MXCuBE status at SOLEIL

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Joint ISPyB and MXCuBE developers meeting at Lund

12th March 2019

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

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

Tunable: 5.5 - 18.5 keV

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

Beam size: 5x10 µm

Area Detector: Eiger X 9M

XRF Detector: Ketek AXAS-M2 H80

OAV Camera: Prosilica GC 1350

Goniometer: MD2 with MK3

Sample Changer: CATS (144 samples)

MXCuBE: Qt4 v2.3 (Ubuntu 14.04)

Proxima 1

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Proxima 2

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Focussing: KB, horizontal PFM

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

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Sample Changer: CATS (144 samples)

MXCuBE: Qt4 v2.3 (Ubuntu 14.04)

Eiger X on Protein Crystallography Beamlines in SOLEIL

- Firmware version: SIMPLON v. 1.6.4
- User operation
 - Eiger X 9M December 2015 on Proxima 2
 - Eiger X 16M October 2018 on Proxima 1
- bslz4 compression
- Max speeds
 - 133Hz @ 16M
 - o 238Hz @ 9M
 - 750Hz @ 4M ROI (stable as of SIMPLON API 1.6.2)

Multiaxis goniometry

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



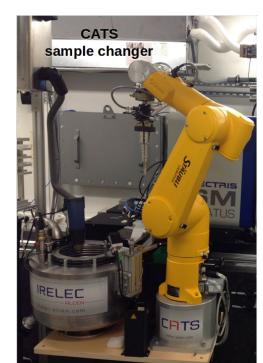
- Minikappa MK3 on Proxima 2 (Arinax)
 - JLIB software accessed through Tango Device server



Sample changers

- CATS robots on both beamlines. Control via PyCats Tango Device Server
- Mature integration
 - Failure rate below 1 per 1000
 - Exchange time 35 seconds





Remote access

- NoMachine servers installed on control computers
- Regularly scheduled on both beamlines for both industrial and academic users (5-10%)

Data handling infrastructure

- 10Gbit network
- Local buffer on the processing server
 - **2.56TB RAM**
 - 3TB RAID 6 SAS (to be upgraded by 16TB SSD)
- Medium and long term storage (Active Circle based), NFS access
 - Local cell: 10TB SSD, 20TB SAS
 - Remote cell: 1PB via 10Gbe

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

- o 8 x XEON E7-8890 v3 @ 2.5GHz, 144 cores, 288 threads
- 2.56 TB RAM (DDR4 1866MHz)
- 4 x 10GBe
- 5.76 TFlops
- \circ spot finding with dials.find_spots and Dozor
- data integration with XDS

MAXIMUM_NUMBER_OF_30BS= 10 MAXIMUM_NUMBER_OF_PROCESSORS= 32



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

Performance of the setup

- ~ 1000 MB/sec download speed
 - Using both 10Gbit ports of the DCU
 - ~600 MB/sec with single 10Gbit port
- ~ 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 Iz4
- 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

For steady processing

sync; echo 3 > /proc/sys/vm/drop_caches

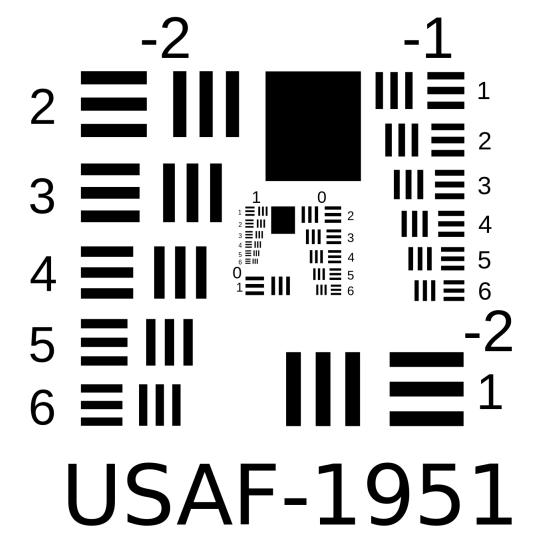
For steady processing

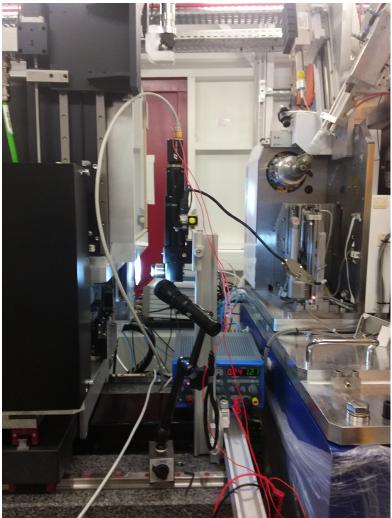
sync; echo 3 > /proc/sys/vm/drop_caches

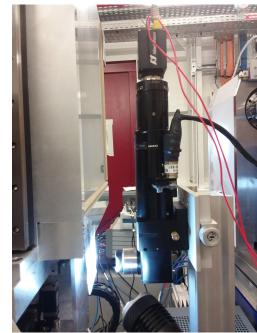
* executed as a cron job every 4 hours

- OAV zoom failure on Proxima 2
 - exchange for a spare and then for a replacement

