Automation of Alignment and 3D Analysis for Neutron Scattering Experiments

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AI for Scattering – UMD

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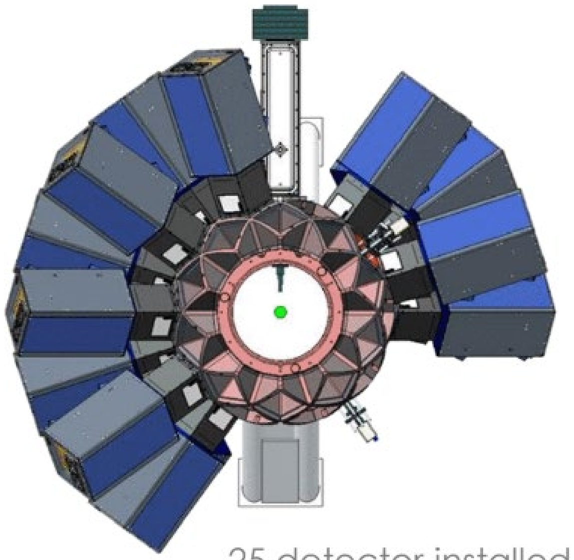
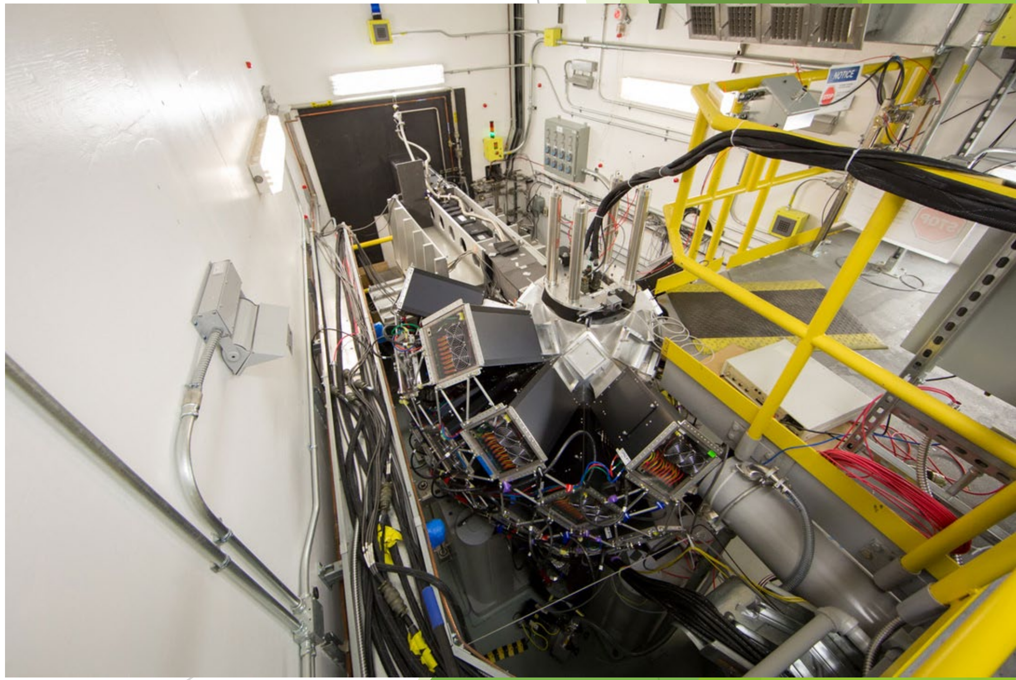
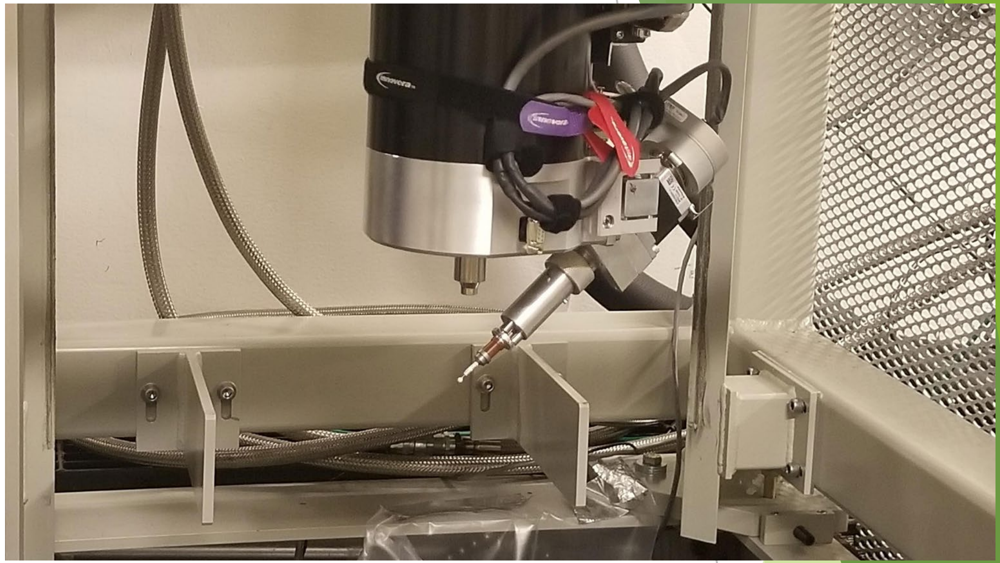
TOPAZ Single -crystal Diffractometer

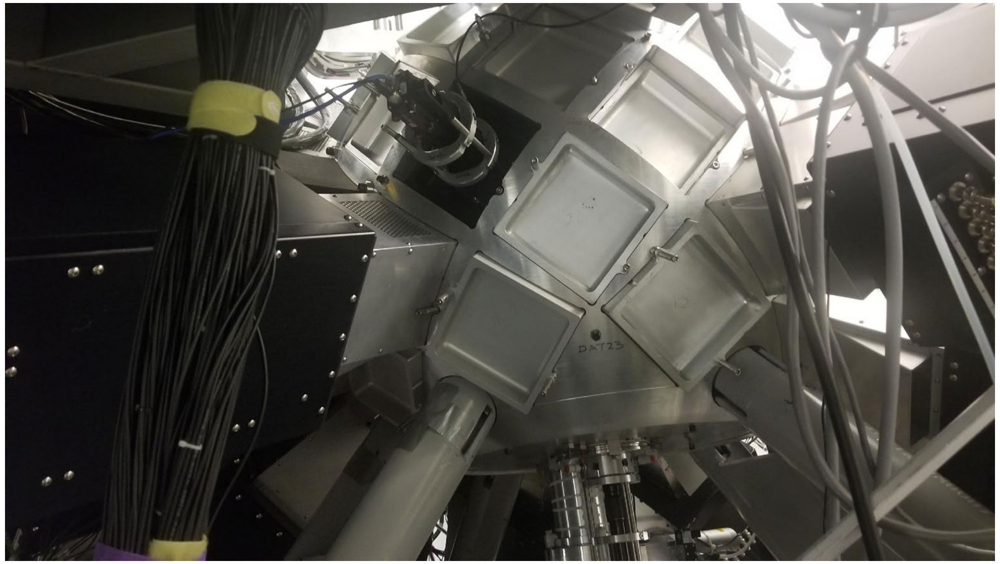
- Located at ORNL and receives neutrons from the Spallation Neutron Source
- Samples can be measured with high precision for volumetric sampling in reciprocal space (momentum measurements)
  - Samples are rotated to measure all aspects of the lattice
  - Temperature control from 5 K- 450 K
  - Broad Q coverage

