Highly Automated Macromolecular Crystallography(AMX) beamline update

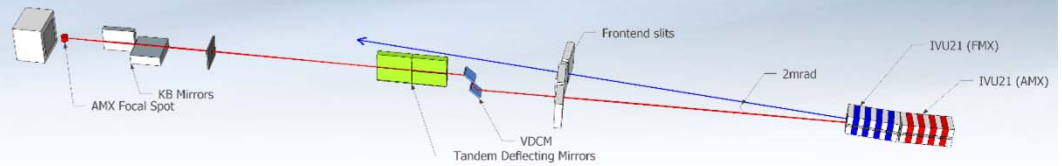
First Light: March 2016
First General User: February 2017
First Paper: TBD

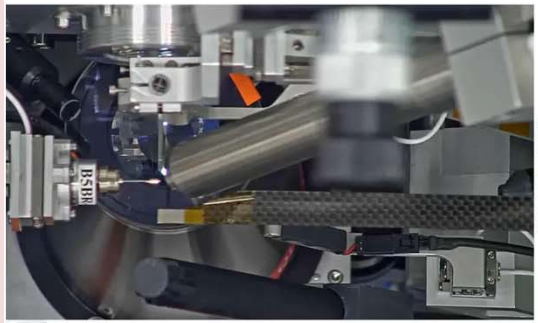
NSLS-II SAC Meeting, September 20th , 2017

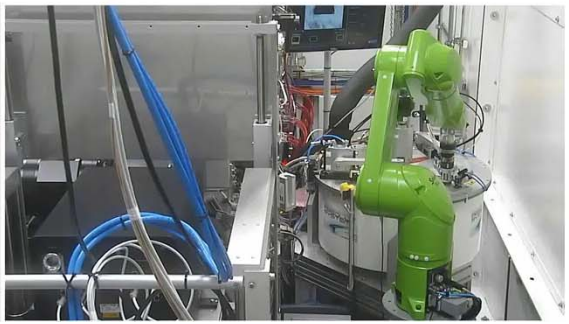
Beamline at a glance

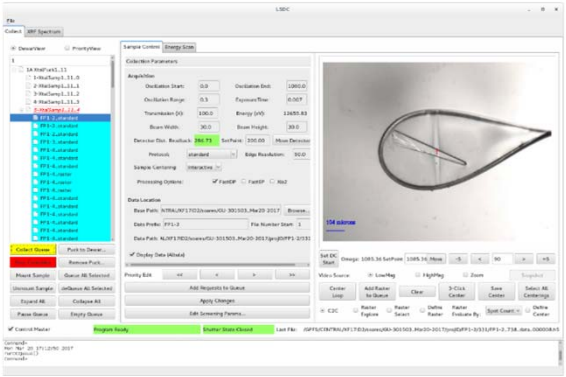
<u>As of July 2017</u>

Beam size: 8 x 10 μm^2 (*<u>5 x 5 μm^2</u>*)
Flux: 4.10^{12} ph.s^{-1} (@1Å)
Energy range: 5-18 keV (0.7- 2.5 Å)
Detector: EIGER 9M (≤238 Hz)
Samples: Spine bases in Unipuck
Capacity: 3 Unipucks at a time
Sample exchange time: < 60 secs (*<u>40</u>*)
Data collection: > 0.5 sec
Automated data processing: < 80 secs

