Likely Evolution of Computational Infrastructure for Bio Beam Lines Over the Next Five Years

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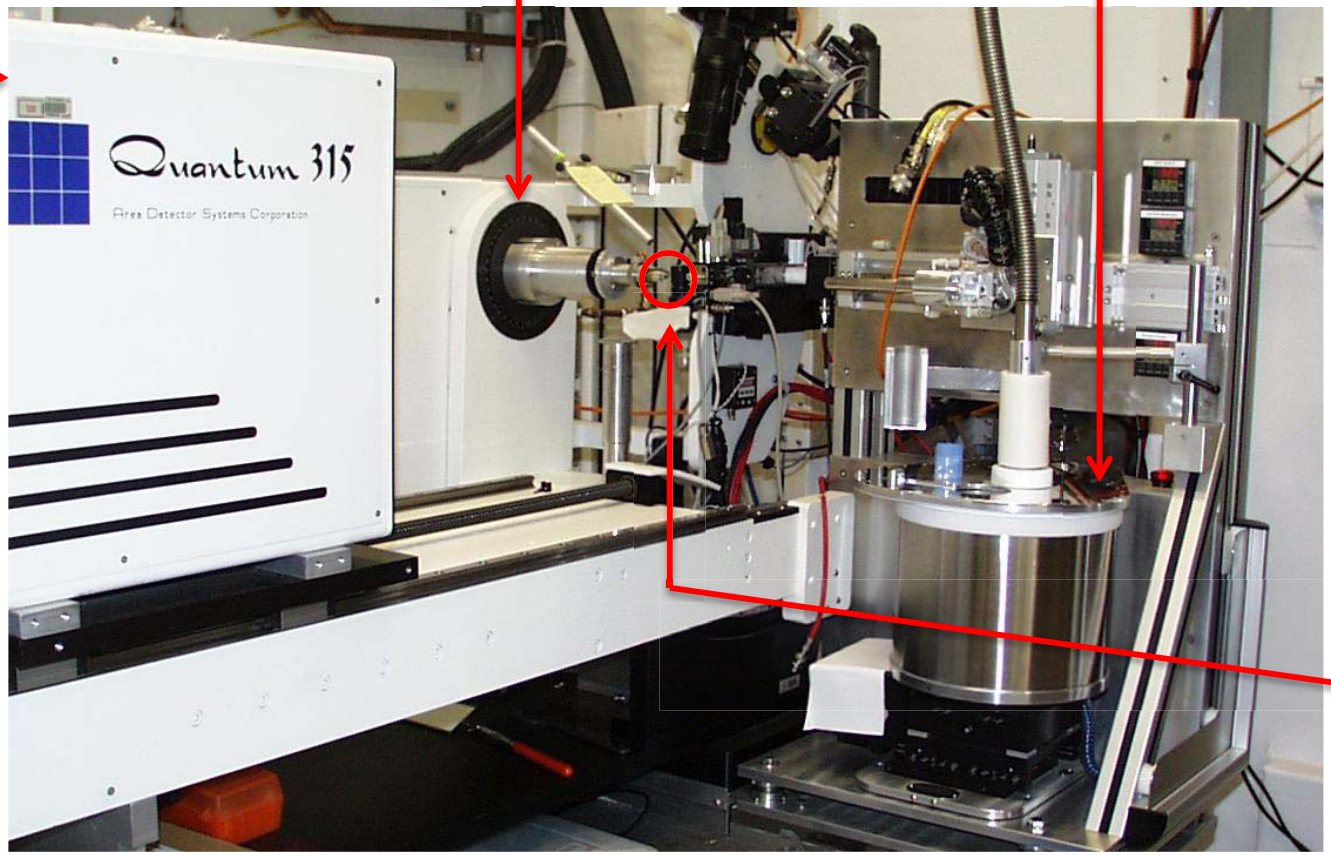
The macromolecular crystallographer's beam line at the NSLS

