SOLEIL status update

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. mxcubecore, mxcubeweb in development (nearly ready)

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: **BZoom**

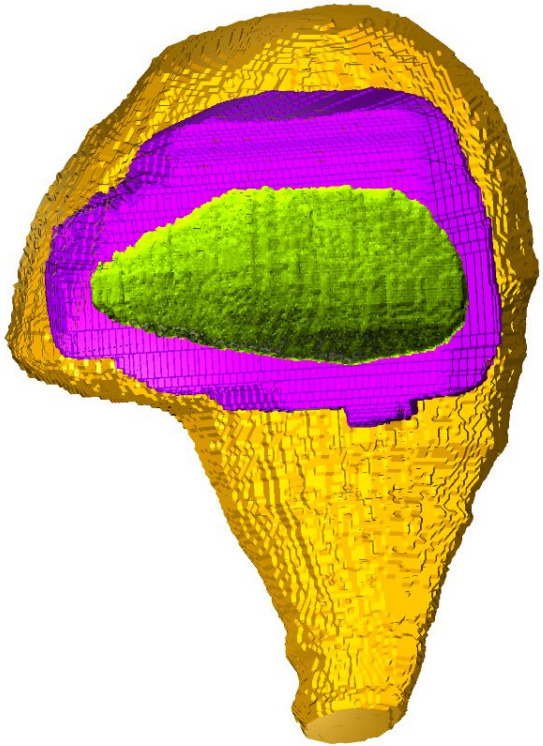
Goniometer: **MD3Up with minikappa (MK3 and HC/REX), Plate Screener**

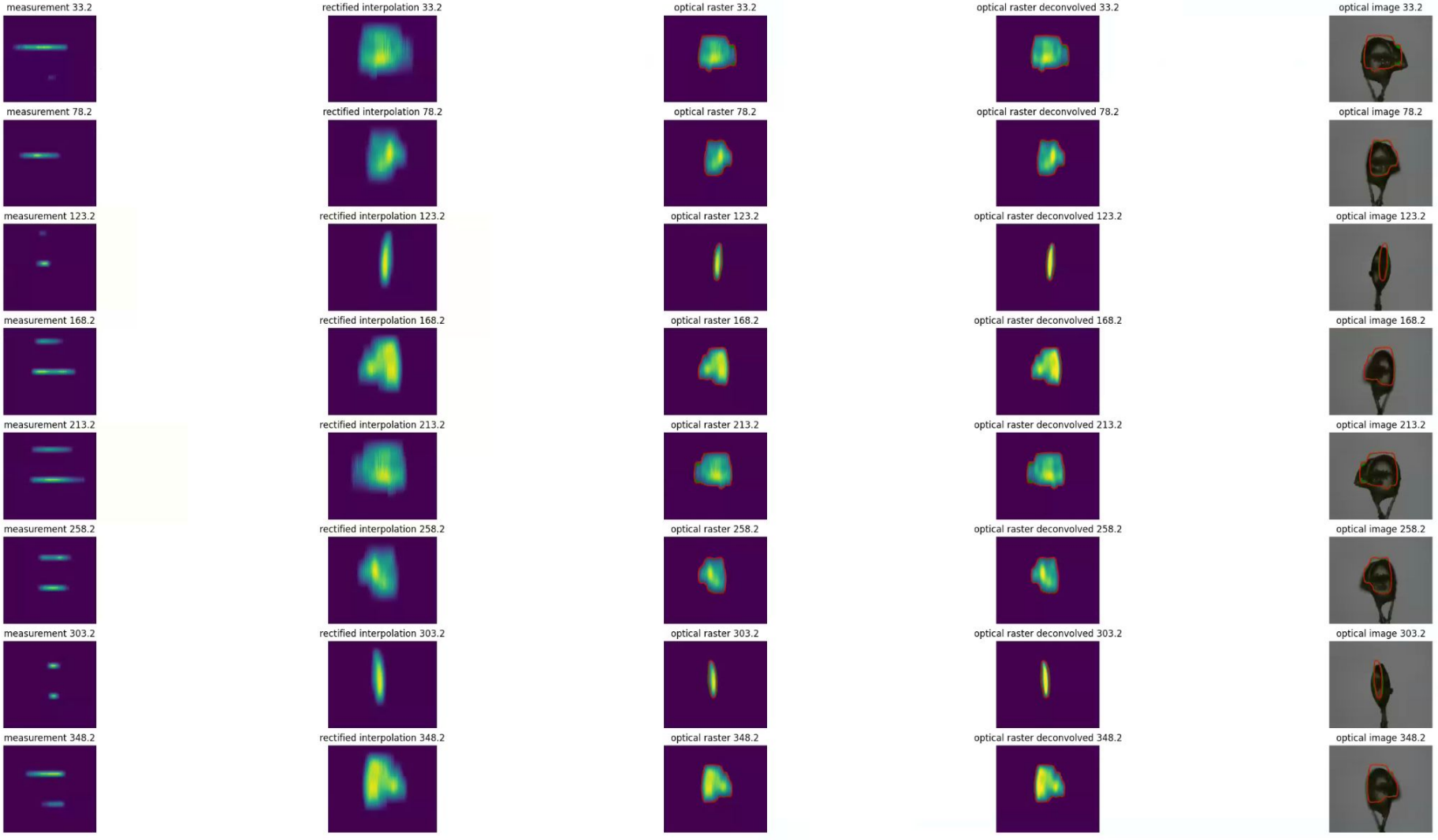
Sample Changer: CATS (**144 cryo, 48 ambient**)

