SOLEIL status update

Dan Costin & Martin Savko

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Synchrotron SOLEIL

- energy: 2.75 GeV
- current: 500 mA
- electron beam lifetime: ~11 hours
- circumference: 354 m
- emittance (horizontal, vertical): 3.7×10^{-9}, 11×10^{-12} m.rad
- brilliance: 10^{20} ph.s^{-1}.mrad^{-1}.mm^{-2} @ 0.1% bandwidth

- founded in 2001, in operation since 2006
- funded jointly by CNRS (72%) and CEA (28%)
- 350 employees

Proxima 1

Source: **U20** in vacuum undulator

Focussing: KB, **CRL**, **20x40 µm, project for new KB mirrors**

Tunable: Si 111 CCM, 5.5 - 15.5 keV

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

Area Detector: **Eiger X 16M**

XRF Detector: Ketek AXAS-M2 **H150** (XIA)

OAV Camera: Prosilica GC 1350 (4.65um, 1360x1024)

Goniometer: **SmarGon**

Sample Changer: CATS (**48 cryo, 16 ambient**) **Looking into getting a bigger dewar !**

MXCuBE: Qt4 v 2.3 (**CentOS 7**), HardwareRepository, Python 2.7

Proxima 2A

Source: **U24** in vacuum undulator

Focussing: KB, **horizontal PFM, 5x10 µm**

Tunable: Si 111 CCM, 5.5 - 18.5 keV

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

Area Detector: **Eiger X 9M**

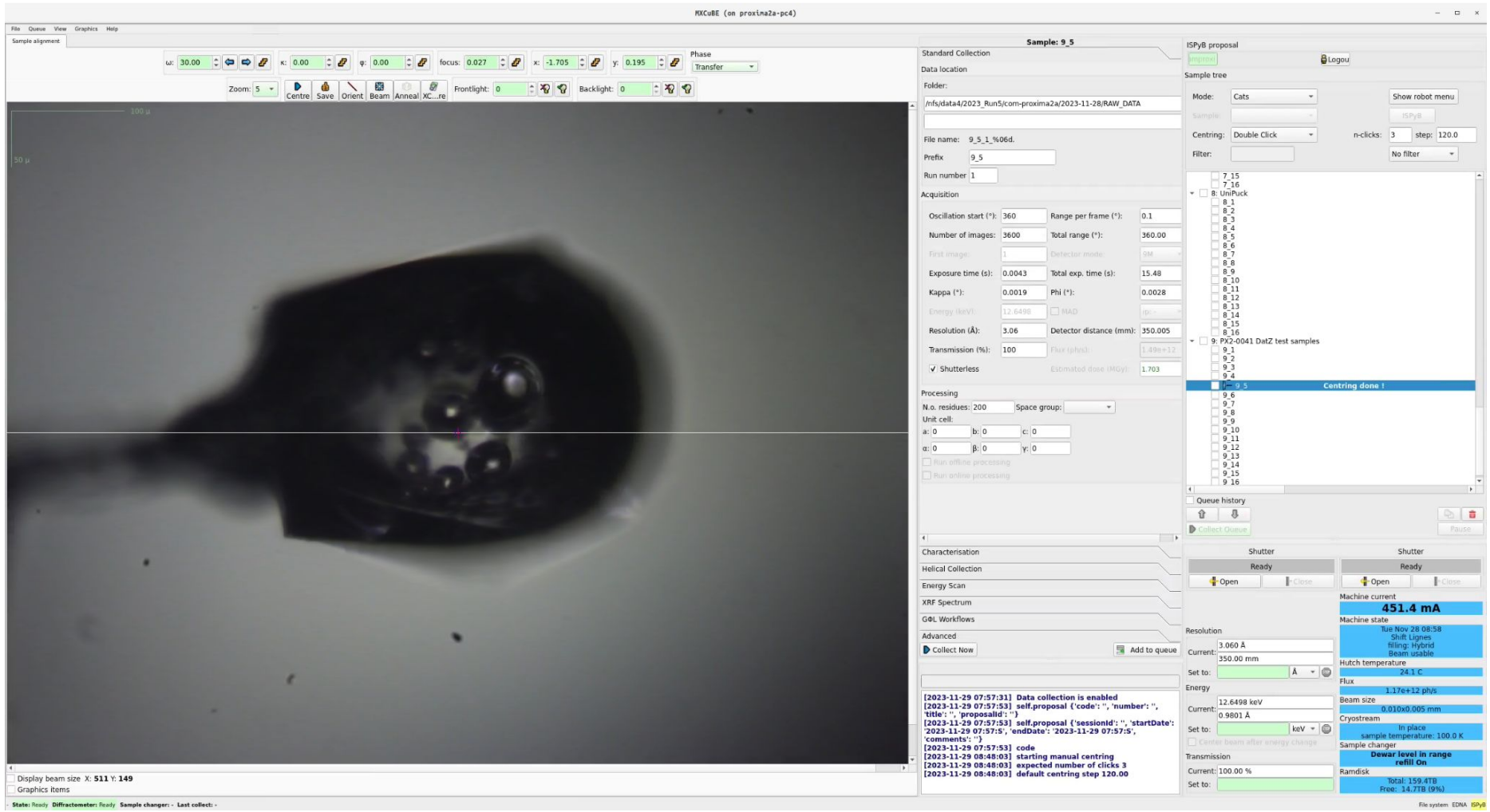
XRF Detector: Ketek AXAS-M2 **H80** (XIA, Xpress3)

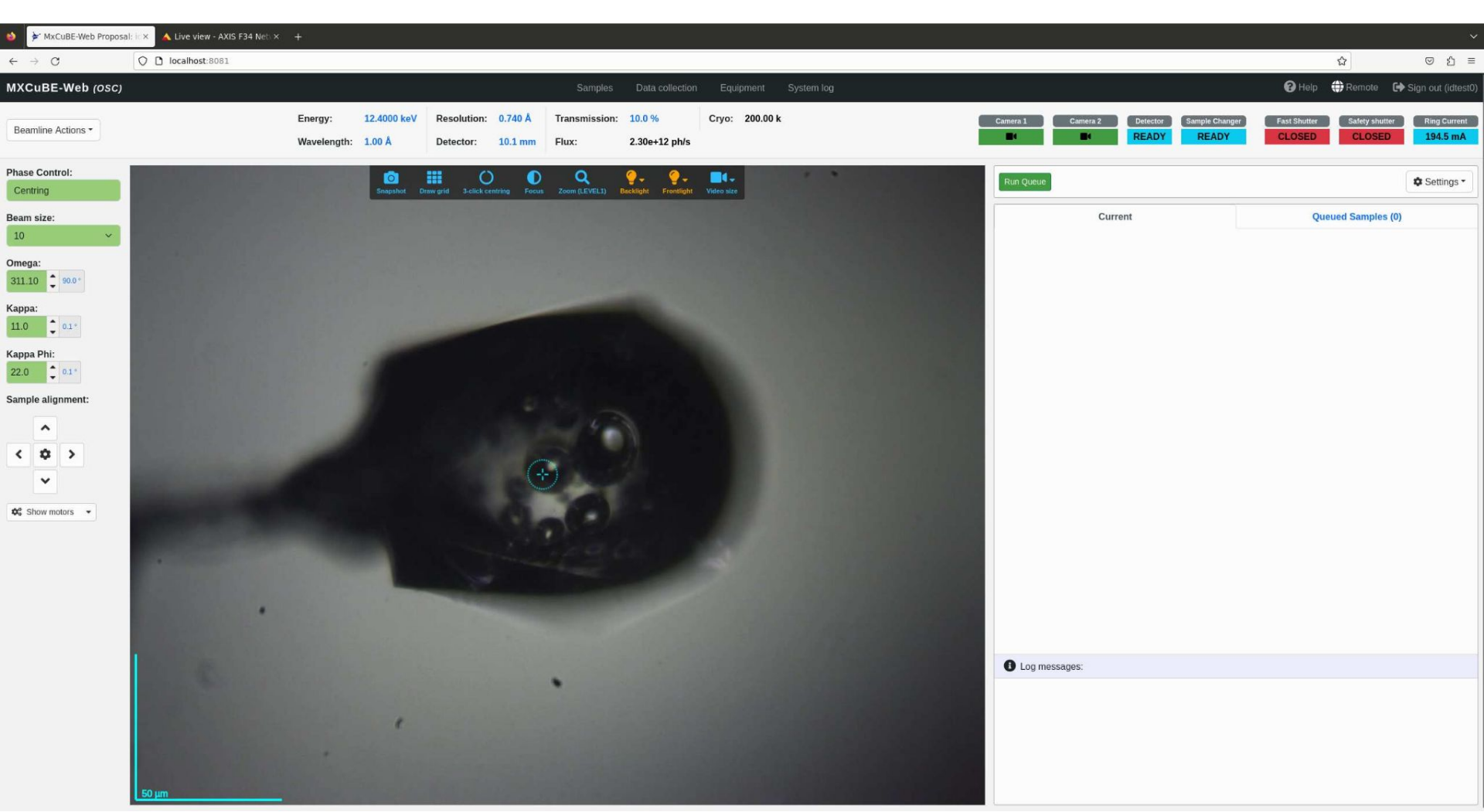
OAV Camera: **MAKO G-192C (4.50um, 1600x1200)**

Goniometer: **MD2 with minikappa (MK3), Plate Screener, HC/REX installed, MD3 coming next December !**

Sample Changer: CATS (**144 cryo, 48 ambient**)

