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MX3 Beamline – Automation

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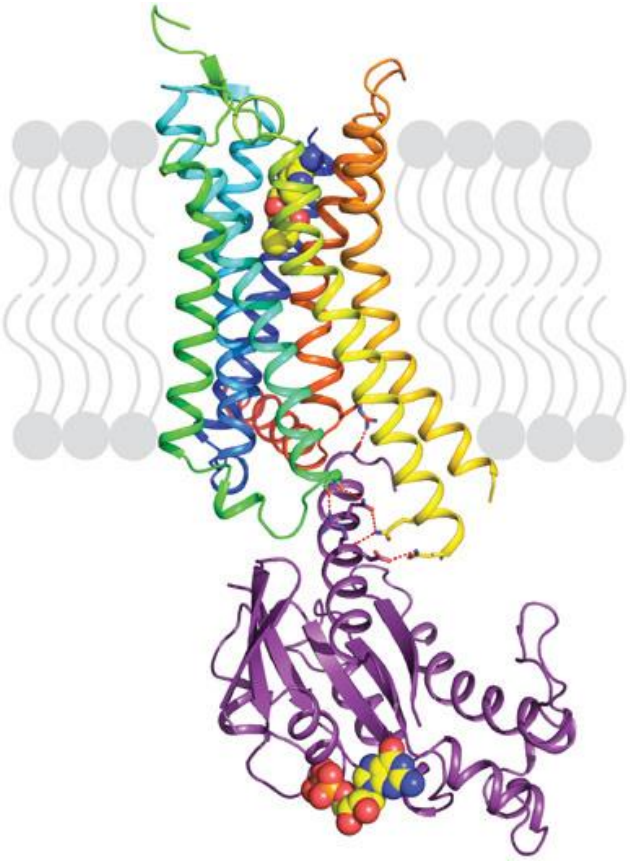
Overview of High performance Macromolecular Crystallography (MX3)



- High Flux Microfocus MX line – first users July 2023.
- Endstation optimised for ***single crystal and serial crystallography***
- Will complement the existing MX1/MX2 beamlines.
  MX3 will be able to measure smaller and more weakly diffracting crystals.
- MX3 will also be capable of ***in-tray screening***, breaking the current bottleneck in crystal production to understand disease pathologies and drug development.
- ***Highly automated (crystal location, data collection and merging).***

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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)

Eiger2 9M

MX2:

3m u22 IVU source

22x12 micron beam, 2.4e12 ph/s flux

MAD capable (5-21 keV energy range)

Eiger 16M

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Current MX Eiger processing system outline

Web app

http://processing/retrigger/submit

8876: zmq reply

8877: zmq pub

Forkintegrate re-written in Python and handles interface to Kubernetes

zmq subscribe

autorun
IP:*.2.44

"START ...."
"IMAGE ...."
"FINISH...."

newdataset.py
IP:*.2.44

Autodataset redis queue

Indexing redis queue

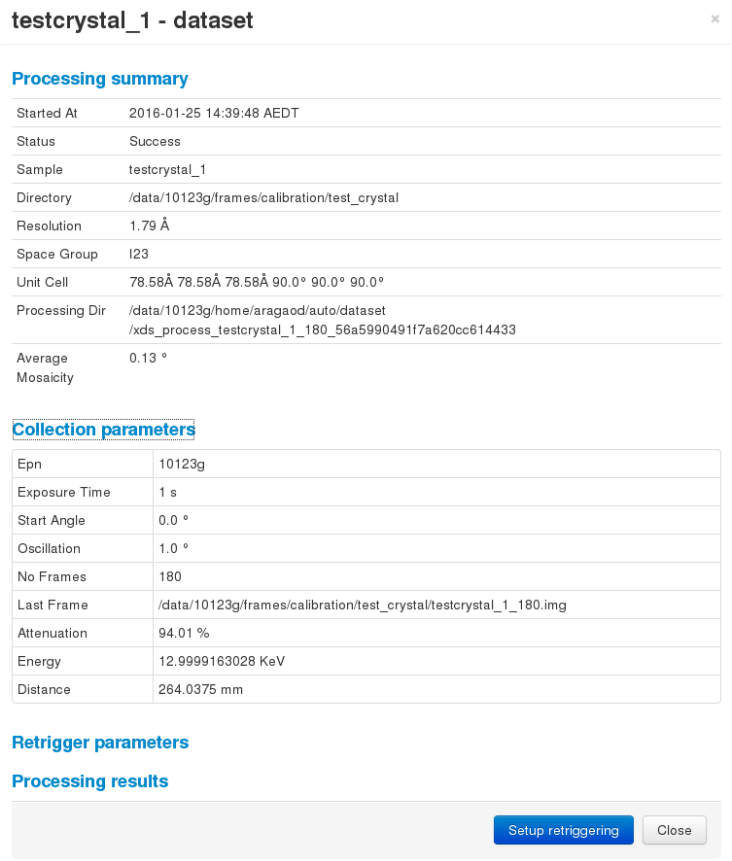
indexing-cpu1,2,3 host:EPU

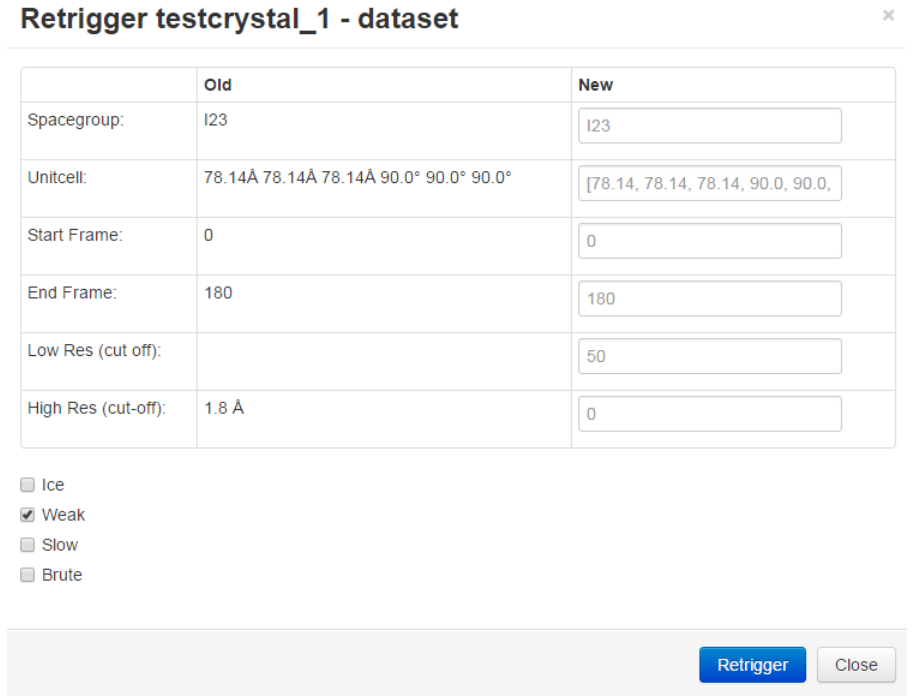
ASCI processing cluster
12x 2xE5-2697 v4 CPUs, 128GB RAM

Data processing is normally ~4X collection time (~72s for an 18s collection) from shutter close. Frequently 2X.