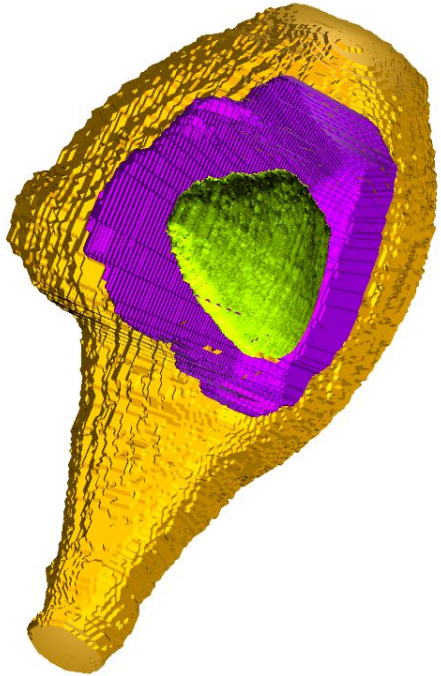
MXCuBE: Qt5 (**Ubuntu 20.04**), mxcubecore, Python 3.8

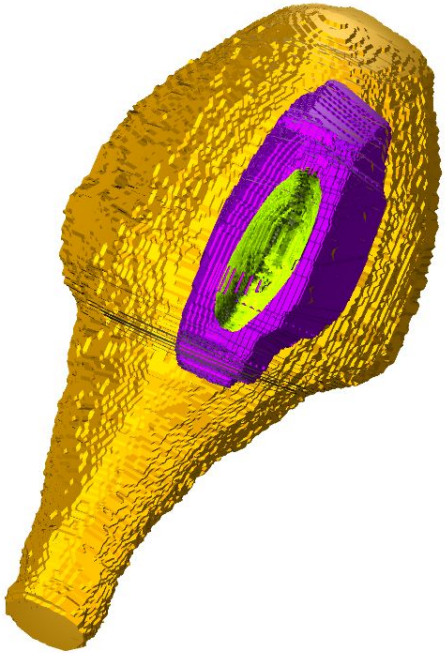
work done over the past 6 months

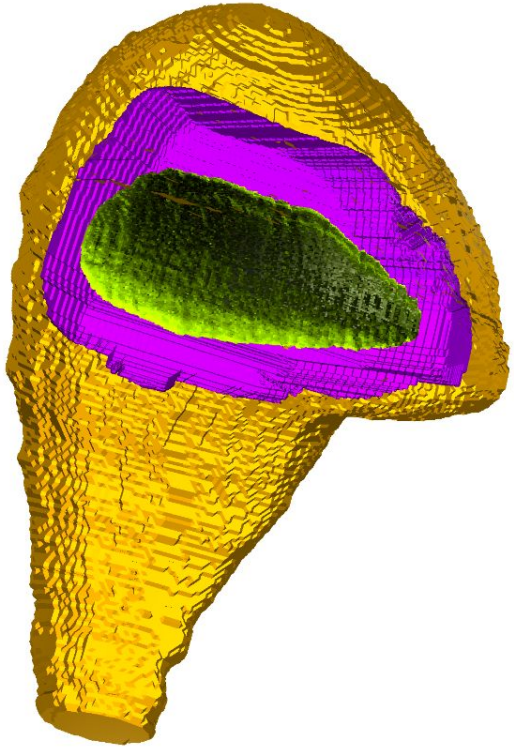
- Concerted push for unattended data collection capability
  - available on both beamlines
  - full ISPyB integration
- Murko
  - deployed on Proxima1 (Arthur Felisaz-Calvino, + 2000 annotated images, excellent performance)
  - working on inclusion of additional targets: diffraction raster scans
    prediction head: learn crystals and ice!, bounding box and key points
    in-network inference
- Volume aware experiments
  - sample shape reconstruction, diffracting volume reconstruction