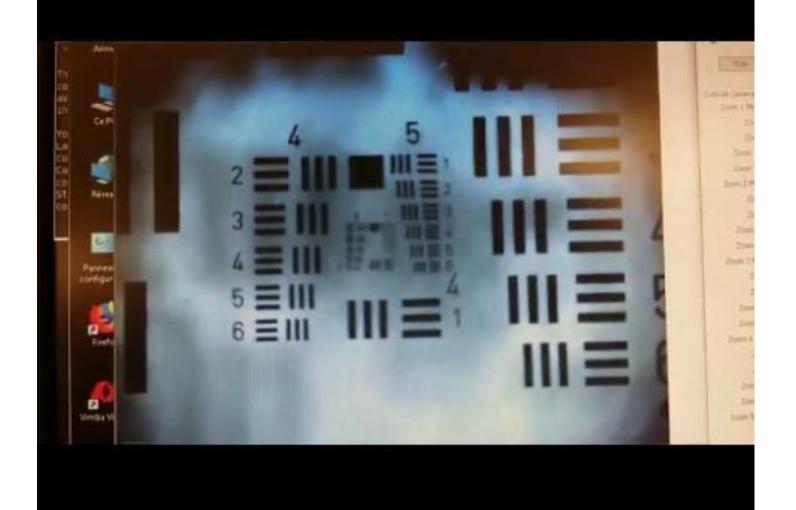
- OAV zoom failure on Proxima 2
 - exchange for a spare and then for a replacement
 - o aligning transfocator optical center and the camera center
 - verifying pixel calibration







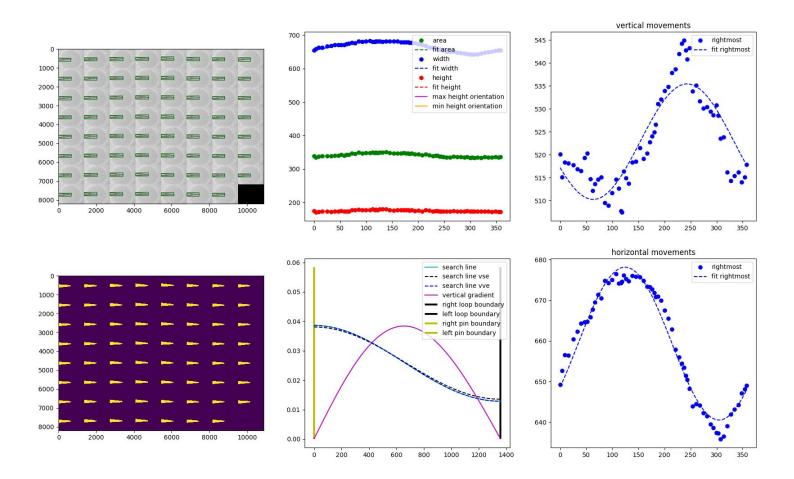


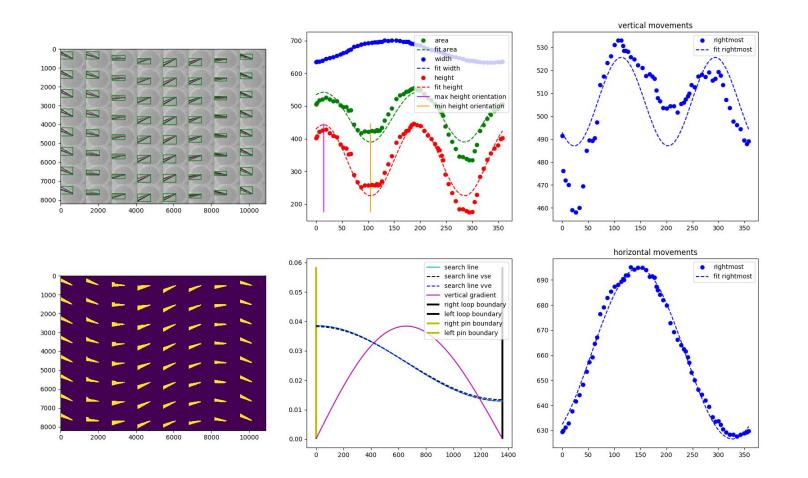


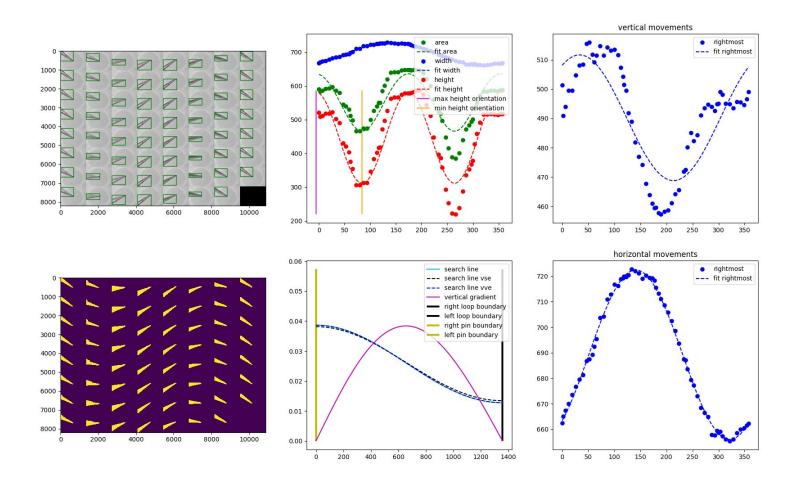
- OAV zoom failure on Proxima 2
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 - aligning transfocator optical center and the camera center
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- Deterioration of sphere of confusion of Omega axis with MK3
 - Discovered during a development session with GPHL in January 2019
 - in vertical from 2.4 um with kappa closed, ~ 10 um with kappa open (< 5um during SAT)
 - horizontal discrepancy of similar magnitude at large kappa