Processing GUI

- Retriggering – automatic processing is run on all data, with best estimates for parameters
  - Retriggering allows the user to feed information back into the system to get a better dataset





MX3 Scientific computing

- A database to manage sample/experiment data (ISpyB)
- User GUI (MXCubev3)
- Tray screening GUI (SynchWeb)
- Python logic code (similar to ZOO[1], some in-house)
- Ophyd+Bluesky
- Autoprocessing code
- Cluster management
- Data management

1: Hirata *et al,* (2018) “ZOO: an automatic data-collection system for high-throughput structure analysis in protein microcrystallography”, *Acta Cryst* D75, 138-150.

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Scientific Capabilities that MX3 will add:

1. In-tray screening
2. High flux micro crystallography (GPCRs)
3. Serial Crystallography
4. Automated crystal location and collection

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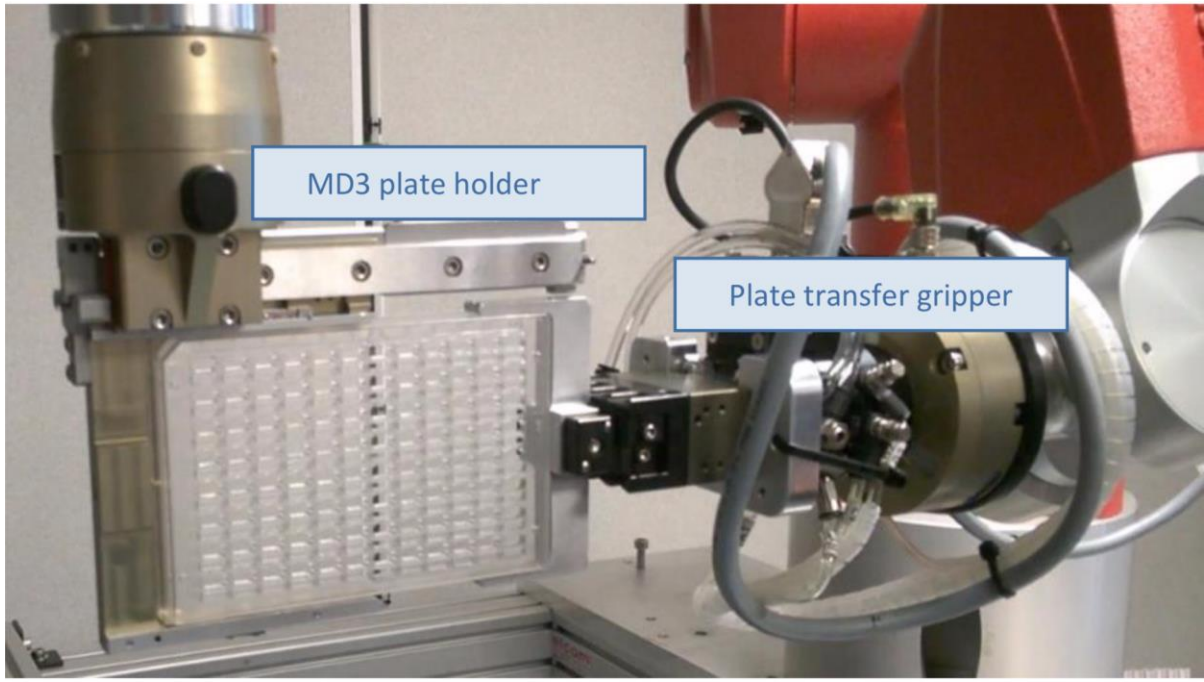
1. In-tray

- ISARA robot will load trays from a 20-tray hotel in the hutch onto the MX3.
- “Tray Tuesdays”
- Tray shipping trial Q1 2012. Trays shipped from users to and from the AS
- Seeking volunteers to take part
- Goal is to develop and test shipper, procedures and tracking software
- Goal is to have a “blanket” proposal for the program = no paperwork for users.