State-of-the-art CCD detector records diffraction patterns

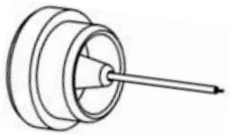
Goniometer centers crystal into beam

Spindle rotates crystal during collections

Automounter handles cryogenic specimen mounted on crystal caps

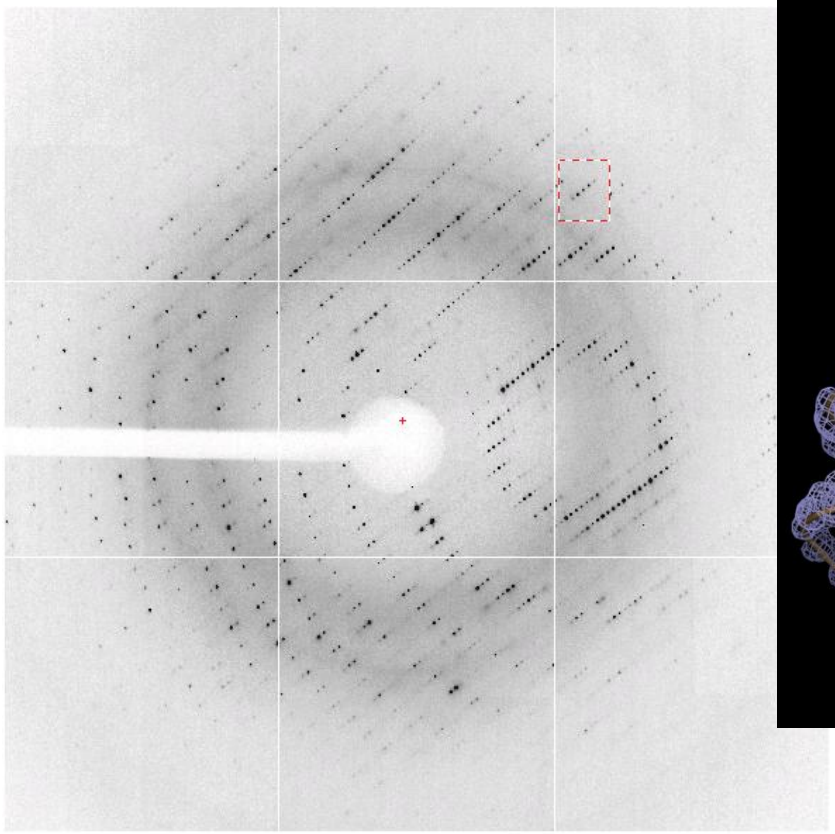


Crystals are pre-mounted and small 10–100 μm

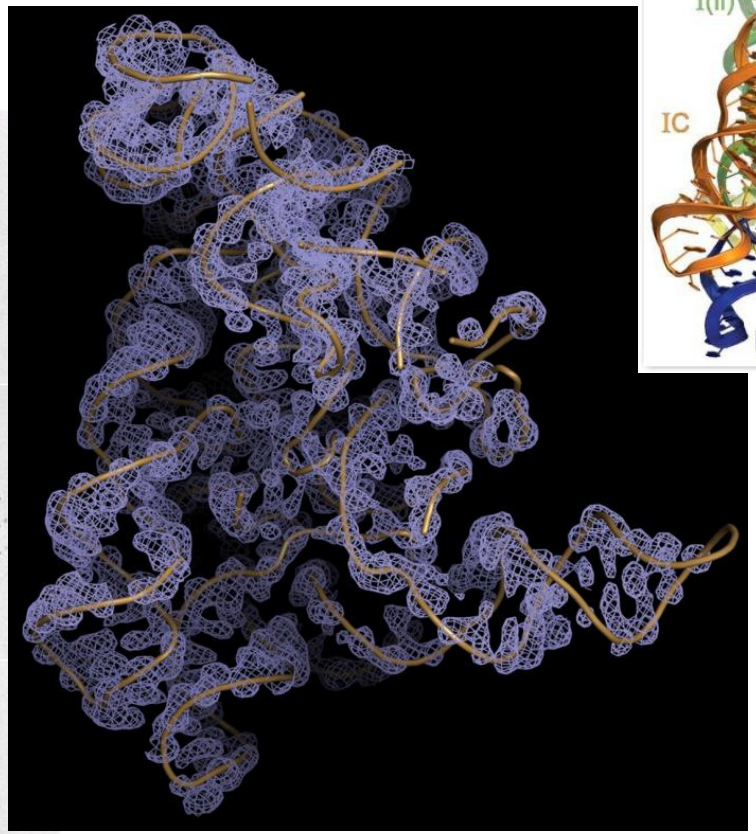


MX experiment from data to structure to print

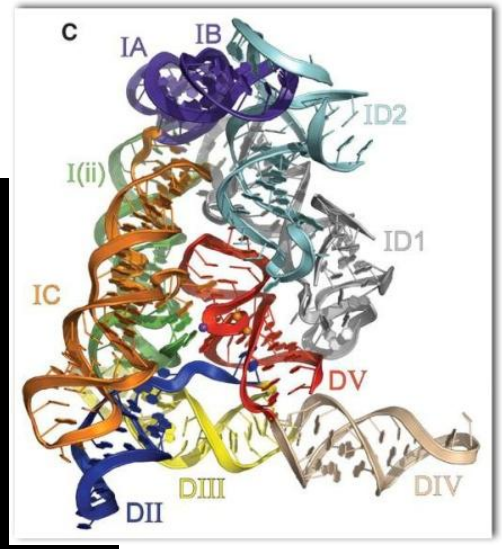
Hundreds of diffraction patterns record thousands of Bragg spots