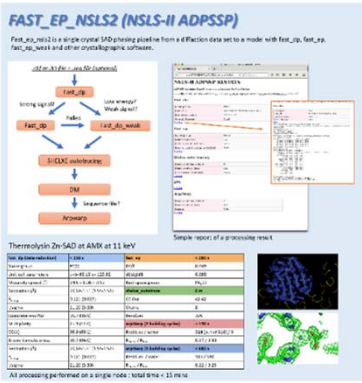




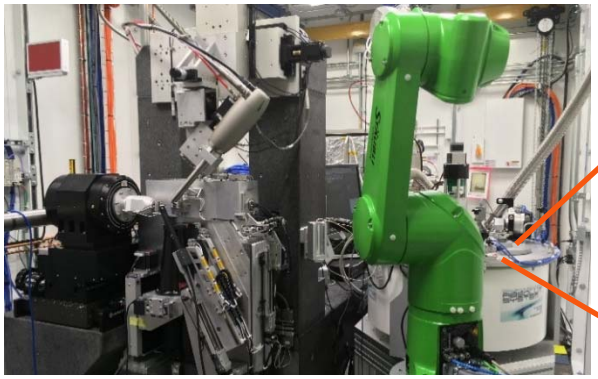




LSDC, ophyd, bluesky, css



Pipelines



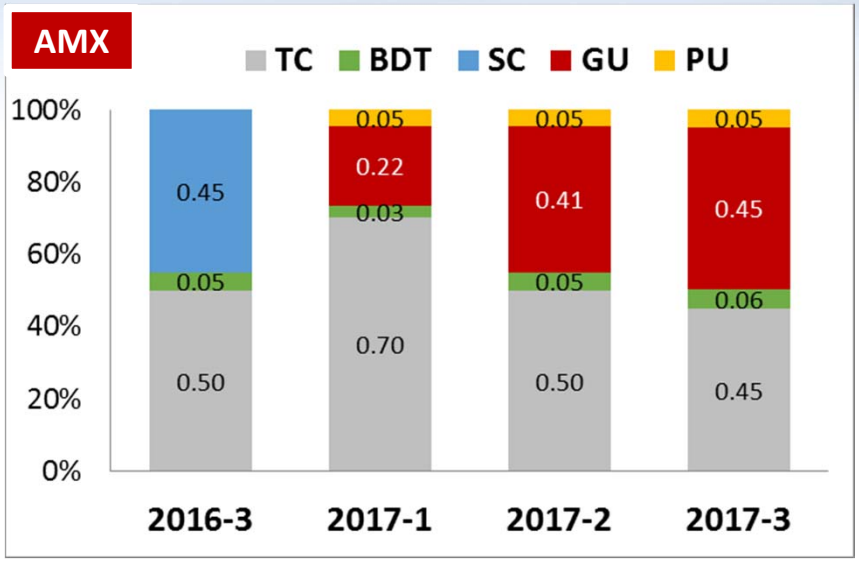
In-House End-Station

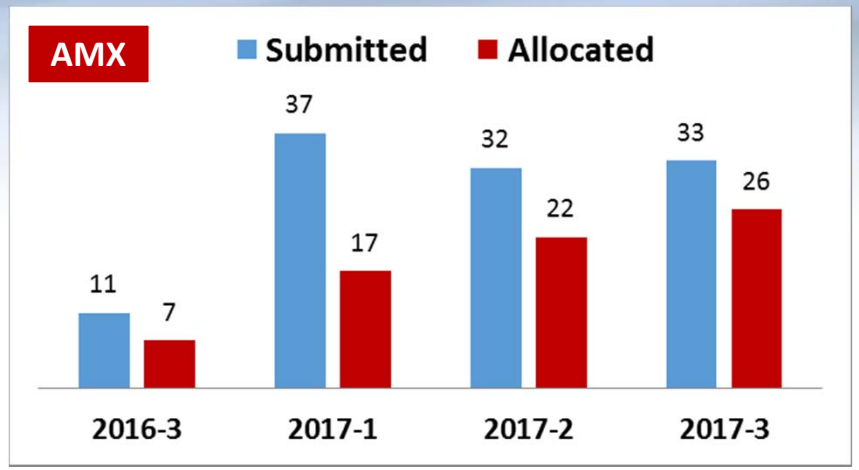
"3 pucks-plate"