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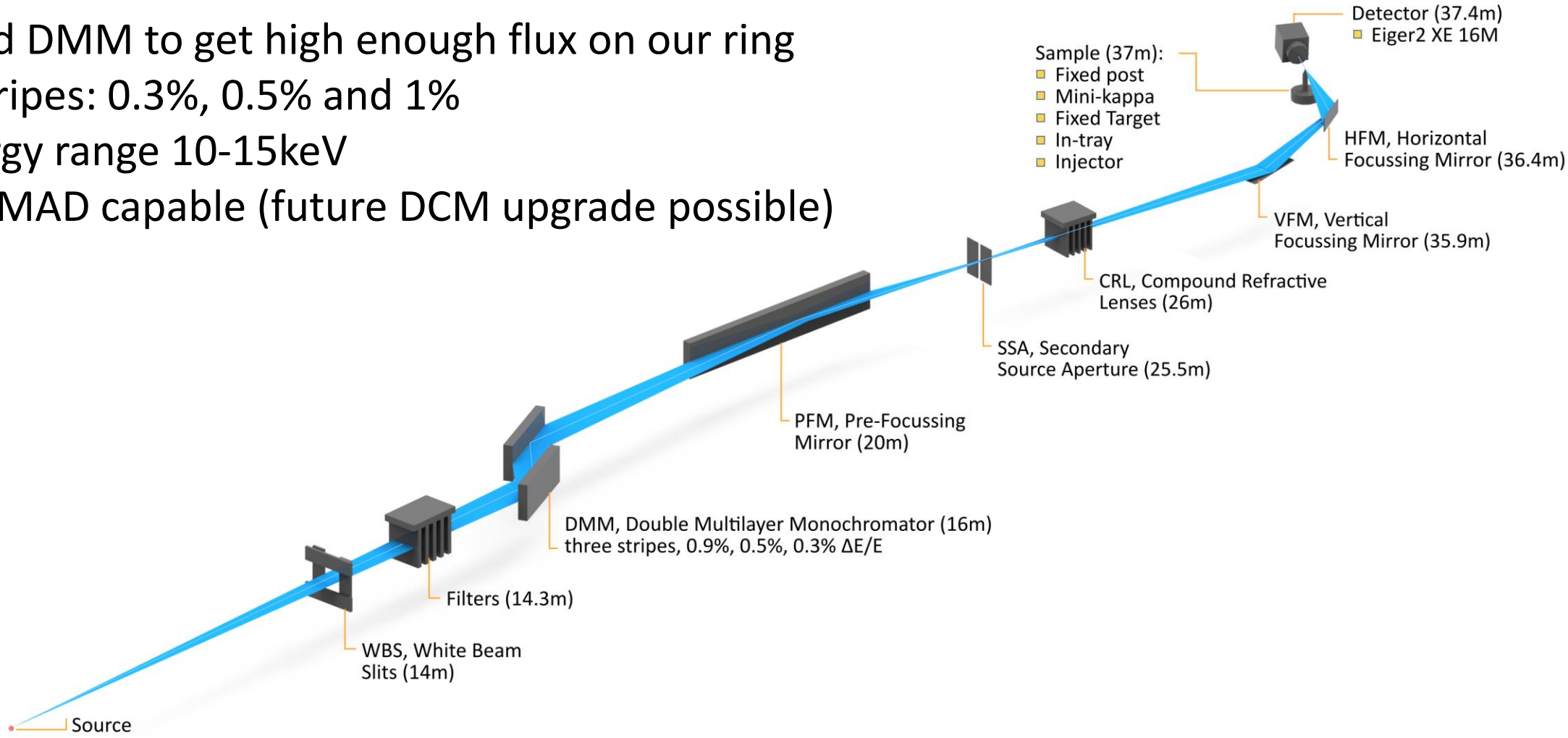
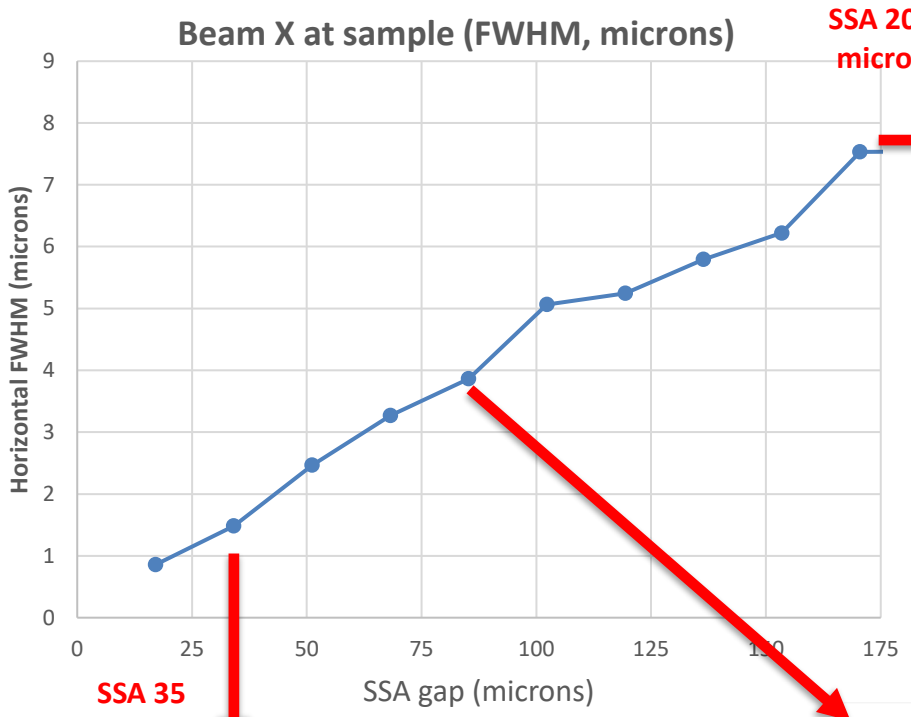
2. High flux micro crystallography

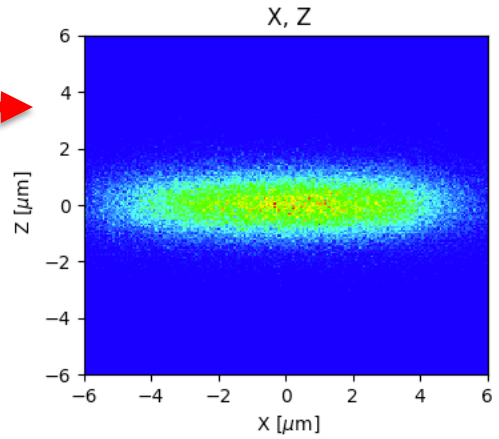
Need DMM to get high enough flux on our ring
3 stripes: 0.3%, 0.5% and 1%
Energy range 10-15keV
Not MAD capable (future DCM upgrade possible)