MXCuBE: Qt5 (**Ubuntu 20.04**), mxcubecore, Python 3.8


MXCuBE (on proxima2a-pc4)
File Queue View Graphics Help
Sample alignment
ω: 30.00 κ: 0.00 φ: 0.00 focus: 0.027 x: -1.705 y: 0.195 Phase Transfer
Zoom: 5 Centre Save Orient Beam Anneal XC...re Frontlight: 0 Backlight: 0
100 µ
50 µ
Display beam size X: 511 Y: 149
Graphics items
State: Ready Diffractometer: Ready Sample changer: - Last collect: -
Sample: 9_5
Standard Collection
Data location
Folder:
/nfs/data4/2023_Run5/com-proxima2a/2023-11-28/RAW_DATA
File name: 9_5_1_%06d.
Prefix 9_5
Run number 1
Acquisition
Oscillation start (°): 360 Range per frame (°): 0.1
Number of images: 3600 Total range (°): 360.00
First image: 1 Detector mode:
Exposure time (s): 0.0043 Total exp. time (s): 15.48
Kappa (°): 0.0019 Phi (°): 0.0028
Energy (keV): 12.6498 MAD
Resolution (Å): 3.06 Detector distance (mm): 350.005
Transmission (%): 100 Flux (ph/s): 1.49e+12
Shutterless Estimated dose (MGy): 1.703
Processing
N.o. residues: 200 Space group:
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0
Run offline processing
Run online processing
Characterisation
Helical Collection
Energy Scan
XRF Spectrum
GΦL Workflows
Advanced
Collect Now
Add to queue
[2023-11-29 07:57:31] Data collection is enabled
[2023-11-29 07:57:53] self.proposal {'code': '', 'number': '', 'title': '', 'proposalId': ''}
[2023-11-29 07:57:53] self.proposal {'sessionId': '', 'startDate': '2023-11-29 07:57:5', 'endDate': '2023-11-29 07:57:5', 'comments': ''}
[2023-11-29 08:48:03] code
[2023-11-29 08:48:03] starting manual centring
[2023-11-29 08:48:03] expected number of clicks 3
[2023-11-29 08:48:03] default centring step 120.00
ISPyB proposal
Logou
Sample tree
Mode: Cats
Show robot menu
Sample:
ISPyB
Centring: Double Click
n-clicks: 3 step: 120.0
Filter:
No filter
7_15
7_16
8: UniPuck
8_1
8_2
8_3
8_4
8_5
8_6
8_7
8_8
8_9
8_10
8_11
8_12
8_13
8_14
8_15
8_16
9: PX2-0041 DatZ test samples
9_1
9_2
9_3
9_4
9_5 Centring done !
9_6
9_7
9_8
9_9
9_10
9_11
9_12
9_13
9_14
9_15
9_16
Queue history
Collect Queue
Pause
Shutter
Ready
Open
Close
Shutter
Ready
Open
Close
Resolution
Current: 3.060 Å
350.00 mm
Set to:
Å
Energy
Current: 12.6498 keV
0.9801 Å
Set to:
keV
Center beam after energy change
Transmission
Current: 100.00 %
Set to:
Machine current
451.4 mA
Machine state
Tue Nov 28 08:58
Shift Lignes
filling: Hybrid
Beam usable
Hutch temperature
24.1 C
Flux
1.17e+12 ph/s
Beam size
0.010x0.005 mm
Cryostream
In place
sample temperature: 100.0 K
Sample changer
Dewar level in range
refill On
Ramdisk
Total: 159.4TB
Free: 14.77TB (9%)
File system EDNA ISPyB


MxCuBE-Web Proposal:
Live view - AXIS F34 Net
localhost:8081
MXCuBE-Web (OSC)
Samples
Data collection
Equipment
System log
Help
Remote
Sign out (idtest0)
Beamline Actions
Energy: 12.4000 keV
Wavelength: 1.00 Å
Resolution: 0.740 Å
Detector: 10.1 mm
Transmission: 10.0 %
Flux: 2.30e+12 ph/s
Cryo: 200.00 k
Camera 1
Camera 2
Detector
READY
Sample Changer
READY
Fast Shutter
CLOSED
Safety shutter
CLOSED
Ring Current
194.5 mA
Phase Control:
Centring
Beam size:
10
Omega:
311.10
Kappa:
11.0
Kappa Phi:
22.0
Sample alignment:
Show motors
Snapshot
Draw grid
3-click centring
Focus
Zoom (LEVEL1)
Backlight
Frontlight
Video size
50 µm
Run Queue
Settings
Current
Queued Samples (0)
Log messages:

Plans for the past 6 months

- Finalizing mxcubeweb adaptation
- Murko
  - diffraction raster scans prediction head: learn crystals and ice!
  - bounding box and key points in-network inference
- Volume aware experiments
  - sample shape reconstruction + 3d sample shape registration
    - expressing points, lines, planes and volumes in intrinsic coordinate system
    - fully automated sample realignment
- Concerted push for unattended data collection capability
  - first simple experimental protocol gradually employing more thorough e.g. using GPhL workflows

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GPhL Workflows integration status

- The workflows available in production since the first run of 2023
  - Development sessions June 2021, December 2021, February 2022, June 2022
  - in-house project (9 shifts, validated by research director), extended for 2023 (6 shifts)
- The newest version of the workflows available to our users.
  - MXCuBE at the most recent version.
  - We will soon boost our processing capacity -- adding 1024 CPU threads and additional GPU cards.

Issues

- Minikappa damaged September 2024
  - fixed in October
  - still some issues with false collision detection
- Monochromator controller failure November 2024
  - operating at fixed energy

Automation?

- Is there a value in automation?
  - consistent and careful evaluation of sample properties
  - encoding best practices
  - consistent and careful evaluation of the instrument performance
- Is there a danger in automation?
  - optimizing for wrong metrics (speed vs. quality)
  - loss of expertise
  - mindless experiments
  - stifling of innovation (difficult to increase capacity of a mind that thinks it is already full of knowledge)

Automation?

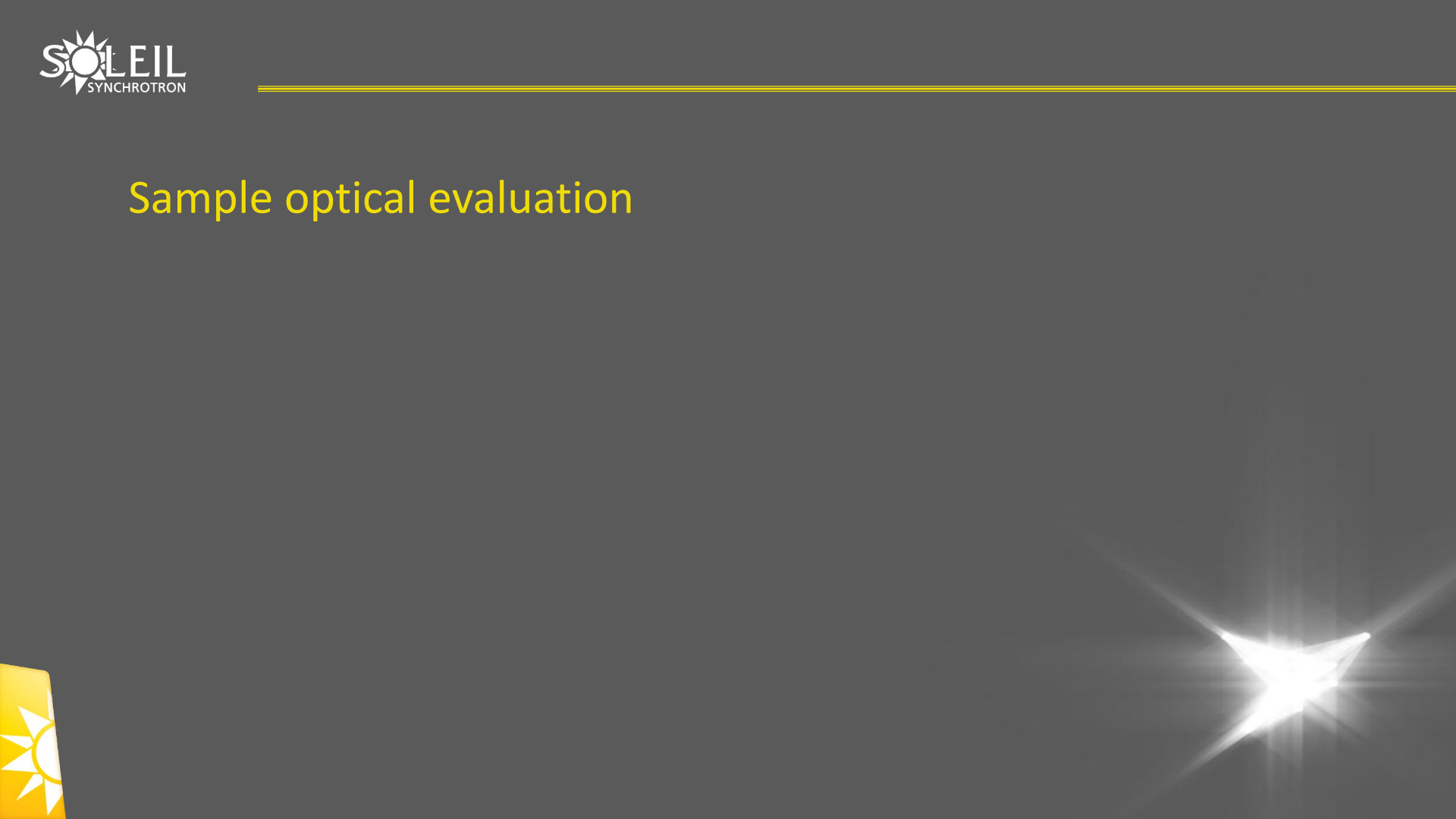
… once we have seen how to mechanize some part of our understanding, then we can also see how transcend this mechanization. [Gödel 1931, Penrose 1989]

What distinguishes reality is our inability to describe it to exhaustion [Lanier 2017]

What do we do?

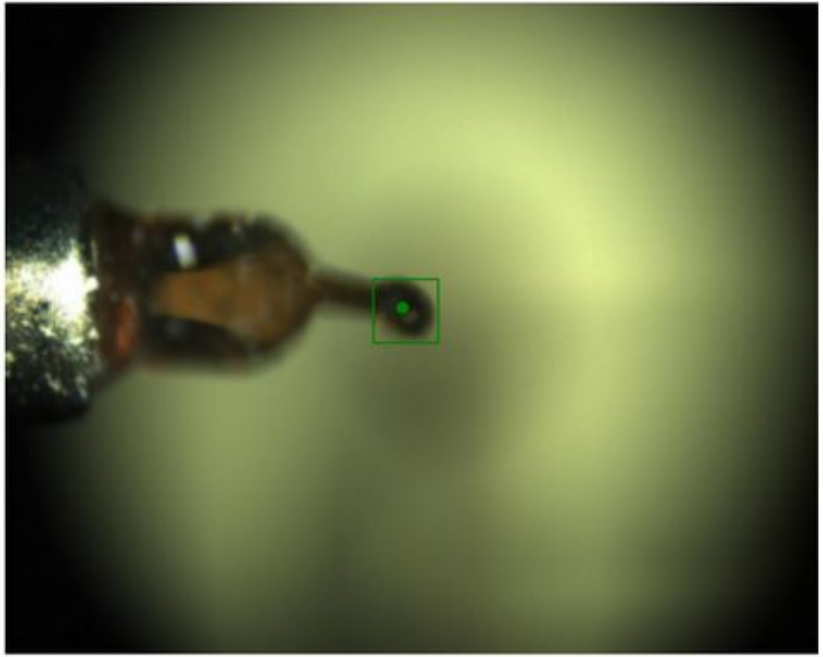
- Sample optical evaluation
  - alignment and centring
  - shape determination
- Diffraction evaluation from stills
  - diffraction tomography
  - diffraction quality mapping
- Diffraction evaluation from oscillation
  - few wedges around 360 degrees of rotation
  - resolution limit
  - strategy determination
- Full reciprocal space mapping
  - single or more sweeps of diffraction at one or more goniometer settings