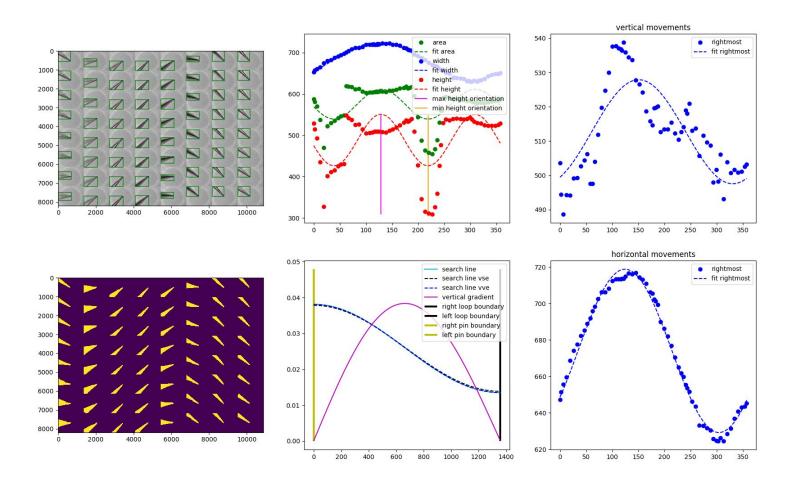
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GPhL Workflows	
Workflow	type
TranslationalCalibration	~
Data loca	tion
Folder:	
/nfs/ruche/proxima2a-spool/2019 Run1/com-proxi	ma2a/2019-03-11/RAW_DATA
Commissioning	
commissioning	
	Browse
Prefix transcal	
Prefix transcal	









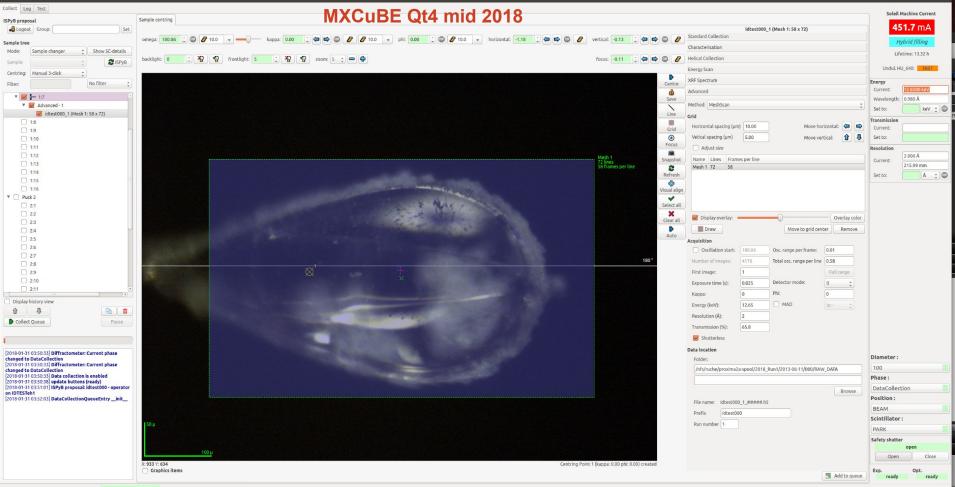
Short history of MXCuBE GUI on Proxima 2