2. MX3 Beam performance (1% stripe)

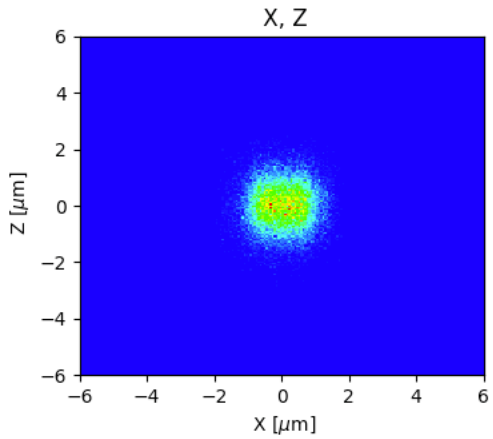


SSA 2000 microns



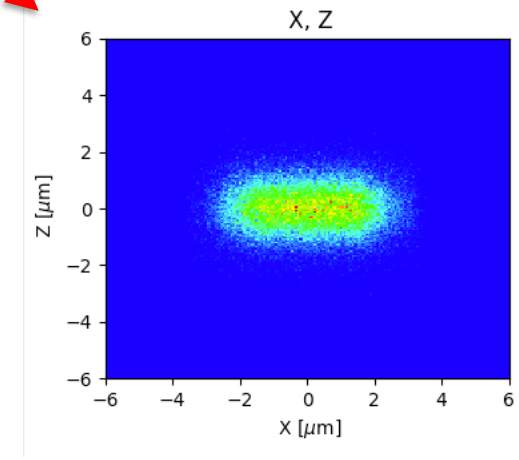
8 x 2 microns
1e^{14} ph/s

SSA 35 microns

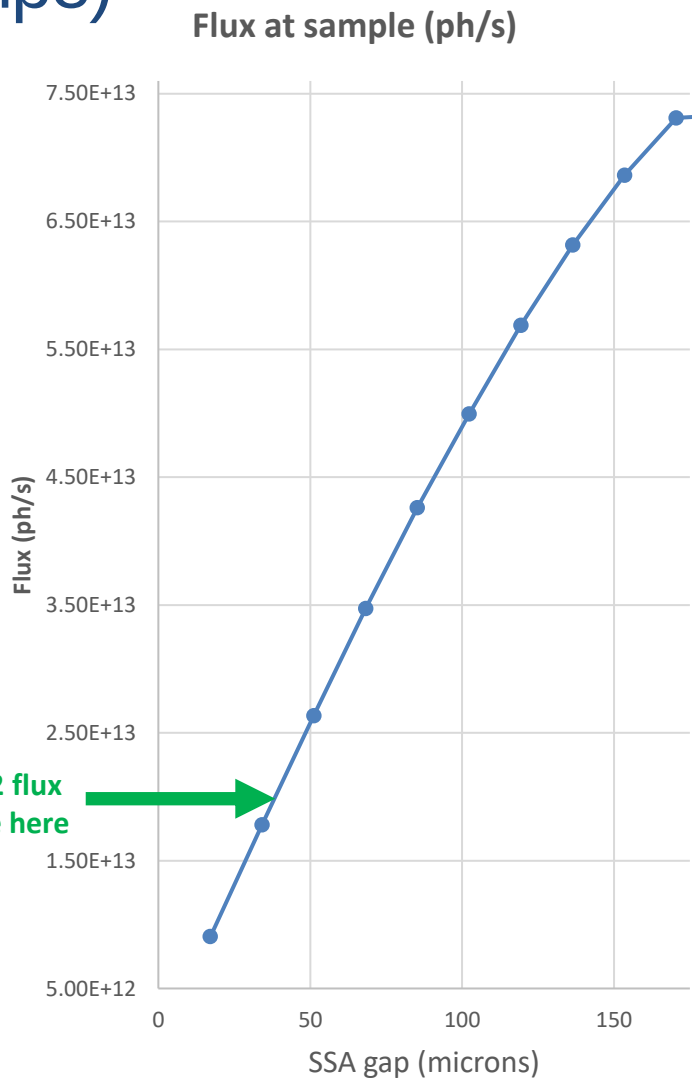


2 x 2 microns,
2e^{13} ph/s

SSA 85 microns



4 x 2 microns,
5e^{13} ph/s



10X MX2 flux would be here

Modelled in shadow3

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2. Making the beam BIGGER

Will use beryllium compound refractive lenses (1D)

Fast

User selectable

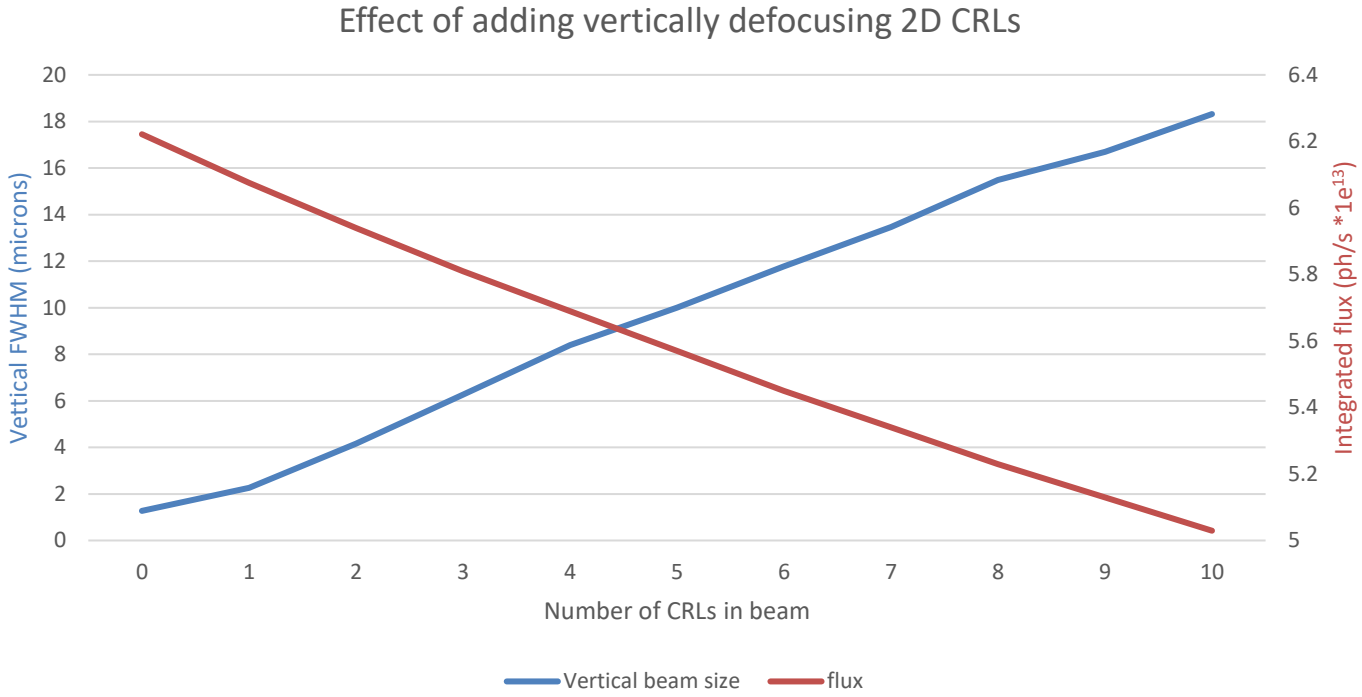
Max beam size now 15x15 microns

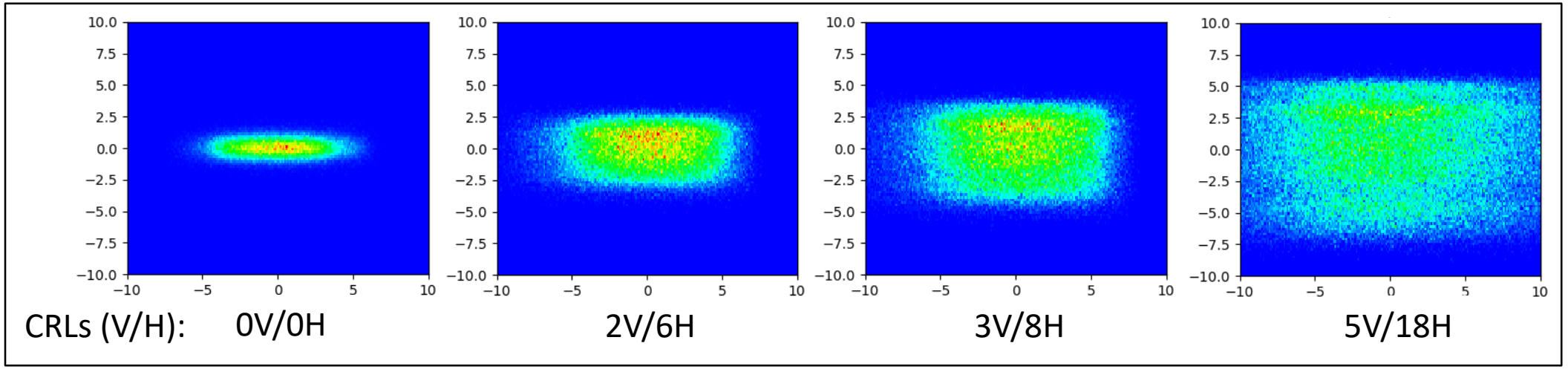
Separate H and V defocus

Vertical defocus costs flux (20% size)

