National Synchrotron Light Source II

Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

Autonomous Synchrotron Experiments

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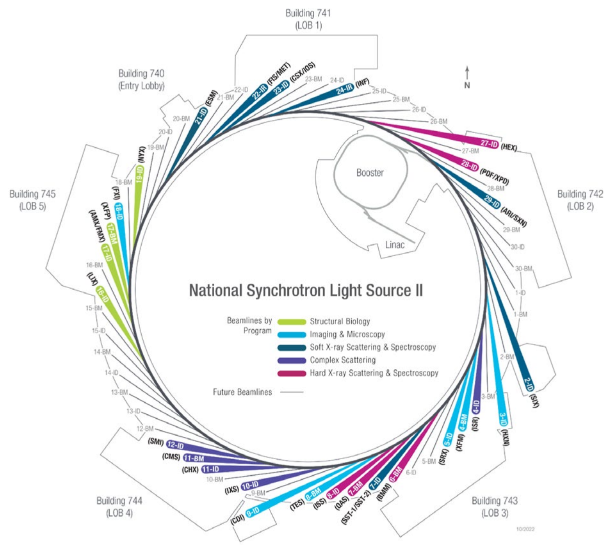
Program Manager

Data Science and Systems Integration (DSSI), NSLS-II

NSLS-II is a state-of-the-art user facility



The Vision: Transparent, remote access to facilities from proposal submission to data acquisition to data interpretation to publication

Original Facility Beamlines Baseline Complete

2007

How do we integrate new technology and AI/ML into our facility?

Integration & infrastructure is the key…

Computing technology has transformed many aspects of our lives.

This transformation has largely been enabled by integration and interoperability which hides the complex details of databases, storage, interfaces, file formats from the end user.

NSLS-II will use the same concept to transform the user’s experiments.

How do we integrate this into a typical experiment?

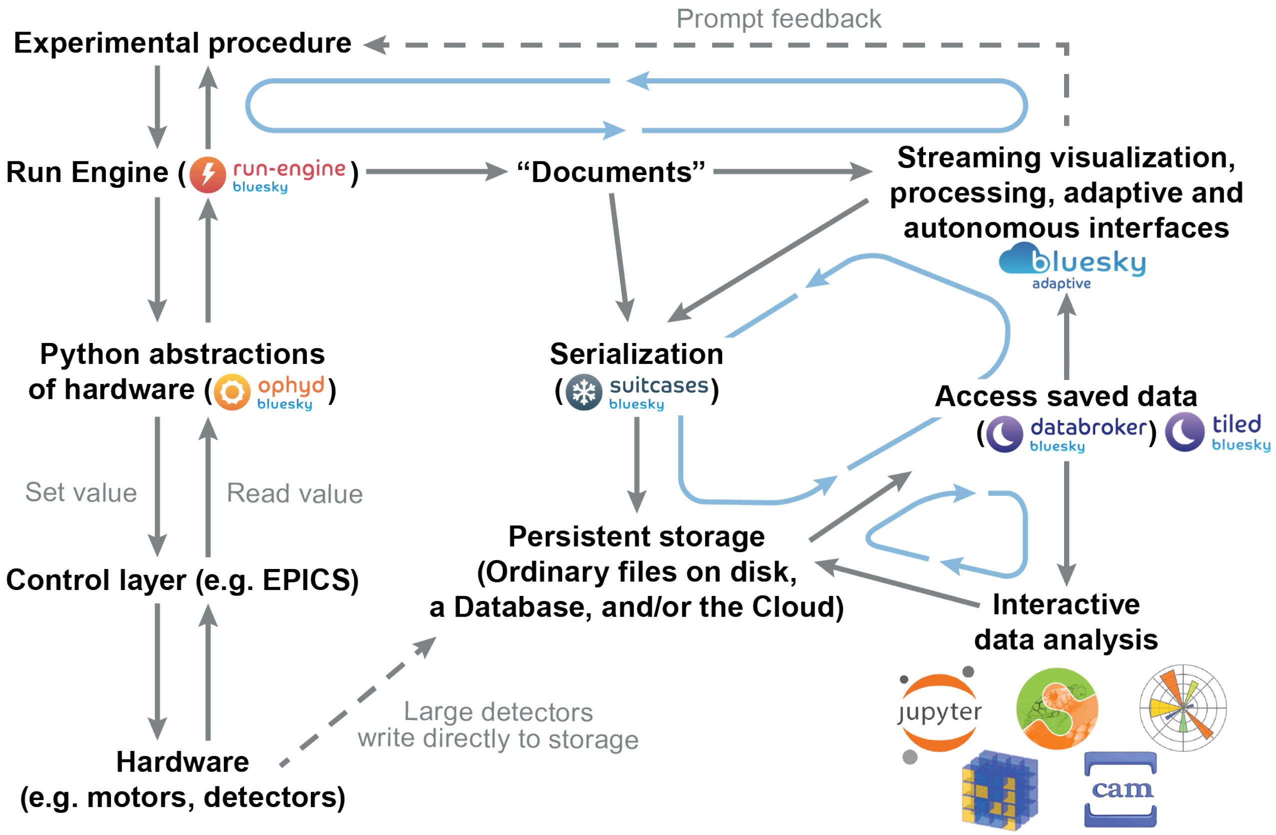
How do we build an ecosystem to allow development?