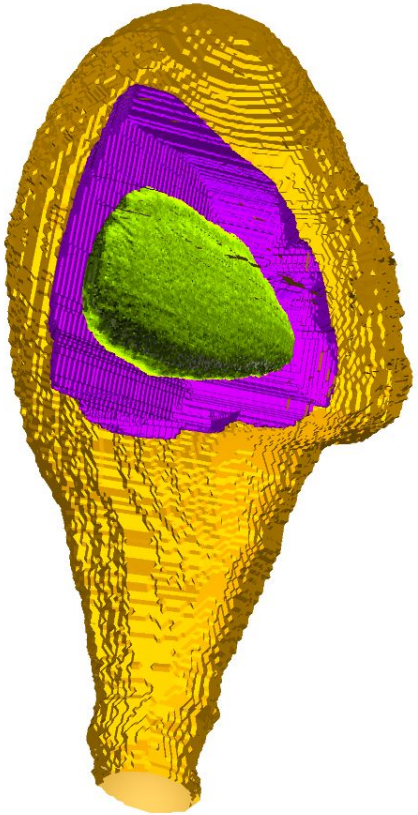


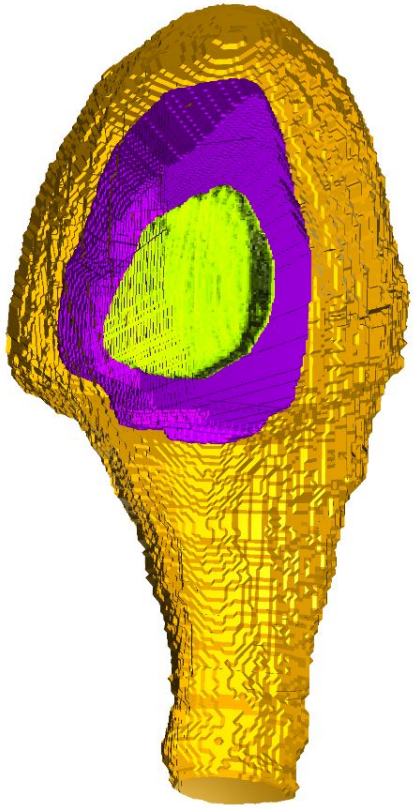

measurement 33.2
rectified interpolation 33.2
optical raster 33.2
optical raster deconvolved 33.2
optical image 33.2
measurement 78.2
rectified interpolation 78.2
optical raster 78.2
optical raster deconvolved 78.2
optical image 78.2
measurement 123.2
rectified interpolation 123.2
optical raster 123.2
optical raster deconvolved 123.2
optical image 123.2
measurement 168.2
rectified interpolation 168.2
optical raster 168.2
optical raster deconvolved 168.2
optical image 168.2
measurement 213.2
rectified interpolation 213.2
optical raster 213.2
optical raster deconvolved 213.2
optical image 213.2
measurement 258.2
rectified interpolation 258.2
optical raster 258.2
optical raster deconvolved 258.2
optical image 258.2
measurement 303.2
rectified interpolation 303.2
optical raster 303.2
optical raster deconvolved 303.2
optical image 303.2
measurement 348.2
rectified interpolation 348.2
optical raster 348.2
optical raster deconvolved 348.2
optical image 348.2