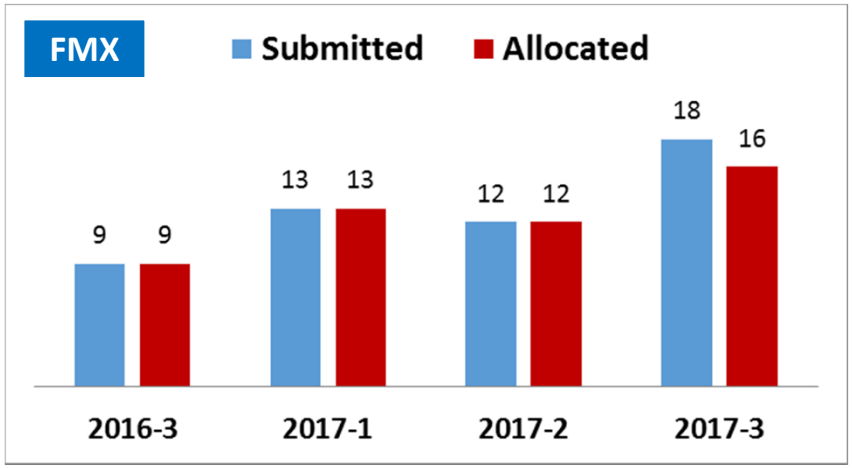
Scientific capabilities

Vast numbers	AMX supports programs that require testing of vast numbers of specimens, e.g. studies of membrane proteins, and drug discovery explorations.
Micro-crystals	AMX provides a "mini" beam and sample delivery and data processing to support efficient structure determination from small crystals and multi crystals or from multi positions on a single crystal.
Large unit cells	AMX supports structure determination of multi-component assemblies, thanks to its "large" beam size of up to 100 µm and its low divergence.
Collect on all	High flux and short data collection times makes it possible to collect on every specimen, assisted by crystallographic decision making software. This is part of the various modes of operation of the beamline.
Specialize and Complement	AMX cover the mini-beam regime and FMX the micro-beam, yet both have complementary and overlapping capabilities
Access Modes	Visiting users, collecting data from AMX or LOB5 dedicated space. Remote data collection from home institutions. Automated crystal screening, followed by USER decision an automated data collection. The level of automation and computing power will enable unattended/automated data collection. We will provide a Rapid Feedback service to users that have few samples and need to know ASAP if they diffract.

User stats

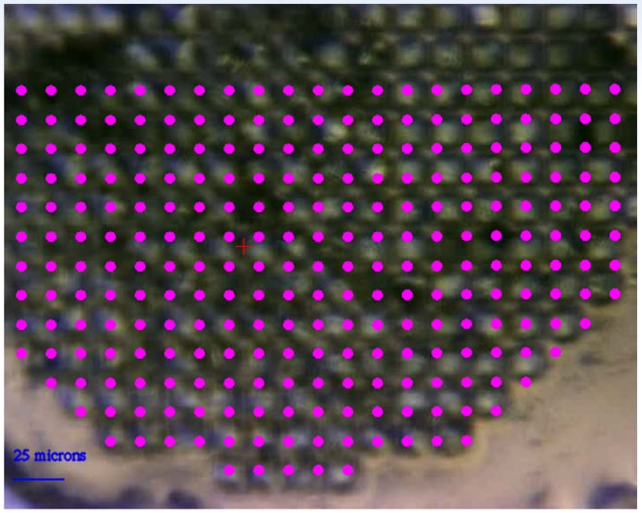


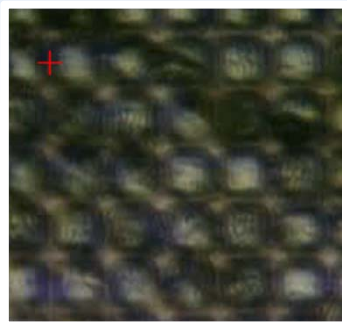




- Equal beam time distributions at AMX and FMX up to cycle 2017-03
- Assignment of proposals to beamline based on measurement and scheduling requirements
- Currently accepting rapid access and proprietary user proposals (2017-3)
- Starting 2017-03 AMX increasing number of available rapid access shifts

Science highlight 1: Structures from 1000s of crystals

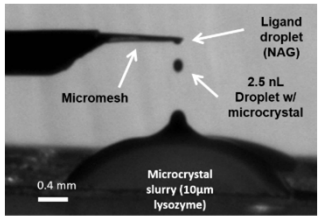




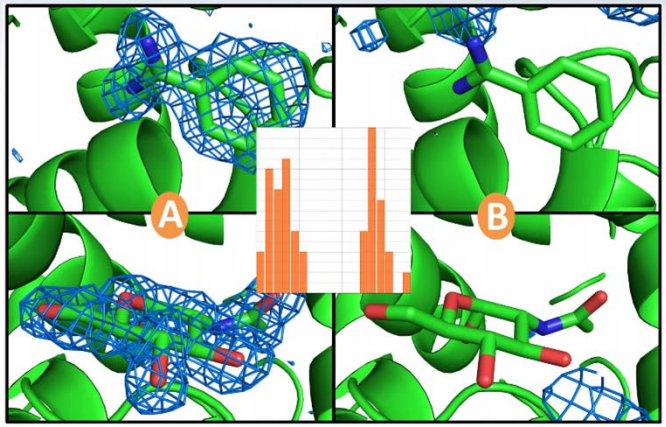
2 types of crystals mixed on meshes.