bluesky

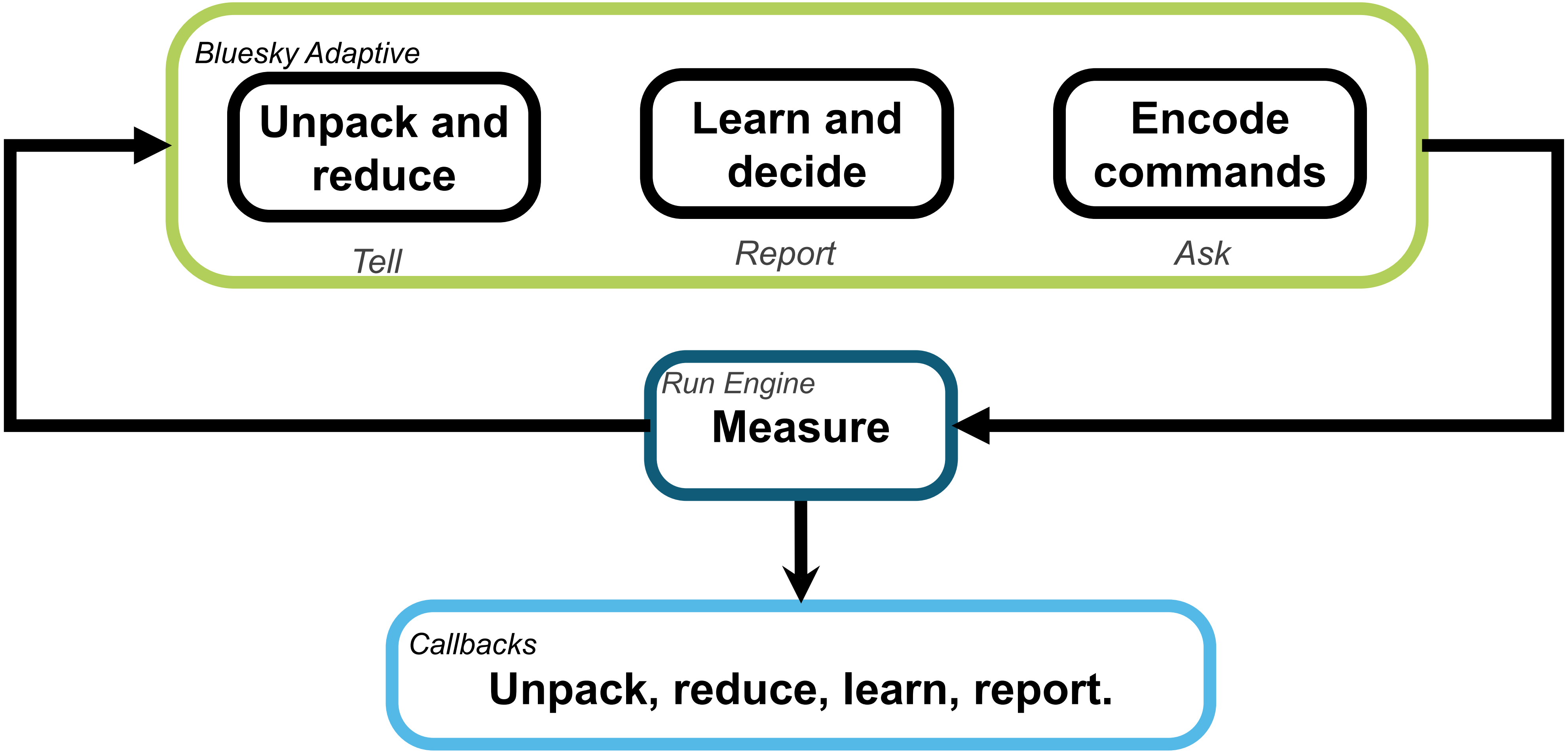
Design of Bluesky readily accommodates both adaptive and autonomous interfaces.