Once phased, they yield electron density map of Macromolecule, and …



then a Science paper



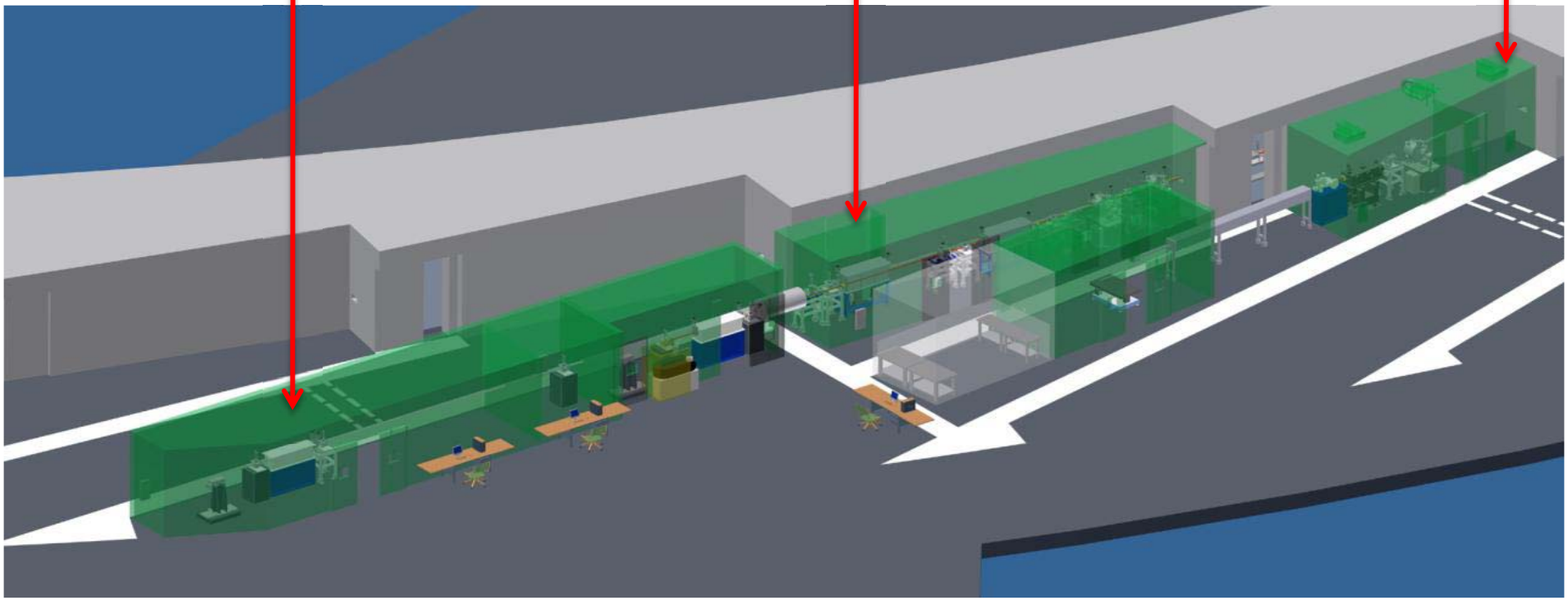
Plans for MX beam lines at NSLS-II

Day 1:

Micro diffraction undulator line

Highly automated undulator line

Complementary methods 3 pole wiggler beam line



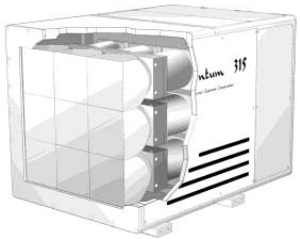
Soon after:

- High energy resolution undulator line
- Complementary methods undulator line
- Screening and training 3PW line

Fully built MX capabilities:

- 4 ID beam lines
- 2 3PW beam lines

New detectors enable new data collection methods



	NSLS	NSLS-II
Detector technology	CCD Composite	Pixel Array
Detector model	ADSC 315r	Pilatus 6M
Effective dynamic range	15 bits	20 bits
Dead time between frames	0.25 s + overhead = 1 s	0.0036 s
Electronic background	0.015 e^-/pixel/s	0