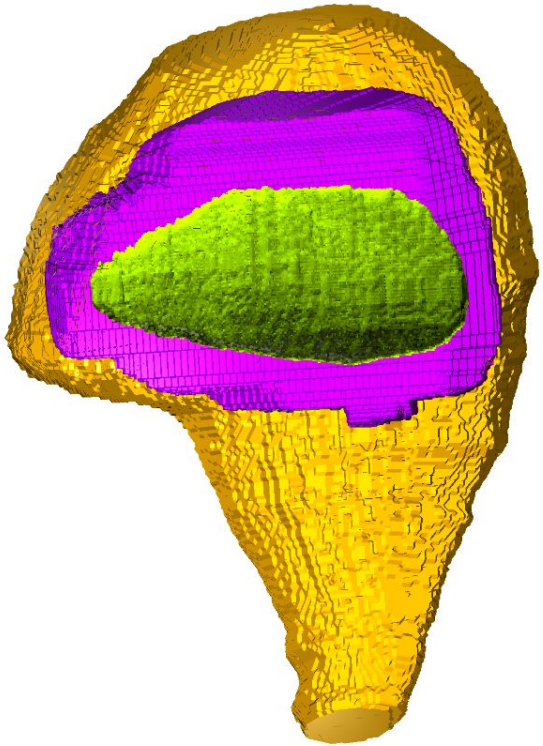


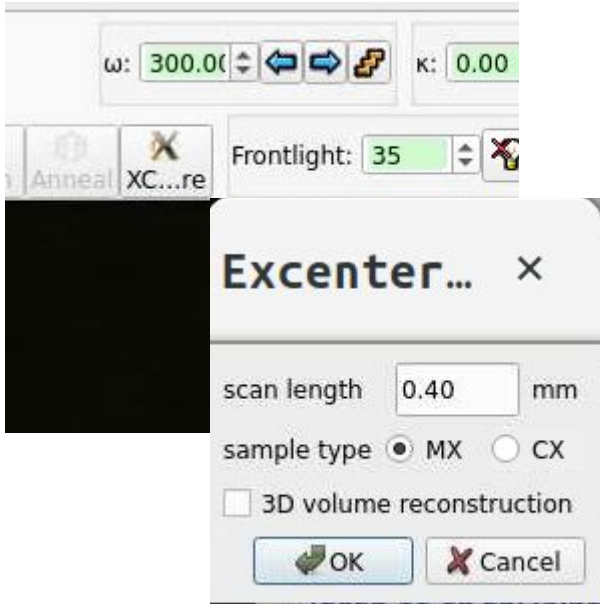











ω: 300.0(
κ: 0.00
Anneal
XC...re
Frontlight: 35
Excenter...
scan length 0.40 mm
sample type MX CX
3D volume reconstruction
OK
Cancel

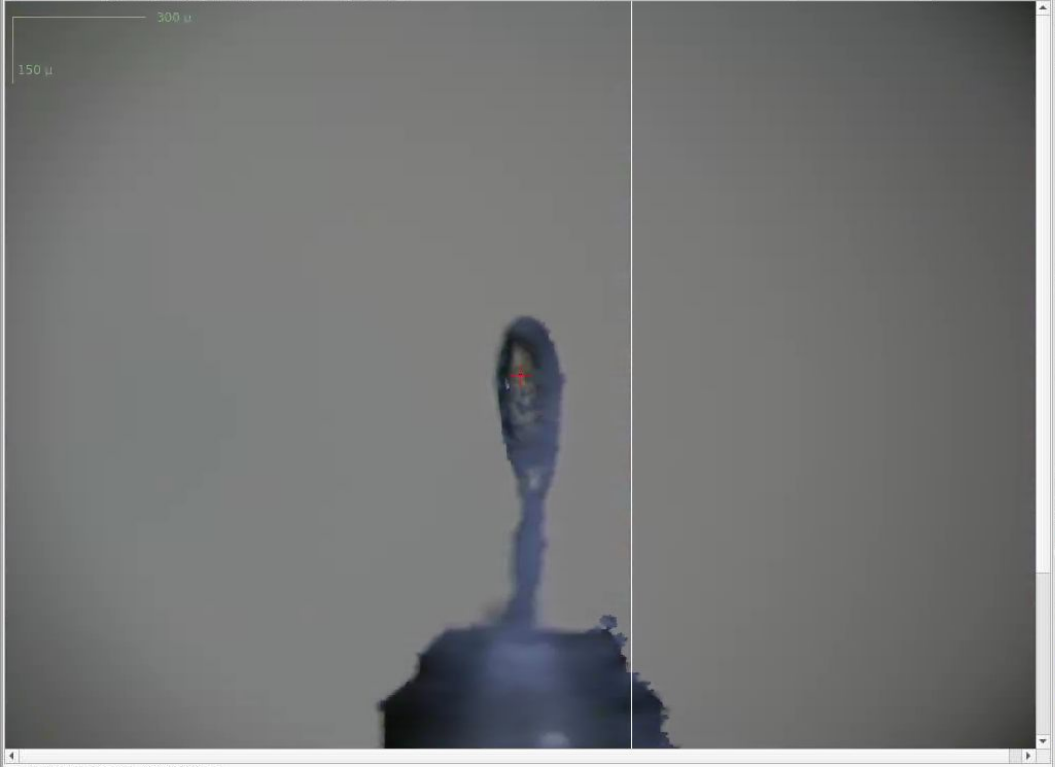
MXCuBE (on proxima2a-pc4)