- Data acquisition system for high-level control and planning
- Collection of co-developed Python libraries (useful a la carte)
- Support both automatic and manual metadata encoding
- Store data/metadata in robust, searchable API called *DataBroker* (now *Tiled*)
- Data emitted in streaming fashion via standard Python structures
- First-class support for adaptive feedback and inline analysis

www.blueskyproject.io



Agents are enabled by Bluesky Adaptive and Run Engine callbacks.

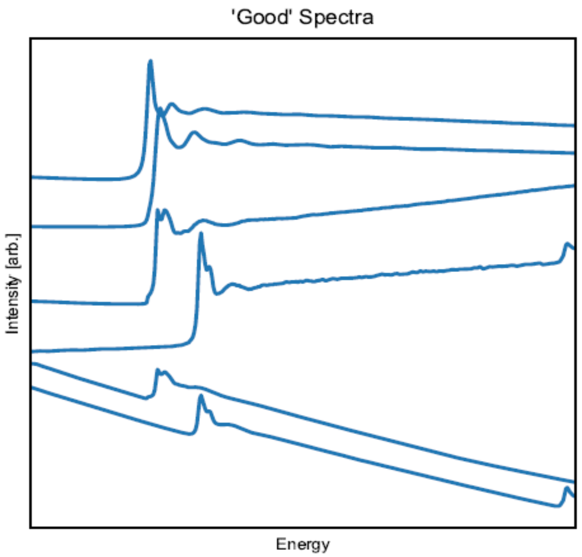


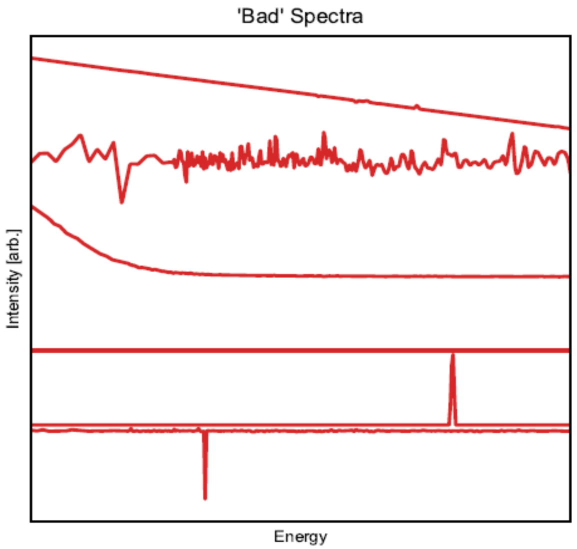
Letting the AI watch the beamline

711 labeled datasets from transmission and fluorescence data of variable quality measured at BMM.

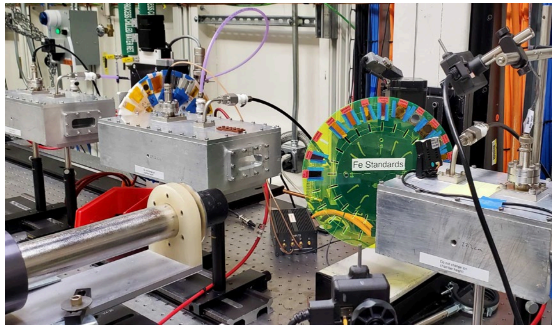
Key feature identified by expert is rising-edge in XAS.

Used as automated 'sanity check' – alerts posted by beamline to slack.