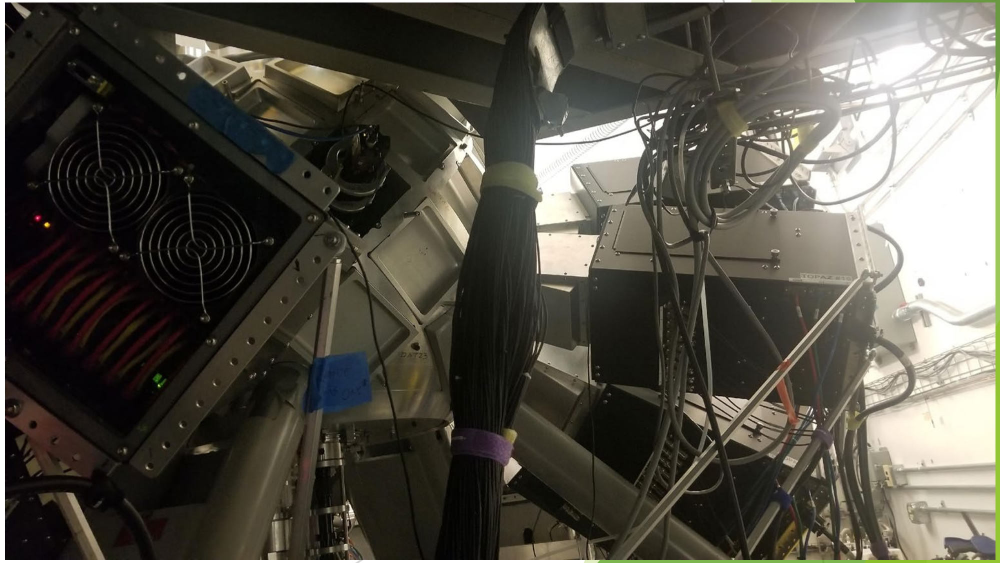

25 detector installed



TOPAZ Single -crystal Diffractometer



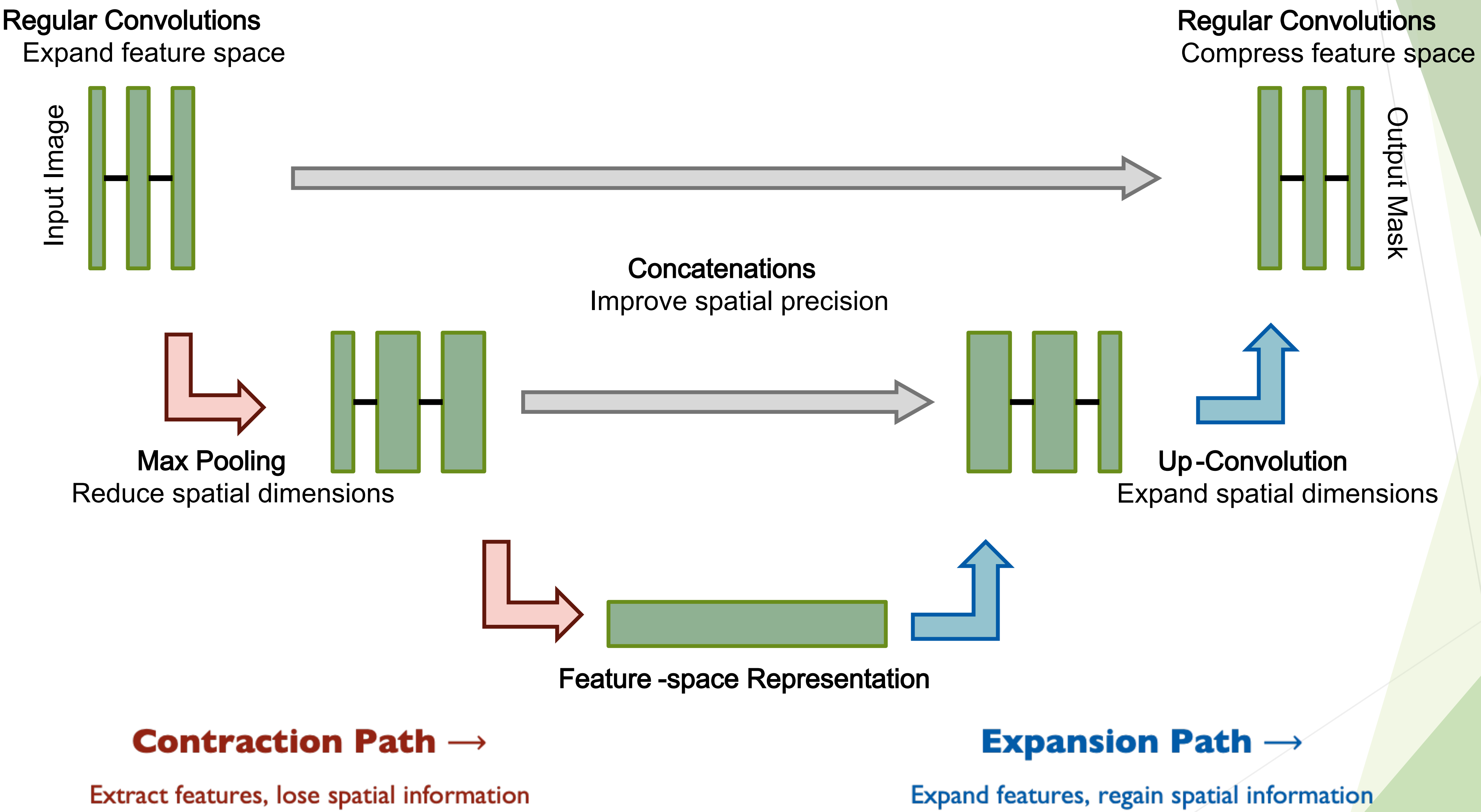




Background & Motivation

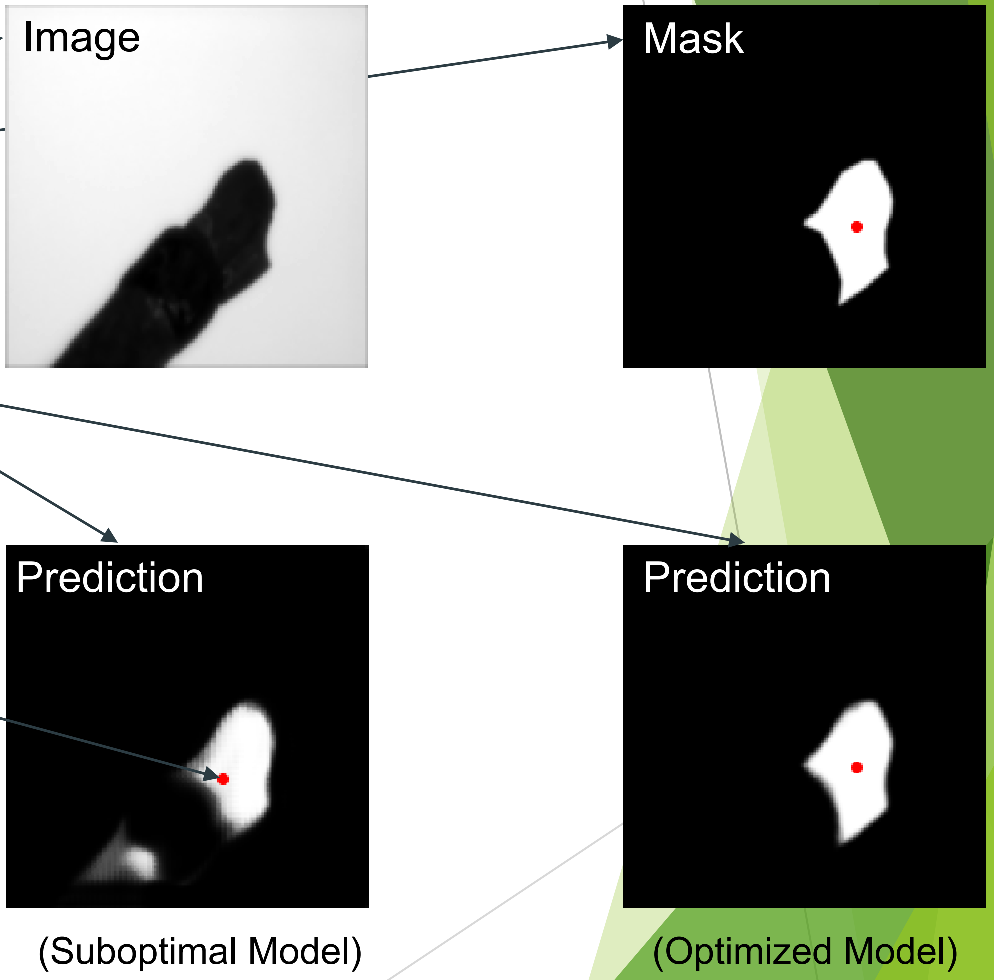
- Sample alignment
  - Neutron production time is limited
  - Some activities require constant realignment, such as temperature scans
  - User facilities especially face schedule constraints
  - Machine learning (ML) is a key automation tool
- Alignment protocols vary between beamlines
  - Opportunity to employ & test models
  - Broad applications for sample alignment