File Queue View Graphics Help

Sample alignment

ω: 135.0 κ: 0.00 φ: 0.00

Zoom: 1 | Centre | Save | Orient | Beam | Anneal | XC...re | Frontlight: 35 | Backlight: 0 | Transfer | oav



Display beam size X: **873** Y: **61**

Graphics items

Sample: 9_11

Standard Collection

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

Data location

Folder:

/nfs/data4/2025_Run5/com-proxima2a/2025-11-18/RAW_DATA

PX2-0046

File name: pos11_1_######.raw

Prefix: pos11

Run number: 1

Parameters

Count time (s): 10

Excitation energy (keV): 15.00

Adjust transmission

GPhL Workflows

Advanced

Collect Now | Add to queue

[2025-11-18 23:49:51] Collection finished
[2025-11-18 23:49:51] Collection: Updating data collection in LIMS
[2025-11-18 23:49:51] Collection: Updating data collection in LIMS
[2025-11-18 23:49:51] Collection finished
[2025-11-18 23:49:51] Characterisation: Please wait ...
[2025-11-18 23:49:51] Characterising, please wait ...
[2025-11-18 23:49:51] Characterisation completed.

ISPyB proposal

Logou

Sample tree

Mode: Cats | Show robot menu

Centring: Auto + n-click | n-clicks: 3 | step 120.0

Filter: | No filter

9_5
9_6
9_7
9_8
9_9
9_10
9_11
Characterisation - 1
ref-pos11_1 (Point - not defined)

Queue history

Collect Queue | Pause

Frontend shutter: closed — Open | Close

Safety shutter: disabled — Open | Close

Resolution

Current: 1.920 Å / 200.00 mm

Set to: Å

Energy

Current: 13.0001 keV / 0.9537 Å

Set to: keV

Center beam after energy change

Transmission

Current: 100.00 %

Set to:

Machine current: **501.0 mA**

Machine state: Wed Nov 19 08:06 Shift Lignes filling: 4/4 Derniere perte : Defaut Profibus Alim QPole Beam usable

Hutch temperature: 21.8 C

Flux: 5.62e+10 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: 3.7TB (2%)

State: Ready **Diffractometer:** Ready **Sample changer:** - **Last collect:** Characterisation : Successful (2025-11-18 23:49:51)

File system EDNA ISPyB

MXCuBE (on proxima2a-pc4)

File Queue View Graphics Help

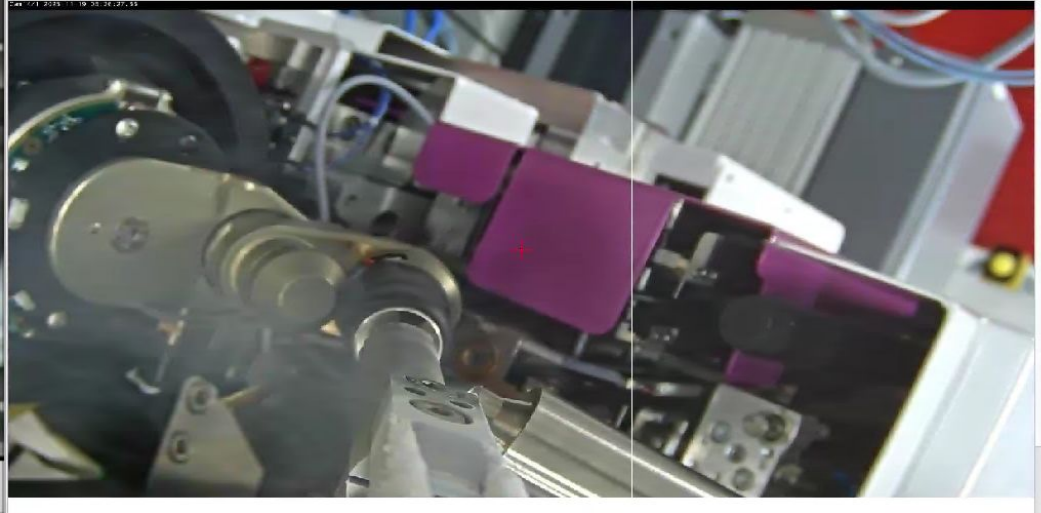
Sample alignment

ω: 0.00 κ: 180.0(φ: 0.00

Zoom: 1 Centre Save Orient Beam Anneal XC...re Frontlight: 35 Backlight: 0 Transfer cam14_1

