MXCuBE status at SOLEIL

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Proxima 1

Source: **U20** in vacuum undulator

Focussing: KB, **CRL**, **20x40 µm**

Tunable: Si111 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**

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, 5x10 µm**

Tunable: Si111 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**

OAV Camera: Prosilica GC 1350

Goniometer: **MD2 with minikappa (MK3)**

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

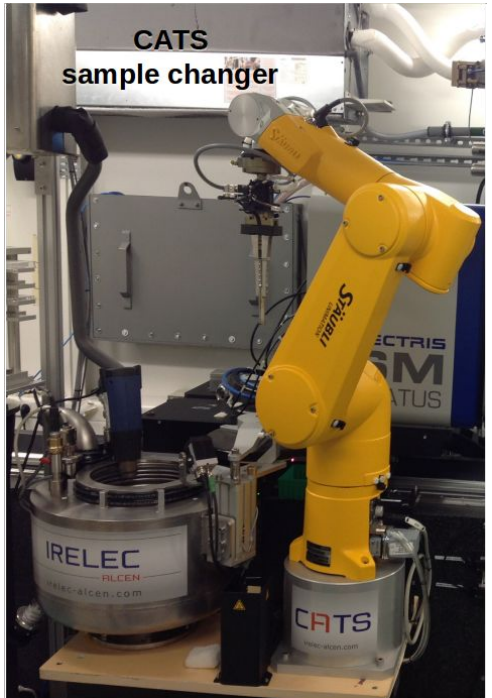
MXCuBE: Qt4 v2.3 (**Ubuntu 14.04**)

X-ray Area Detectors at SOLEIL's MX beamlines

- Eiger X, 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

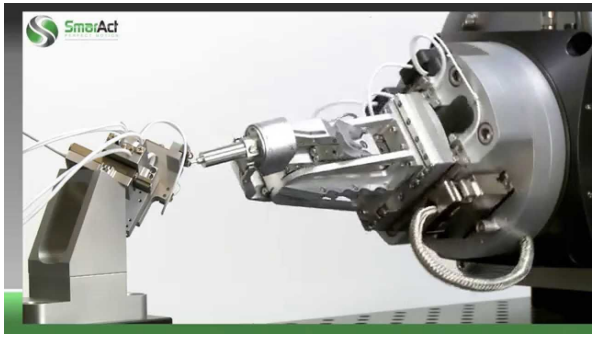
Sample changers

- CATS robots on both beamlines. Control via PyCats Tango Device Server
- Mature integration
  - Failure rate below 1 per 4000
  - Exchange time 35 seconds
  - Mounting ~10k samples per year



