Australian Synchrotron
Turning bright ideas into brilliant outcomes

Current and planned MX Beamline computational and network capabilities at the Australian Synchrotron.

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Supported by

Australian Government

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The MX Team

MX Team

- **Daniel Eriksson - Scientist**
- **Steve Harrop - Scientist**
- **Rachel Williamson- Scientist (0.6)**
- **Santosh Panjikar - Scientist**
- **David Aragao – Scientist**
- **Jason Price – Scientist**
- **Jun Aishima – Postdoc**
- **Sofia Macedo – Scientist (0.6)**

Engineering

- **Mark Clift – Controls Engineer**
- **Robbie Clarken – Developer**
- **Hima Cherukuvada – Mechanical Engineer**

Motion Solutions

Staff at SLS, LBL and SLAC for code, help and advice!

In particular, James Holton, Aina Cohen, Meitian Wang, Zac Panepucci, Simon Ebner & James Leuenberger.

Background

- Two MX beamlines at the AS

	MX1	MX2
Source	Bending Magnet	In-vacuum undulator
Beam size (HxV microns)	180x150	22x12
flux	3.6e11 ph/s	2.1e12 ph/s
energy range (keV)	6 to 18	4.8 to 21
Sample Robot	SAM	SAM
Detector	ADSC Q210r CCD	ADSC Q315r CCD
Micro-collimator	No	Yes (20,10, 7.5m apertures)
Role	General Use	Micro-focus
First Users	June-07	December-08

- Both beamlines have SAM robots installed inc remote access.
- Both detectors are ADSC CCDs (MX1=Q210r, MX2=Q315r).

- Goal is fastest route to structure.

Eiger 16M

- Eiger 16M ordered May 2016.
- EPU ordered as part of package.

- Scheduled for installation in early 2017.

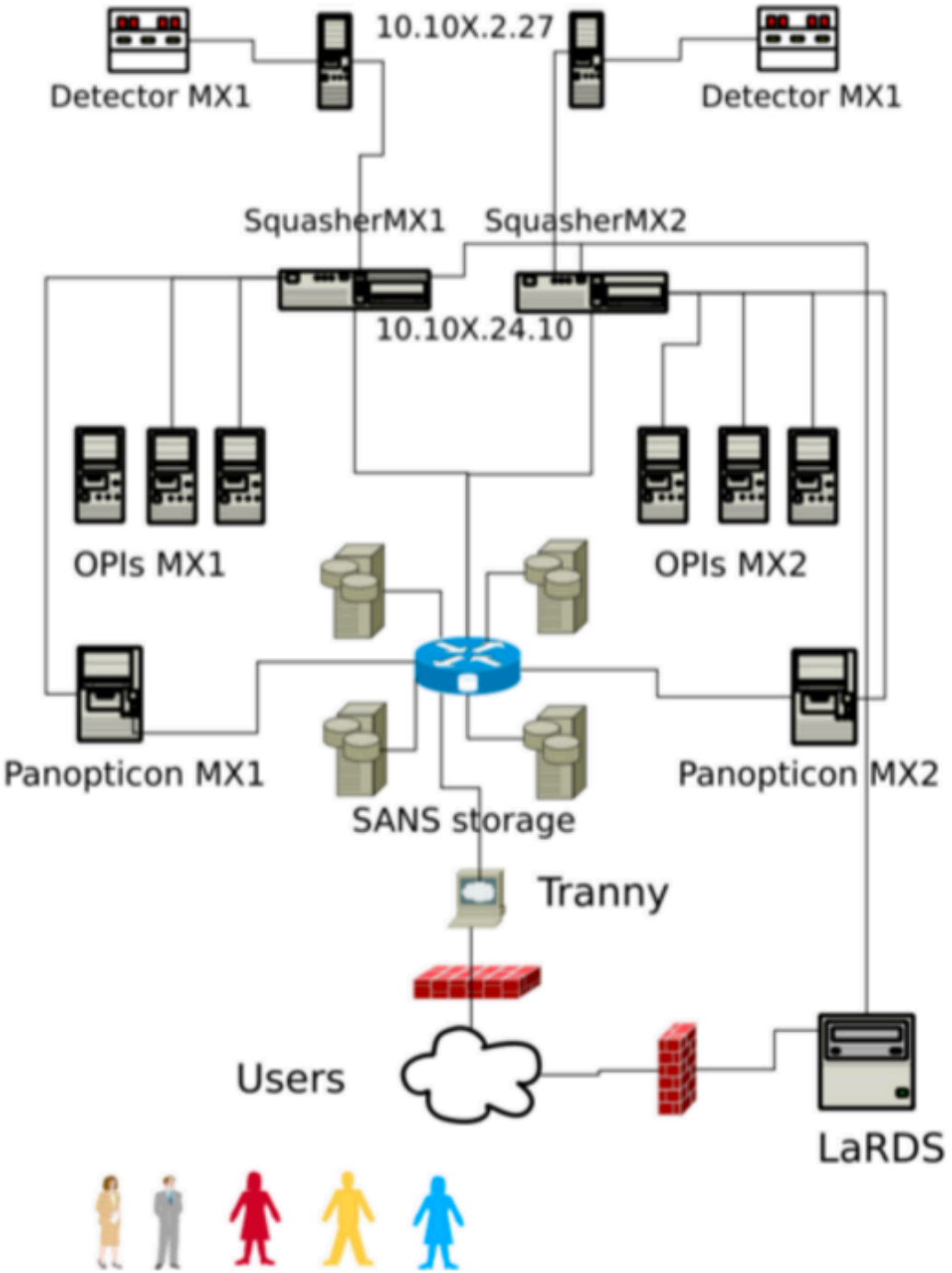
Beamline networks and data flow.

