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 (4.65um, 1360x1024)

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, 5x10 µm**

Tunable: Si111 CCM, 5.5 - 18.5 keV

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

Area Detector: **Eiger X 9M**

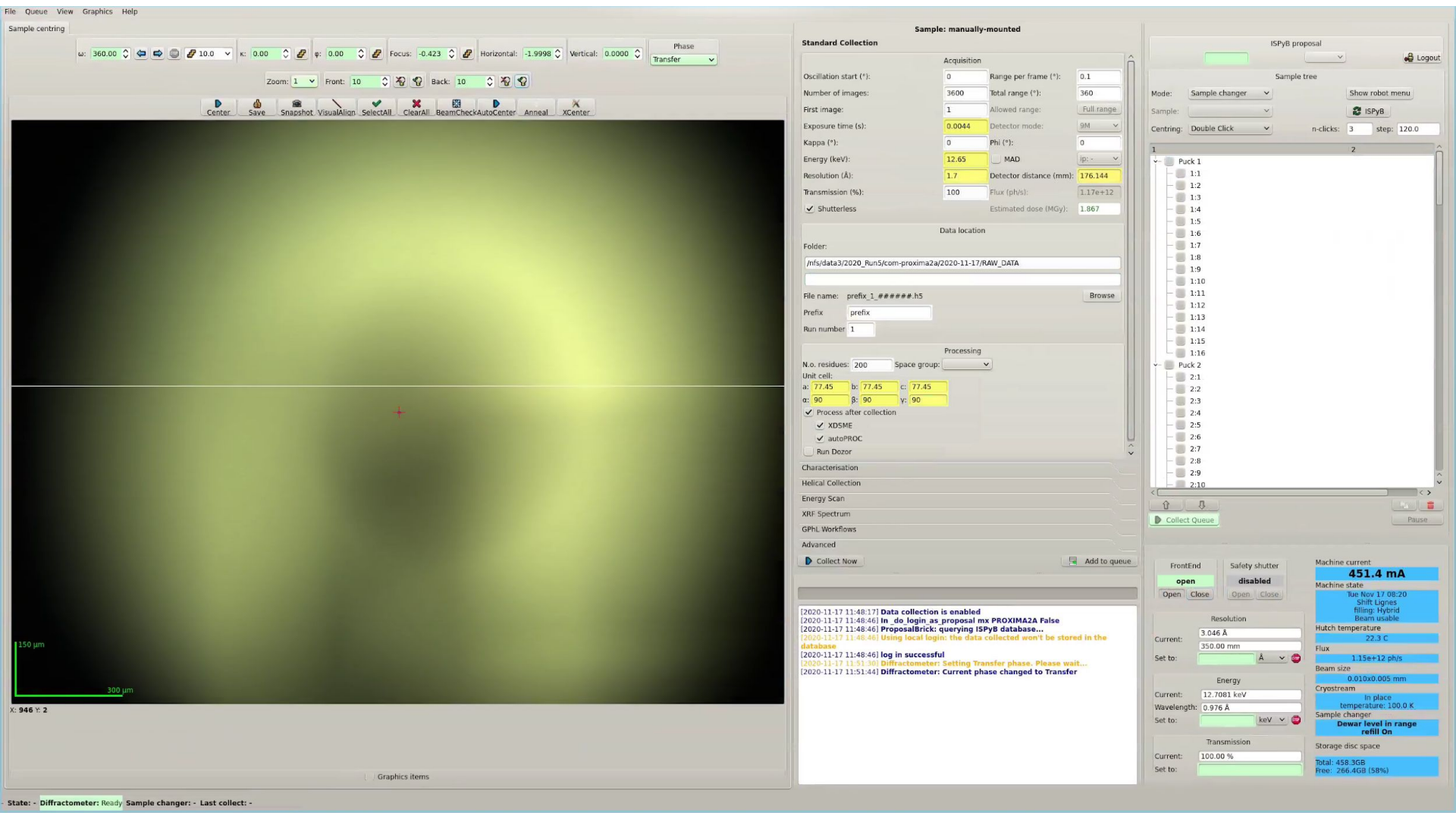
XRF Detector: Ketek AXAS-M2 **H80**

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

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

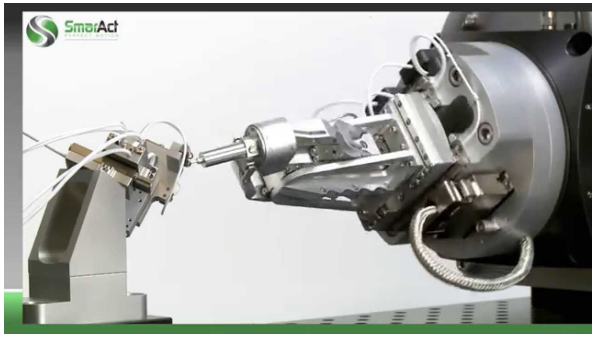
Sample Changer: CATS (**144 samples**)