	Raw Spectra		Engineered Features	
Models	Uniform Validation F1-Score	Unique Validation F1-Score	Uniform Validation F1-Score	Unique Validation F1-Score
RF	0.986	0.829	0.990	0.874
SVM	0.995	0.807	0.990	0.982
MLP	1.00	1.00	0.986	0.957
k-Neighbors	0.995	0.807	0.990	0.947
GP	0.990	0.803	0.986	0.988



Digital Discovery (2022)

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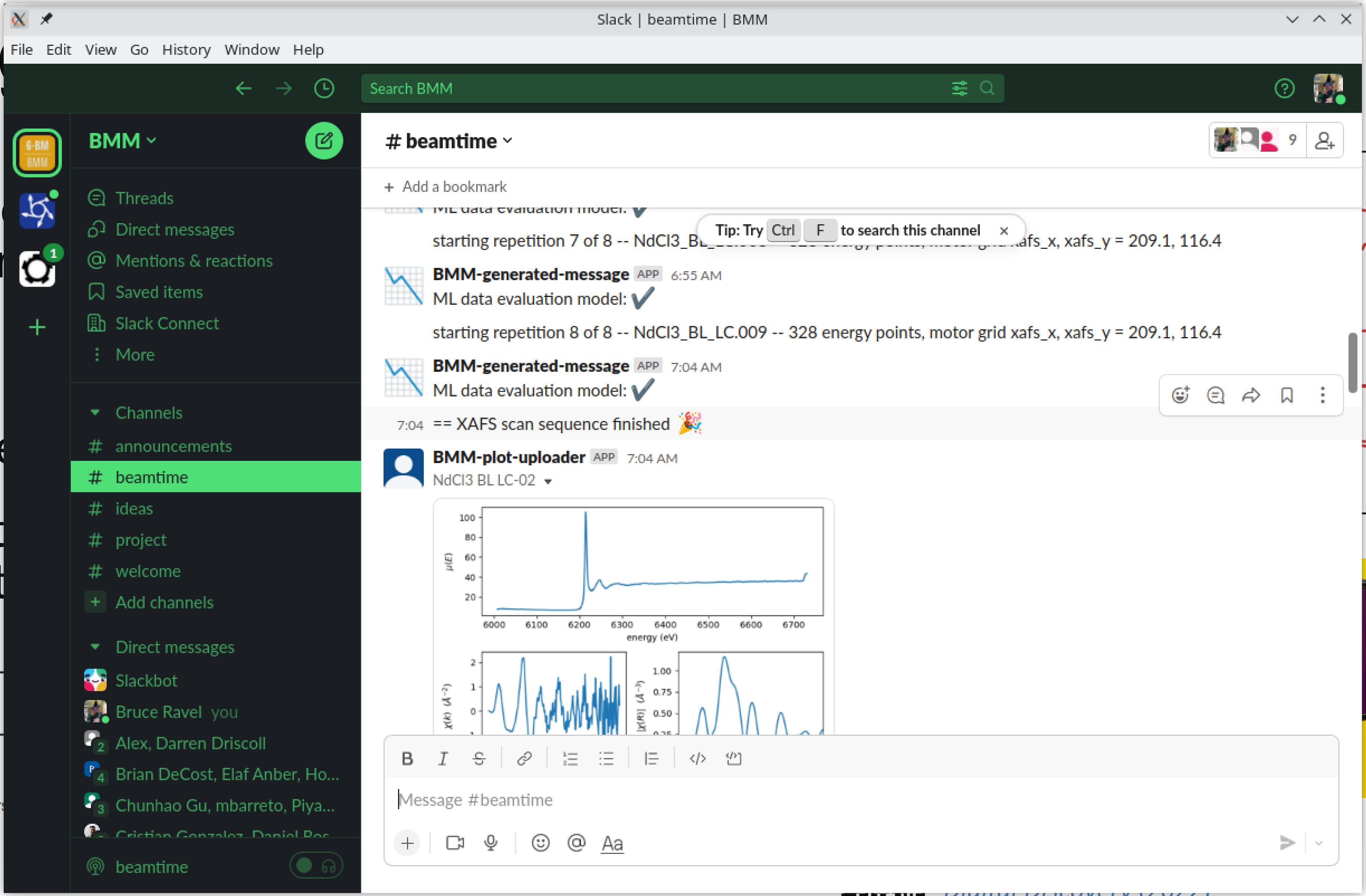


National Institute of Standards and Technology
U.S. Department of Commerce

Digital Discovery (2022)