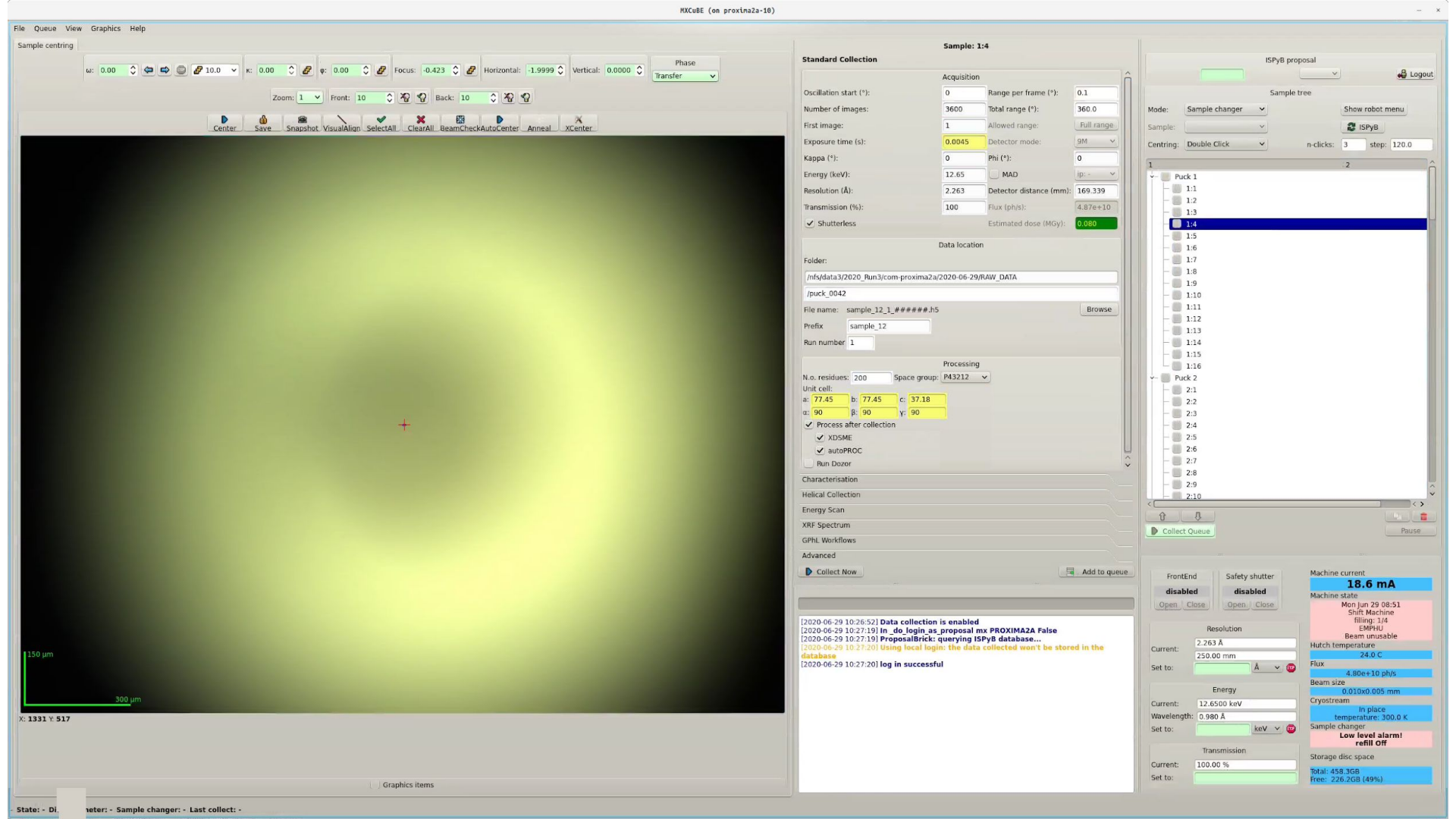
Goniometry

- Smargon on Proxima 1 (SmarAct)
  - SmarAxis Tango Device Server (C++) developed at SOLEIL
  - Series of repairs over the past years
  - **More stable recently**
- MD2 with minikappa on Proxima 2A (Arinax)
  - JLIB software accessed through Tango Device server
  - Sphere of confusion deterioration resolved
  - **Slip ring replaced during the winter shutdown**
    - resolving occasional sample detection malfunction



COVID-19

- Site shut down March 16 - May 16
  - currently 50% of staff on site
- Almost exclusively remote operation on MX beamlines in Run 3 (May-July)
- Return to standard operation expected on August 31st

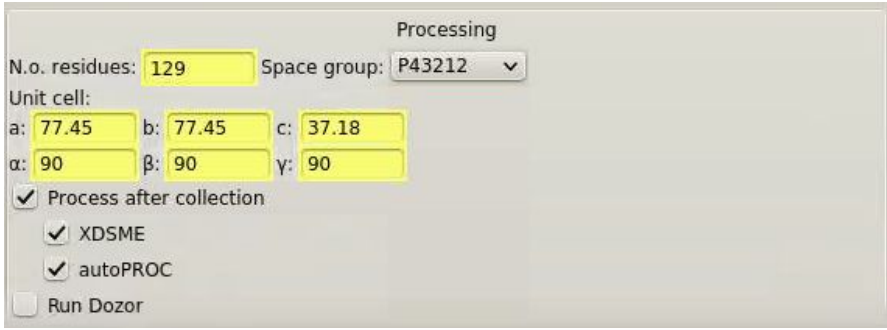

MXCuBE (on proxima2a-10)
File Queue View Graphics Help
Sample centring
ω: 0.00 10.0 κ: 0.00 φ: 0.00 Focus: -0.423 Horizontal: -1.9999 Vertical: 0.0000
Phase
Transfer
Zoom: 1 Front: 10 Back: 10
Center Save Snapshot VisualAlign SelectAll ClearAll BeamCheck AutoCenter Anneal XCenter
150 µm
300 µm
X: 1331 Y: 517
Graphics items
Sample: 1:4
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): 0.0045
Detector mode: 9M
Kappa (°): 0
Phi (°): 0
Energy (keV): 12.65
MAD
Resolution (Å): 2.263
Detector distance (mm): 169.339
Transmission (%): 100
Flux (ph/s): 4.87e+10
Shutterless
Estimated dose (MGy): 0.080
Data location
Folder:
/nfs/data3/2020_Run3/com-proxima2a/2020-06-29/RAW_DATA
/puck_0042
File name: sample_12_1_######.h5
Browse
Prefix sample_12
Run number 1
Processing
N.o. residues: 200
Space group: P43212
Unit cell:
a: 77.45 b: 77.45 c: 37.18
α: 90 β: 90 γ: 90
Process after collection
XDSME
autoPROC
Run Dozor
Characterisation
Helical Collection
Energy Scan
XRF Spectrum
GPhL Workflows
Advanced
Collect Now
Add to queue
[2020-06-29 10:26:52] Data collection is enabled
[2020-06-29 10:27:19] In _do_login_as_proposal mx PROXIMA2A False
[2020-06-29 10:27:19] ProposalBrick: querying ISPyB database...
[2020-06-29 10:27:20] Using local login: the data collected won't be stored in the database
[2020-06-29 10:27:20] log in successful
ISPyB proposal
Logout
Sample tree
Mode: Sample changer
Show robot menu
Sample:
ISPyB
Centring: Double Click
n-clicks: 3 step: 120.0
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
2:8
2:9
2:10
Collect Queue
Pause
FrontEnd
disabled
Open Close
Safety shutter
disabled
Open Close
Resolution
Current: 2.263 Å
250.00 mm
Set to:
Energy
Current: 12.6500 keV
Wavelength: 0.980 Å
Set to:
keV
Transmission
Current: 100.00 %
Set to:
Machine current
18.6 mA
Machine state
Mon Jun 29 08:51
Shift Machine
filling: 1/4
EMPHU
Beam unusable
Hutch temperature
24.0 C
Flux
4.80e+10 ph/s
Beam size
0.010x0.005 mm
Cryostream
In place
temperature: 300.0 K
Sample changer
Low level alarm!
refill Off
Storage disc space
Total: 458.3GB
Free: 226.2GB (49%)
State: - Di... meter: - Sample changer: - Last collect: -