File Beamline script Checks Admin Help				Expert mode
Collect XRF spectrum Log	g Chat (1)			
- User		Sample centring Sample changer MXCuBE Qt3 mid 2018		1
User: mx-com-proxima2a Group:	Set 🔑 Logou		Collection method	Soleil machine current
- Sample list		Omega の の の 会 <i>P P</i> 45.0 ッ Front Light 5 会 物 の Fist 発 物 の Focus 5 会 物 の Focus	Standard Collection	450.9 mA
Mode: Sample changer •	Hide SC-details		Standard concettori	Lifetime: 13.23 h
Centring: Manual	Synch ISPyB		0.1	Undul. HU_640:
			0.1 1	
- 1:1 - 1:2	<u> </u>			
- 1:3			1.0	Energy
- 1:4			12.65 Ip: P	12.650 keV
- 1:6			4.286	Current: 0.980 Å
e Standard - 1	Centring done !		100.0	Move to: keV 🔹 🌑
L C cpbs_26	Collection done			- Detector distance
E Standard - 2	Collection done			Current: 4.286 Å
🗄 🗖 Standard - 4	_			499.94 mm
□ cpbs_28 □ □ Standard - 5	Collection done			Move to: mm 🔹 🥘
L C cpbs_29	Collection done			Current: 100.00%
Standard - 6	Collection done		pxima2a-spool/2018_Run1/2018-01-30/com-proxima2a/RAW_DATA /Commissioning/CPBS	Set to:
E Standard - 7			peonini ano iniger us	Aperture
□ cpbs_31 □ □ Standard - 8	Collection done			Diameter :
└─ □ cpbs_32 ⊖- □ Standard - 9	Collection done		cpbs	50 V Transfer
└-□ cpbs_33	Collection done		38	
E □ Standard - 10	Collection done			Position : Scintillator :
E- C Standard - 11			200	BEAM V PARK V
└ □ cpbs_35 E-□ Standard - 12	Collection done			
L C cpbs_36	Collection done			
E □ Standard - 13	Collection done		0 0	
- 1:8 - 1:9				Guillotine
- 🗆 1:10				extract insert
- 1:11				
- 🗆 1:13				
- 1:14				
- 1:16				Frontend shutter
- 2:1				open
1 2.3	<u>ح</u>			
û IJ	1			Safety shutter
↔	<u> </u>			
Collect Queue	Pause			Fast shutter
[2018-01-31 03:05:07] Starting conected	hofore collect			out
[2018-01-31 03:05:13] Setting resolutio				
detector. [2018-01-31 03:05:13] Capillary beamst	stop in the beam			LN2 Regulation
path, starting to collect. [2018-01-31 03:05:15] Moving the deter	ector done.	100 µm		ON
[2018-01-31 03:05:15] Setting resolutio [2018-01-31 03:05:15] Capillary beamst	on done.		Characterization in the second s	Optical hutch Experimental hutch ready ready
path, starting to collect.	The second s	x: 1303 Y: 656	Characterisation Helical Collection	Current users
[2018-01-31 03:05:26] Collection compl [2018-01-31 03:07:20] CATS: Power On		Centre i Saachet BaanPachin Aneturalien Add Center Paint i	Energy Scan	Current users
[2018-01-31 03:08:22] Manual centring user to center sample	and the second second second	Centre Snapshot BeamPosition ApertureAlign Add Center Point	Advanced	E Colorting pives control
[2018-01-31 03:09:30] Centring saved [2018-01-31 03:10:16] Manual centring				Selecting gives control Allow timeout control
user to center sample [2018-01-31 03:10:53] Centring saved	and the second		Add to queue	Ask for control
[2016-01-31 03:10:53] Centring saved	<u> </u>	4		My name: proxima2a-5

8 🗢 🗊 MXCuBE			
Collect Log Test			Soleil Machine Current
ISPyB proposal	Sample centring MXCuBE Qt4 mid 2018		
Logout Group: Set		Sample: 1:7	450.3 mA
Sample tree	omega: 181.94 🙄 🖉 90.0 💌 —— kappa: 0.00 🙄 🖨 🖨 🖉 🖉 10.0 💌 horizontal: 1.11 🙄 🖨 🖨 🦉 🖉 vertical: 10.14 🙄		Hybrid filling
Mode: Sample changer 🛟 Show SC-details		Acquisition Oscillation start: 181.94 Osc. range per frame: 0.1	Lifetime: 13.41 h
Sample:	backlight: 25 🗧 🖓 🔞 frontlight: 5 📮 🎝 🔞 zoom: 5 🛫 🖶 🖨	Number of images: 3600 Total osc. range: 360.0	and the second second
Centring: Manual 3-click		First image: 1 Full range	Undul. HU_640: EAST
Filter: No filter ‡		Centre	Energy
* D - 1:7			Current: 12.6500 keV Wavelength: 0.980 Å 76
V Standard - 1			Set to: keV :
test_26_1 (Point 1) Collection		Line Energy (kev).	Transmission
▼ Standard - 2 test_26_2 (Point 1) Collecti		Crid	Current: 50.00 %
1:8		Transmission (%): 50	Set to:
1:9		Focus Shutterless	Resolution
1:10		Snapshot Data location	Current:
1:11		Folder:	215.99 mm
1:13		Refresh /nfs/ruche/proxima2a-spool/2018_Run1/2013-06-11/000/RAW_DATA	Set to:
1:14		Visual align	
1:15		Select all	
▼ □ Puck 2		File name: Uest_20_3_######.ns	
2:1		Clear all Prefix test_26	
2:2		Auto Run number 3	
2:4		Processing	
2:5		N.o. residues: 200 Space group: \$ 1 Unit cell:	
2:6			T
2:8	e experience a second	a: 0 β: 0 γ: 0	
2:9		Run processing after collection	
Display history view		Run parallel processing	
û 🤑 💼			
Collect Queue Pause			
1			
[2018-01-51 05:51:10] Collection: Getting sample inro			Diameter :
[2018-01-31 03:31:10] Getting loaded sample coords [2018-01-31 03:31:10] Collection: Moving to centred	and the second se		50
position [2018-01-31 03:31:10] Collection: Taking 1 sample			Phase :
snapshot(s) [2018-01-31 03:31:10] Collection: Setting transmission			DataCollection
to 50.00 [2018-01-31 03:31:10] Collection: Setting energy to			Position :
12.6500 [2018-01-31 03:31:10] Collection: Setting resolution to			BEAM
2.000 [2018-01-31 03:31:10] Collection: Updating data	ton.	Characterisation	Scintillator :
collection in LIMS [2018-01-31 03:31:10] Collection: started		Helical Collection	PARK
[2018-01-31 03:31:10] get_distance_from_resolution 1: resolution 1.9999922402, wavelength 980.11159619,		Energy Scan	Safety shutter
radius None [2018-01-31 03:31:10] get_distance_from_resolution 2:		XRF Spectrum	Open Close
[2018-01-31 03:31:10] get_distance_rrom_resolution 2: resolution 1.9999922402, wavelength 0.98011159619, radius None	X: 907 Y: 602 Point 1 (happa: 0.00 phi: 0.00) sele		
[2018-01-31 03:33:01] Collection finished	Graphics Rems	🚍 Add to queue	Exp. Opt. ready ready
			2

com-proxima2a@PROXIMA2A State: Ready Diffractometer: Ready Sample changer: - Last collect: OSC: Successful (2018-01-31 03:33:01)





com-proxima2a@PROXIMA2A State: - Diffractometer: Ready Sample changer: - Last collect: -