MXCuBE: Qt5 (**Ubuntu 20.04**); Qt4 (Unbuntu 14.04)


File Queue View Graphics Help
Sample centring
ω: 360.00 10.0 κ: 0.00 φ: 0.00 Focus: -0.423 Horizontal: -1.9998 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: 946 Y: 2
Graphics items
Sample: manually-mounted
Standard Collection
Acquisition
Oscillation start (°): 0
Range per frame (°): 0.1
Number of images: 3600
Total range (°): 360
First image: 1
Allowed range: Full range
Exposure time (s): 0.0044
Detector mode: 9M
Kappa (°): 0
Phi (°): 0
Energy (keV): 12.65
MAD ip: -
Resolution (Å): 1.7
Detector distance (mm): 176.144
Transmission (%): 100
Flux (ph/s): 1.17e+12
Shutterless
Estimated dose (MGy): 1.867
Data location
Folder:
/nfs/data3/2020_Run5/com-proxima2a/2020-11-17/RAW_DATA
File name: prefix_1_######.h5
Browse
Prefix: prefix
Run number: 1
Processing
N.o. residues: 200
Space group:
Unit cell:
a: 77.45 b: 77.45 c: 77.45
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
[2020-11-17 11:48:17] Data collection is enabled
[2020-11-17 11:48:46] In_do_login_as_proposal mx PROXIMA2A False
[2020-11-17 11:48:46] ProposalBrick: querying ISPyB database...
[2020-11-17 11:48:46] Using local login: the data collected won't be stored in the database
[2020-11-17 11:48:46] log in successful
[2020-11-17 11:51:30] Diffractometer: Setting Transfer phase. Please wait...
[2020-11-17 11:51:44] Diffractometer: Current phase changed to Transfer
ISPyB proposal
Logout
Sample tree
Mode: Sample changer
Show robot menu
Sample:
ISPyB
Centring: Double Click
n-clicks: 3
step: 120.0
1
2
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
open
Open Close
Safety shutter
disabled
Open Close
Resolution
Current: 3.046 Å
350.00 mm
Set to:
Å
Energy
Current: 12.7081 keV
Wavelength: 0.976 Å
Set to:
keV
Transmission
Current: 100.00 %
Set to:
Machine current
451.4 mA
Machine state
Tue Nov 17 08:20
Shift Lignes
filling: Hybrid
Beam usable
Hutch temperature
22.3 C
Flux
1.15e+12 ph/s
Beam size
0.010x0.005 mm
Cryostream
In place
temperature: 100.0 K
Sample changer
Dewar level in range
refill On
Storage disc space
Total: 458.3GB
Free: 266.4GB (58%)
State: - Diffractometer: Ready Sample changer: - Last collect: -

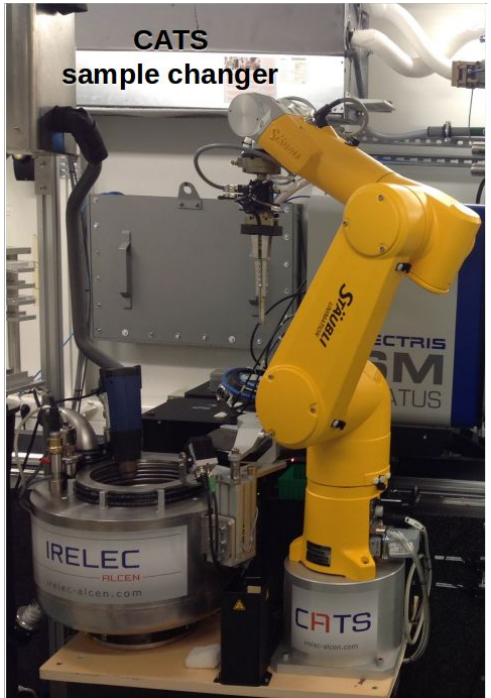
Goniometry

- Smargon on Proxima 1 (SmarAct)
  - SmarAxis Tango Device Server (C++) developed at SOLEIL
  - Series of repairs over the past years
  - **More stable since past year**
- MD2 with minikappa on Proxima 2A (Arinax)
  - JLIB software accessed through Tango Device server
  - Sphere of confusion deterioration resolved
  - **No problems since slip ring replacement last winter**