1. The beamline networks are segmented.
2. Each has dual bonded 10Gb fibre links to the facility server network (SAN, cluster).
3. Data is processed on a fast local server inside the beamline network.
4. After the experiment is complete data is compressed using squashfs and the squashfile is moved to the facility SAN. After validating this move the raw data is deleted.

MX Data flow.

SANS Storage is a 0.5Pb array.

Will be replaced with 2Pb CEPH cluster.



Experiment control and Data Processing.

- BluICE[1] user GUI.
- EPICS for instrument control.
- Python beamline library used for logic and execution
- Areadetector used for detector control.
- Files processed from disk
- Triggering and processing using ZeroMQ
- Automated integration and scaling using XDS[2] (via xdsme[3]), pointless[4] and Aimless[5].
- Results displayed on Python web-app (Flask).
- Fast indexing results.
- Reasonably fast integration results.

1. McPhillips, T.M. J Sync. Rad. (2002).
2. Kabsch, W. Acta Cryst. D66, 125-132 (2010).
3. Legrand, P. https://github.com/legrandp/xdsme
4. Evans, P.R Acta Cryst. D62, 72-82 (2006).
5. Evans, P.R. Acta Cryst. D69, 1204-1214 (2013)

Proposed Eiger Experiment control and Data Processing.

- Areadetector and ADEiger plugin used for detector control.
- Fast processing with EPU
- Encoder position capture using Galil 4080.
- Triggering and processing using ZeroMQ
- Data processed in RAM as stream.
- Automated integration and scaling TBA (testing code from SLS)
- Results displayed on Python web-app (Flask).
- Very Fast indexing results.
- Fast integration results.
- Fast rastering
- Serial crystallography
- Beam-based crystal location.

Planned new structure

1. Use kit supplied by Dectris (DCU and EPU).
2. Add additional local processing hardware (many fast cores, lots of RAM, little GPU) as needed.
3. Add storage to new facility CEPH cluster as needed.
4. Move compressed data to CEPH cluster after experiments

Development

1. Collaborate with SLS and other light sources on community fast processing code (not reinvent the wheel).
2. Contribute to new data standards and HDRMX methodologies.
3. Be flexible. New equipment will be purchased as needed to reach performance goals.
4. We have one full time developer (Jun Aishima) on new pipelines and automation. Will be hiring a second developer on a 3-year contact soon.

Summary:

1. Replacing CCD with Eiger.
2. Separate beamline networks
3. Fast local hardware
4. Flexible and keen to collaborate.
5. Intend to implement new pipelines using community code and practices.

Questions?