Collect Log							
ISPyB proposal		Sample centring	MVCuDE Otd October 200	10			ty shutter Machine current
Code: mx v - Password:	Login	Omega stage	MXCuBE Qt4 October 201		Transfer (100)	open Open Close O	open 449.8 mA Machine state
Sample tree Mode: Sample changer	Show SC-details	Omega: 360.00 🗘 ——	📾 🛃 10.0 👻 Kappa: 0.00 🗘 🍠 SampX: 0.000 🗘 SampY: 0.000 🗘	Front: 15 🕻 🏹 🌚	Transfer the design of the de	Resolution	Thu Jun 21 17:38, Shift Lign filling: Hybrid
Sample:	😂 ISPyB					2.658 Å	Beam usable
Centring: Manual 3-click		X: -0.423 🗘 Y: -1.027	Z: -0.050 C Phi: 0.00 C Focus: 0.000 C Vertical: 0.000 C	Back: 0 🗘 🏠 🌚	Zoom 1 🛟 🚍 🔂	Current: 300.00 m	Hutch temperature 21.8 C
Filter:	No filter 💲	Sample video				Set to:	A the Flux Remeasure flux!
Puck 1						Transmission Current: 12.75 %	Cryostream
Puck 2 Puck 3						Set to:	In place sample temperature: 100.0
Puck 3 Puck 4						Energy	Sample changer Low level alarmi, refill Of
Puck 5						Current: 12.6531	
Puck 6 Puck 7						Wavelength: 0.980 Å	
Puck 8						Set to:	keV 🛫 🔤
Puck 9							
						DataCollection [2018-06-22 10:00:17] Di	iffractometer: Current phase changed to
						Transfer [2018-06-22 10:03:26] Di	iffractometer: Current phase changed to
						DataCollection [2018-06-22 10:07:28] Di	iffractometer: Current phase changed to
(4()))					Transfer [2018-06-22 10:10:39] Di	iffractometer: Current phase changed to
Queue history							iffractometer: Current phase changed to
						Transfer [2018-06-22 10:26:39] Di	iffractometer: Current phase changed to
Collect Queue	Pause		and the second se		35		iffractometer: Current phase changed to
1			+			Transfer [2018-06-22 10:46:14] Di	iffractometer: Current phase changed to
Sample: manually-mounted	d		All			DataCollection [2018-06-22 11:01:23] Di	iffractometer: Current phase changed to
Standard Collection		States of Concession, Name				Transfer [2018-06-22 11:04:38] Di	iffractometer: Current phase changed to
Acquisition Oscillation start: 360 Osc. range per	r frame: 0.1						iffractometer: Current phase changed to
Number of images: 1800 Total osc. range						Transfer [2018-06-22 11:14:18] Di	iffractometer: Current phase changed to
First image: 1	Full range					DataCollection [2018-06-22 11:22:01] Di	iffractometer: Current phase changed to
Exposure time (s): 0.025 Detector mode						Transfer [2018-06-22 11:26:26] Di	iffractometer: Current phase changed to
Kappa: 0.0009 Phi:	0.0028			2 -		DataCollection [2018-06-22 11:30:50] Di	iffractometer: Current phase changed to
Energy (keV): 12.6531 MAD	ip:- ‡			1000		Transfer [2018-06-22 11:32:13] Di	iffractometer: Current phase changed to
Resolution (Å): 2.658							iffractometer: Current phase changed to
Transmission (%): 12.745						Transfer [2018-06-22 11:44:14] Di	iffractometer: Current phase changed to
Shutterless						DataCollection [2018-06-22 11:53:01] Di	iffractometer: Current phase changed to
Data location						Transfer	
Folder:							
/nfs/data/testQt4/2018-06-21/local-user/RAW_DATA	·						
Characterisation							
Helical Collection							
Energy Scan							
XRF Spectrum		X: 662 Y: 265		× × •			
Advanced			Centre Save Line Grid Focus Snapshot Refresh Alig			-)(
Collect Now	Add to queue	Graphics items				Say:	Send