Horiz

flux (·





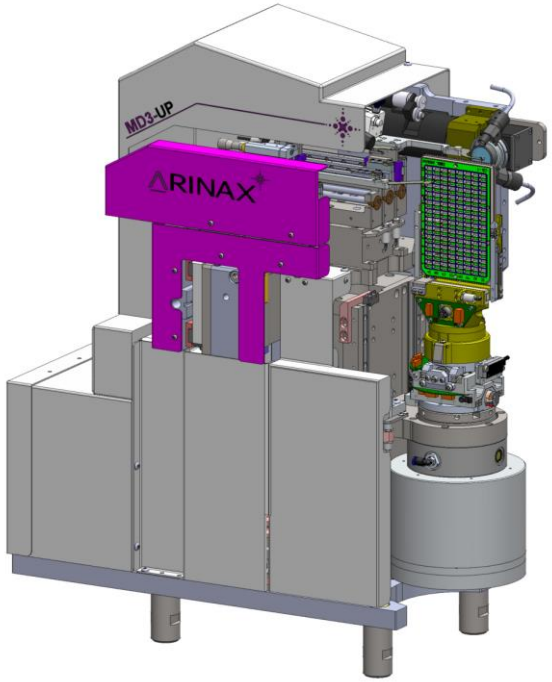
2. Goniometer

High performance goniometer

- MD3 ordered Jan 2021.
- Single axis, kappa and tray-holder heads

Static target systems

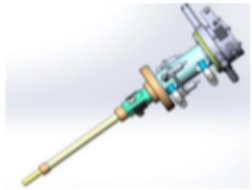
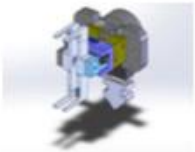
- In tray screening using MD3
- Tray hotel in cabin (20 trays)
- Robot can transfer trays from hotel to goniometer.



Arinax

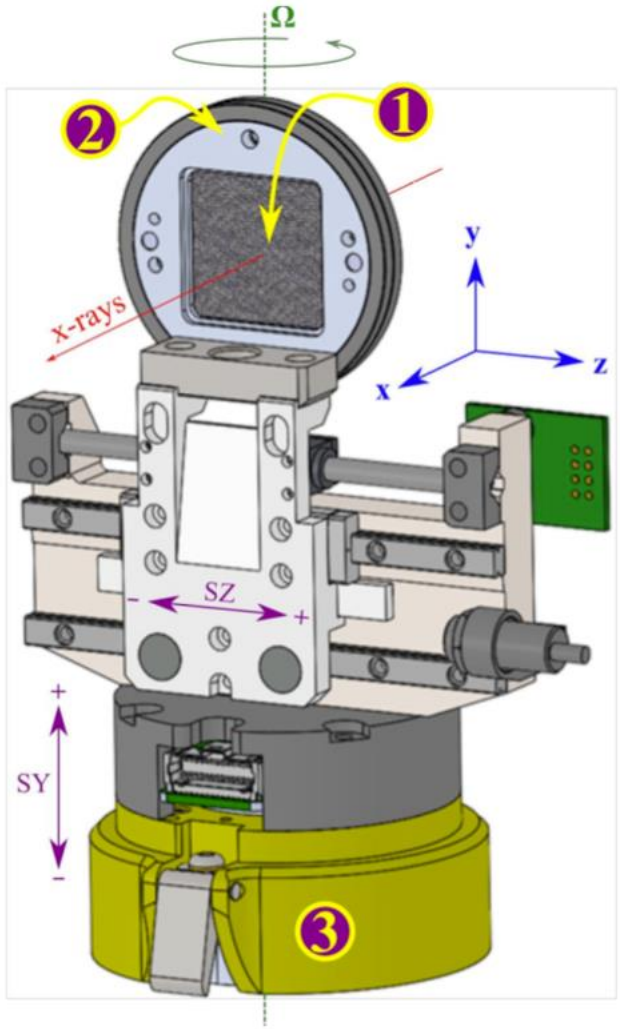
2. MX3 Robot

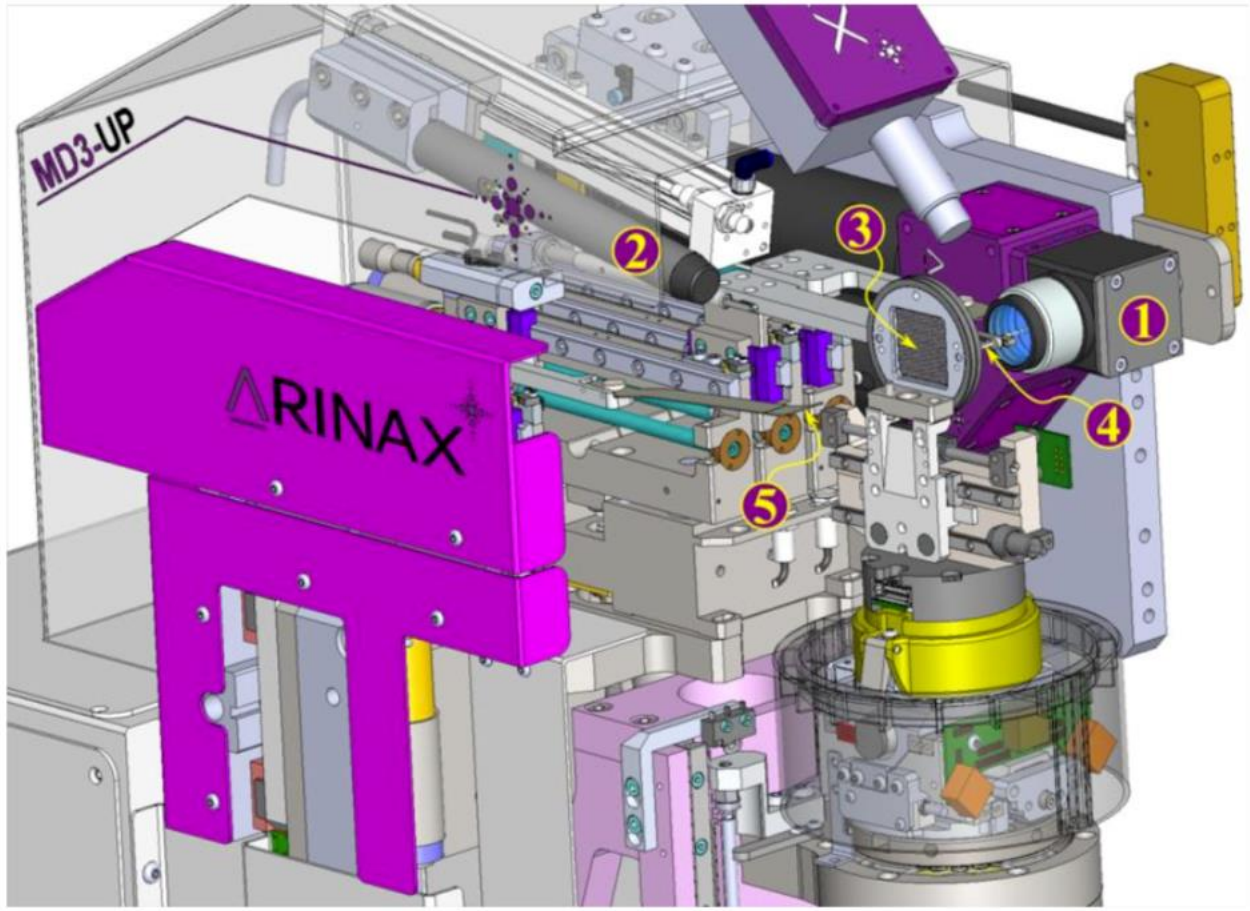
ISARA robot from Irelec ordered Jan 2021.
Dewar capacity is 29 pucks (pin-up).
Integration with MD3 and ISARA is well established.

