Interactive Automated Bragg Peak Identification with 3D Neutron Scattering Data

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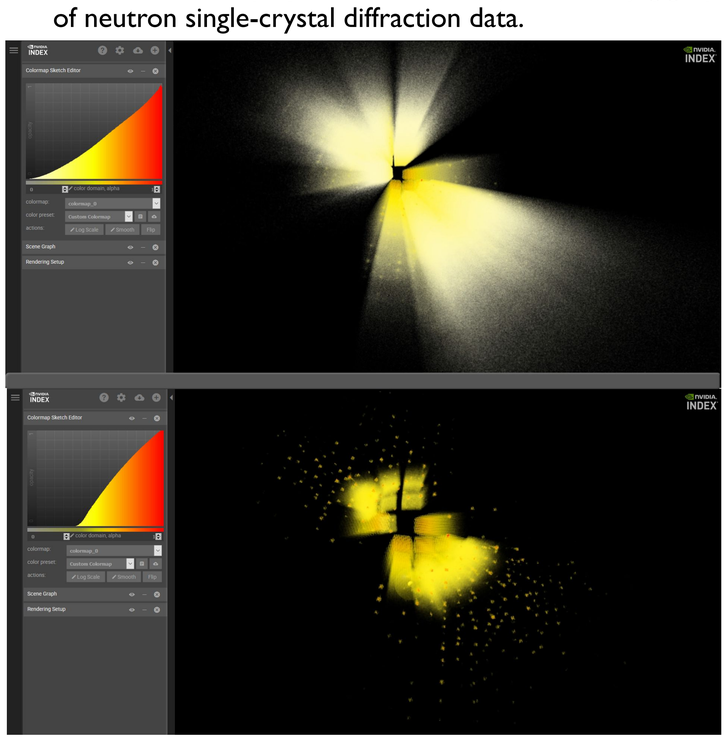
Summary

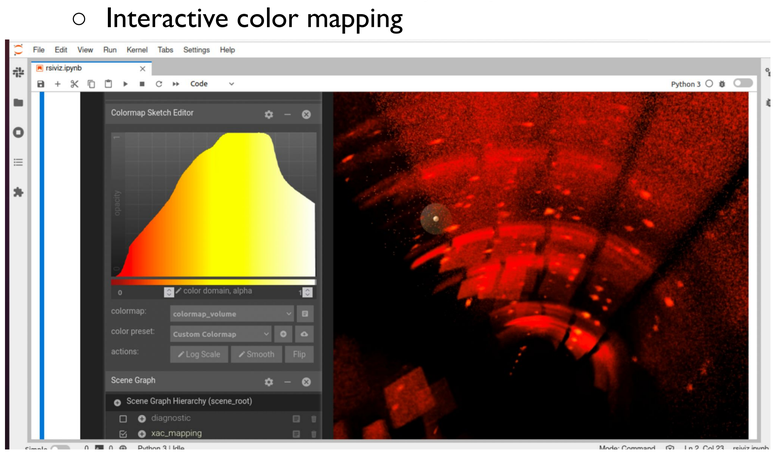
- Fast, interactive 3D rendering of reciprocal space
  - in your browser via NVIDIA's IndeX technology
- Automated identification of Bragg peaks
  - DBSCAN clustering distinguishes peaks from noise
  - more accurate and robust than Mantid algorithms
- Mantid uses DBSCAN peaks for UB matrix & hkl indices
  - predicts 100% of the indices within 0.15 tolerance
  - Mantid-only approach yields 76.5% within tolerance
- Statistical fit on the cluster size can distinguish a complex diffuse background from both noise and Bragg peaks
- Complete analysis of 5 different types of crystal lattices with accurate automated Bragg peak finding

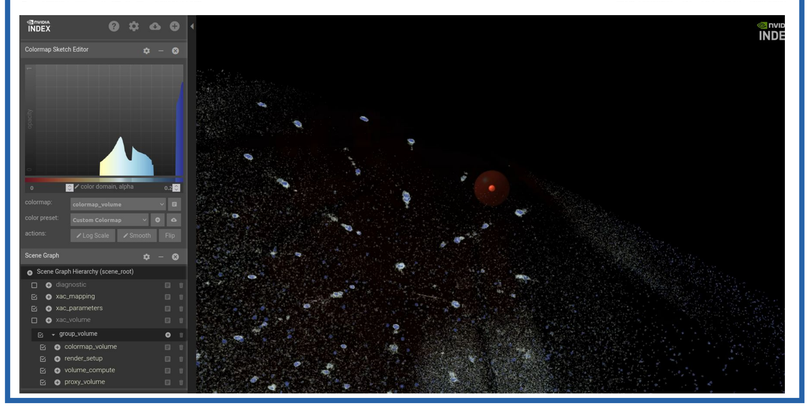
IndeX Visualization

- NVIDIA IndeX technology [3]
  - 3D browser based volumetric interactive framework
  - Scientists can interact with massive data sets
  - Make real-time modifications
  - Navigate to the most pertinent parts of the data in real time
- Our implementation of IndeX
  - Docker based deployment Interactively view many gigabytes of neutron single-crystal diffraction data.



