

MXCuBE status at SOLEIL

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Proxima 1

Source: U20 in vacuum undulator

Focussing: KB

Tunable: 5.5 - 15.5 keV

Flux: 2.0×10^{12} ph/s @ 500mA @
12.65keV

Beam size: 20x40 μm

Detector: Pilatus 6M

Goniometer: SmarGon

Sample Changer: CATS

MXCuBE: Qt3 v 2.1

Proxima 2

Source: U24 in vacuum undulator

Focussing: KB, HPM

Tunable: 5.5 - 18.5 keV

Flux: 1.6×10^{12} ph/s @ 500mA @
12.65keV

Beam size: 5x10 μm

Detector: Eiger X 9M

Goniometer: MD2 with MK3

Sample Changer: CATS

MXCuBE: Qt3 v 2.1

User: mx-com-proxima2a Group: [] Set Logou

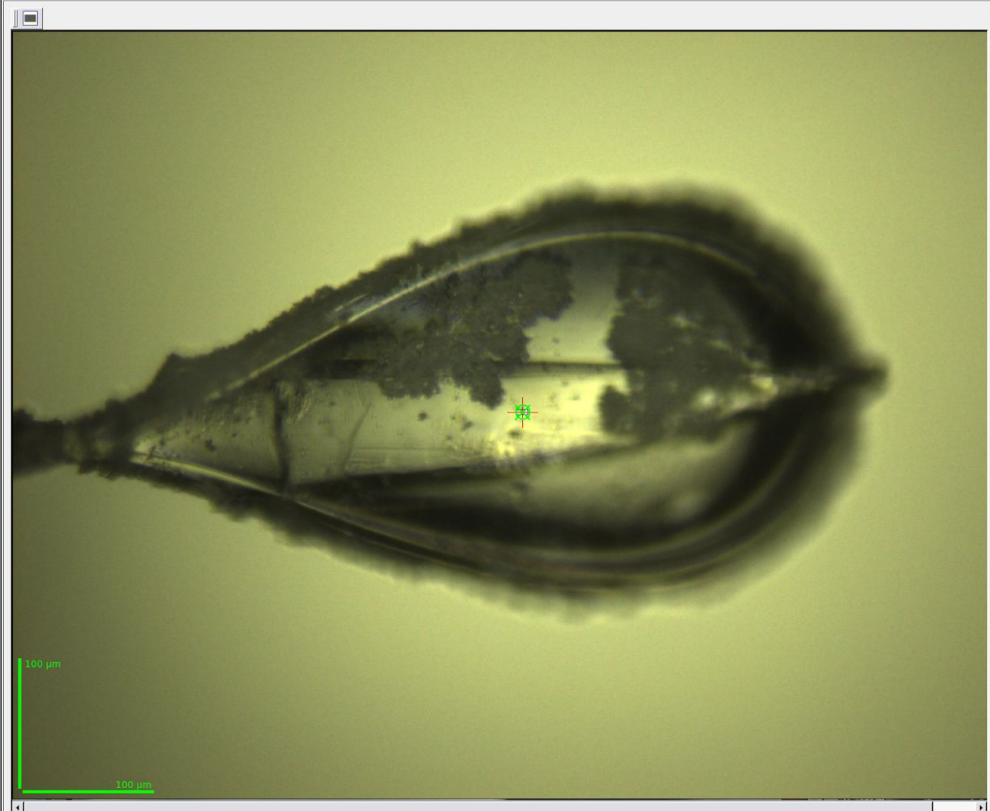
Sample list: Mode: Sample changer | Hide SC-details | Centring: Manual | Synch ISPyB

- 1:1
- 1:2
- 1:3
- 1:4
- 1:5
- 1:6
- 1:17 **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

Collect Queue | Pause

[2018-01-31 03:02:07] 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, 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

Sample centring | Sample changer
 Omega: 0.00 | Front Light: 5 | Back Light: 15 | Exposure: 0.050 | Focus: -0.110 | zoom: 5



X: 1303 Y: 656

Centre | Snapshot | BeamPosition | ApertureAlign | Add Center Point

Collection method: Standard Collection

0.1 | 1
 1.0 | 1
 12.65 |
 4.286 |
 100.0 |

ixima2a-spool/2018_Run1/2018-01-30/com-proxima2a/RAW_DATA
 /Commissioning/CPBS

cpbs | 38 | 200
 0 | 0 | 0
 0 | 0 | 0

Soleil machine current
450.9 mA
 Hybrid filling
 Lifetime: 13.23 h
 Undul. HU_640:

Energy
 Current: 12.650 keV
 0.980 Å
 Move to: keV

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

Transmission
 Current: 100.00%
 Set to:

Aperture
 Diameter: 50 | Phase: Transfer
 Position: BEAM | Scintillator: PARK

Guillotine
 insert
 extract | insert

Frontend shutter
 open

Safety shutter
 open

Fast shutter
 out

LN2 Regulation
 ON
 Optical hutch: Experimental hutch
 ready ready

Characterisation
 Helical Collection
 Energy Scan
 Advanced
 Add to queue
 Current users
 Selecting gives control
 Allow timeout control
 My name: proxima2a-5

