MX3 Beamline Update

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Existing MX beamlines at the AS:

MX1:

BM source

180x150 micron beam, 3.4e11 ph/s flux.

MAD capable (6-18 keV energy range)

MX2:

3m u22 IVU source

22x12 micron beam, 2.4e12 ph/s flux
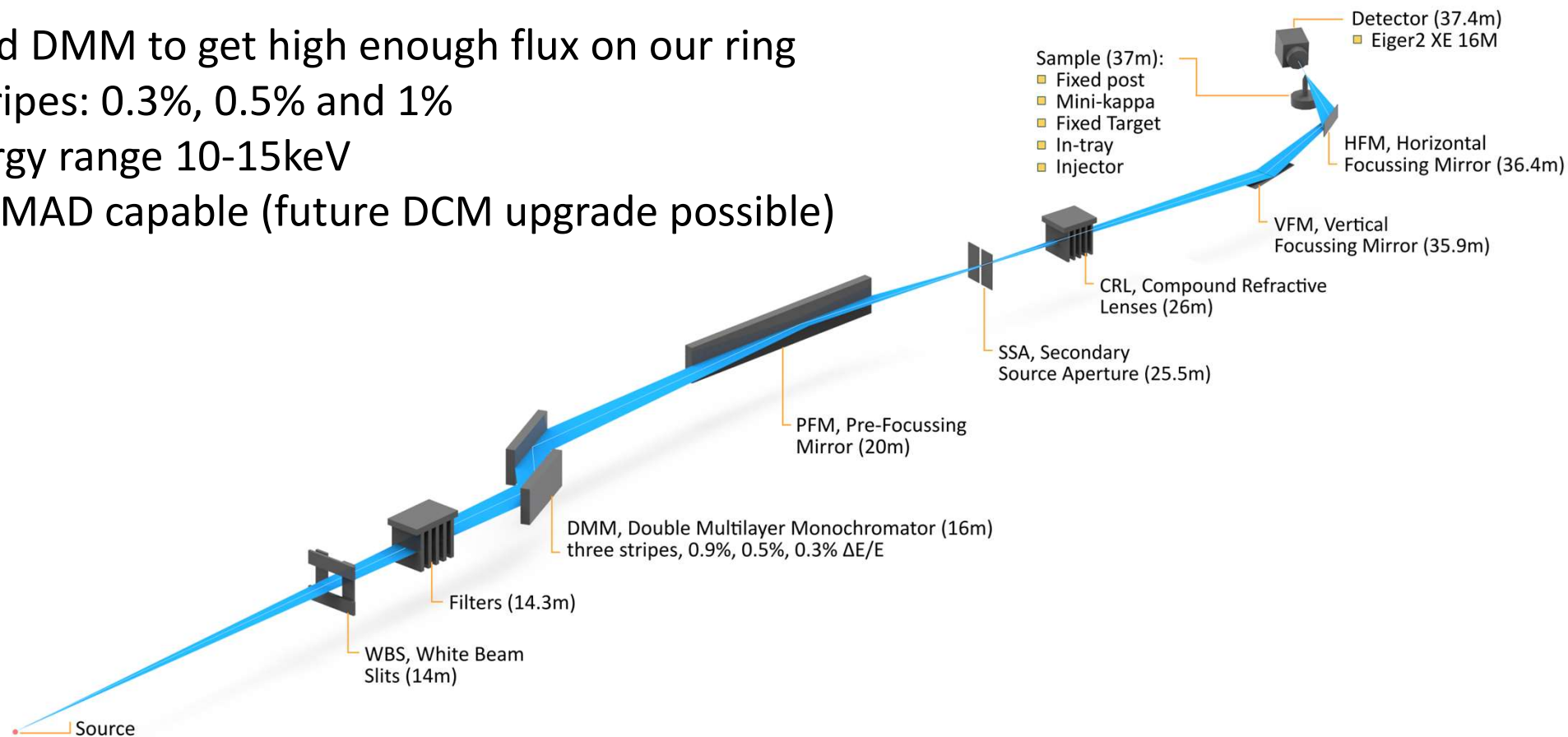
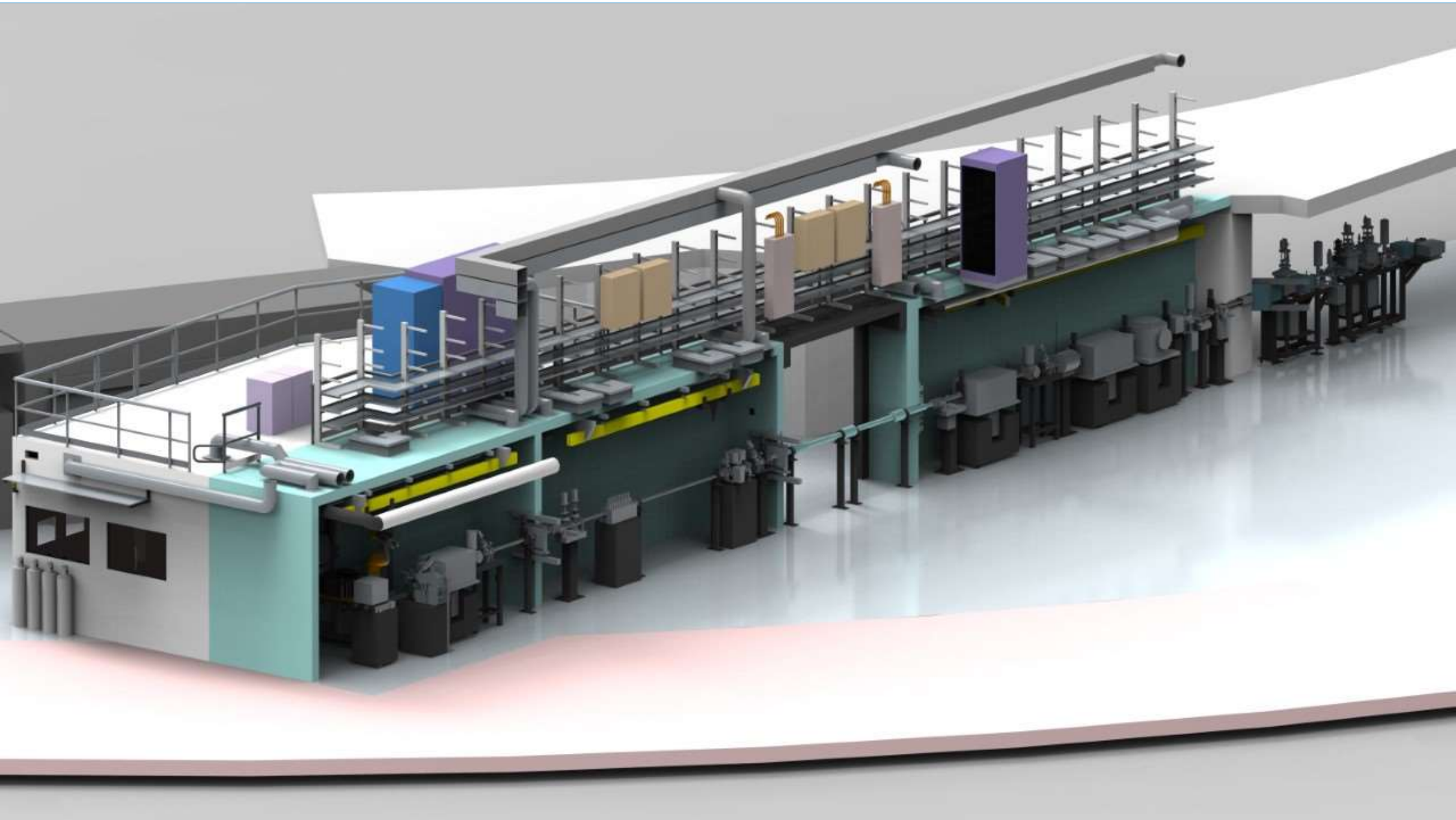MAD capable (5-21 keV energy range)