300 µ

150 µ



Display beam size X: **775** Y: **12**

Graphics items

Sample: 9_11

Standard Collection

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

Data location

Folder:

/nfs/data4/2025_Run5/com-proxima2a/2025-11-18/RAW_DATA

PX2-0046

File name: pos11_1_######.raw

Prefix pos11

Run number 1

Parameters

Count time (s) 10

Excitation energy (keV) 15.00

Adjust transmission

GPhL Workflows

Advanced

Collect Now Add to queue

[2025-11-18 23:49:51] Collection finished
[2025-11-18 23:49:51] Collection: Updating data collection in LIMS
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[2025-11-18 23:49:51] Characterisation: Please wait ...
[2025-11-18 23:49:51] Characterising, please wait ...
[2025-11-18 23:49:51] Characterisation completed.

ISPyB proposal

Logou

Sample tree

Mode: Cats Show robot menu

Centring: Auto + n-click n-clicks: 3 step 120.0

Filter: No filter

9_5
9_6
9_7
9_8
9_9
9_10
9_11
Characterisation
pos11_1 (Beam - not defined)

Queue history

Collect Queue Pause

Frontend shutter: closed — Open Close

Safety shutter: disabled — Open Close

Machine current: **500.1 mA**

Machine state: Wed Nov 19 08:06 Shift Lignes filling: 4/4 Derniere perte : Defaut Profibus Alim QPole Beam usable

Hutch temperature: 21.8 C

Flux: 5.62e+10 ph/s

Beam size: 0.010x0.005 mm

Cryostream: Unknown sample temperature: 100.0 K

Sample changer: **Dewar level in range refill On**

Ramdisk: Total: 159.4TB Free: 3.7TB (2%)

Resolution

Current: 1.920 Å / 200.00 mm

Set to: Å

Energy

Current: 13.0001 keV / 0.9537 Å

Set to: keV

Center beam after energy change

Transmission

Current: 100.00 %

Set to:

State: Ready **Diffractometer:** Preparing the Transfer position for Sample Changer **Sample changer:** - **Last collect:** Characterisation : Successful (2025-11-18 23:49:51)

File system EDNA ISPyB

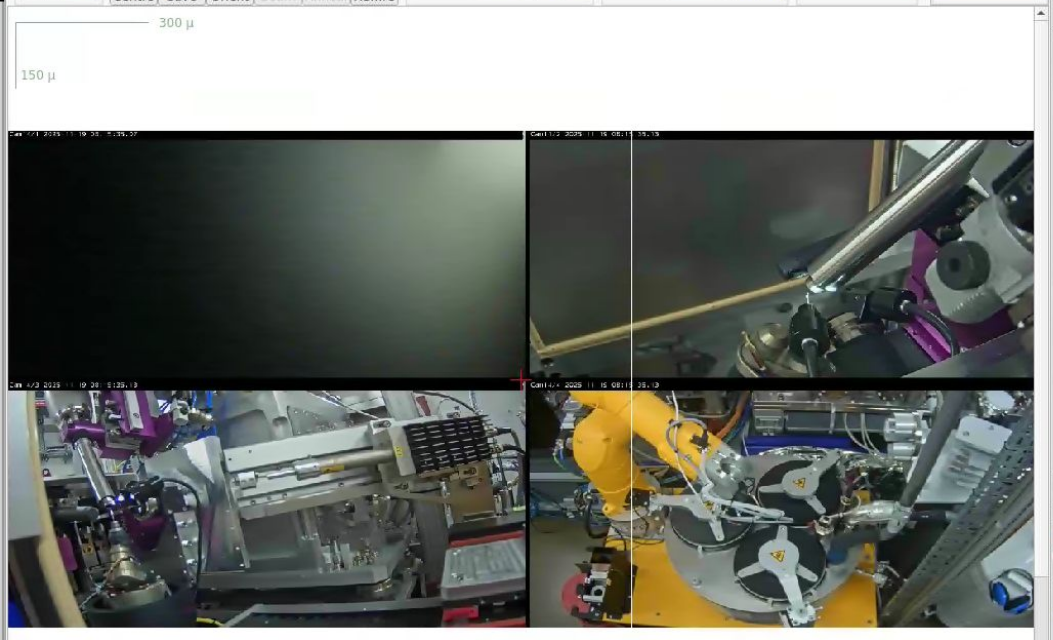
MXCuBE (on proxima2a-pc4)