UNet Architecture for Image Segmentation

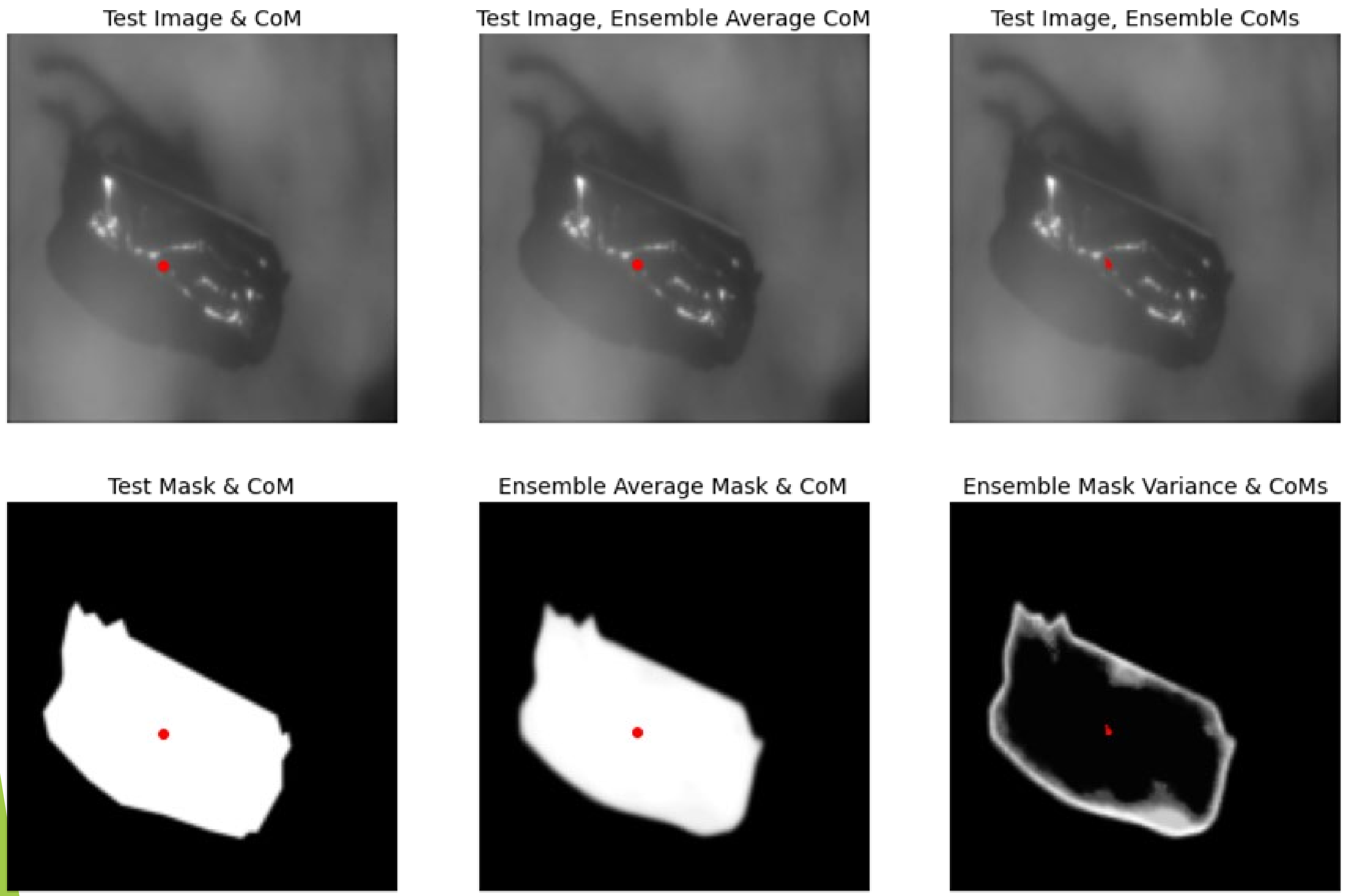


Machine Learning for Sample Identification

- Supervised learning problem
  - Input images come from optical camera
  - Beamline scientist / expert identifies the sample mask
- Train neural network model to learn the image to mask relationship
- Find the sample CoM



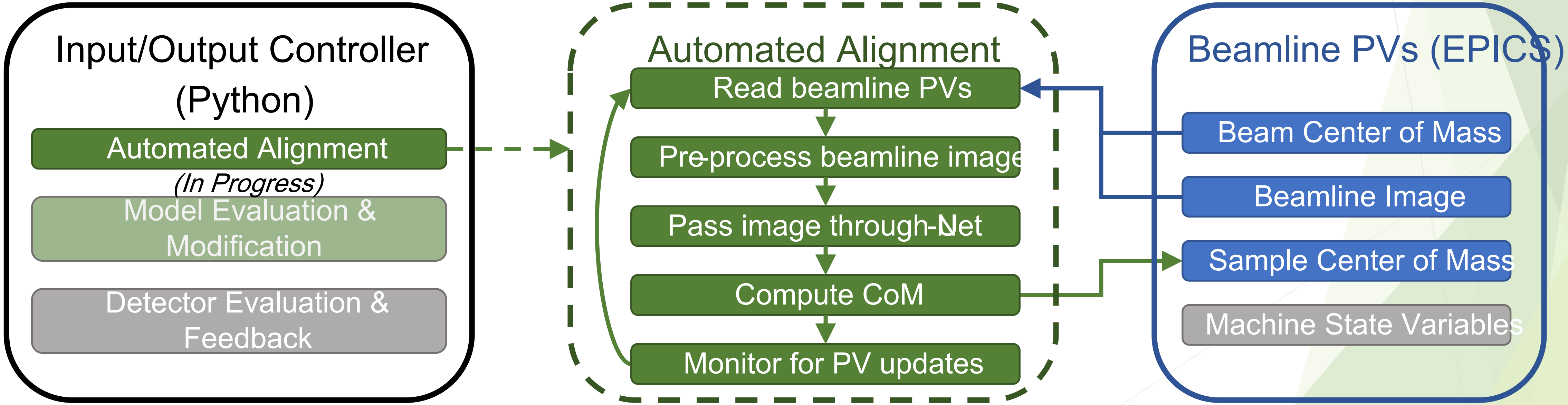
Uncertainty Quantification