High flux micro crystallography

Need DMM to get high enough flux on our ring
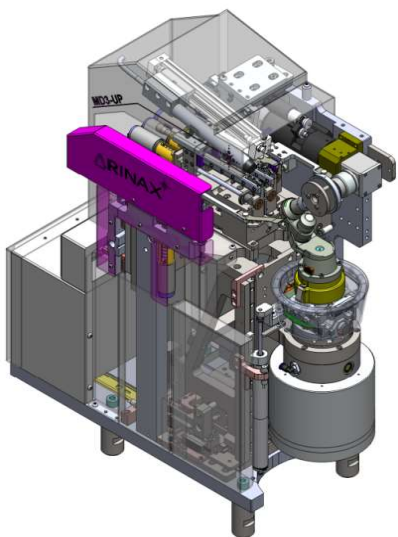3 stripes: 0.3%, 0.5% and 1%
Energy range 10-15keV
Not MAD capable (future DCM upgrade possible)

Detector (37.4m)
Eiger2 XE 16M

Sample (37m):
- Fixed post
- Mini-kappa
- Fixed Target
- In-tray
- Injector

HFM, Horizontal
Focussing Mirror (36.4m)

VFM, Vertical
Focussing Mirror (35.9m)

CRL, Compound Refractive
Lenses (26m)

SSA, Secondary
Source Aperture (25.5m)

PFM, Pre-Focussing
Mirror (20m)

DMM, Double Multilayer Monochromator (16m)
three stripes, 0.9%, 0.5%, 0.3% ΔE/E

Filters (14.3m)

WBS, White Beam
Slits (14m)

Source

Four main modes of collecting data

Single crystal goniometer

Tray screening and collecting

Fixed target

Sample motion

X-rays
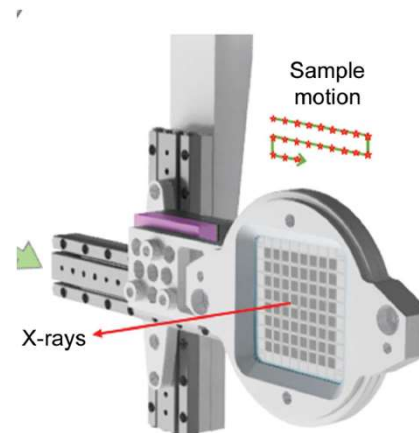
Injector

?

In-house expertise

ANSTO

Automation, the core problem

At modern data rates humans can't keep up:

- What sample is this?
- Typing info into a GUI
- Writing notes
- Assessing data quality
- Making good collection decisions
- Automated crystal location
- Automated collection plans

MX3 Scientific computing

Confidence

- A database to manage sample/experiment data (ISPyB vs in-house)
- User GUI (MXCubev3 vs in-house)
- Tray screening GUI (SynchWeb vs in-house)
- Python logic code (similar to ZOO, some in-house)
- Ophyd+Bluesky
- Autoprocessing code
- Cluster management
- Data management

ANSTO

Thank you!

~~Questions?~~

Questions!

- ISPyB with IceBear?
  - w/o IceBear?

- MongoDB vs SQL?
  - Flexibility vs speed?

- Going from single to serial xtallography?
  - Lessons learned?

- Injector data processing?
  - Or, how to drink from the fire-hose?