File Queue View Graphics Help

Sample alignment

ω: 135.0(κ: 0.00 φ: 0.00

Zoom: 1 | Centre | Save | Orient | Beam | Anneal | XC...re | Frontlight: 35 | Backlight: 0 | Transfer | cam14_quad



Display beam size X: **873** Y: **61**

Graphics items

Sample: 9_11

Standard Collection

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

Data location

Folder:

/nfs/data4/2025_Run5/com-proxima2a/2025-11-18/RAW_DATA

PX2-0046

File name: pos11_1_######.raw

Prefix: pos11

Run number: 1

Parameters

Count time (s): 10

Excitation energy (keV): 15.00

Adjust transmission

GPhL Workflows

Advanced

Collect Now | Add to queue

```
[2025-11-18 23:49:51] Collection finished
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[2025-11-18 23:49:51] Characterisation: Please wait ...
[2025-11-18 23:49:51] Characterising, please wait ...
[2025-11-18 23:49:51] Characterisation completed.
```

ISPyB proposal

mproxi | Logou

Sample tree

Mode: Cats | Show robot menu

Samples | ISPyB

Centring: Auto + n-click | n-clicks: 3 | step 120.0

Filter: | No filter

- 9_5
- 9_6
- 9_7
- 9_8
- 9_9
- 9_10
- 9_11
  - Characterisation - 1
    - ref-pos11_1 (Point - not defined)

Queue history

Collect Queue | Pause

Frontend shutter: closed — Open | Close

Safety shutter: disabled — Open | Close

Resolution

Current: 1.920 Å

Current: 200.00 mm

Set to: Å

Energy

Current: 13.0001 keV

Current: 0.9537 Å

Set to: keV

Center beam after energy change

Transmission

Current: 100.00 %

Set to:

Machine current: **500.5 mA**

Machine state: Wed Nov 19 08:06 Shift Lignes filling: 4/4 Derniere perte : Defaut Profibus Alim QPole Beam usable

Hutch temperature: 21.8 C

Flux: 5.62e+10 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: 3.7TB (2%)

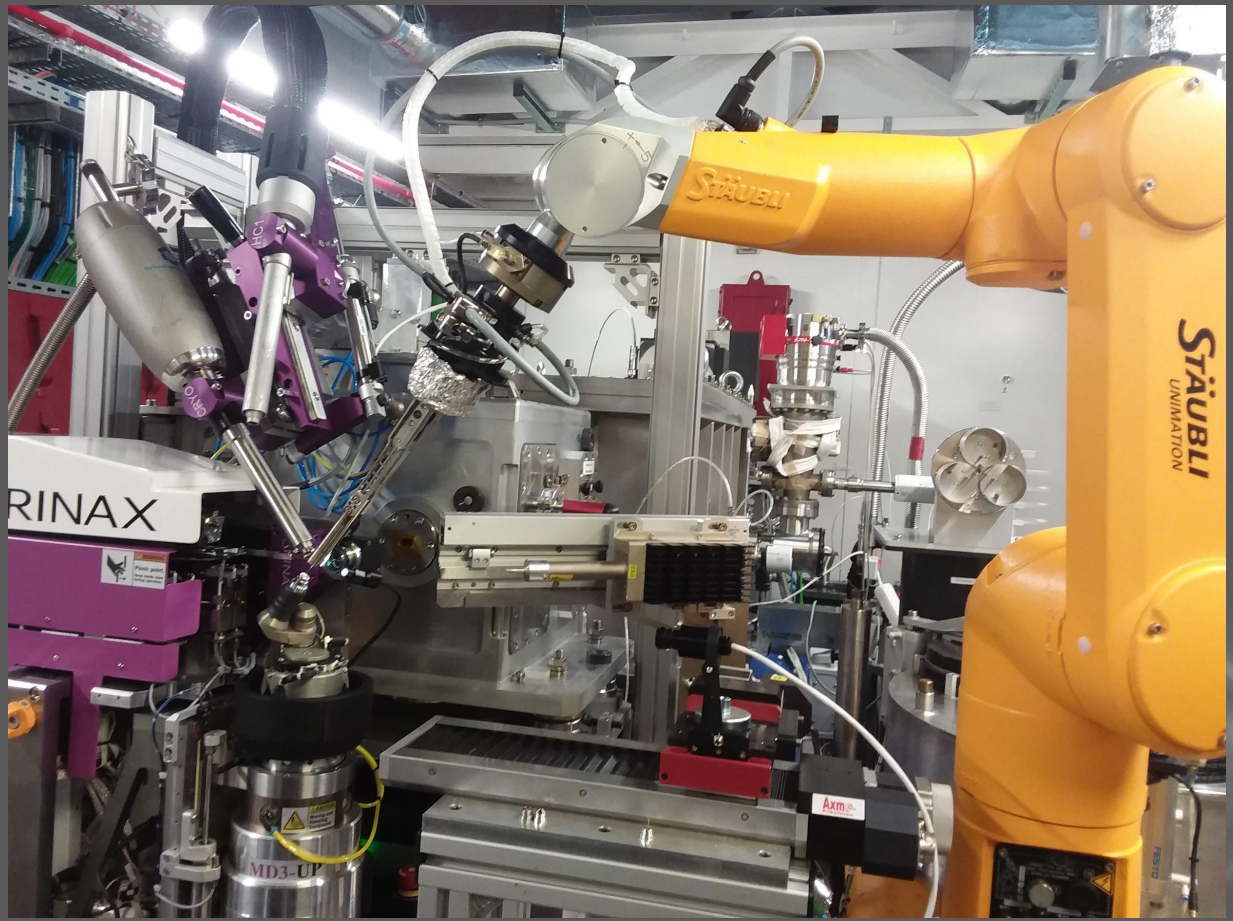
State: Ready **Diffractometer:** Ready **Sample changer:** - **Last collect:** Characterisation : Successful (2025-11-18 23:49:51)