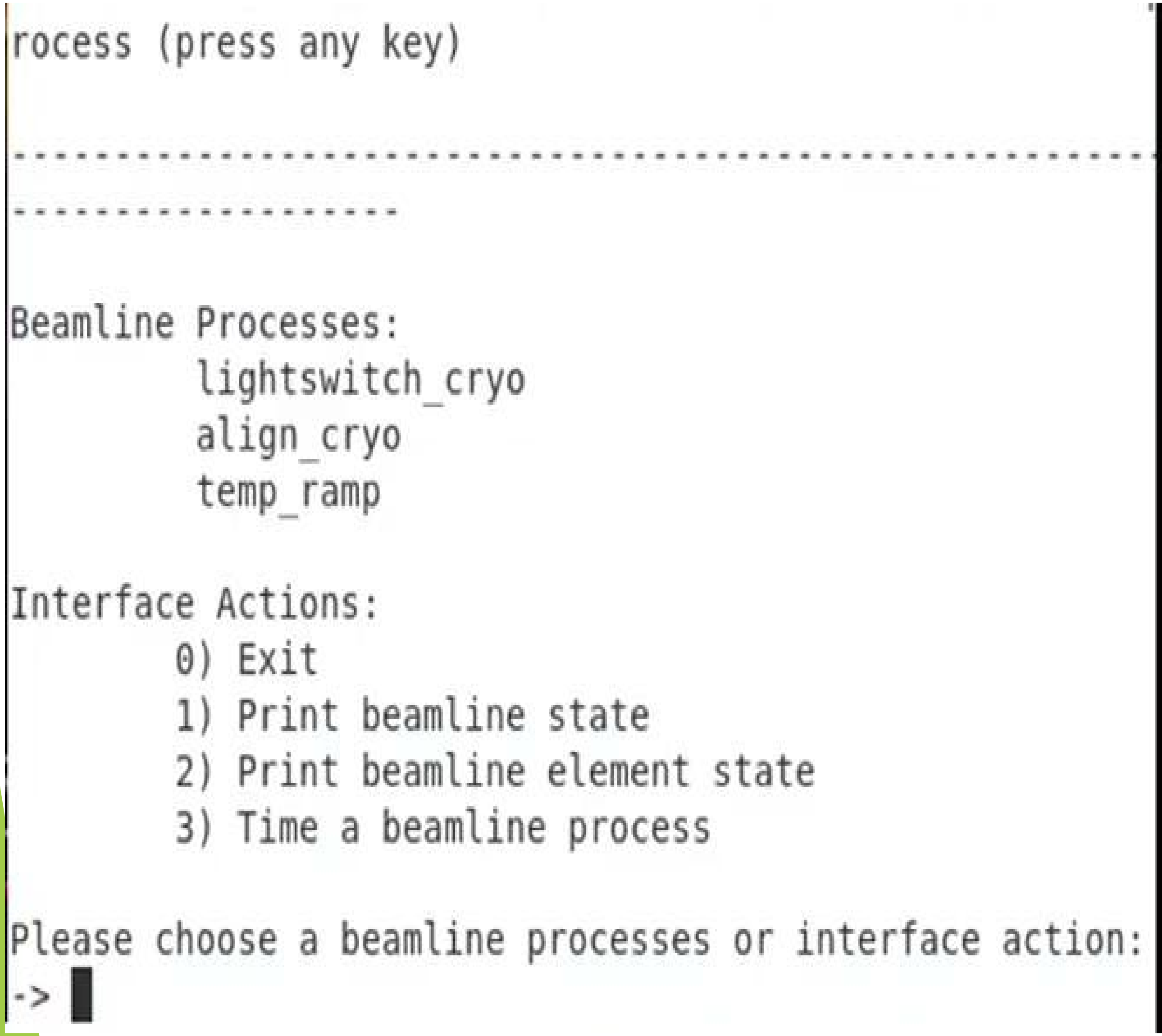
- During supervised training
  - Real error compared to human defined masks
- During testing and operations
  - Ground-truth data not available
  - Employ statistics from ensemble predictions
  - Variance between many trained models
- Takeaways
  - Excellent CoM prediction
  - Negligible ensemble spread with low uncertainty
  - Mask variance is restricted to edges