Sample optical evaluation

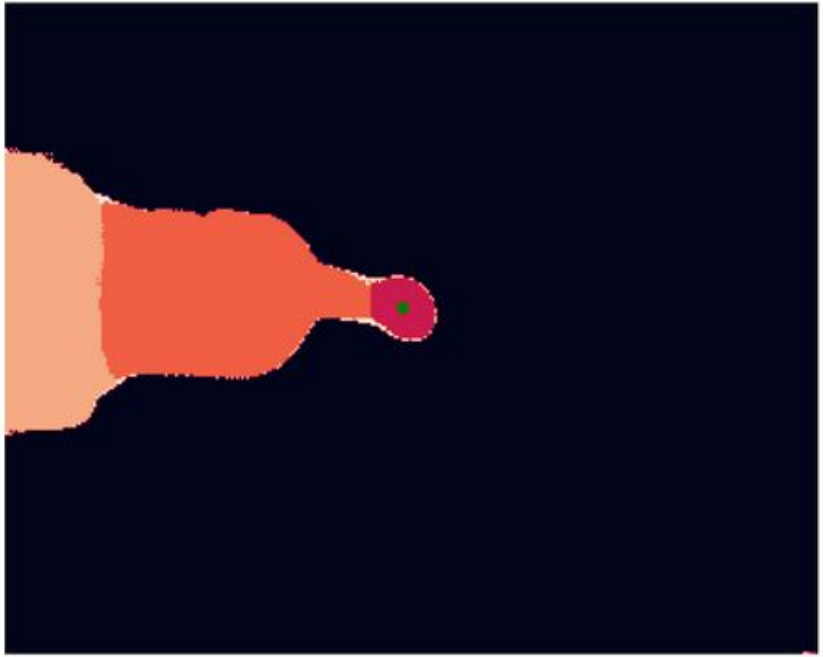


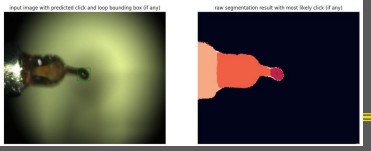
Murko - making sense of sample image

input image with predicted click and loop bounding box (if any)



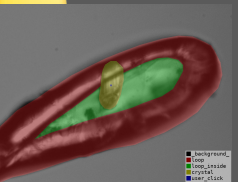
raw segmentation result with most likely click (if any)





Murko updates

- Artificial neural network based model
  - https://github.com/MartinSavko/murko
  - 103 convolutional layers, 3M parameters
  - inference time
    - ~65 ms per single image
    - ~15 ms in batch mode
  - Deployment
    - 0MQ server receives images
    - returns segmentation maps
  - New branches
    - develop, develop_keras_v3, gpu_docker
  - Collaborations
    - DESY, SLS, DLS, EMBL, MAX IV, BESSY



MartinSavko / **murko** Public

Notifications | Fork 1 | Star 0

Code | Issues | Pull requests | Actions | Projects | Security | Insights

main | Go to file | Code

Martin Savko new model example performance ... 19 minutes ago 73

examples	new model example performance	19 minutes ago
LICENSE	Initial commit	5 months ago
README.md	Update README.md	4 months ago
model.h5	update model	28 minutes ago
murko.py	move get_predictions back to murko	last month
parameters.png	param count png	5 months ago
predict.py	remove debug prints	last month
predict_server.py	update model	28 minutes ago
requirements.txt	Update requirements.txt	4 months ago

README.md

Goal

This projects aims to develop a tool to help make sense of optical images of samples people typically work with in macromolecular crystallography experiments. An approach employed at the current stage is the one using an artificial neural network. The current model is based on the architecture, normalization technique, loss definition and other key ideas from the research described in the following papers:

- The One Hundred Layers Tiramisu: Fully convolutional DenseNets for Semantic Segmentation, arXiv:1611.09326
- Xception: Deep Learning with Depthwise Separable Convolutions, arXiv:1610.02357
- Micro-Batch Training with Batch-Channel Normalization and Weight Standardization arXiv:1903.10520
- Focal loss: Focal loss for Dense Object Detection arXiv:1708.02002