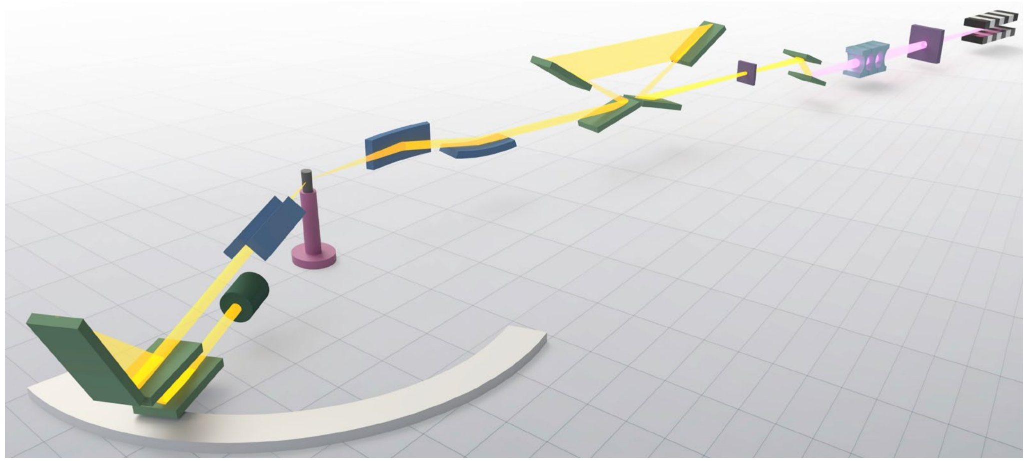
AI-assisted Alignment and Simulations via Bluesky

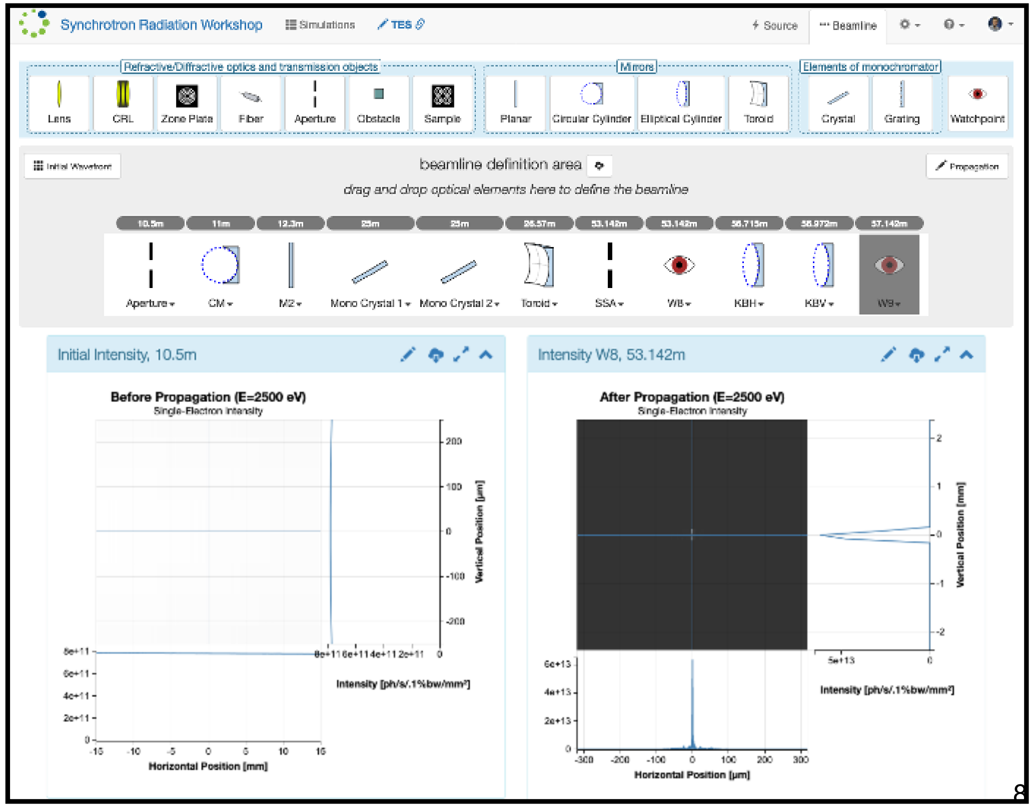
Suite of beamline simulation tools exists (Sirepo, OASYS, LUME)