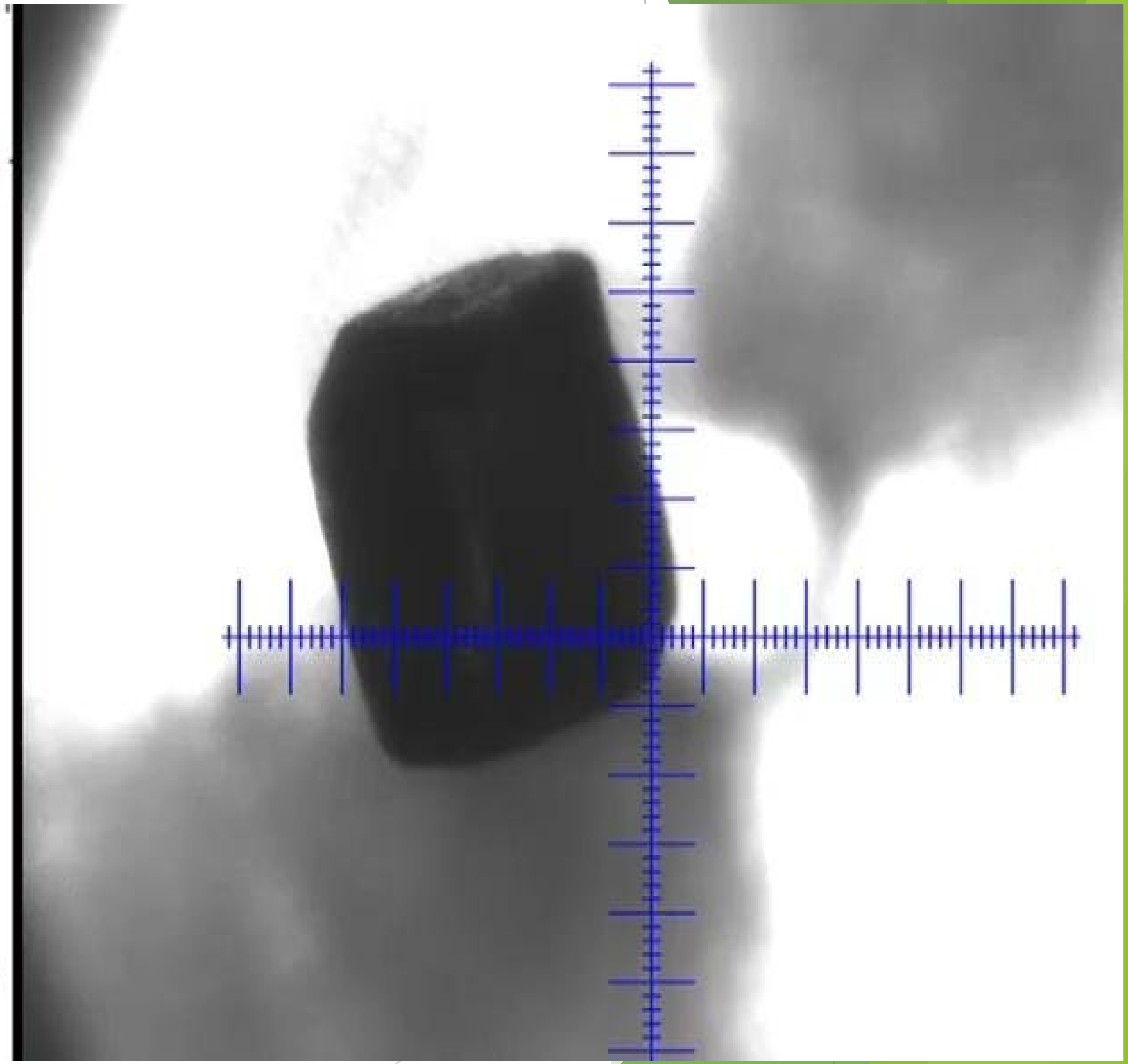
Controls Problem

- Pass images through ML model
  - Retrieve predicted mask & center of mass
  - Retrieve uncertainty measurement
- Evaluate quality of predictions/state of controls
- Pass values back to beamline controls
  - Sample/beam center of mass offsets
  - Human intervention needed?
- Retrain networks with feedback from cycle



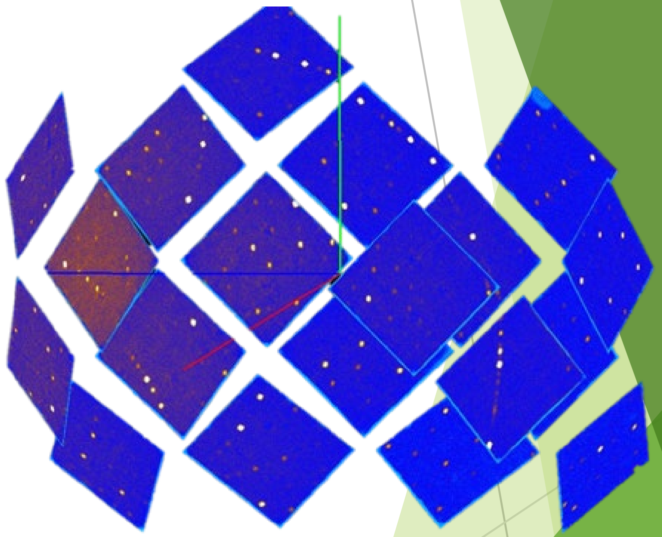
Automated Alignment





Analysis methods for TOPAZ data

- Mantid
  - Open source community developed application
  - Algorithms use raw data processed within 2D slices of the 3D data
- Some challenges faced by the community
  - Large datasets can be up to 100 Gb in size and current tools limit interactivity
  - Displaying data requires a high level of user interaction
  - 2D slices may miss key features of the diffraction data
  - May be slow to run due to optimization shortfalls