Fast readout and zero e-background make it possible to collect data

- without operating shutter in a
- continuous sweep of the crystal spindle

The high flux at NSLS-II and fast detectors will tax cheep networking

	NSLS	NSLS-II
Beam intensity on crystal	10^{11} ph/s/µm^2	>10^{12} ph/s/µm^2
Detector model	ADSC 315r	Pilatus 6M
Frames per data collection	360 x 1° (wide slicing)	1800 x 0.2° (fine slicing)
Exposure time per frame	1 s	0.083 s @12Hz
Time per collection	720 s = 12 min	150 s = 2.5 min
Detector format in pixels	3088 x 3088 (I*2)	2463 x 2527 (I*4)
Size per frame	19 MB	25 MB (uncompressed)
Size of 360° data set	6.9 GB	45 GB (uncompressed)
Stored size of 360° data set	6.9 GB	11 GB (compressed 4X)
Data transfer rate	0.076 Gb/s	1.3 Gb/s

This is beyond the bandwidth of Gigabit networking !

Data rate assessment with more appropriate 2015 detector

	NSLS	NSLS-II
Beam intensity on crystal	10^{11} ph/s/µm^2	>10^{12} ph/s/µm^2
Detector model	ADSC 315r	**Eiger class detector**
Frames per data collection	360 x 1° (wide slicing)	1800 x 0.2° (fine slicing)
Exposure time per frame	1 s	**0.020 s @ 50 Hz (max 200)**
Time per collection	720 s = 12 min	36 s ~ 0.5 min
Detector format in pixels	3088 x 3088 (I*2)	**5 M pixel (I*4)**
Size per frame	19 MB	**20 MB** (uncompressed)
Size of 360° data set	6.9 GB	**36 GB** (uncompressed)
Stored size of 360° data set	6.9 GB	**9 GB** (compressed 4X)
Data transfer rate	0.076 Gb/s	**2 Gb/s**

This is within bandwidth of 10 Gigabit networking !

Additional factors demanding high network bandwidth

High performance MX beam lines will employ next generation pixel-array detectors to fully exploit available flux and optimized data collection methods.

- The estimated network rate bandwidth will be needed.

We propose to operate the highly automated MX beam line in a multi-user time-shared mode. Every data collection will be analyzed asynchronously.

- This will demand sustained high data transfer capacity.

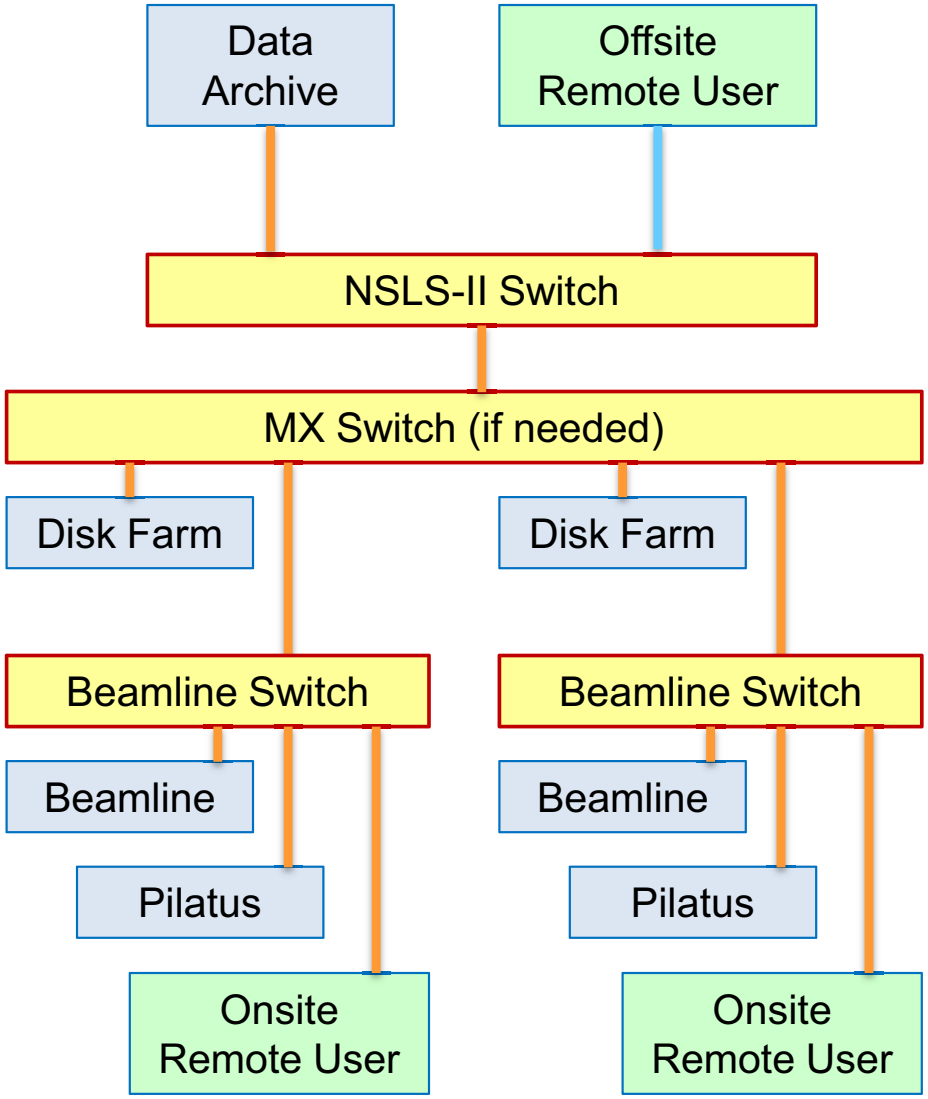
We propose to lay out data processing nodes in duplicate in support of the multi-user time-shared concept.