Sample changers

- CATS robots on both beamlines. Control via PyCats Tango Device Server
- Mature integration
  - **Failure rate below 1 per 4000**
    - **fine tuning approach depth in the dewar**
  - Exchange time 35 seconds
  - Mounting ~10k samples per year



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
  - PERC 840H
  - 192TB local RAID5 filesystem
- XDSME, autoPROC, **TIOGA/DOZOR since last month**

Processing infrastructure

- System dedicated to a single beamline
  - Keeping data close to source
  - Tailor processing power to the detector
  - Minimizing administrative overhead
- DELL Precision 7920 Tower
  - 2 x XEON Gold 6290R @ 2.1GHz, 52 cores, 104 threads
  - 377 MB RAM (DDR4 2934 MT/s)
  - 2 x 10GBe
  - 52TB local RAID5 filesystem
  - **2 x Quadro RTX 6000**

Commissioning Global Phasing workflows

- elusive bug discovered, and **solved!** -> after strategy is calculated, crystal is duly position and centring requested and recorded, but mysteriously (sometimes) kappa, and phi move by a certain delta just before the collection … **Solution**: Do not rely on internal position dictionary (self.current_motor_positions) but call the low level device for fresh values (call is not expensive).
  - queue_entry, DataCollectionQueueEntry class, collect_dc method
- strategy calculation sometimes fails -> tracked down to slow nfs partition (1Gbe) solved by moving machine to a faster network (10Gbe)

TINE/TIOGA/DOZOR

- Contacting EMBL HH at the beginning of April
- Code graciously shared and explained by Marina and Gleb
- Added support for Eiger 9M
- Compiled for CentOS 7 and Ubuntu 20.04
- Setting up minimum TINE environment on our control network
- Configured for Huawei FusionServer (288 threads, 2.56TB memory) for production
    - dedicating 144 threads and 258GB of RAM to TIOGA
    - Eiger 9M@238Hz get processed and gzipped cbfs appear on the filesystem ~211Hz (1GB/s)

Updates

- Running Eiger Stream and FileWriter simultaneously
- currently on 1.6.6 Simplon firmware
  - stable when using FileWriter only
  - exhibits some instability when Stream and FileWriter enabled at the same time
- updating to 1.8.0 Simplon firmware
  - our detector control unit is based on DELL PowerEdge R820
    - not thoroughly tested with the new firmware
    - installation and tests forseen for the next week
  - currently supported DCU platform based on PowerEdge R940

Acknowledgements

- GPhL team: Rasmus Fogh and Gérard Bricogne
- EMBL HH team: Marina Novikova and Gleb Bourenkov

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

…New developments

- integration of X-ray centring into queue on PX2
- speeding up automated optical centring
  - deepen understanding of what we see
  - there goes a strange attractor ...

Robot breakdown and working around it

- After 8 years of operation of our CATS axis no 4. started to malfunction as of the end of last run
  - Problem debugged with staubli support remotely
  - What seems to have happened was the loss of a step due to the distribution belt slippage.
  - Tightening of the distribution belt screws and diminishing the speed (75-50%) got us out of the water for the last weekend of user operation
  - After further tweaking extensive tests during the shutdown ~1600 samples successfully mounted (0 failed)
  - Thorough check-up planned with Staubli for the entire TX60 arm.

New developments

- Beamline operating with refactored mxcubecore
  - current master
    - best ever
    - decreasing complexity and number of SOLEIL specific objects
    - github.com/MartinSavko/{mxcubecore:px2_production, mxcube:px2_production}
  - aim to phase it in production over the next run (starting Today!)
- Python 3.8.5
  - all sequences ported
- Ubuntu 20.04,
  - base python from apt, most of the libraries through pip
  - tango vs PyTango
- PyQt5
  - almost transparent except:
    - wheel signals

```
diff --git a/mxcubecore/HardwareObjects/QtGraphicsLib.py b/mxcubecore/HardwareObjects/QtGraphicsLib.py
index 35d810a9..cab4d09c 100644
--- a/mxcubecore/HardwareObjects/QtGraphicsLib.py
+++ b/mxcubecore/HardwareObjects/QtGraphicsLib.py
@@ -2696,7 +2696,10 @@ class GraphicsView(qt_import.QGraphicsView):
         :param event:
         :return:
         """
-        self.wheelSignal.emit(event.delta())
+        if qt_import.qt_variant == 'PyQt5':
+            self.wheelSignal.emit(event.angleDelta().y())
+        else:
+            self.wheelSignal.emit(event.delta())
```