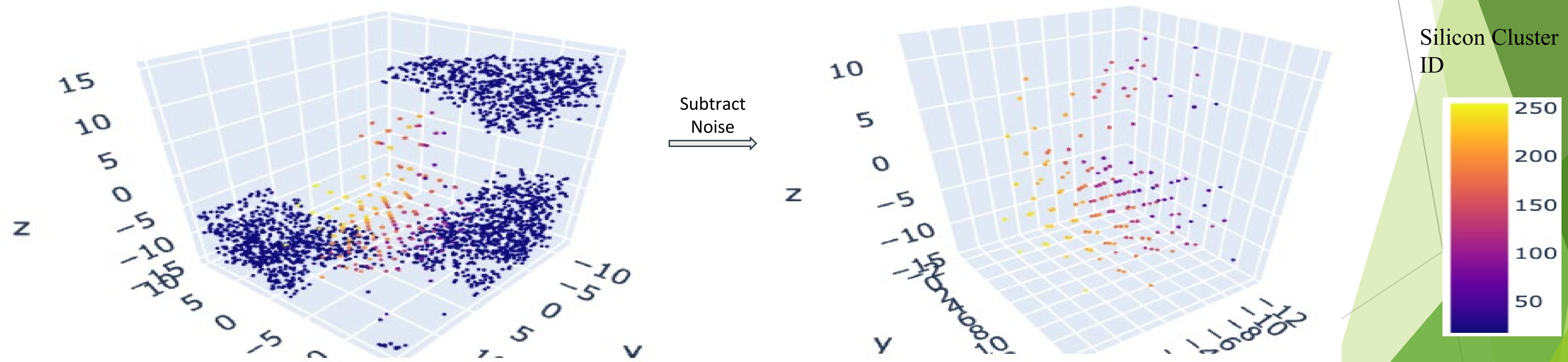
- Working collaboratively to leverage Mantid
  - Machine learning DBSCAN
    - Reduces user interaction
    - Automated Bragg peak identification
- Also improving the interactivity of the data viz
  - Close collaboration with the NVIDIA IndeX development team (Berlin)

- Working towards combination of 3D viz and automated analysis

https://www.mantidproject.org/

Analysis of Scattering Data for a Single Silicon Crystal

- Preprocessing the data
  - Measurements of the particles in momentum space
    - Looking for pockets of constructive interference
  - Measurements projected onto a 3D mesh
- DBSCAN is a density based clustering algorithm
  - Can identify oblong clusters and attribute data to noise if it doesn’t match anything
  - Sparse background can be removed easily



https://scikit-learn.org/stable/modules/generated/sklearn.cluster.DBSCAN.html#sklearn.cluster.DBSCAN

Comparison Cluster Identification with Mantid

- Peak locations
  - Fast Fourier Transform (FFT) to calculate UB matrix (orientation matrix) and predict Miller indices
- Limitations of Mantid peak finding
  - Needs to be told how many peaks to look for
  - Use the number of peaks that is found by DBSCAN

$$\underbrace{Q_s}_{\text{Measured Peaks}} = 2\pi \cdot \underbrace{UB}_{\text{Calculated with FFT from Mantid}} \cdot \underbrace{\begin{pmatrix} h \\ k \\ l \end{pmatrix}}_{\text{Predicted Miller Indices}}$$

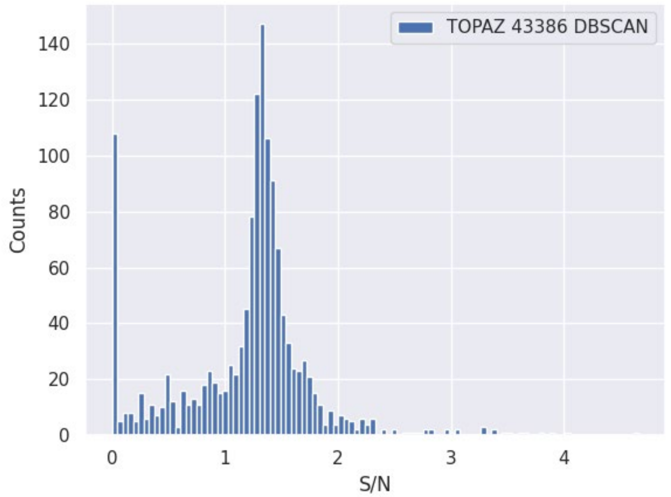
- What do we compare?
  - UB matrix is not unique
    - Due to the symmetry of the Bragg peaks you can rotate the matrix and still predict the peaks in the proper location
  - Miller indices are not unique
    - Due to the rotation of the UB matrix different hkl indices can map to the same peak
    - Confirm values are ‘close’ to an integer value
  - Compare peak locations
    - Clean with Signal-to-noise

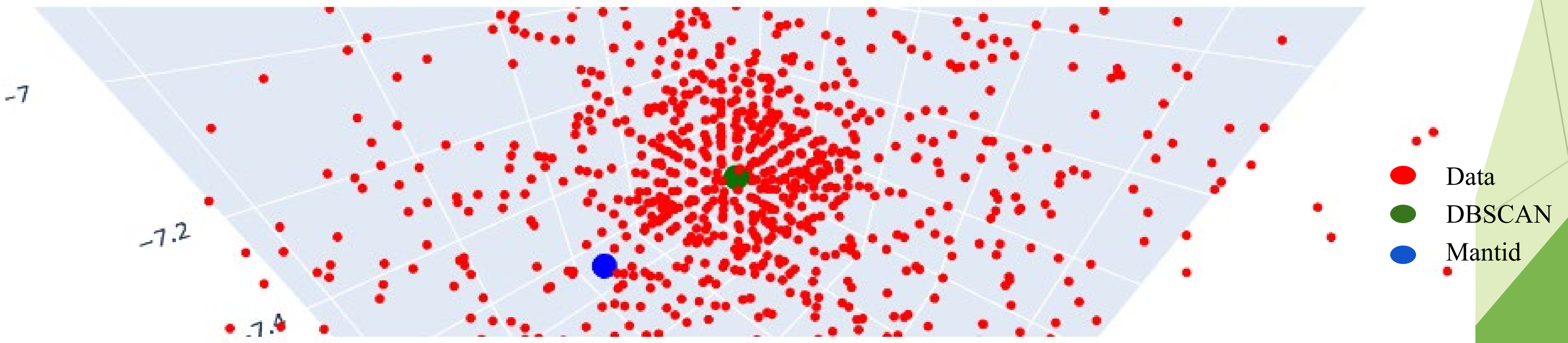
https://docs.mantidproject.org/v4.0.0/algorithms/FindUBUsingFFT-v1.html
https://docs.mantidproject.org/v4.0.0/concepts/Lattice.html#lattice