- This will further tax networking bandwidth.

Solutions:

- 10 Gigabit networking is required
- Reduce data transfers by processing in detector CPU: TB memory

Networking and remote access to MX beam lines



Given the speed of data collections

- xtal screening will mostly vanish
- data evaluation will be asynchronous
- users will work remotely

Onsite remote users work from LOBs and office using NX/Q client served by NX server, as John Skinner demonstrated on Monday

Offsite remote users will control experiment asynchronously in quasi real-time using simple web-based interfaces

A bit about software and computing hardware

Continue to use crystallographic software developed by others thus leveraging proven performance and community acceptance. Build these modules into local architecture.

For data reduction consider detector controller-associated CPU equipped it with vast memory (TB).

Several reduction packages are already parallelized (i.e. xds, d*trek) and tested. This will help in getting fast feedback to rank frames, assess radiation damage, and make strategy decisions.

Use processors with GPUs, rather than clusters, for data scaling, integration, and solving etc. Works for Global Phasing.

Serve only occasional aggregates of data frames (i.e. 10X) for users inspection.

Will need truly fast new software that is competent and reliable in crystallographic decision making.

Archiving is a challenge

Fast paced data collections demands reliable archiving

On the 24-hour scale raw data should be available
at the beam line as if in real time
Volume 9 GB/min x 1440 min/day = 13 TB/day/beamline
Assume 2 lines at full throttle, 2 at half, and 2 at ¼ = 45 TB/day

On the one week scale data should be available on short recall
for reprocessing. Volume: 318 TB/week
Per beam line this amounts to 4 units of 30TB 48 disk modules.

Data should be held for one year to match the experiment to PDB
and publication cycle, and to allow critical systems analysis.
Volume: 17,464 TB/year 17 PB/year

- Long-term archiving is an institutional size task.
- Given the modest size of a dataset of 9 GB,
  users may still carry away raw data on solid media.

MX beam lines will need a dedicated specialized software team

NSLS experience shows that an MX group needs a cross-trained team that together can fill any of the following jobs:

1. A software architect directing integration of software developed by crystallographers and others in the field
2. A specialist to build, tune, and advance network and systems performance and attend to the development of first-class remote capabilities
3. A systems analyst to maintain the 100+ nodes of a group of MX beam lines
4. A specialist concentrating on database programming
5. A specialist for device level EPICS programming and device integration
6. A creative member to drive developments such as advanced GUIs, applications of machine vision, or initiatives in robotics

Common interests of MX villagers and NSLS-II facility staff

Remote

Remote participation and asynchronous data collection will be the rule from day one and requires that offsite and onsite remote users have unimpeded simple access to beam line computers and station monitors.

Staff

A dedicated MX software and computing staff is required to drive continuous upgrades and maintain uninterrupted service to the MX community.

This staff and their colleagues at NSLS-II will benefit from close and organized interactions focused on training, collaborations, and career development.

Networking

To provide optimal data exchange and experimenter mobility between MX beam lines these should be on one facility-independent high-bandwidth network of the 10 Gigabit class.

Archiving

Long-term archiving of raw diffraction data should be provided through an institutional mechanism.