About

Making sense of MX sample optical image

Readme
AGPL-3.0 license
0 stars
2 watching
1 fork
Report repository

Releases

No releases published

Packages

No packages published

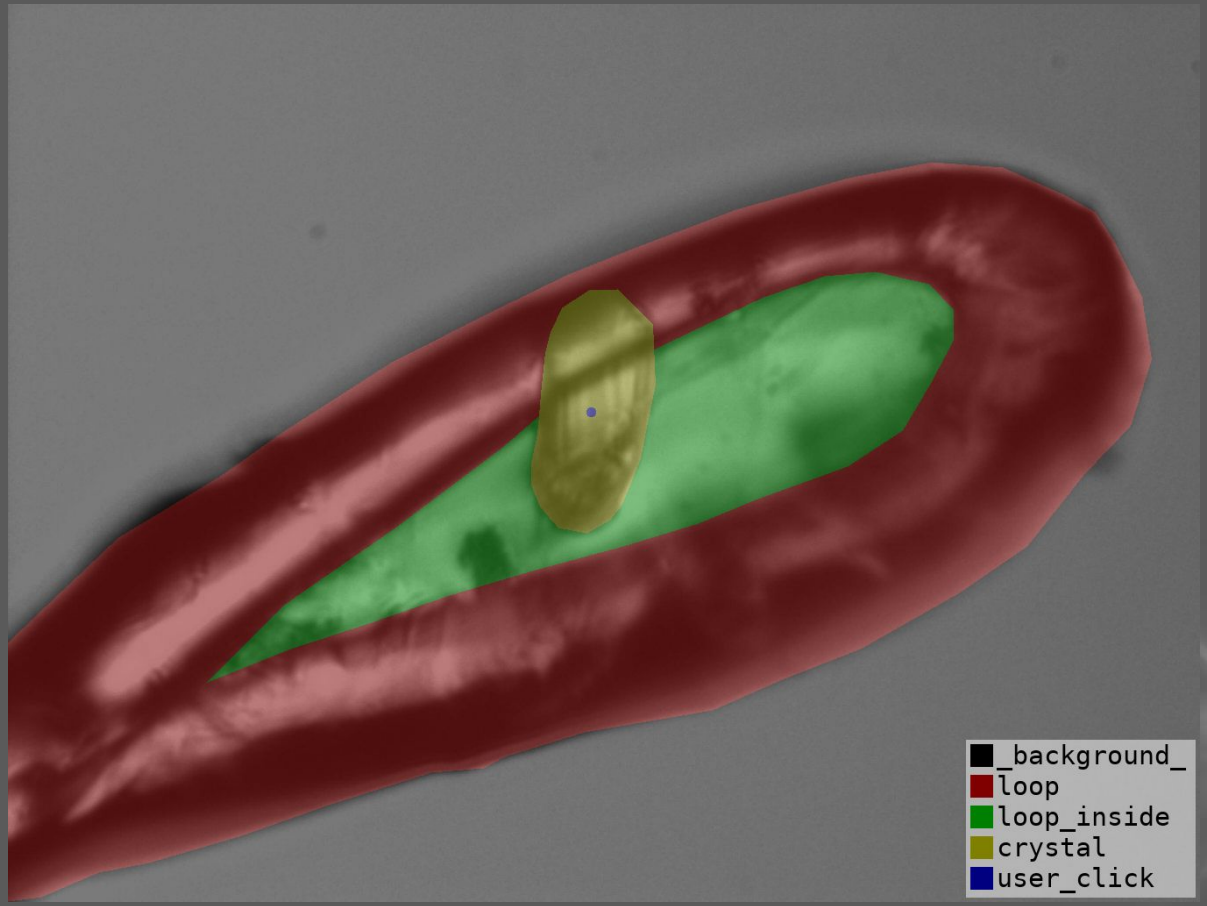
Contributors 2

MartinSavko Martin Savko
agruzinov

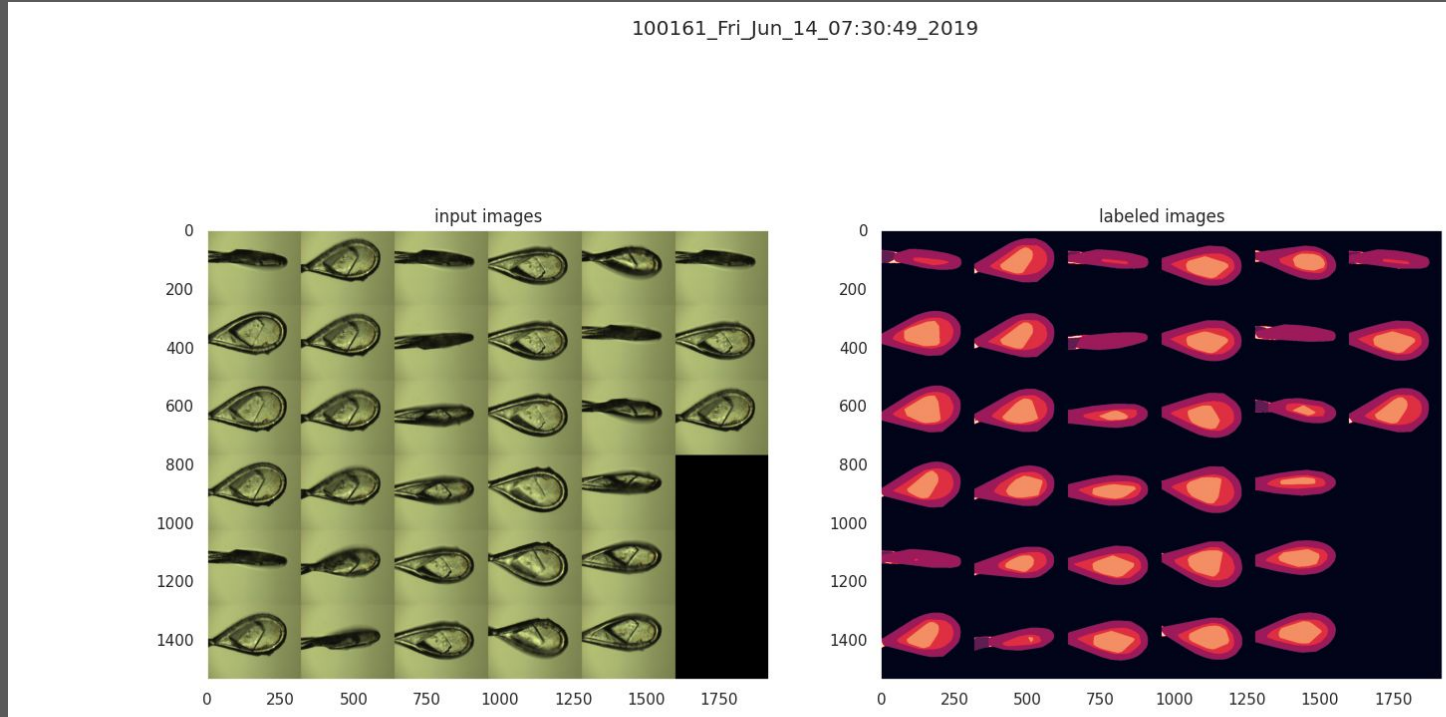
Languages

Python 100.0%

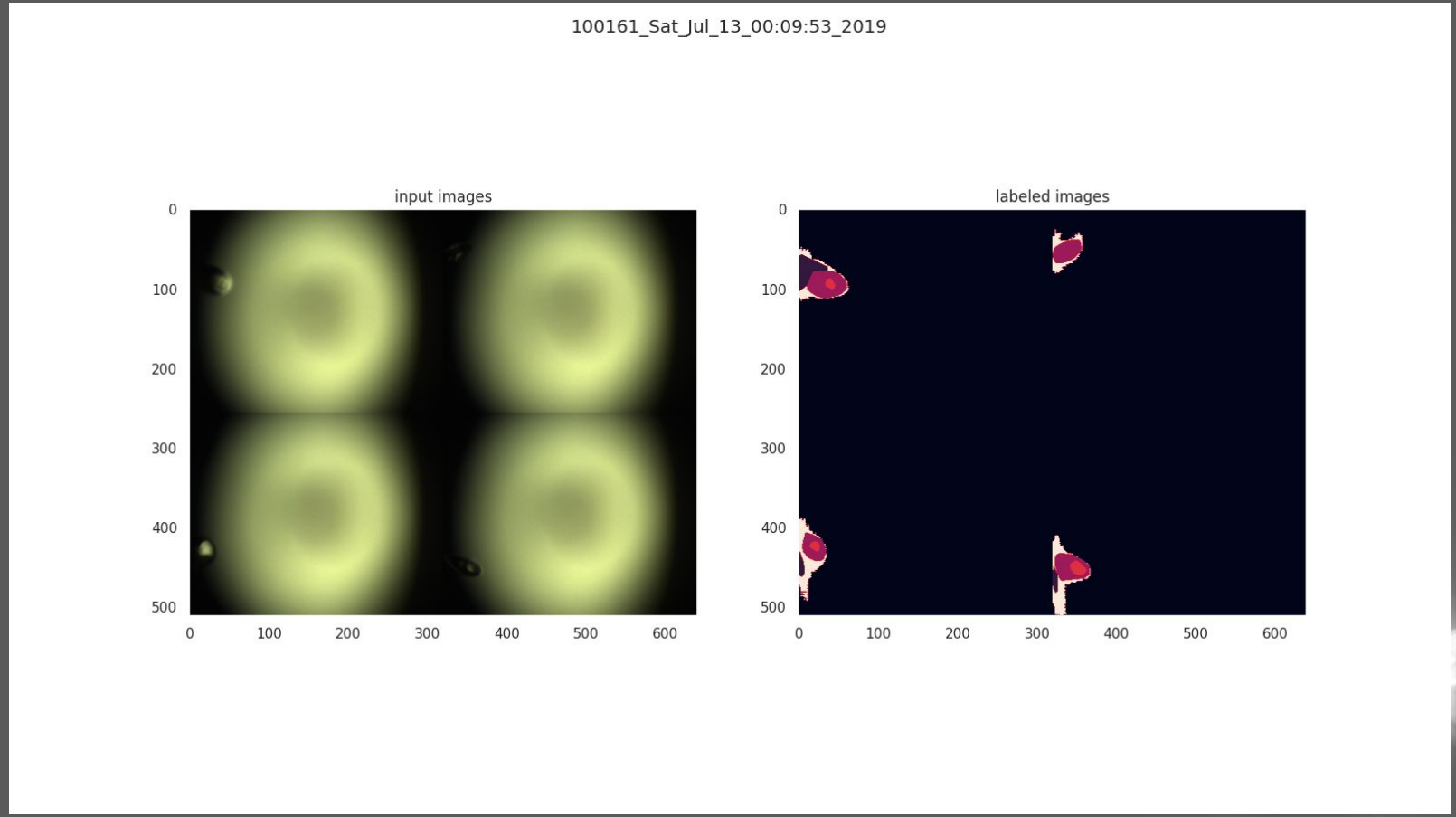
Pixelwise annotated images…



Performance

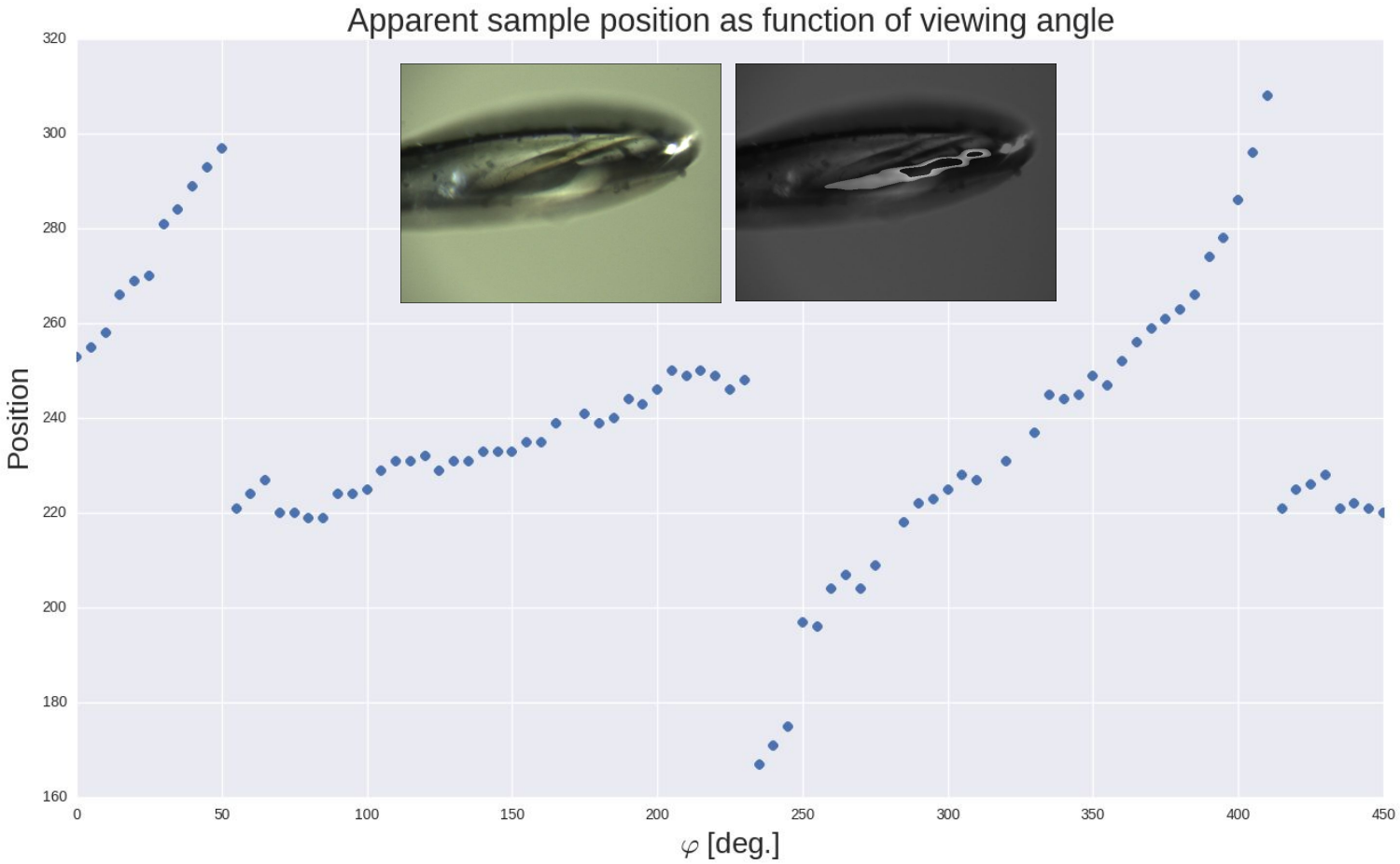


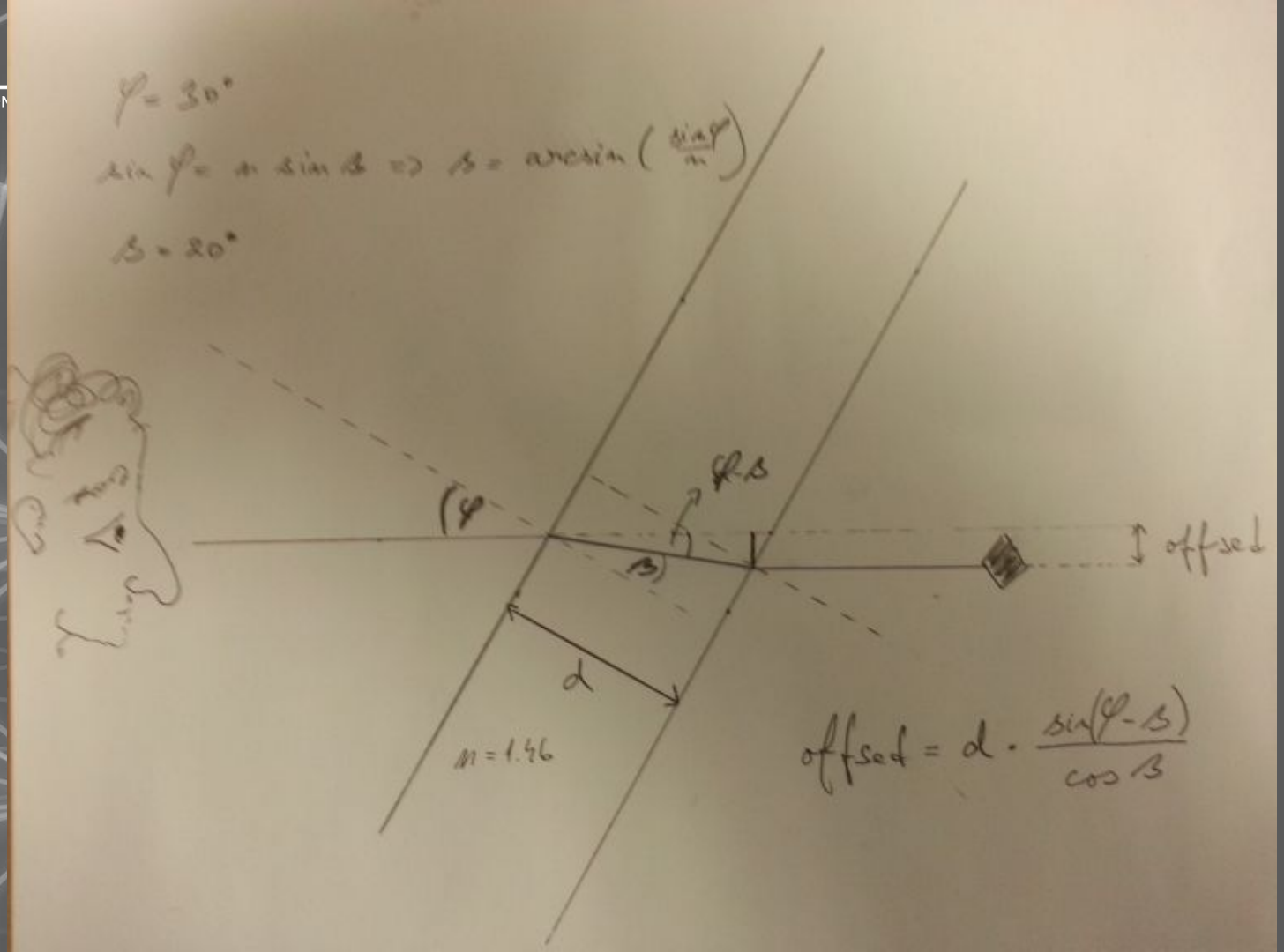
Performance



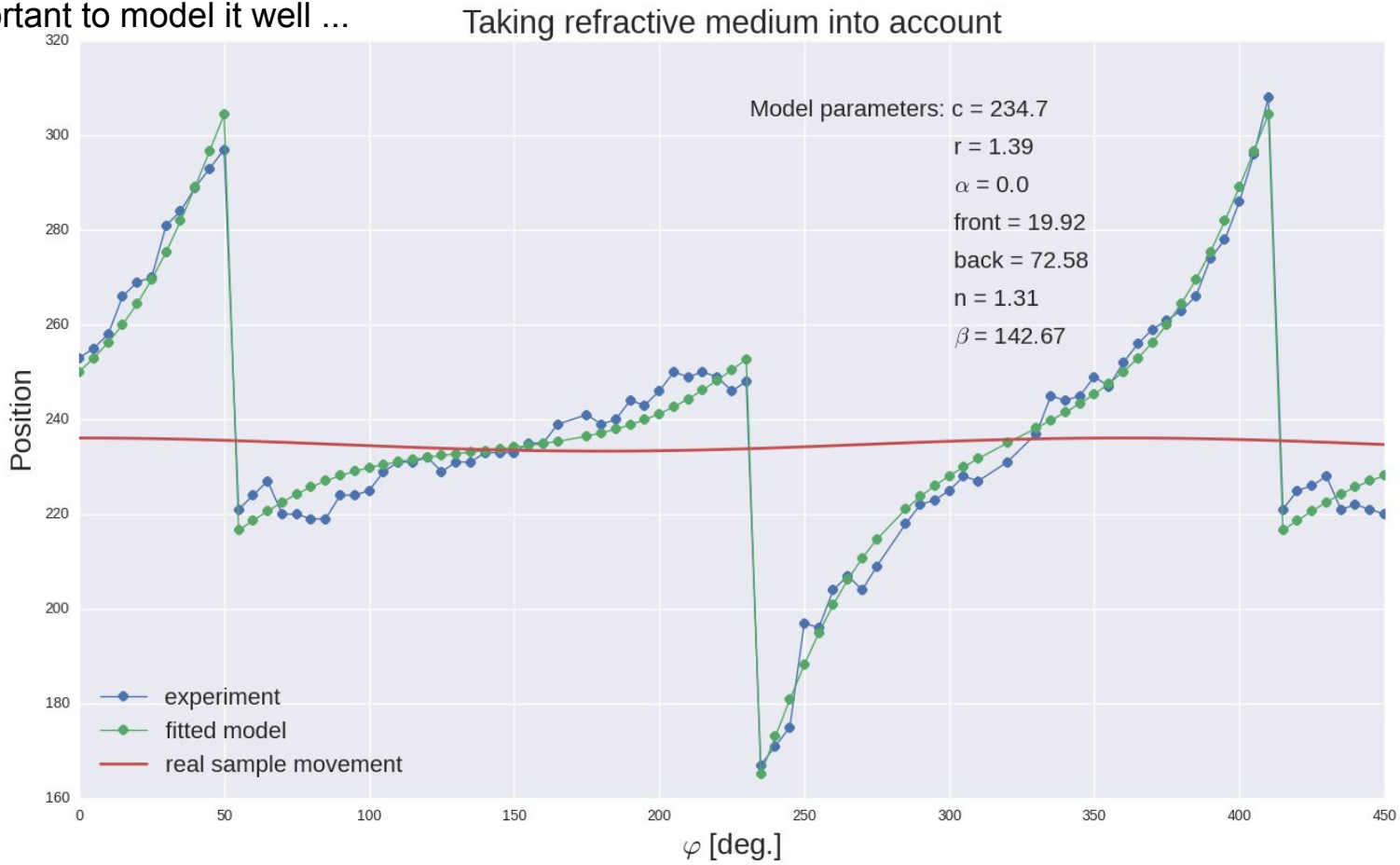
We sometimes need more accurate models of sample image movement …