Improvements

- speeding up x-ray centring
  - consider x-ray centring as a tomography experiment - estimate shape of the crystal
  - sped up analysis and acquisition -- total run+analysis time <1min (>3 min previously)
  - significant increase in use
- fixing Ctrl-2 shortcut bug
  - the most efficient users do not bother to click -- they actually use shortcuts to gain time
  - this one was not properly tested -- instead of just saving the position it triggered slight (~7 um on average) move of the sample (single click centring). Troublesome for thin samples (more in Gerard's presentation)
- More efficient handling of sample tree updates
  - set_sample_pin_icon(self) in dc_tree_widget.py
    - ask location of current loaded sample once
  - more efficient handling of triggers from sample_changer (do not send signal for both lid and pin change, but combine)
  - sample_changer.get_component_by_address() called up to 896 times each time (for 144 samples on Proxima2A)
    - increase efficiency through memoization

Proxima 1

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Area Detector: **Eiger X 9M**

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OAV Camera: Prosilica GC 1350

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

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

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

COVID-19

- Almost exclusively remote operation on MX beamlines (NoMachine). On-site user visits kept to minimum.
- PX2 shutdown for a week due to a visit by a user attained by the CoViD last July.
- To lower the risk of beamline shutdown we have set up a separate room for on-site users to collect from.

Limitations of our current interfaces ...

- Beamline is used less efficiently in remote
  - NX layer not invisible -- some operations are up to 3 times compared to local situation, for some users
- Cool features not exploited enough
  - kappa realignment
  - alignment with refraction taken into account
  - x-ray centring
- Majority of users default to very simply designed experiments
  - strategy recommendation followed only by experienced users
- The weight of the software interface significantly increases in the world without human face to face contact ….

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

*

- Both beamlines are equipped with fast local storage 250TB DAS attached to the main processing server (288 threads, 2.5 TB RAM).
- ~10 TB of raw data per day on average
- ~1PB raw data per year, ~100TB with bslz4 compression

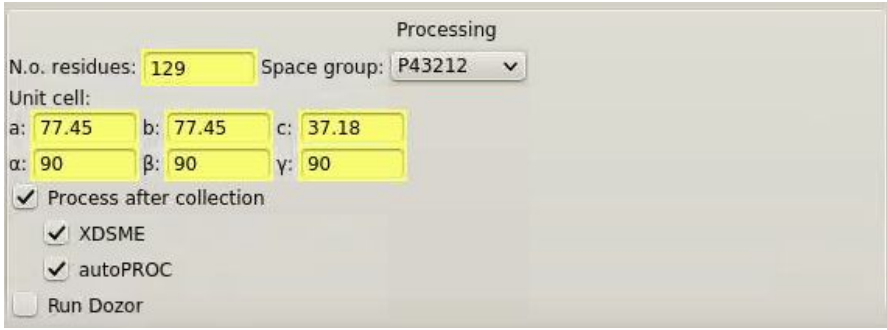
* http://e.huawei.com/en/products/cloud-computing-dc/servers/rh-series/rh8100-v3

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 production, developed by Vicente Rey
  - full integration of the results into overlays -- to be ported to PX2
- Automated data processing … on next slide

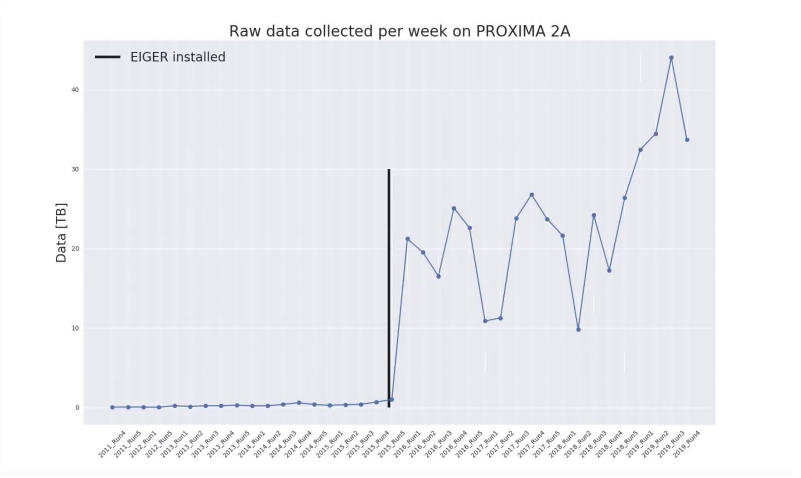
Automated data processing

- 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)

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