Flux
4.13e+10 ph/s
Beam size
0.010x0.005 mm
Cryostream
In place
temperature: 300.0 K
Sample changer
Dewar level in range
refill On
Storage disc space
Detector distance
Current: 1.729 Å
180.04 mm
Set to:
mm
Energy
Current: 12.6500 keV
Wavelength: 0.980 Å
Set to:
keV
Transmission
Current: 100.00 %
Set to:



Alignment duration
Frequency
0
500
1000
1500
2000
2500
3000
3500
4000
5
10
15
20
25
30
35
Duration [seconds]
# data points = 37868 (last five runs)


Alignment models: duration and relative frequency of use
circular
refractive
# data points = 9645 (last two runs)
# circular = 8716 (90.37%)
# refractive = 929 (9.63%)
Frequency
1000
800
600
400
200
0
5
10
15
20
25
30
35
Duration [seconds]

```python
if self.centring_method != CENTRING_METHOD.REFRACTIVE:
    initial_parameters = [4.0, 25.0, 0.05]
    fit_y = minimize(
        self.circle_model_residual,
        initial_parameters,
        method="nelder-mead",
        args=(angles, vertical_discplacements),
    )

    c, r, alpha = fit_y.x
    c *= 1e-3
    r *= 1.0e-3
    v = {"c": c, "r": r, "alpha": alpha}

else:
    initial_parameters = lmfit.Parameters()
    initial_parameters.add_many(
        ("c", 0.0, True, -5e3, +5e3, None, None),
        ("r", 0.0, True, 0.0, 4e3, None, None),
        ("alpha", -np.pi / 3, True, -2 * np.pi, 2 * np.pi, None, None),
        ("front", 0.01, True, 0.0, 1.0, None, None),
        ("back", 0.005, True, 0.0, 1.0, None, None),
        ("n", 1.31, True, 1.29, 1.33, None, None),
        ("beta", 0.0, True, -2 * np.pi, +2 * np.pi, None, None),
    )

    fit_y = lmfit.minimize(
        self.refractive_model_residual,
        initial_parameters,
        method="nelder",
        args=(angles, vertical_discplacements),
    )
```

```python
def circle_model(self, angles, c, r, alpha):
    return c + r * np.cos(angles - alpha)

def i(self, t, n):
    return np.arcsin(np.sin(t) / n)

def planparallel_shift(self, depth, t, n, sense=1):
    i = self.i(t, n)
    return -depth * np.sin(sense * t - i) / np.cos(i)

def shift(self, t, f, b, n, beta):
    t = t - beta
    dt = np.degrees(t)
    s = np.zeros(dt.shape)
    t_base = t % (2 * np.pi)
    mask = np.where(((t_base < 3 * np.pi / 2) & (t_base >= np.pi / 2)), 1, 0)
    s[mask == 0] = self.planparallel_shift(f, t_base[mask == 0], n, sense=1)
    s[mask == 1] = self.planparallel_shift(b, t_base[mask == 1], n, sense=-1)
    return s
```

```python
def refractive_model(self, t, c, r, alpha, front, back, n, beta):
    return self.circle_model(t, c, r, alpha) - self.shift(t, front, back, n, beta)
```

https://github.com/mxcube/HardwareRepository/blob/master/HardwareObjects/SOLEIL/PX2/PX2Diffractometer.py

# Acknowledgements

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- Lidia Ciccone
- Adam Simpkin
- Igor Chaussavoine
- Denis Duran
- Patrick Gourhant
- Idrissou Chado