- although sample moves on a circle as omega axis changes, its image almost never does (only if there is just material of refractive index of 1 around it). It follows much stranger law. Law nonetheless -- one just needs more parameters to model it …


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


φ = 30°
sin φ = n sin β ⇒ β = arcsin(sin φ / n)
β = 20°
φ
β
offset
d
n = 1.46
offset = d · sin(φ − β) / cos β

This is example of a sample aligned almost perfectly. It's image is moving across many microns … it is important to model it well ...



The Slab Model

$$i = \varphi - \beta$$

$$t = \arcsin(\frac{sin(i)}{n})$$

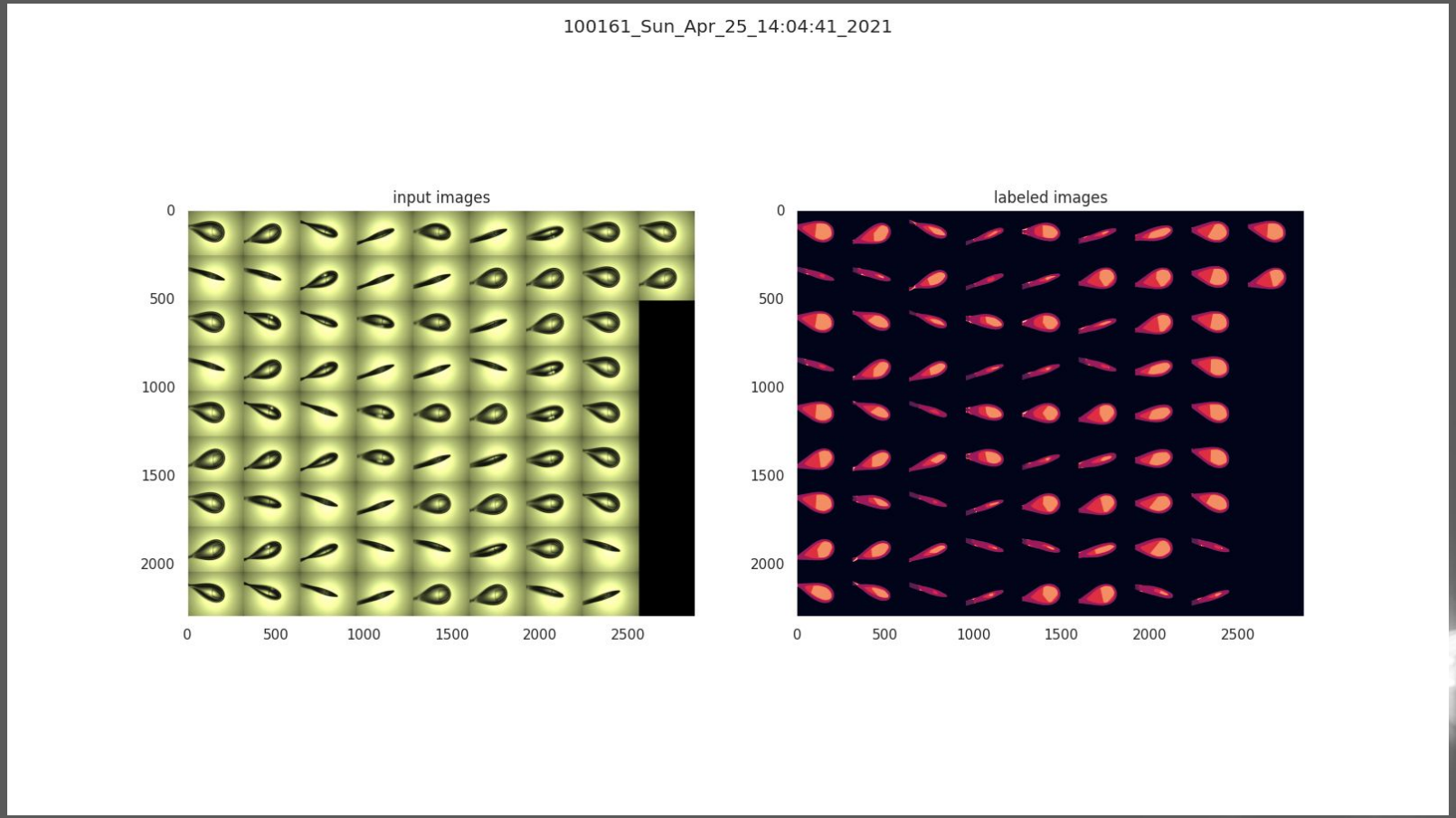
$$y_{slab} = y - \frac{d\sin(i-t)}{cos(t)}$$