- State: - Diffractometer: Ready Sample changer: - Last collect: -

Sample centring		5li	w manually-mounted				
	M now (ma	Sample	: manually-mounted	ISPyB p Code:		Password:	🕹 Login
	14 NOW (Ma			Sample			
		Oscillation start:	0 Range per frame: 0.1			•	Show SC-details
Front: 0 ; 70 9 Back: 10 ; 70 9 Centre Save Line Grid Snapshot Select all Clear all Beam Auto Anneal Excenter	Phase	Number of images:	1800 Total range: 0	Samp			😂 ізРув
Front: 0	Transfer 🛟	First image:	1 Fi	l range			
		Exposure time (s):	0.025 Detector mode: 9M	Cent	ring: Manual n-clicks	:	n-clicks: 3 step: 120.0
		Kappa:	0.0012 Phi: 360	Filter	ŧ		No filter 🛟
		Energy (keV):	12.65 MAD ip:	: •	Puck 1		G
		Resolution (Å):	6.776		1:1		
		Transmission (%):	20		1:2		
		Shutterless			□ 1:3 □ 1:4		
		Data location			1:5		
		Folder:			1:6		
		/nfs/ruche/proxima2a-spool/2019_Run1/com	-proxima2a/2019-03-08/RAW_DATA		1:7		
					1:8 1:9		
		File name: prefix_1_######.h5			1:10		
		Prefix prefix			1:11		
		Run number 1			1:12		
					□ 1:13 □ 1:14		
A REAL PROPERTY OF THE RE		Processing N.o. residues: 200 Space group:	-		1:15		
		Unit cell:	•)		1:16		
		a: 0 b: 0 c: 0			Puck 2		
	269°	α: 0 β: 0 γ: 0			2:2		
		Run processing after collection			2:3		
		🔲 Run Dozor			2:4		
		Characterisation			2:5		
		Helical Collection			2:7		
		Energy Scan			- m))))
		XRF Spectrum			eue history		
		GPhL Workflows			<u>0</u>		
					ollect Queue		Pause
		Advanced Collect Now	Add	0.0000			
		Confect Now	EB Add	Fron			Machine current
					disabled disable		0
		1			Open Close Open	Close	Machine state
		[2019-03-08 16:19:25] Data collection is enable	ed	Resol	ution		None Hutch temperature
				Curr	6.776 Å		21.7 C
150 µm					800.00 mm		Flux
				Set	.0:		Remeasure flux!
				Transi	mission		Cryostream In place
300 µm				Curr	ent		temperature: 290.0 K
X 77 ¥ 41				Set	.0:		Sample changer Low level alarm!
				Energ	v		refill Off
				Curr			Storage disc space
				Wav	elength: 0.980 Å		
Graphics items				Set	0:	keV 🛫 😂	

Improving ergonomy of the interface

making number of clicks and centring ste	p easily visible and c	configurable
	Standard Collection	Code: my

	Standard Collection		Code: mx v	- Pacword:	😂 Login
u: 270.00 🕻 🖨 🖨 🕲 🏉 10.0 👻 K: 0.00 🗍 🧬 K: 360.00 🕻 🏉 Focus: -0.137 🕻 🖉 Zoom: 1 🚊	Acquisition		Sample tree		
	Oscillation start:	0 Range per frame: 0.1		ample changer 👘	
	Number of images:	1800 Total range: 0	Mode: Sa	ample changer 🛫	Show SC-details
Front: 0 , 2 2 Back: 10 , 2 2 Centre Save Line Grid Snapshot Select all Clear all Beam Auto Anneal Excenter Transfer ;	First image:	1 Full range	Sample:		срув
	Exposure time (s):	0.025 Detector mode: 9M	Contring: M	anual n-clicks	n-clicks: 3 step: 120.0
	Карра:	0.0012 Phi: 360	Filter:		No filter 💲
	Energy (keV):	12.65 MAD ip:-	V D Puck 1		
	Resolution (Å):	6.776	1:1		
	Transmission (%):	20	1:2		
	Shutterless		□ 1:3 □ 1:4		
	Data location		1:4		
	Folder		1:6		
	/nfs/ruche/proxima2a-spool/2019_Run1/com-	-proxima2a/2019-03-08/RAW_DATA	1:7		
			1:8		
	File name: prefix_1_######.h5	Browse	1:10		
	Prefix prefix				
	Run number 1		1:12		
	Processing		1:14		
	N.o. residues: 200 Space group:	\$	1:15		
NULL CARDEN	Unit cell:		1:16 V Puck 2		
	a: 0 b: 0 c: 0 α: 0 β: 0 γ: 0		2:1		
269	Run processing after collection		2:2		
	Run Dozor		2:3		
			2:5		
	Characterisation		2:6		
A N L S	Helical Collection		2:7		
	Energy Scan		Queue history	,	
	XRF Spectrum		Û .		
	GPhL Workflows		Collect Que	Je	Pause
	Advanced				
	Collect Now	🗏 Add to queue	FrontEnd	Safety shutter	Machine current
			disabled	disabled	0
	6		Open Clo	ose Open Close	Machine state
	[2019-03-08 16:19:25] Data collection is enable	ed	Resolution		None
	for the second se			6.776 Å	Hutch temperature 21.7 C
150 µm			Current:	800.00 mm	Flux
12 yuu			Set to:	A 🔅 😂	Remeasure flux!
			Transmission		Cryostream In place
300 µm			Current:		temperature: 290.0 K
×77×41			Set to:		Sample changer Low level alarm!
			Energy		refill Off
				12.6500 keV	Storage disc space
			Wavelength:		
Graphics items			Set to:	keV 💲 🤤	

Sample centring

making number of clicks and centring step easily visible and configurable

	20100023		Logout	Group:			
nple tree							
Mode:	Manually mounted	*			Sho	w SC-details	
Sample:		÷	_		2	SPyB	
Centring:	Manual n-clicks			n-clicks:	3	step: 12	20.0
Filter:					No fil	ter	\$
	manually-mounted						
▼ 👿 s	itandard - 1 Manual centring (Skipp	ed				
8	mx20100023_1 (Colle	cting				

