

HDRMX LUND MARCH 2017

DIAMOND / EIGER STATUS UPDATE



ACKNOWLEDGEMENTS

- Worldwide developers for e.g. EPICS drivers
- Software developers - XDS, DIALS, xia2, ...
- Funding - CCP4, EU, Diamond, Wellcome, ...
- Infrastructure support - science computing, data acquisition, data analysis, beamline staff, ...



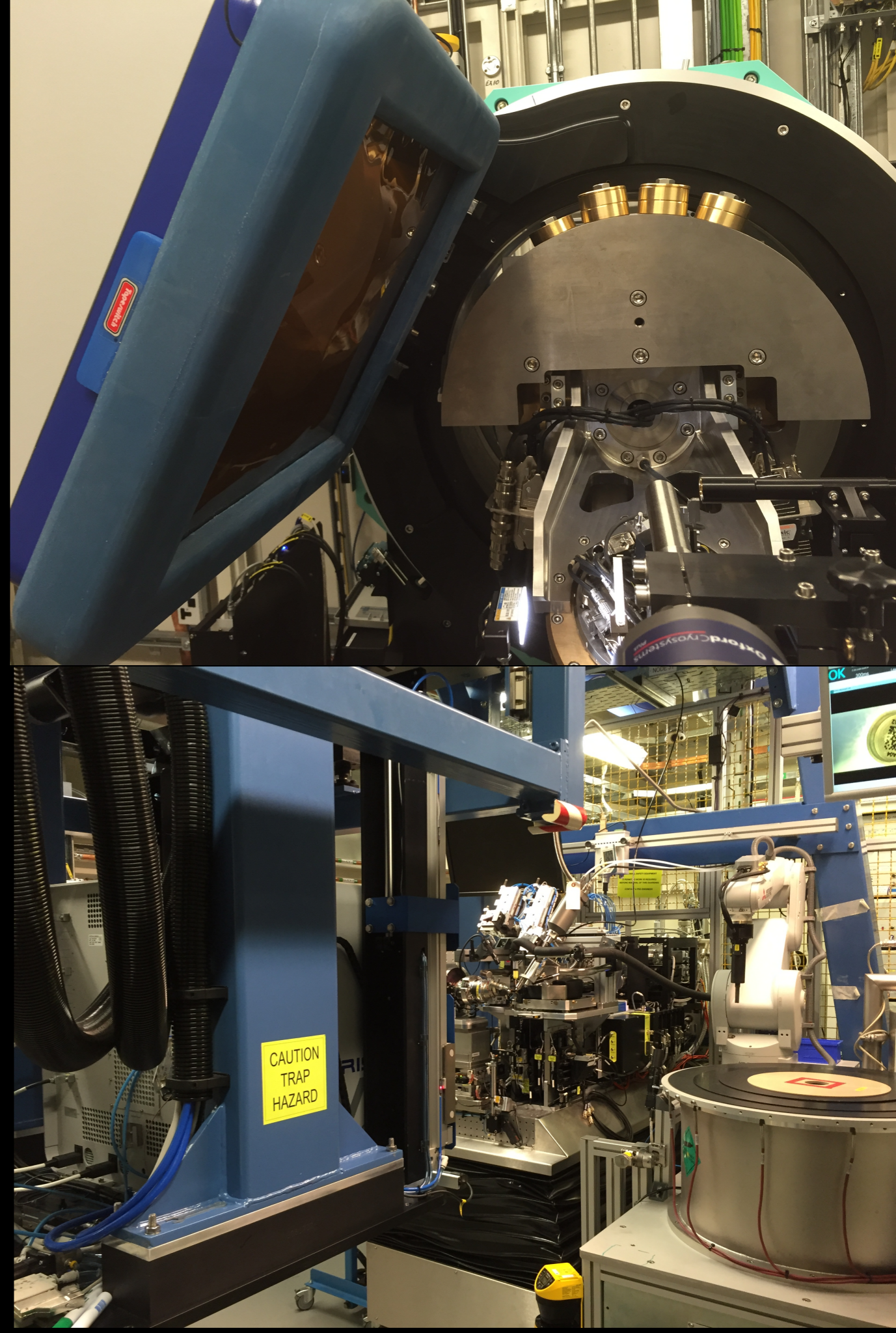
diamond

xia2



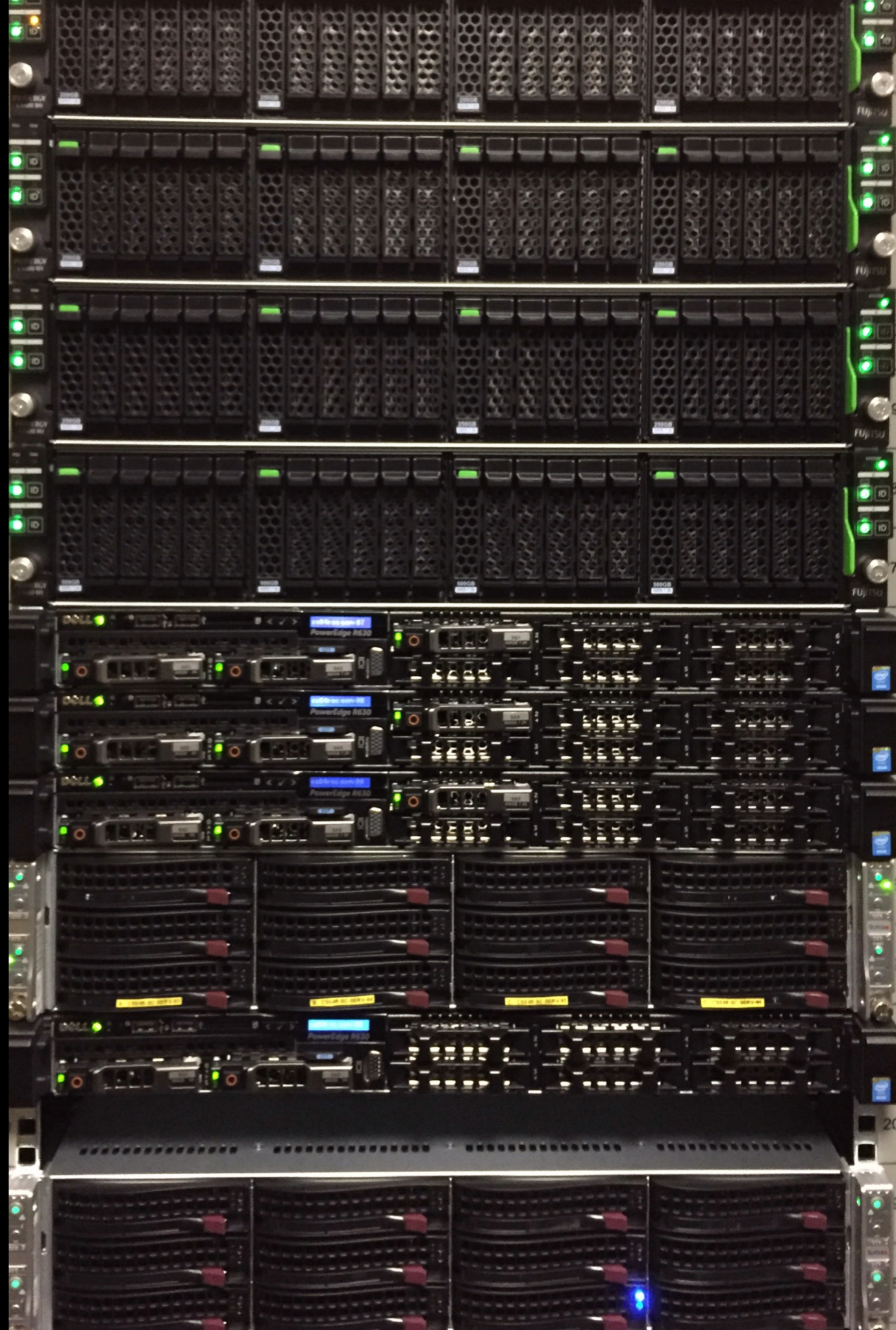
DIAMOND BEAMLINES

- All MX / MX-like beamlines have pixel array detectors
- 2 x Pilatus3 6M @ 100Hz
- 3 x Pilatus2 6MF @ 25 Hz
- 1 x Pilatus2 12M @ 12 Hz
- 1 x Pilatus2 2M @ 30Hz
- Aggregate around 2GB/s