Standard	Gripper	
Unipuck 	*Simple Unipuck gripper* 	*Double Unipuck grippers*  *designed for MD3-Down*
MiniSpine / Newpin  *same Dewar interface as for the Unipuck*	*MiniSpine gripper* 	*Double MiniSpine gripper* 
Crystallization Plates (SBS standard) 	*Plate Gripper* 	*Gripper for transferring plates onto the goniometer*  *adapted to EMBL plate holder to be mounted on MD3*

3. Serial Crystallography – Large Fixed Target

Now run on MD3 (same system as new ID29 at ESRF)





[1]Sherrel D. A. et al. "A modular and compact portable mini-endstation for high-precision, high-speed fixed target serial crystallography at FEL and synchrotron sources". Journal of Synchrotron Radiation. Volume 22| Part 6| November 2015| Pages 1372-1378

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4. 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

https://blogs.gartner.com/andrew-lerner/2019/01/07/2019-network-resolution-invest-in-network-automation/

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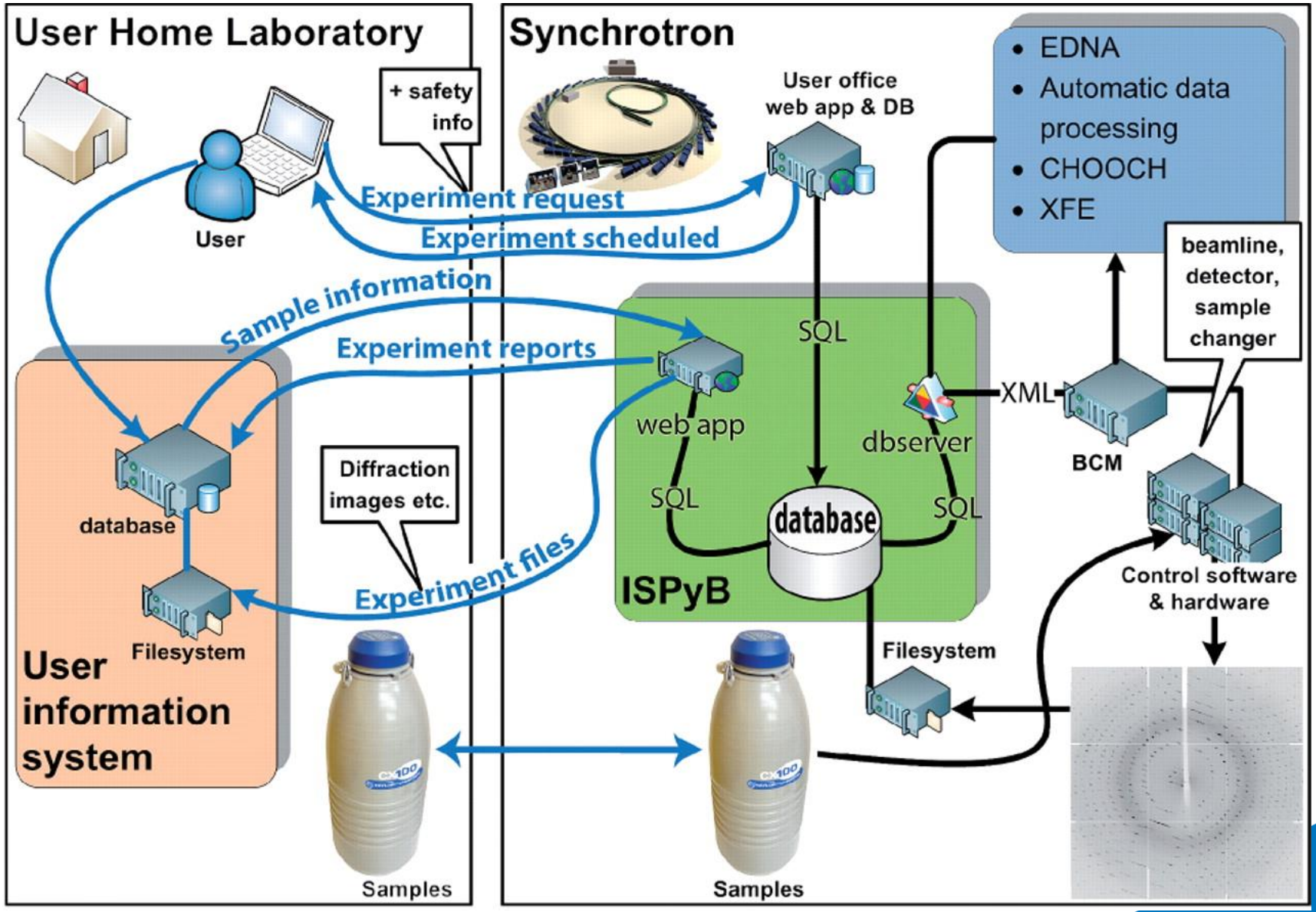
ISPyB

Interest in Python re-write of IspyB backend

Has possible use across more new beamlines at AS (we are building 8)

Ideally deployed to MX1/2 as well.