Sample centring annealing dialog							
	Standard Collection	e: manually-mounted		Code: mx		word:	Login
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Graphics items				Set to:	keV		

- State: - Diffractometer: Ready Sample changer: - Last collect: -

Sample centring annealing dialog						
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Front 0 2 20 Back 10 2 20 Centre Save Line Crid Stapshot Select all Clear all Beam Auto Annea Excenter Transfer :	First image:	1	Full range			n-clicks: 3 step: 120.0
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anneal for 1.0 seconds	/nfs/ruche/proxima2a-spool/2019_Run1/com	-proxima2a/2019-03-08/RAW DATA		1:7		
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269*	Run processing after collection			2:2		
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			CPhL Workflows Advanced Collect Now (2019-03-08 16:19:25) Data collection i		Add to queue	Collect Que FrontEnd Gopen Cl Resolution Current: Set to: Transmission Current: Set to: Energy Current:	ue Safety shutter disabled Open Close 6.776 Å 800.00 mm Å 12.6500 keV 0.980 Å	Machino Hutch tu Flux Remeas Cryostro Sample	Pause current 0 state None urrefture 21.7 C ure fluxt mperature temperature 20.0 K
	Construct all Clear all Beam	Second Length 0.1	Scan length 0.1 mm Cancel OK	Sector Sector Scan length 0.1 Scancel OK Sector Sector Scancel OK Sector Sector <th>Scandength 0.1 max Cancel OK Marketenado See graph Scandength 0.1 Marketenado See graph Marketenado</th> <th>Image: receive rece</th> <th>Image: real real real real real real real real</th> <th>Image: Image: Image</th> <th>Image: Image: Image</th>	Scandength 0.1 max Cancel OK Marketenado See graph Scandength 0.1 Marketenado See graph Marketenado	Image: receive rece	Image: real real real real real real real real	Image: Image	Image: Image

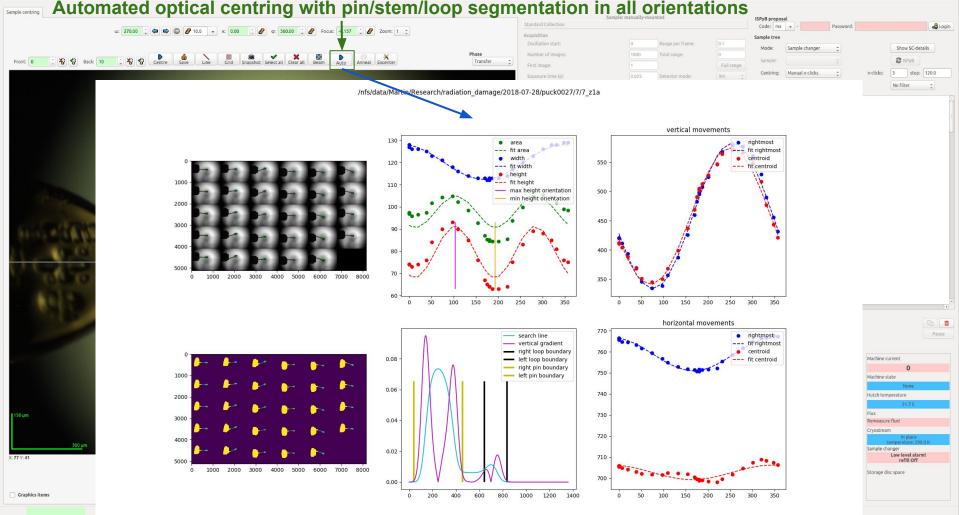
- - -



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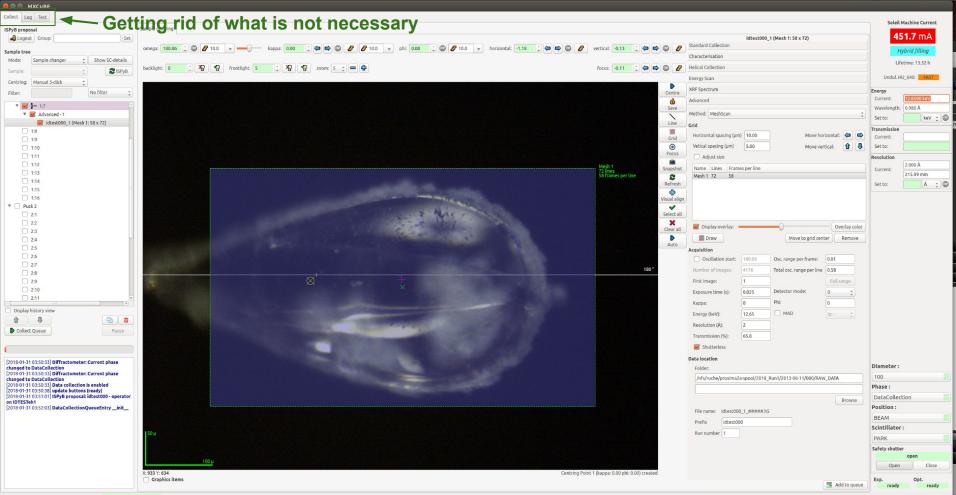
- State: - Diffractometer: Ready Sample changer: - Last collect: -



State: - Diffractometer: Ready Sar

Rapid beam realignment -- steering small beam to the center of the camera (optical center of the OAV)