Energy	8
Flux	5.3 x 10^{11} ph/sec (85 % attenuation)
Total oscillation	5 deg./spot
Osc. width	0.2 deg./frame
Exp. time	0.04 sec./frame (P6M)

Y. Yamada, KEK, Japan, H. Bernstein, RIT.



ADE
A. Soares

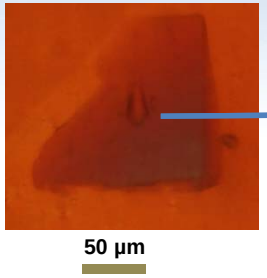


Lysozyme crystals +/- 2 ligands (unit cell / CC filtering)

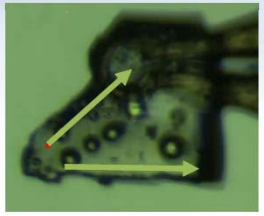
When increasing the number of forms from 2 to 4: current software and methods fail.

<u>R21 application (Oct 2017)</u>

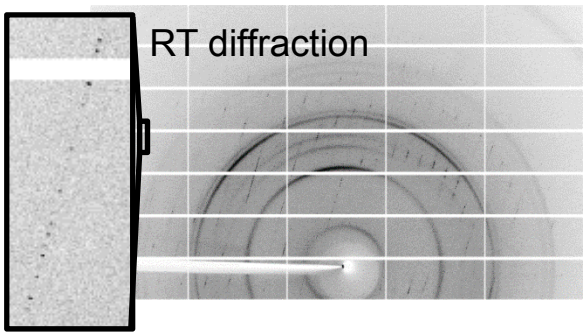
Science highlight 2 : PBP5 R. Page (Brown U., U. Arizona)

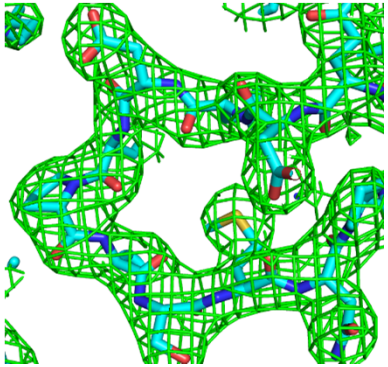


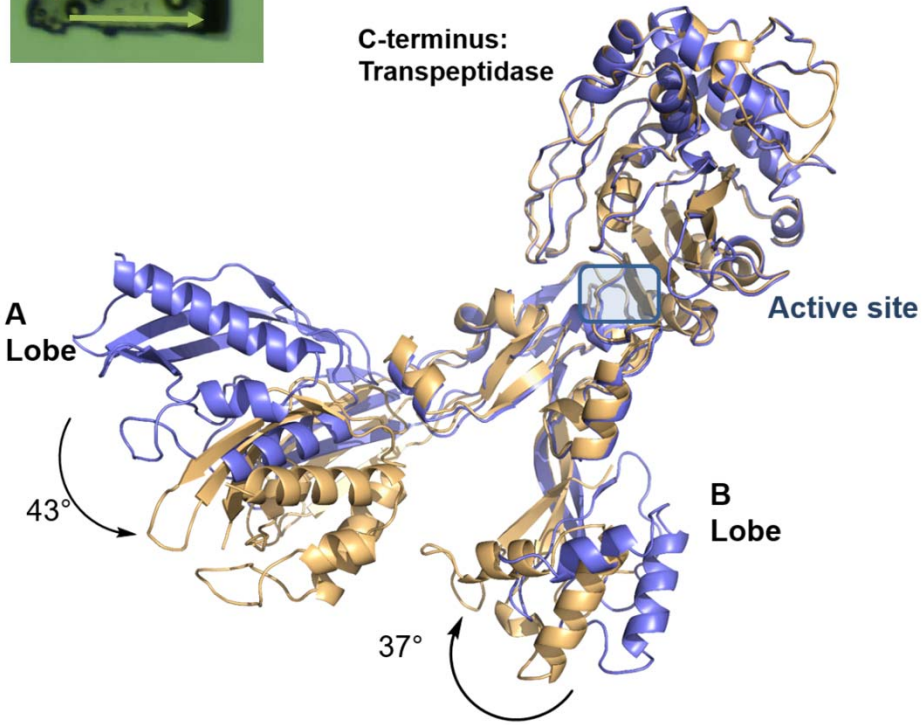
Initial
RT Screening
(radiation damage)