NETWORK / COMPUTE

- Dedicated per beamline 2 x 10Gb link to GPFS / Lustre storage
- 4PB fast parallel storage
- 2160 cores available to MX for auto processing (12, 16, 20 core nodes) - connected by infiniband to storage



XCHEM - HIGH THROUGHPUT

- Beamline dedicated to unattended experiments - automount, centre, collect, unload
- 500 - 700 samples / day
- 40s sample exchange
- Full data set in 60s: 1500 images @ 25 Hz / 0.12°

09-03-2017 08:10:12 - FALZ

Sample: FALZA-x0438	Flux: NaN
Ω Start: 0.0°	Ω Osc: 0.12°
Ω Overlap: 0°	No. Images: 1500
Resolution: 1.50Å	Wavelength: 0.9282Å
Exposure: 0.040s	Transmission: 100.00%
Beamsize: 0x0µm	Type: SAD
Comment: (119376,79,283) Aperture: 70um	

Auto Processing

Downstream Processing

09-03-2017 08:09:28 - Robot loading puck 35 pin 8 (Bar

09-03-2017 08:08:23 - FALZ

Sample: FALZA-x0437	Flux: NaN
Ω Start: 0.0°	Ω Osc: 0.12°
Ω Overlap: 0°	No. Images: 1500
Resolution: 1.50Å	Wavelength: 0.9282Å
Exposure: 0.040s	Transmission: 100.00%
Beamsize: 0x0µm	Type: SAD
Comment: (119850,-195,207) Aperture: 70um	

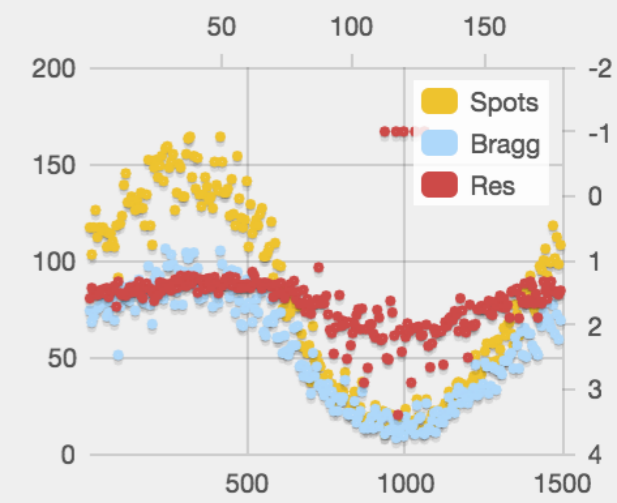
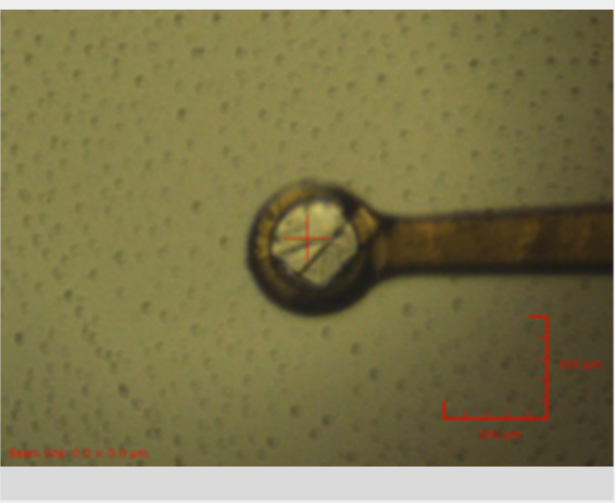
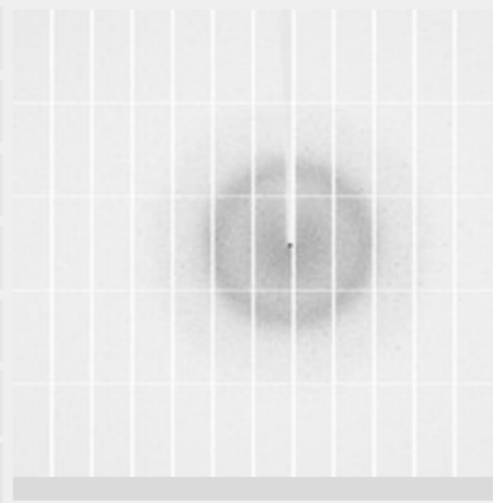
Auto Processing