Bluesky can be used to drive both real- and simulated-beamlines

Simulated data stored in DataBroker

Demonstrated work on TES beamline using Differential Evolution methods

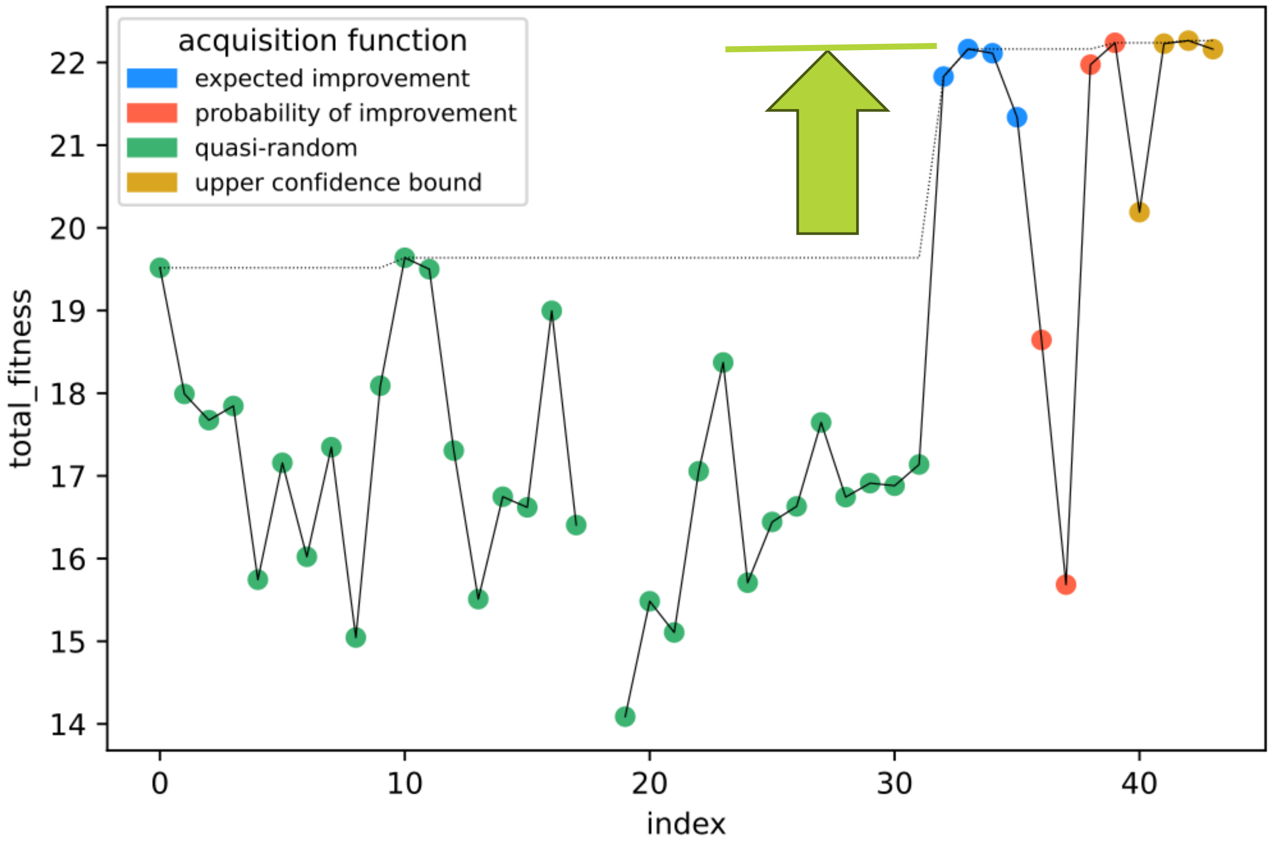




Rakitin, M.S., *et al.* "Introduction of the Sirepo-Bluesky interface and its application to the optimization problems." *Advances in Computational Methods for X-Ray Optics V*. Vol. 11493. International Society for Optics and Photonics, 2020.