File system EDNA ISPyB

MD3 integration

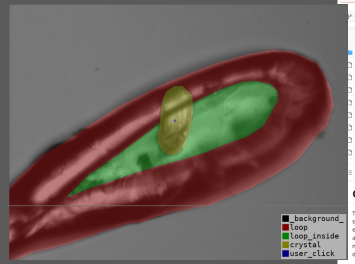
- Excellent performance of the new goniometer
  - FATs Dec 2024; SATs Jan 2025
  - SOC ~ 150nm
  - MK3 necessary for sample exchange (at 180 deg)
  - Non ideal position of the Cryostream with respect to the sample -- varying cross section of the cold stream with pin at non zero Kappa.
  - Nearly instantaneous zoom changes.

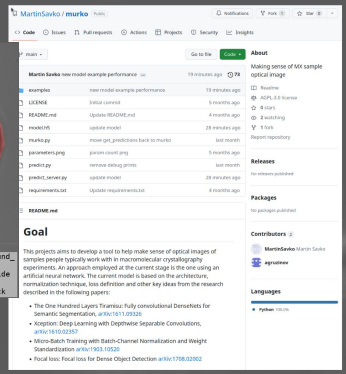
Commissioning new goniometer!



Plans for the next 6 months

- Finalizing mxcubeweb adaptation
  - Dan Costin
- Minikappa & GPhL workflows with MD3
- Murko
  - github.com/MartinSavko/murko.git
  - deploy model version with additional outputs
    - diffraction raster scans prediction head: learn crystals and ice!
    - bounding box, key points and explicit shape encoding in-network inference
- Volume aware experiments
  - rational spread of the dose (multi sweep experiments)





Acknowledgements

- GPhL team: Rasmus Fogh, Peter Keller, Clemens Vonrhein, Claus Flensburg and Gérard Bricogne
- EMBL HH team: Marina Novikova and Gleb Bourenkov
- Murko collaboration: Andrey Gruzinov and Thomas White (DESY), Didier Nurizzo (ESRF), Arthur Felisaz-Calvino (SOLEIL); David Aragao and Ralf Fleig (DLS), Annie Heroux & Nicola Demitru (Elettra), Jie Nan and Isak Lindé (Max IV), Roeland Boer (Alba), Tom Crosskey (Bessy), Kate Smith and Ezequiel Panepucci (formerly SLS), Scott Classen (ALS)
- SOLEIL team: Bill Shepard, Serena Sirigu, Rémi Soen, Damien Jeangerard, Eric Larquet, Pierre Legrand, Tatiana Isabet, Robin Lener, Andrew Thompson, Dan Costin, Arthur Felisaz-Calvino

What do we do in automated mode?

- 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