Detectors

- Eiger X 9M on Proxima 2
 - In operation since 2015
- Pilatus 6M on Proxima 1
 - In user operation since mid 2011
 - Passing to Eiger X 16M mid 2018

Multiaxis goniometry

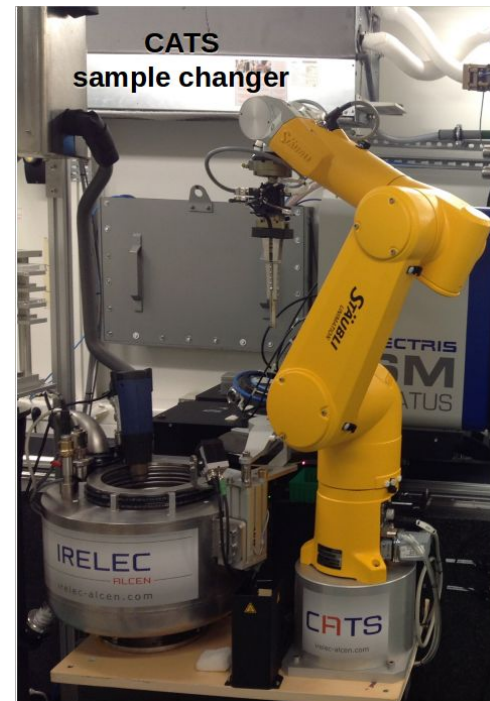
- Smargon goniometer on Proxima 1 (SmarAct)
 - SmarAxis Tango Device Server (C++) developed at SOLEIL

- 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
 - Automated resolution of occasional problems
 - Failure rate below 1 per 1000
 - Ready for remote access



Processing infrastructure

- 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 (estimated)
- 8U form factor

- System dedicated to a single beamline

- large memory -- data for on-line processing will be kept in ramdisk
- spot finding with `dials.find_spots` at 80Hz
- processing with XDS



```
MAXIMUM_NUMBER_OF JOBS= 10
MAXIMUM_NUMBER_OF_PROCESSORS= 32
```

Remote access

- NoMachine Enterprise servers installed on beamline control computers.
- External users on Proxima 1 and Proxima 2 since Autumn 2017.
- Regularly scheduled on Proxima 1 for the next proposal period.

Autoprocessing (on going work)

- Collaboration with Olof Svensson (ESRF)
- Passerelle EDM server based solution (both Proxima 1 and Proxima 2)
- Local adaptations by Frederic Picca
- Analysis via MXCuBE controlled scripts where real time processing required

Passing to Qt4 version, groundwork for MXCuBE3

- Finishing port of complete functionality Qt3 version
 - Tests ongoing on both beamlines
- Code cleanup
 - Inheriting from Abstract and Generic classes
 - GenericDiffractometer (Smargon and MD2+MK3)
 - AbstractCollect
 - AbstractMotor (TangoDCMotor, MicrodiffMotor)
 - Following master, v 2.3 of HardwareObjects
- Testing during Run 1 2018, production for Run 2 (Mid March)

Sample centring

omega: 181.94 90.0 kappa: 0.00 phi: 0.00 10.0 horizontal: -1.11 vertical: -0.14

backlight: 25 frontlight: 5 zoom: 5 focus: -0.11



X: 907 Y: 602

Point 1 (kappa: 0.00 phi: 0.00) selected

- 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
 - 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
- 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 1.999922402, wavelength 980.11159619,
radius None
[2018-01-31 03:31:10] get_distance_from_resolution 2:
resolution 1.999922402, wavelength 0.98011159619,
radius None
[2018-01-31 03:33:01] Collection finished
  
```

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 Full range

Exposure time (s): 0.025 Detector mode: 0

Kappa: 0.0005 Phi: 0

Energy (keV): 12.65 MAD

Resolution (Å): 2

Transmission (%): 50

Shutterless

Data location

Folder: /Infs/ruche/proxima2a-spool/2018_Run1/2013-06-11/000/RAW_DATA

/Commissioning/test2 Browse

File name: test_26_3_#####.h5

Prefix: test_26

Run number: 3

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 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: **FAST**

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

Passing to Qt4 version, groundwork for MXCuBE3

- Finishing port of complete functionality Qt3 version
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- Code cleanup
 - Inheriting from Abstract and Generic classes
 - GenericDiffractometer (Smargon and MD2+MK3)
 - AbstractCollect
 - AbstractMotor (TangoDCMotor, MicrodiffMotor)
 - Following master
- Testing during Run 1 2018, production for Run 2 (end of February)
- New features
 - Mesh scan integration
 - X-ray centring integration
 - Alignment of beamline components

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

Detector: **Eiger X 16M**

Goniometer: SmarGon

Sample Changer: CATS

MXCuBE: **Qt4 v 2.3**

Proxima 2

Source: U24 in vacuum undulator

Focussing: KB + pre focussing mirror

Tunable: 5.5 - 18.5 keV

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

Beam size: 5x10 μm

Detector: Eiger X 9M

Goniometer: MD2 with **MK3**

Sample Changer: CATS

MXCuBE: **Qt4 v 2.3**

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