The Slab Model -- two faces/two thicknesses

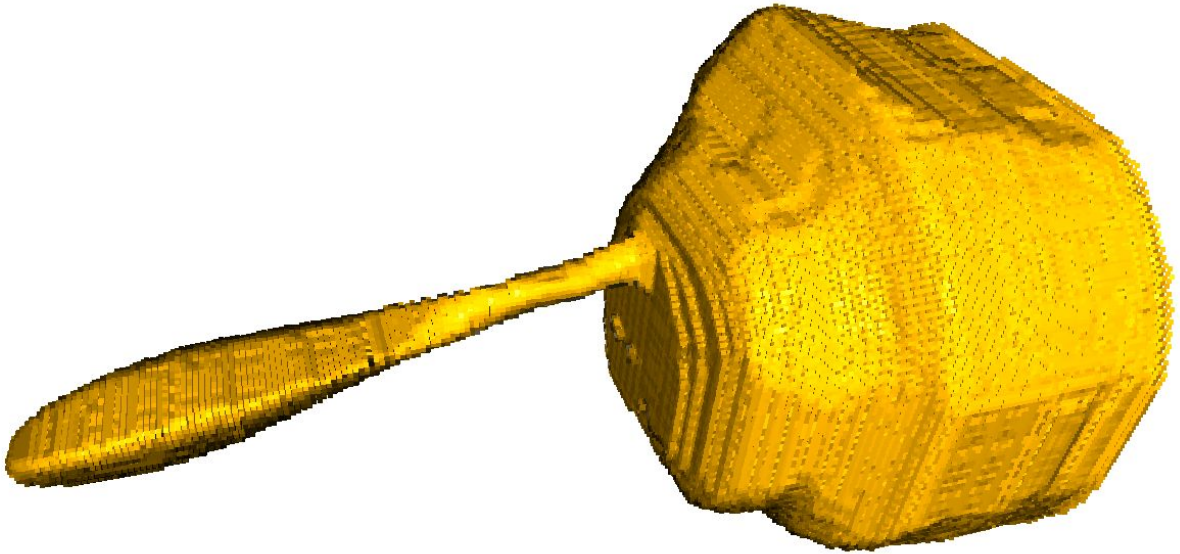
$$y_{slab} = y - \frac{d_1 \sin(i - t)}{\cos(t)} \qquad -\frac{\pi}{2} < i \leq \frac{\pi}{2}$$

$$y_{slab} = y - \frac{d_2 \sin(-i - t)}{\cos(t)} \qquad \frac{\pi}{2} < i \leq \frac{3\pi}{2}$$

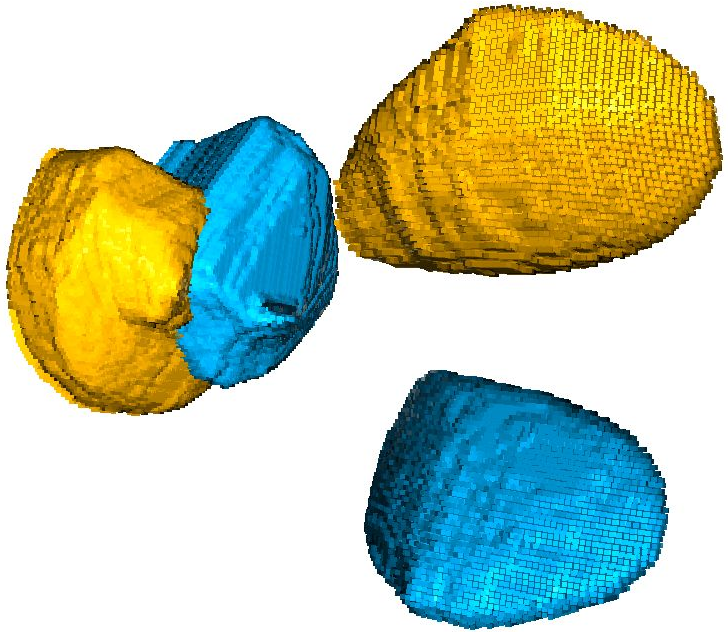
Performance



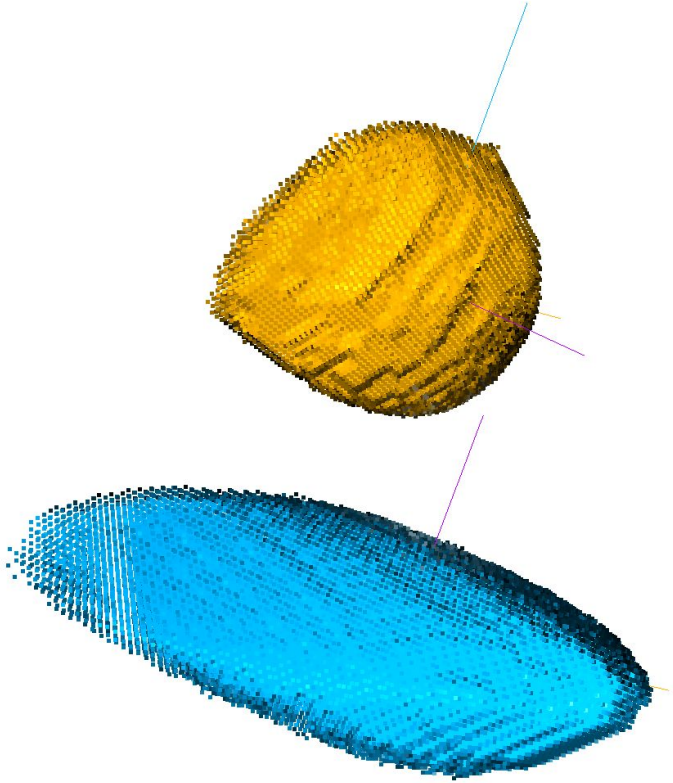
Reconstructed sample shape



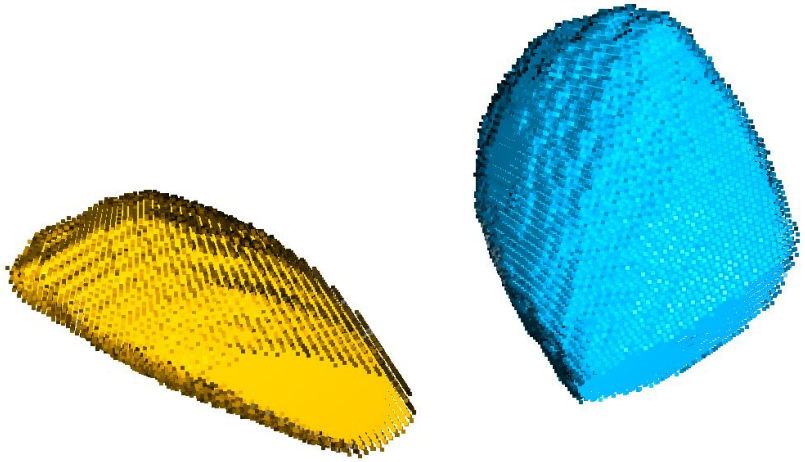
Perfect realignment: input volumes



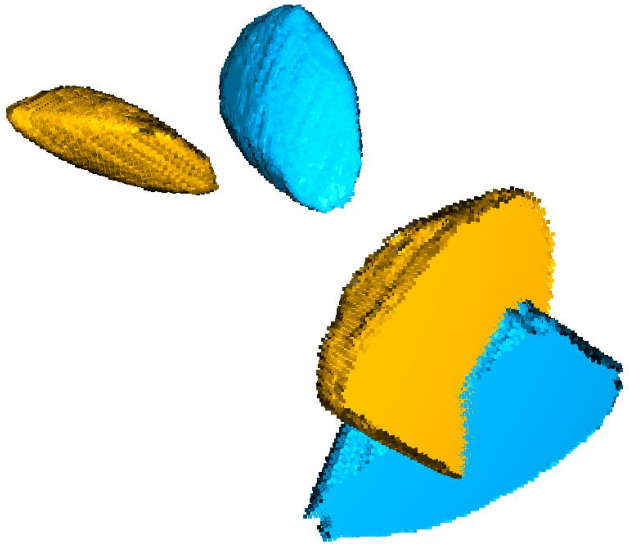
Perfect realignment: parts in focus



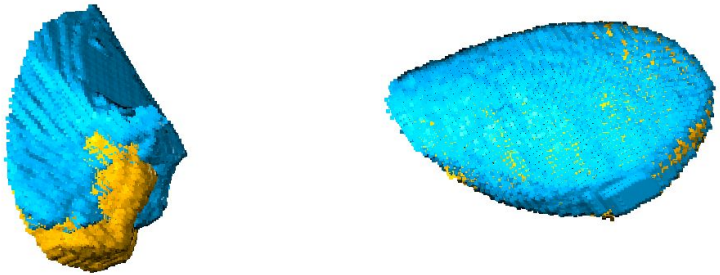
Perfect realignment: in focus, equal volumes