Downstream Processing

AUTO PROCESSING

09-03-2017 08:10:12 - FALZA/FALZA-x0438/FALZA-x0438_1_####.cbf

Sample: <u>FALZA-x0438</u>	Flux: NaN
Ω Start: 0.0°	Ω Osc: 0.12°
Ω Overlap: 0°	No. Images: 1500
Resolution: 1.50Å	Wavelength: 0.9282Å
Exposure: 0.040s	Transmission: 100.00%
Beamsize: 0x0µm	Type: SAD
Comment: (119376,79,283) Aperture: 70µm	



Auto Processing Fast DP: Xia2:

Fast DP XIA2 3d XIA2 3d XIA2 DIALS XIA2 3dii XIA2 3dii XIA2 DIALS autoPROC

Beam Centre	X	Y
Start	212.50	250.90
Refined	212.65	251.11
Δ	-0.15	-0.21

[MTZ file](#)
[Log file](#)
[Archive](#)
[Radiation Damage](#)
[Lookup Cell](#)

Space Group	A	B	C	α	β	γ
C 1 2 1	112.04	27.37	38.19	90.00	96.01	90.00

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
outerShell	2083	1596	1.15 - 1.18	0.850	0.6	14.1	52.0	1.3	12.1	1.1	0.0
innerShell	1538	508	5.13 - 27.86	0.025	35.3	99.8	99.0	3.0	87.9	1.8	5.7
overall	98693	38421	1.15 - 27.86	0.064	8.2	99.7	92.3	2.6	57.2	1.6	0.6

Downstream Processing Fast EP: Dimple: MrBUMP: Big EP:

All autoindexing results:

Lattice	a	b	c	alpha	beta	gamma
mC	112.00	27.40	38.20	90.00	96.00	90.00
aP	27.40	38.20	57.60	95.90	103.70	90.00

Mosaic spread: 0.09 < 0.13 < 0.14

Happy with sg# 5

112.20	27.40	38.20	90.00	96.10	90.00
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Low resolution	27.86	27.86	1.18
High resolution	1.15	5.13	1.15
Rmerge	0.064	0.025	0.850
I/sigma	8.20	35.30	0.60
Completeness	92.3	99.0	52.0
Multiplicity	2.6	3.0	1.3
CC 1/2	99.7	99.8	14.1
Anom. Completeness	57.2	87.9	12.1
Anom. Multiplicity	1.6	1.8	1.1
Anom. Correlation	0.6	5.7	0.0
Nrefl	98693	1538	2083
Nunique	38421	508	1596
Mid-slope	0.958		
dF/F	0.138		
dI/sig(dI)	0.940		