2 Complete sets
At 100 K







$P4_32_12$
a=b=63Å c=381Å
Resolution 2.8Å
Partial data.
Pilatus 6M.

$P4_32_12$
a=b=63Å c=371Å
Resolution 2.9 Å
Complete data.
8/25/16 (~ 20 um beam)

Article in preparation.

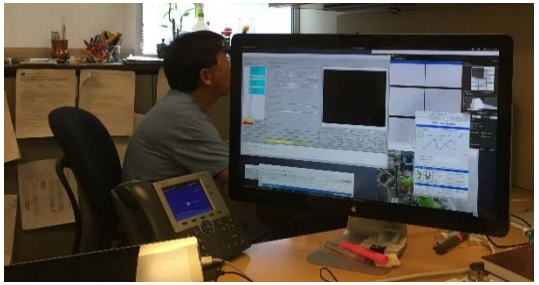
Future plans (automation / structure solution)

Short term (< 6 months):
Access from all sample positions (24x16=384)
Unattended data collection from single crystals (standard then strategy based collection)
Optimized code for spot finding (used for crystal location / characterization)
Test remote access: NX client as a 1st implementation.

Medium term (<12 months):
Automated structure solution pipelines (compute nodes & user input required/database front end)
Data collection in the 5-7 keV range (S-SAD): optimized transmission using He flight path
Remote access data collection
2-3 beam sizes (5x5; 15x15)
Room Temperature data collection from compact InSitu trays

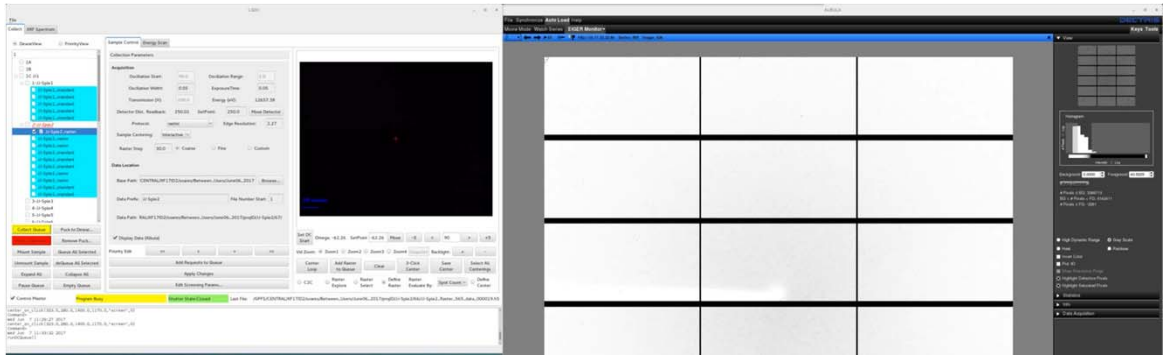
Long term (< 18 months):
Enable post-processing of data
Unattended data collection from many small crystals in a loop/mesh
Deploy, automated data collection and remote access data collection via database front end: hybrid mode.

Summary



Beamline is up and running: positive feedback
Adding features/capabilities in timely manner
Rapid access / Remote access: increasing demand
Future Workshops: training expert users and prepare for remote (NYU, SB, teachers, proprietary)

Challenges:
24/6 operation.
Facility computing to speed up rate of discovery (providing partially refined models).



Current implementation of fast rastering.