Quantifying the validity of Bragg peaks

- Calculate a Signal-to-Noise for each matched peak
  - A Bragg peak should have a large S/N ratio
  - Background events result in a minimal ratio
  - Tunable cut to allow for optimized data cleaning

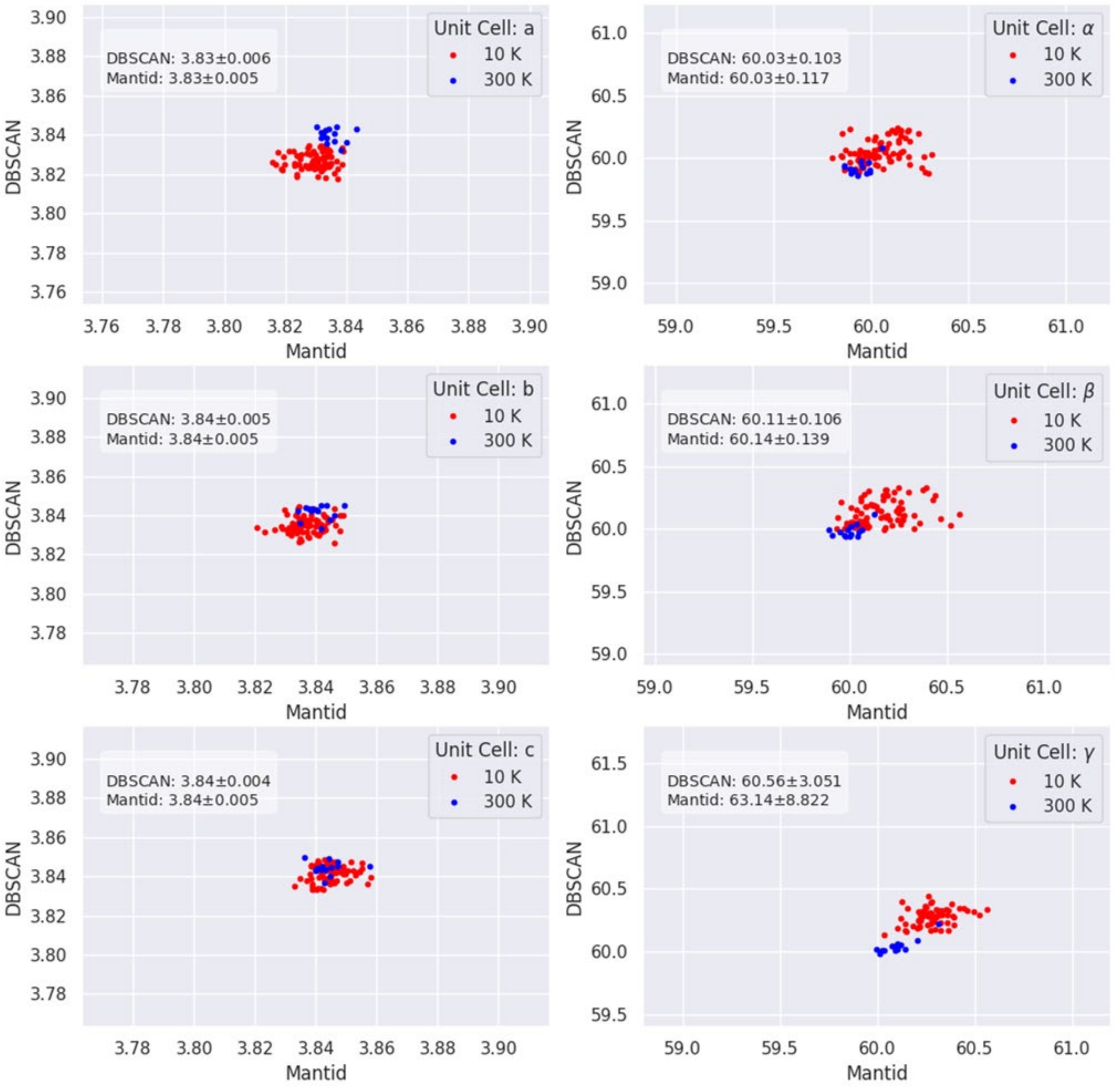
$$\frac{S}{N} = \frac{I_{\delta S}}{\sqrt{I_{\delta B}^2 + N_S}}$$





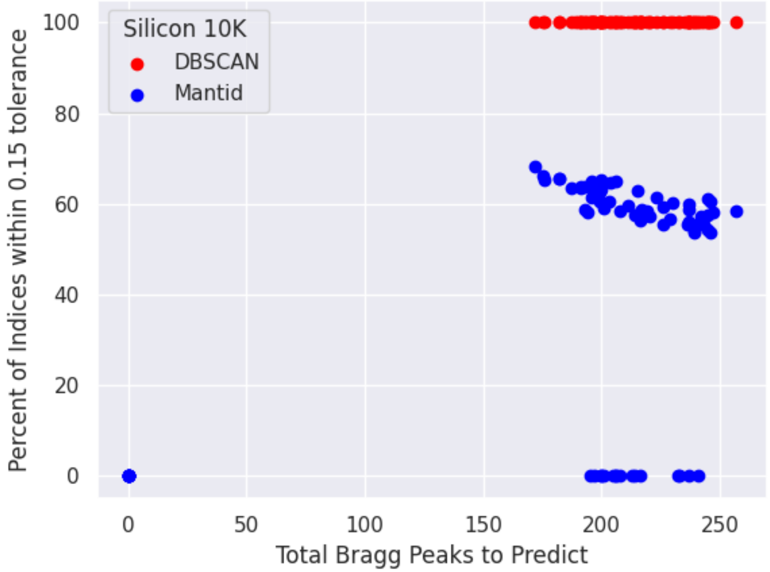
Silicon 10K and 300K unit cell (reduced) parameters