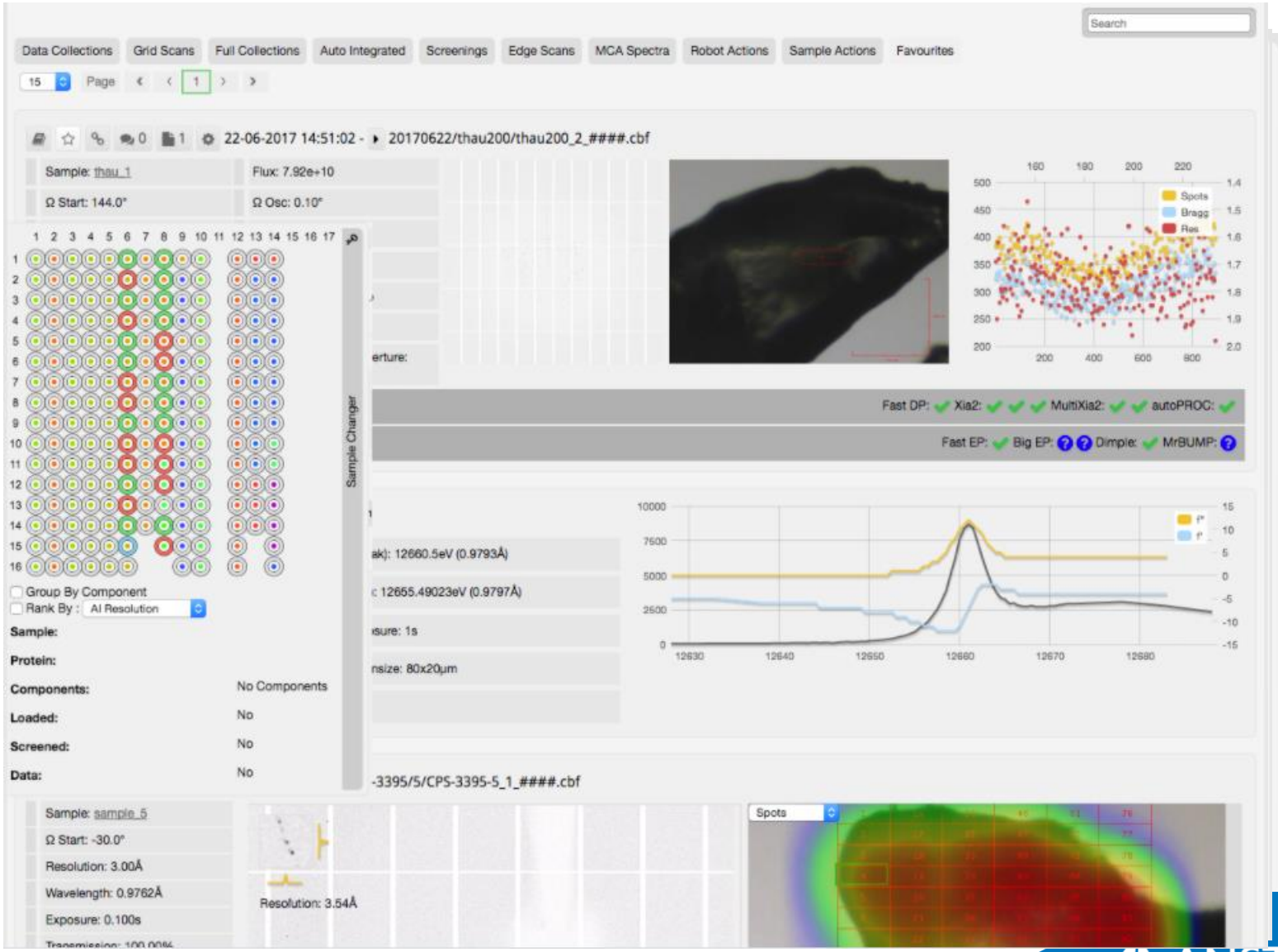


Bioinformatics, Volume 27, Issue 22, 15 November 2011, Pages 3186–3192, https://doi.org/10.1093/bioinformatics/btr535

GUIs – ISPyB, SyncWEB etc etc

SynchWEB – WebAPP (PHP).

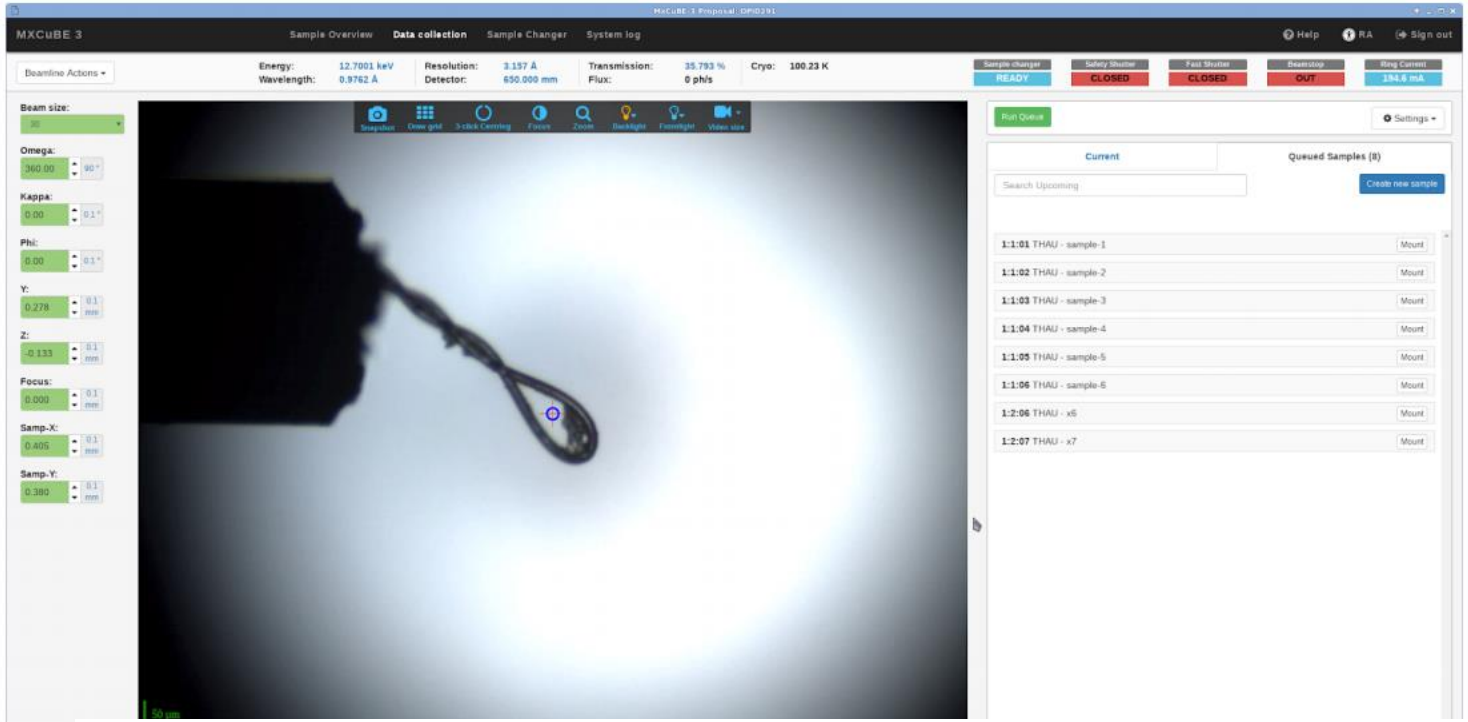
(https://github.com/ispyb/ispyb-js-api)