Merging point group: C 1 2 1

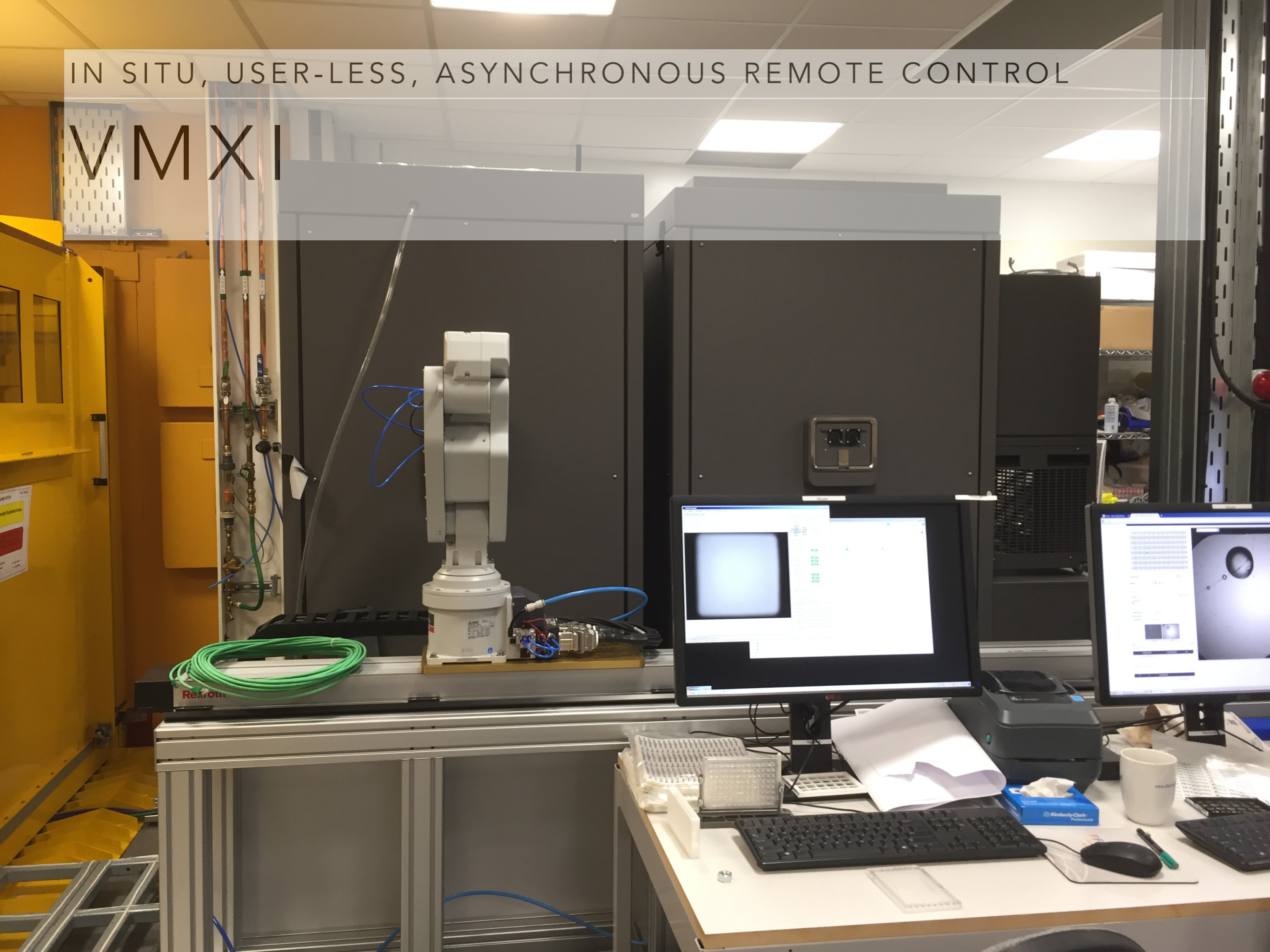
Unit cell: 112.04 27.37 38.19 90.00 96.01 90.00

Processing took 00h 00m 30s (30 s) [98693 reflections]