Recent advances

- Increasing the default data collection speed on PX2
  - default frame rate: 220Hz with rotation speed: 22deg/s, 16.2 seconds per turn
  - conservative default dose: < 2MGy per median crystal size and composition
    - Beware of the defaults though! With beam shape and flux well calibrated -- BEST strategies allow to collect superior data with a much lower dose.
  - slicing 0.1 deg/frame
  - This move was allowed by resolving issue with neggia plugin mishandling of unmasked bad pixels of 16bit Eiger images. Thanks to Clemens Vonrhein of Global phasing!
- Porting automated optical alignment program from PX2 to PX1
  - still some challenges -- main problem is the background with very different statistics
- X-ray centring and mesh scans on PX1
  - in development, with help from Vicente Rey
  - full integration of the results into overlays -- to be ported to PX2
- Automated data processing … on next slide

Automated data processing

- Pipelines integration (by Fred Picca)
  - XDSME
  - autoPROC
  - DIALS via XIA2 under development



- Characterization
  - spot finding and resolution estimation with DOZOR and dials.find_spots
  - data integrated with XDSME
  - BEST strategy calculation (upon successful integration)

Fixing annoying bugs

- Stop button triggering strange instability -- next collect would crash entire application (sometimes). Solved in DataCollectionQueueEntry.collect_dc().

```
except gevent.GreenletExit:
    log.warning("Collection stopped by user.")
    list_item.setText(1, 'Stopped by user')
    self.collect_hwobj.ready_event.wait()
    self.collect_hwobj.ready_event.clear()
    raise QueueAbortedException('queue stopped by user', self)
```

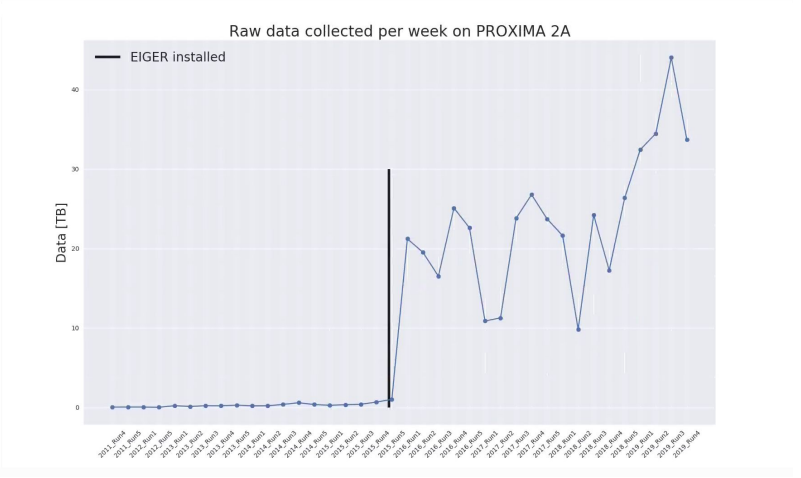
- Gradual slow down of procedures (standard collect or characterization)
  - self.parameter_fields attribute was defined as a class attribute and kept growing without limits

```
if hasattr(self, 'parameter_fields'):
    self.parameter_fields += omega_scan.specific_parameter_fields
else:
    self.parameter_fields = omega_scan.specific_parameter_fields[:]
```

The team

- Bill Shepard
- Serena Sirigu
- Damien Jeangerard
- Pierre Legrand
- Tatiana Isabet
- Robin Lener
- Leo Chavas
- Andrew Thompson
- Frédéric Picca
- Elke de Zitter
- Lidia Ciccone
- Adam Simpkin
- Igor Chaussavoine
- Idrissou Chado
- Bixente Rey
- Olof Svensson

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

Performance of the setup

- ~ 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

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
```

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