Perfect realignment: parts in both, for validation

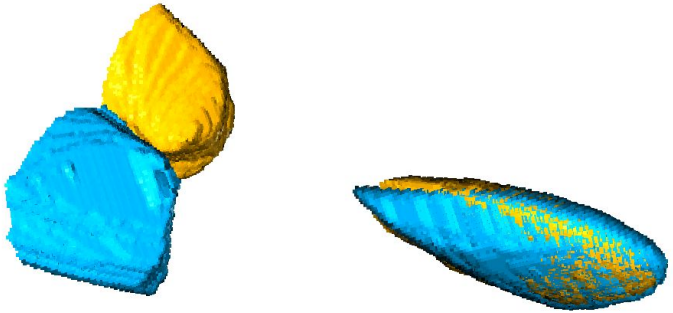


Perfect realignment: coherent axis direction



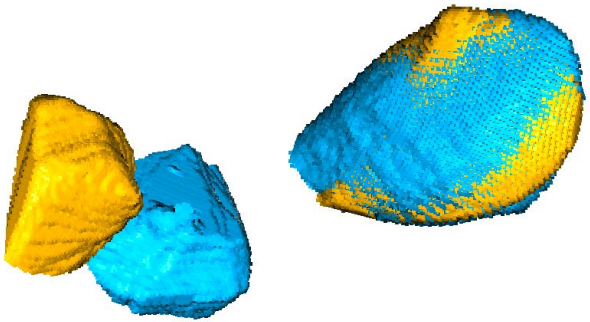
rmsd: 0.0093

Perfect realignment: coherent axis direction



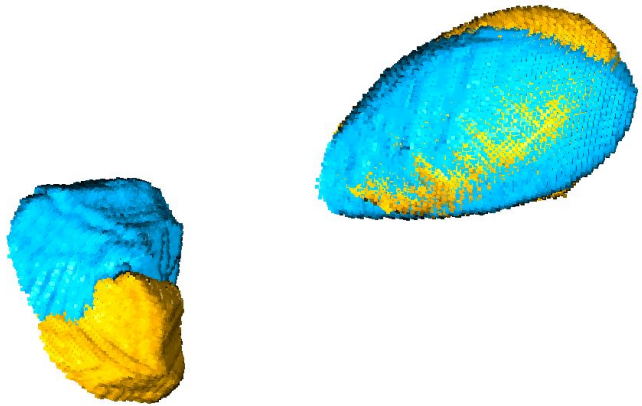
rmsd: 0.0787

Perfect realignment: coherent axis direction



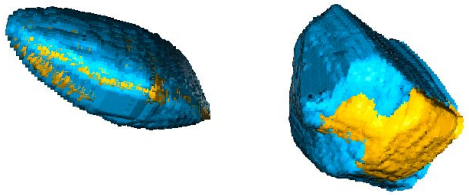
rmsd: 0.0888

Perfect realignment: coherent axis direction



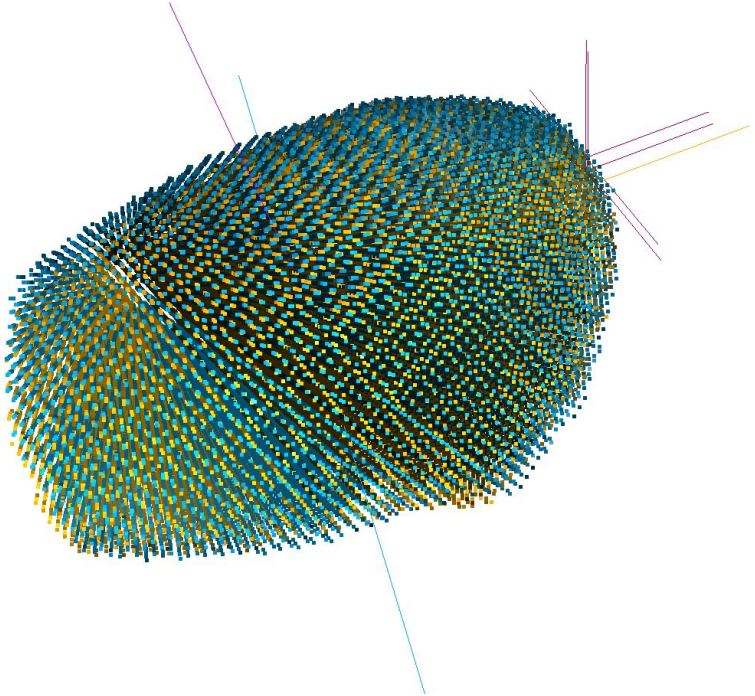
rmsd: 0.0229

Perfect realignment: coherent directions found!



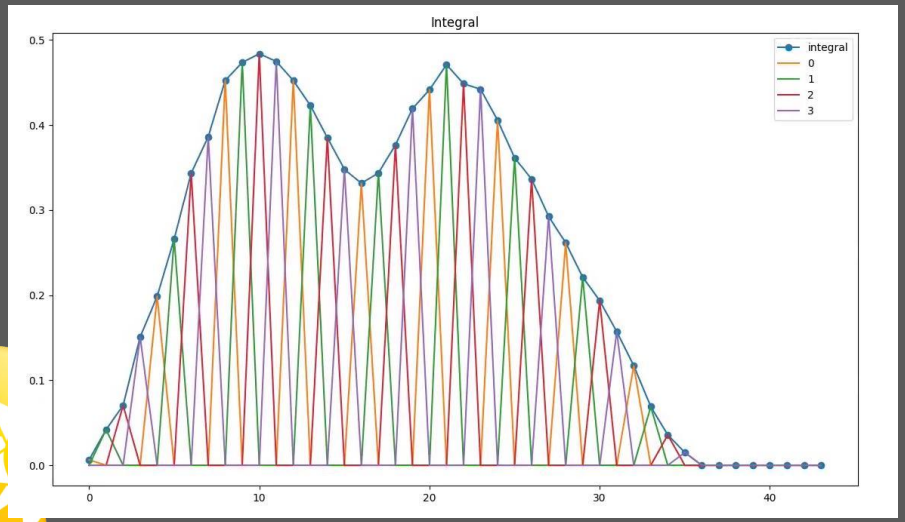
rmsd: 0.0093

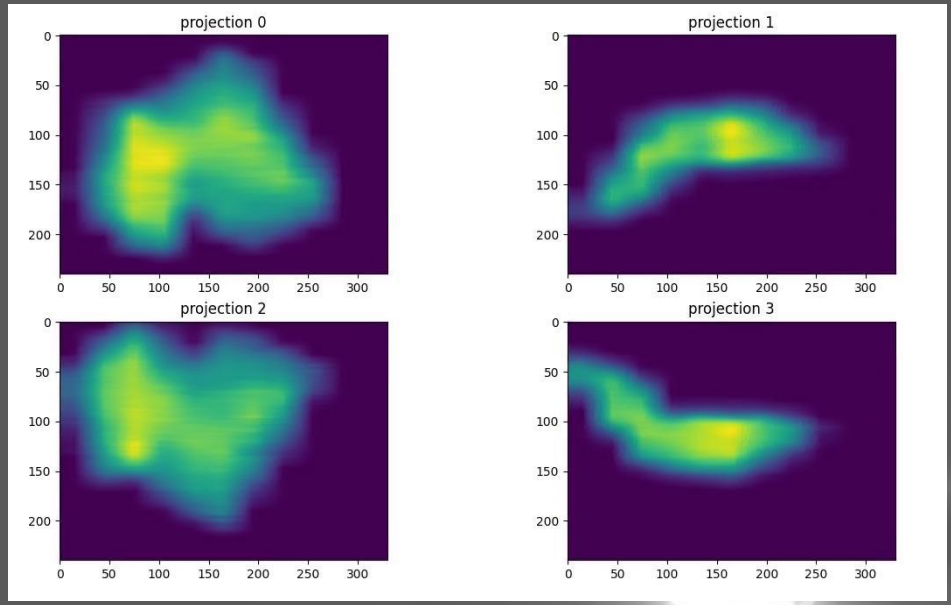
Perfect realignment: done!



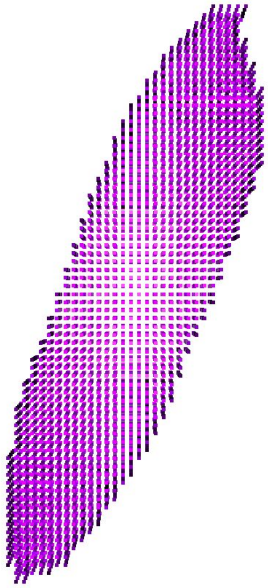
Sample evaluation from diffraction stills

Sample evaluation from diffraction stills

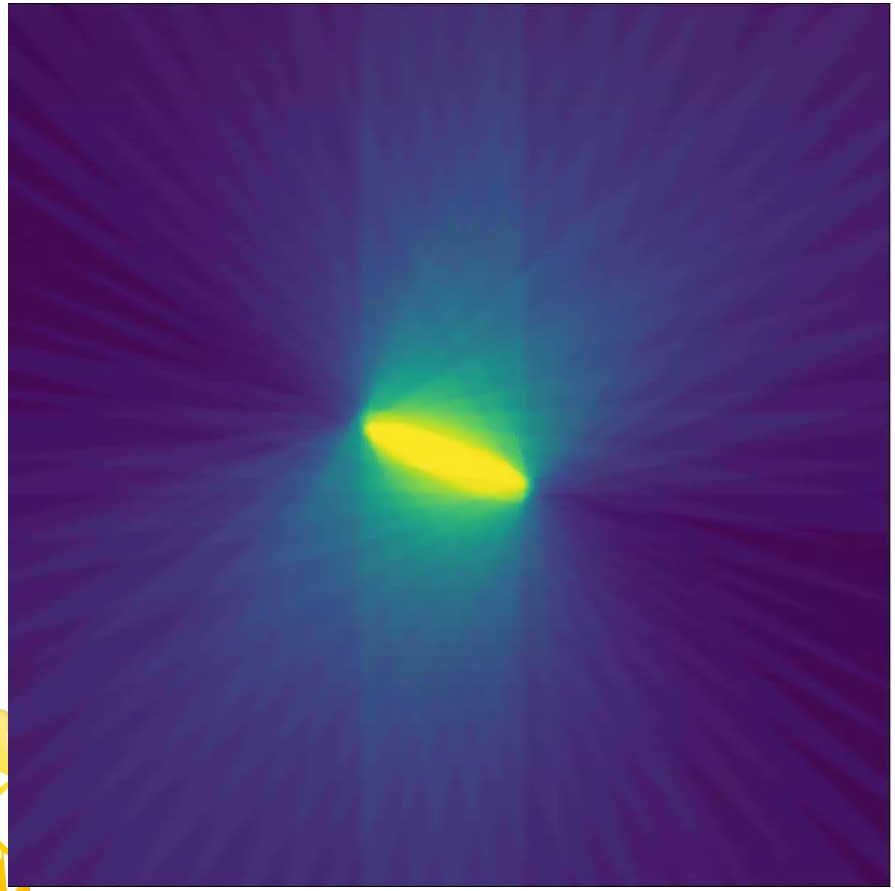




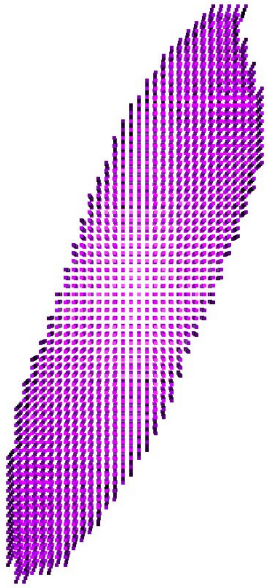
Reconstructed crystal shape (36 projections)