		Standard Collection				Code: mx		Password:		🕹 Log	gin
uz 270.00 📮 🖨 🏟 🕲 🧬 10.0 👻 🖈 🔞 360.00 🛊 🌮 95.000 🛊 🥙 Focus: -0.137 🗦 🥔 Zoom: 1 🛫		Acquisition				Sample tree					
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		Exposure time (s):	0.025	Detector mode:	9M 🛟	Centring:	Manual n-clicks	:	n-clicks: 3	step: 120.0	
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com-proxima2a@PROXIMA2A State: - Diffractometer: Ready Sample changer: - Last collect: -

Getting rid of what is not necessary		Sample: ma	anually-mounted		ISPyB proposal				
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			20		1:2				
		Shutterless			1:3				
		Data location			1:4				
		Folder:			1:6				
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		File name: prefix_1_######.h5		Browse	1:10				
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HE STATE A DECEMBER OF STATE		Unit cell:			1:16 V				
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	269°	Run processing after collection			2:2				
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		Characterisation			2:6				
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ቆ Login

step: 120.0

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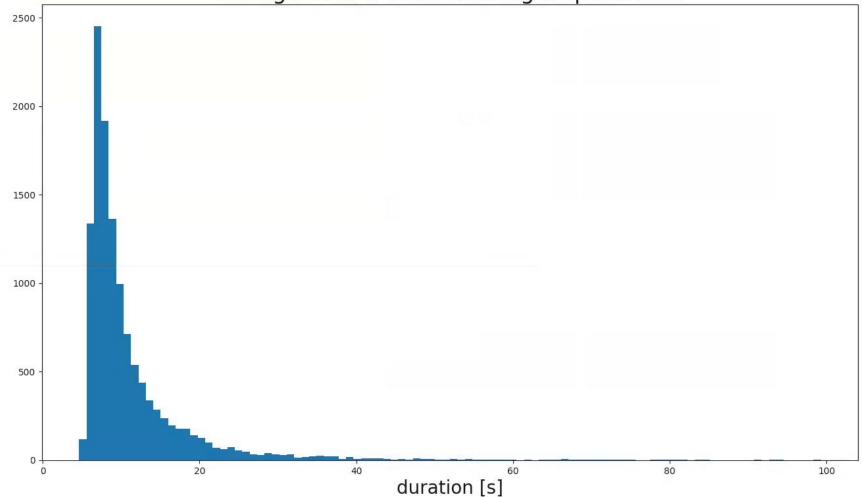
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Other developments

- Shuterless Energy Scan
 - faster acquisition while not losing accuracy
 - <u>https://github.com/MartinSavko/chooch_python_translation</u>
 - translating mucal.c and chooch.c into python
- Adding excitation energy parameter for XRF
 - Useful information when performing the fit
 - Automated fit of the most common scatterers
- Learning from users about centring
 - database of 15k centring for last couple of runs

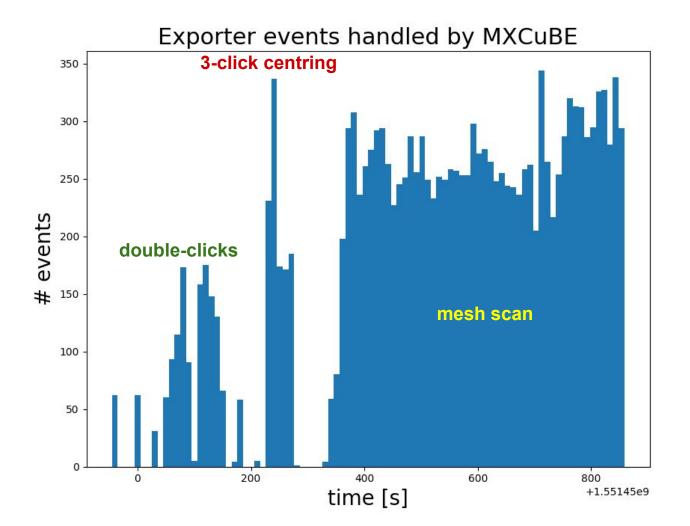
XRF Spectrum	
Data location	
Folder:	
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/XRF	
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Prefix Sample X	
Run number 1	
Parameters	
Count time (s): 10	
Excitation energy (keV): 15.00	
✓ Adjust transmission	

Histogram of n-click centring elapsed time



empression g		Sample: manually-mounted			ISPyB proposa					
		Standard Collection			Code: mx	· -	Password:		4	
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150 µm				_	Cables		A :	Flux		
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300 µm		Thanke by	arel		Current:				nperature: 290.0 K	
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					Wavelength					
					Set to:	0.700 A	keV 🛊 😂			
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😂 Login



Wrap up

- Improving smoothness ergonomics of the GUI
 - tango with events (with exception of sample changer)
 - exporter events for MD2
- resolved problem with MD2 stutter
 - problems stabilising Omega axis at the end of movements
 - executing startSimultaneousMoveMotors() as opposed to writing to an attribute
- stripped down non essential components
 - start-up time 15 seconds (down from about 55 second at the beginning of the campaign)
- focus on ergonomy
 - three column design
- making the useful features obvious
 - x-ray centring, n-click centring options, automated alignment

MXCuBE is embodiment of Experimenter's dream of performing a perfect experiment

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