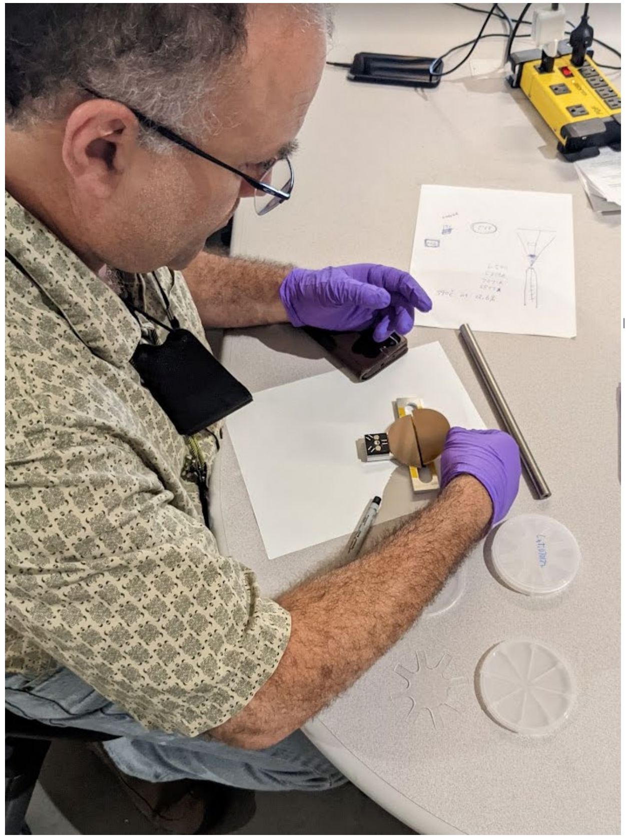
Testing beamline auto-alignment

- NSLS-II
  - TES: aligning KB mirrors + toroidal mirror (8 dims)
  - ISS: optimizing flux, optimizing spectrometer resolution
  - IOS: KB mirrors (forthcoming)
- ALS
  - BL 5.3.1: aligning toroid and monochromator (4 dims)
- Benchmarking on Sirepo backend with SRW and Shadow3



Above: optimizing the flux density of the KB mirror system of the simulated TES beamline (4 dims). After 32 random initialization points, we rapidly find the global optimum. This takes 2-3 minutes at the real TES beamline. The fitness is log-scaled, so ~20 times more flux density than at the start.