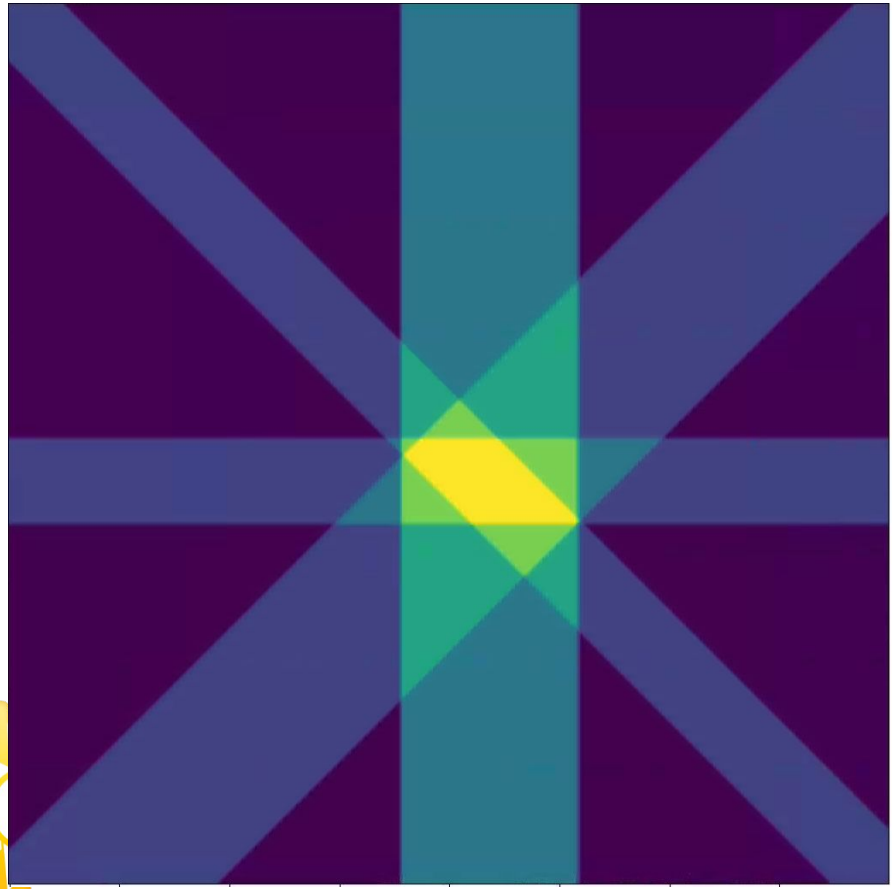
Reconstructing crystal shape (36 projections)

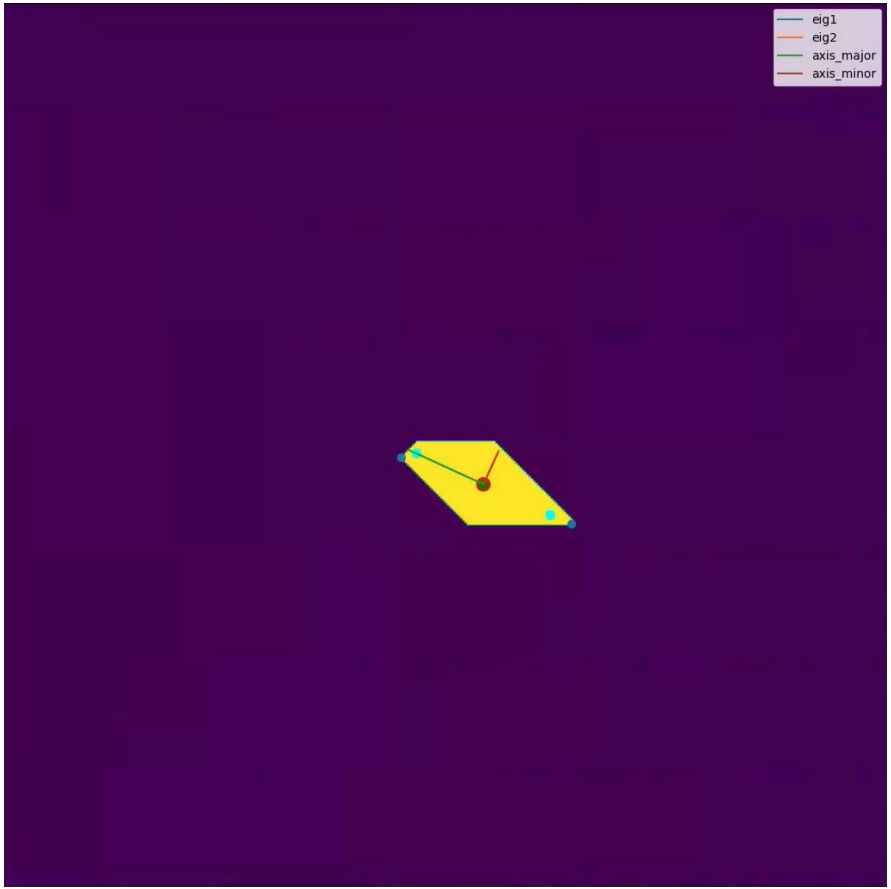


Reconstructed crystal shape (36 projections)

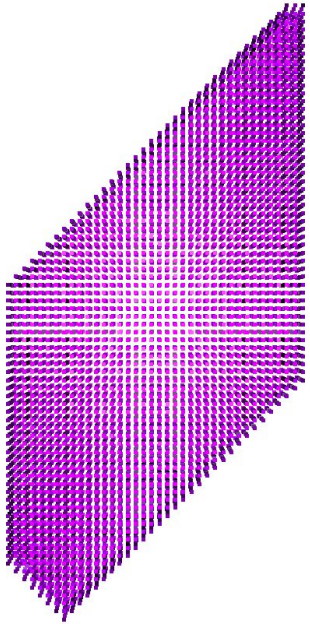


Reconstructed crystal shape (4 projections)



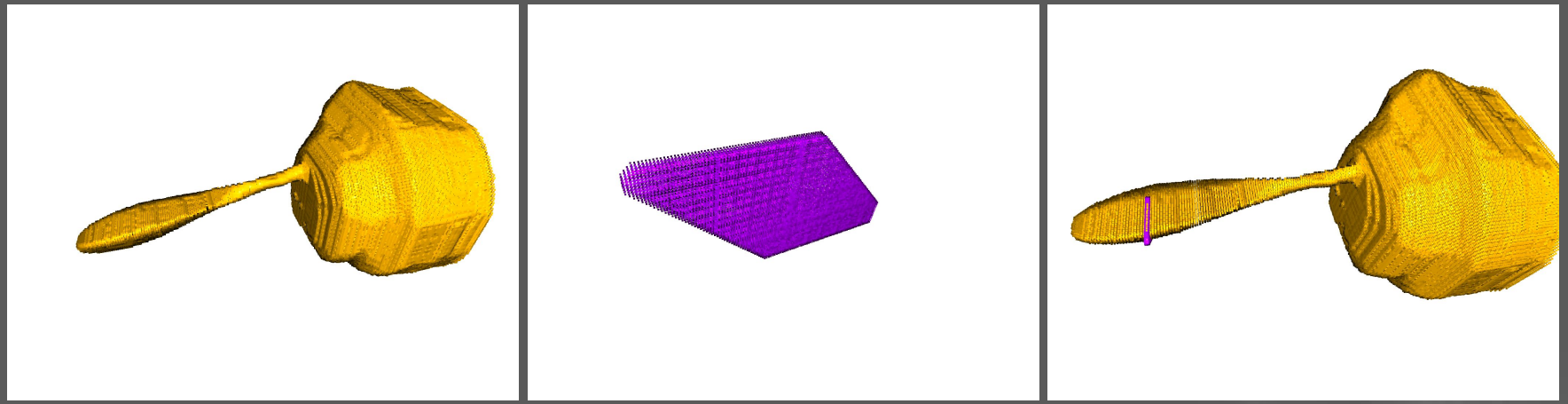


Reconstructing crystal shape (4 projections)



Solution

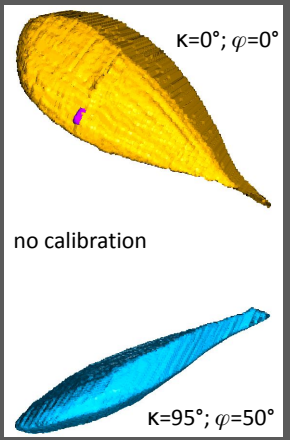
Merging optical and X-ray information

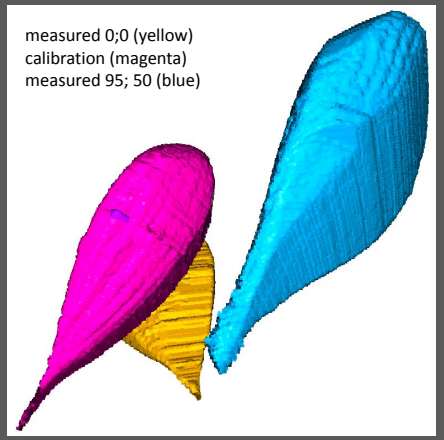


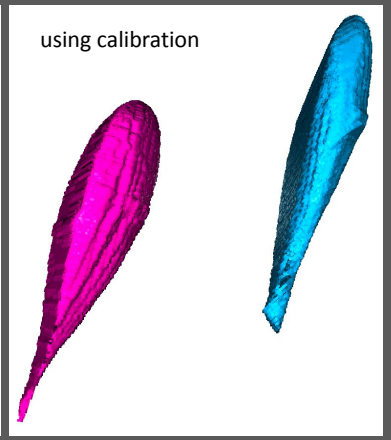
Combining optical and diffraction contrast tomography then expressing the coordinates of objects in the sample's intrinsic frame of reference

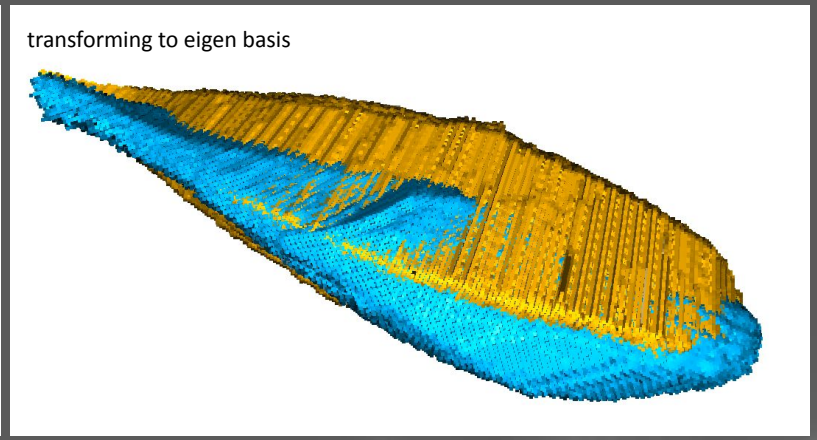
Perfect realignment !

Merging optical and X-ray information









Combining optical and diffraction contrast tomography then expressing the coordinates of objects in the sample's intrinsic frame of reference

Diffraction evaluation from oscillation

Full reciprocal space mapping

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- ThermoFisher Scientific Titan KRIOS G4
  - Eric Larquet, Pierre Legrand, Andy Thompson
- Polaris beamline
  - open to users !