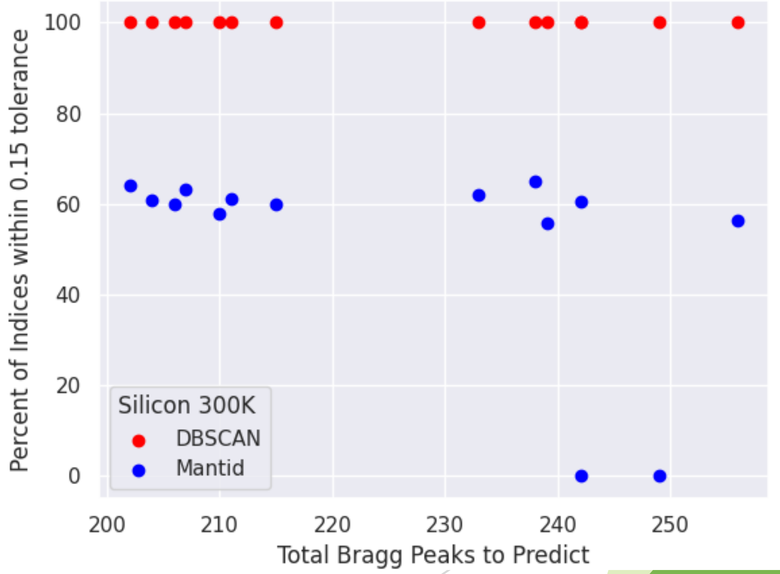
- Good agreement
  - Mantid and DBSCAN methods show the same lattice parameters for Silicon
  - Standard deviation is comparable!
- DBSCAN datasets
  - Automated peak finding allows for similar results to Mantid only methods
  - Files with only DBSCAN results are shifted from the normal results
  - All lattice parameters agree with the theoretical value of Silicon



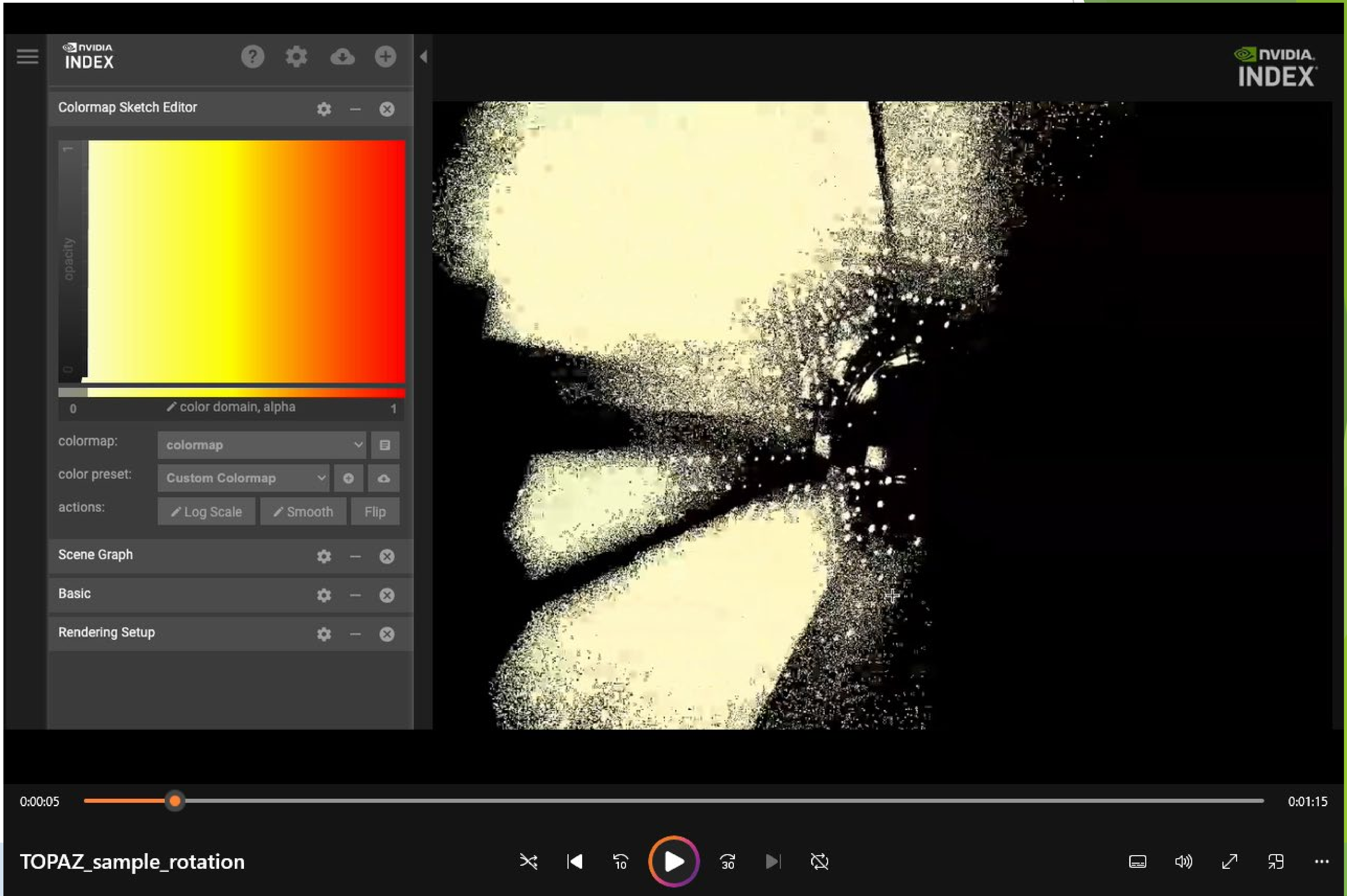
Silicon 10K and 300K

- Predict UB matrix with identified Bragg peaks
  - DBSCAN finds 100% of Bragg peaks within tolerance
  - Mantid finds 55–65% of Bragg peaks within tolerance
  - Silicon 10K
    - 24 3D silicon datasets could not find a UB matrix with Mantid peaks
  - Silicon 300K
    - 2 3D silicon datasets could not find a UB matrix with Mantid peaks





ADARA Live Streaming into NVIDIA's IndeX



Summary

- Take the user out of the loop
  - Automated sample identification
  - Real time sample visualization and analysis
  - Information at your fingertips

- 3D visualization
  - Integrated on a single GPU
  - Interactive analysis

- Open-source collaboration
  - Applications to many real time 3D datasets
  - Broad applications to samples within a beamline

THANK YOU!

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