RPS: 3224.9

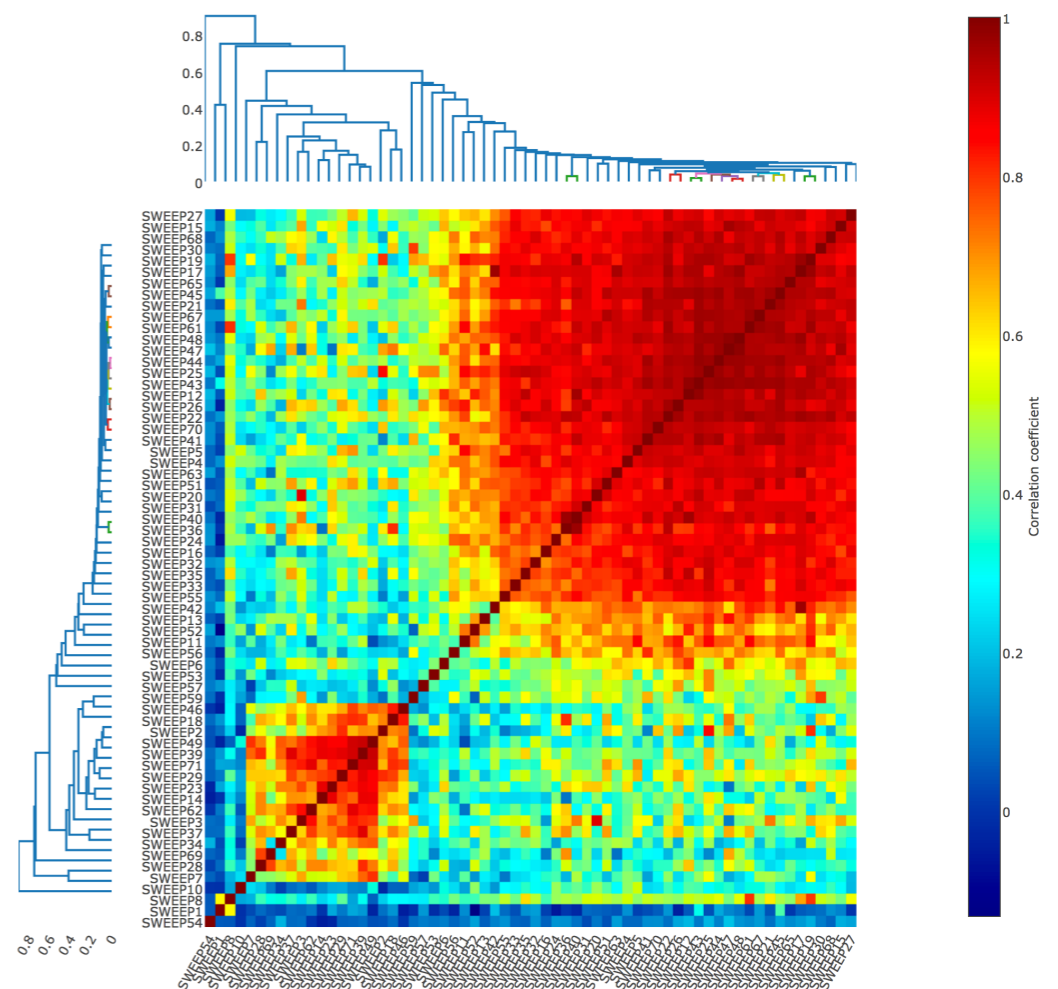
IN SITU, USER-LESS, ASYNCHRONOUS REMOTE CONTROL

VMXI



VMXI COLLECTION

- Automated UV / vis plate imaging
- In situ data collection
- Grid scans
- 5 micron beam
- DCM 2×10^{12} / DMM 10^{14}
- #1 Diamond Eiger detector - 4M @ 750 Hz (Q2 2017)



PHASED SOFTWARE STRATEGY

- Phase 0: adapt xia2 / DIALS to work with Eiger HDF5 - done
- Phase 1: adapt existing tools for fast processing - fast_dp - to use CBF images from Eiger detector, parallel unpack to network scratch area for processing - done
- Phase 2: adapt DIALS to replace XDS in fast_dp, re-implement per-image-analysis for HDF5 - ongoing...

TIMELINE (CURRENT)

- Q2 2017 Eiger 4M / VMXi - MX
- Q2 2018 Eiger 16M / i04 - MX
- Q3 2018 Eiger 4M / B21 - SAXS
- Q4 2018 Eiger 16M / i03 - MX



CHALLENGES

- Container format, moving data, storage
- SynchWeb data view
- Live beamline data view
- High multiplicity / low dose data collection - TB / hour reasonable
- In situ possibility - 1mm x 1mm grid @ 0.01mm @ 750 Hz x 96 wells - 1,000,000 x 4MP images in < 30 minutes
- Automated collection - removing the human from the loop - XCHEM, VMXi



ARE WE PREPARED?

- We don't know how these detectors will be used
- Best case - similar to Pilatus
- Worst case - previous slide
- Truth - probably somewhere in the middle