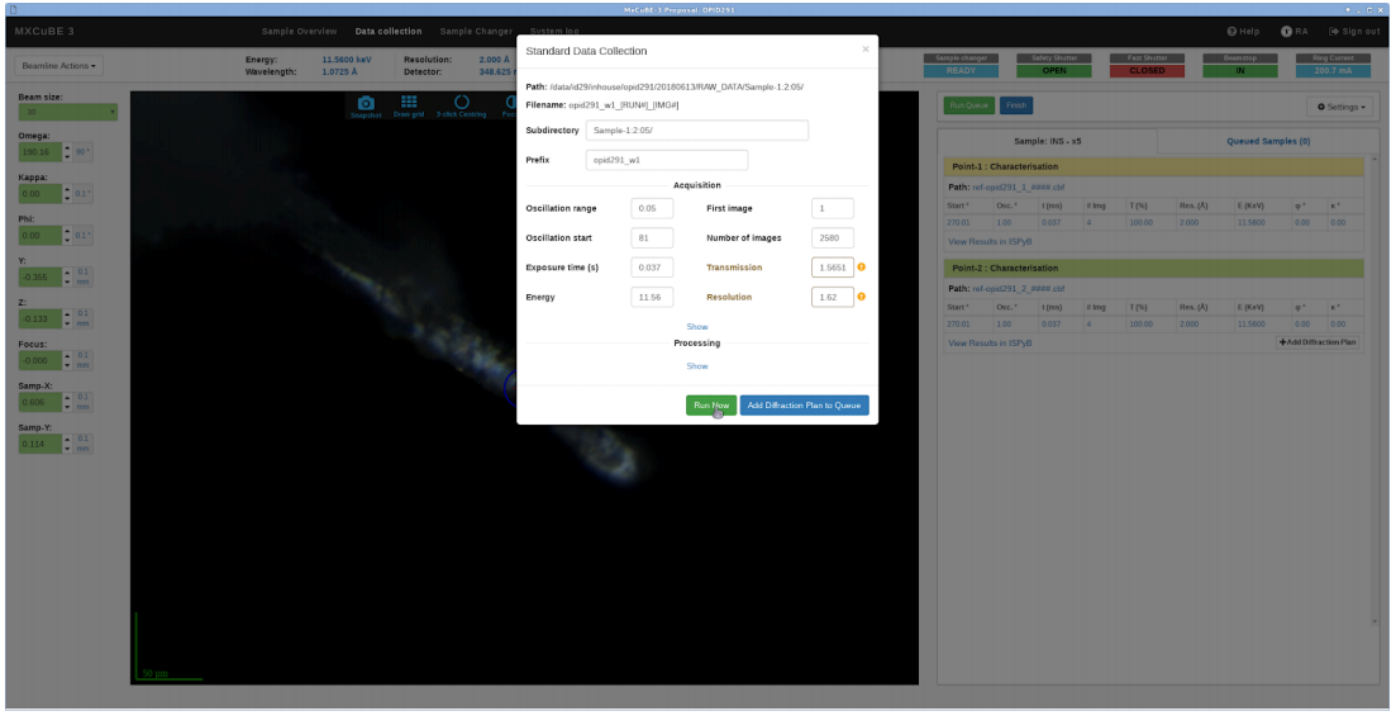


https://diamondlightsource.github.io/SynchWeb/

MXCUBEv3

1. WebAPP
2. Backend: Python-flask , SocketIO, REST API
3. Aligns with new code architecture for BRIGHT beamlines.
4. Deployed on ESRF MX lines now





http://esrf.eu/files/live/sites/www/files/UsersAndScience/Experiments/MX/Software0/MXCuBE3/MXCuBE3%20manual%20v0.1.1.pdf

We need automation!

1. MX3 will be the most highly automated beamline at the AS
2. Scientific computing will drive the useability and thoughput of the beamline
3. Plan is to join ISpyB and MXCUBE consortiums
4. Automated (no-user) queued collection.

The Team

MX

Alan Riboldi-Tunnicliffe

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Jun Aishima (now at NSLS II)
David Aragao (now at Diamond)
Kate Smith (now at PSI)
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Santosh Panjikar
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Stephen Harrop
Eleanor Campbell
Stephanie Boer
Nathan Mudie
Sofia Macedo

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Robert Grubb
Mark Colclough

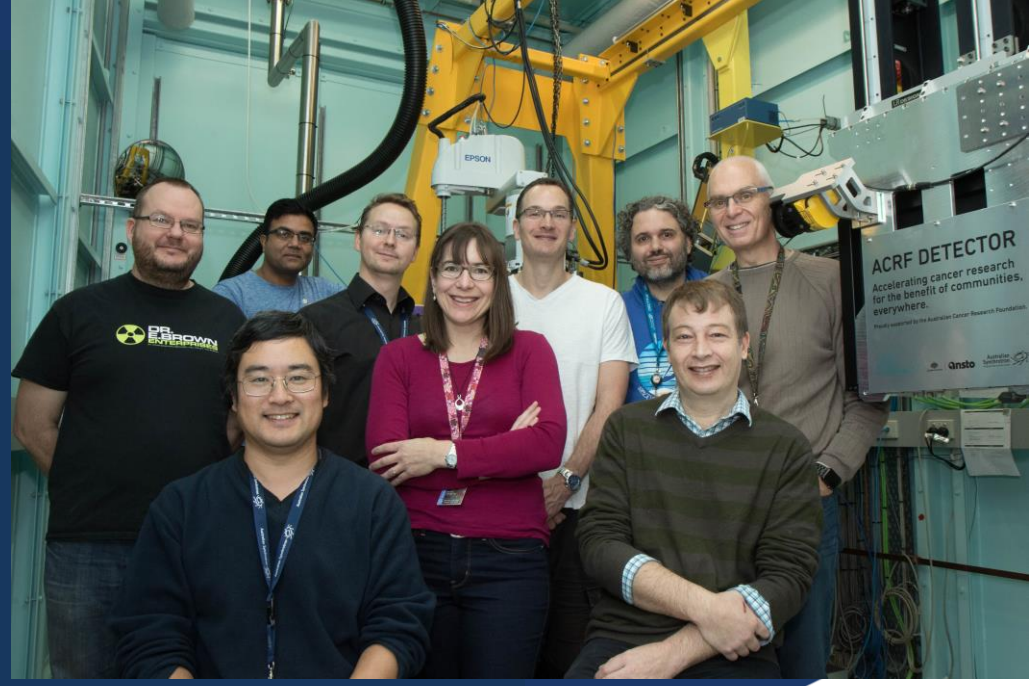
IT Group

Uli Felzmann (now at UniMelb)
Robbie Clarken (now at BOSCH)
Ron Bosworth

Scientific Computing

Andreas Moll
John Marcou

Dectris – Andreas Forster, Diego Gaemperle
SLS – Simon Ebner, Zac Panepucci, Meitian Wang
HDRMX – http://hdrmx.medsbio.org
NSLS2 – Bruno Martins for AD Eiger



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Thank you!

Questions?