Wafer example

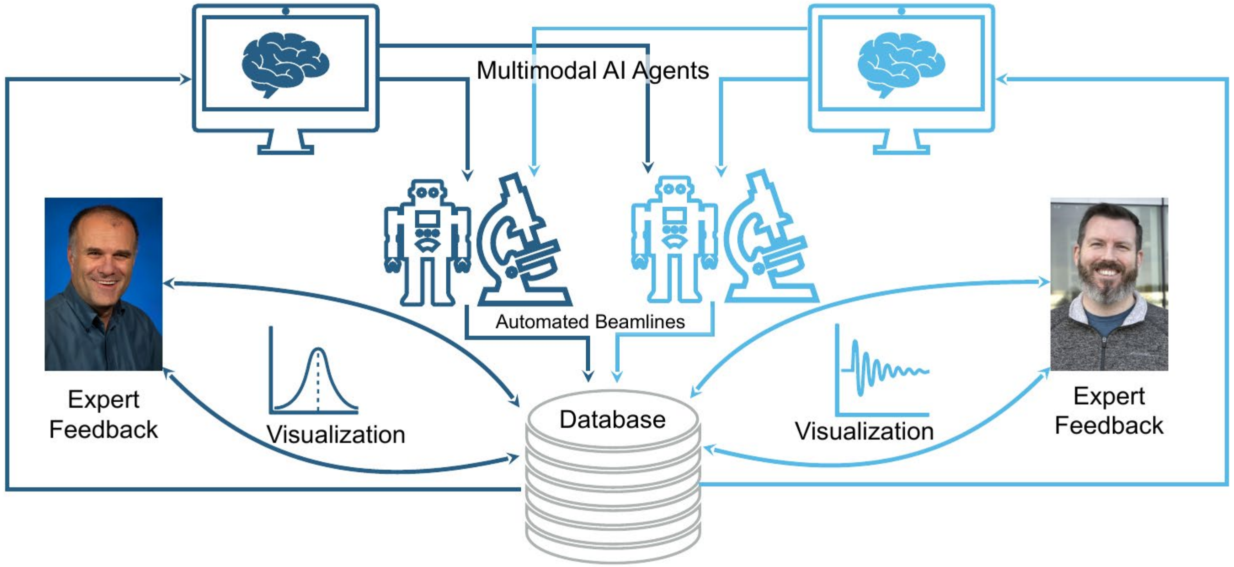


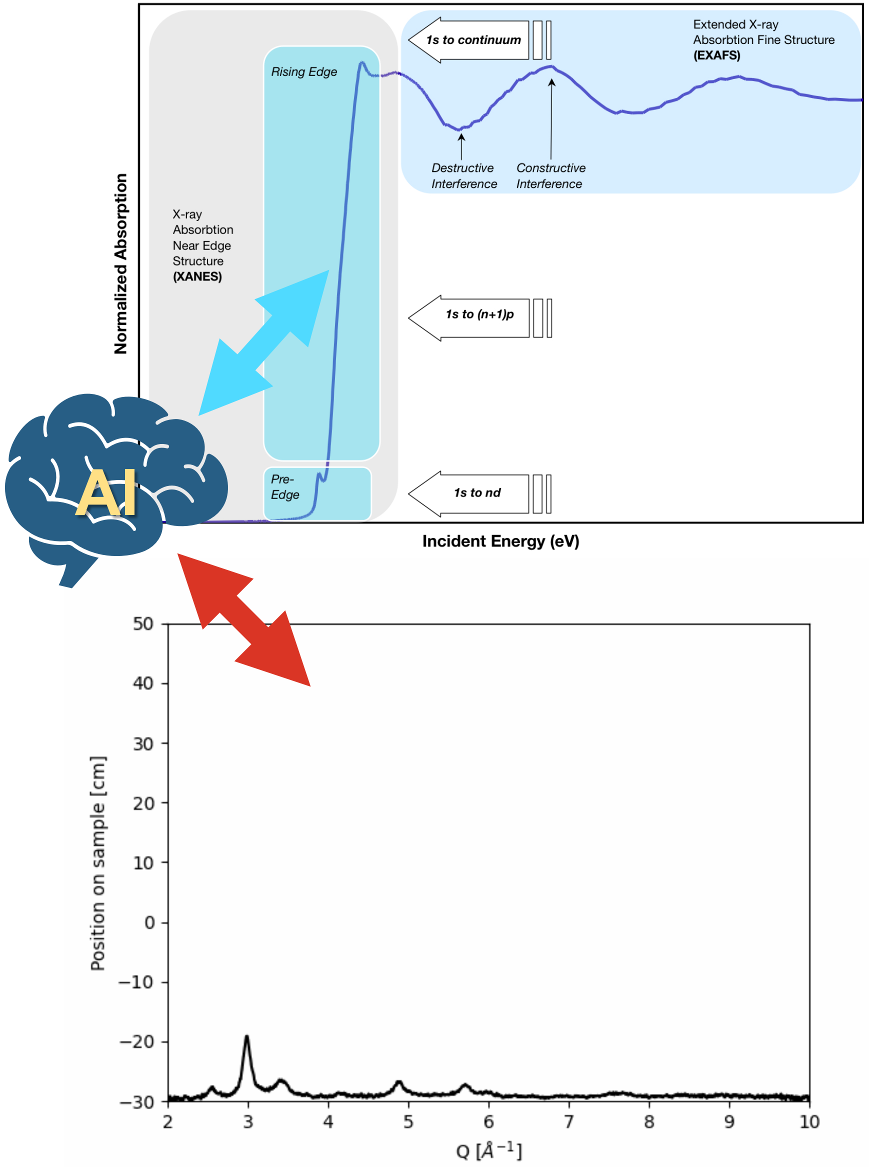
- Identical PtZr wafers loaded at BMM and PDF.
- While measuring diffraction (fast), we apply multiple machine learning methods to select promising regions to probe with spectroscopy (slow), and vice versa.
- Phases are determined by real-time ML analysis of XAFS and diffraction.

This demonstrates a world's first truly multimodal light source measurement, with AI performing both real-time analysis and control of multiple beamlines simultaneously.

AI-Driven, Real-Time, Multimodal Science

Goal: Autonomously and simultaneously drive both beamlines while continuously leveraging all information possible.





The Next Generation Synchrotron

The next (large) gains in science and facility upgrades are going to be in the data and the automation of data collecting, processing and analysis as well as (x-ray) brightness.

AI/ML Coupled with modern, scalable infrastructure will accelerate synchrotron science.

Out goal is to develop an ecosystem which enables this transition.