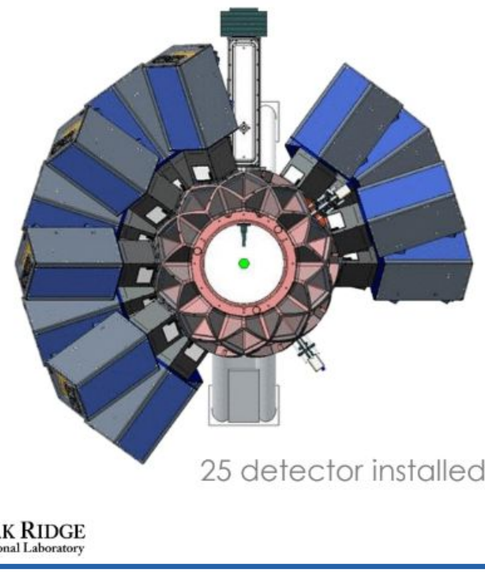
- **Live Data Streaming!**
  - Successful implementation of IndeX at ORNL with live data
  - Interactive neutron intensity analysis
  - Interactive color mapping

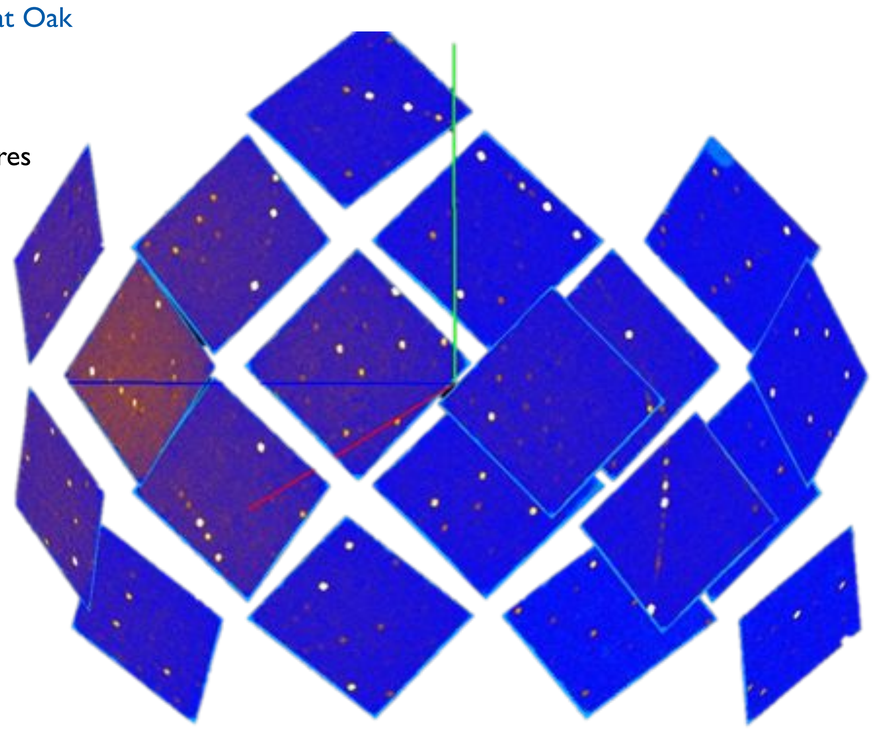




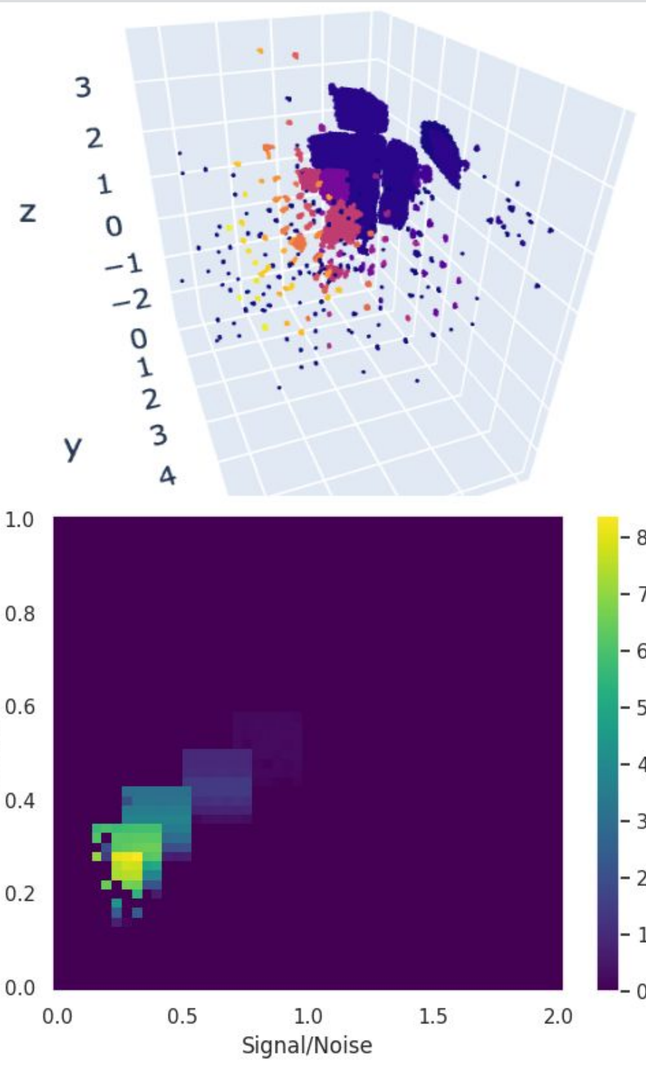
Background

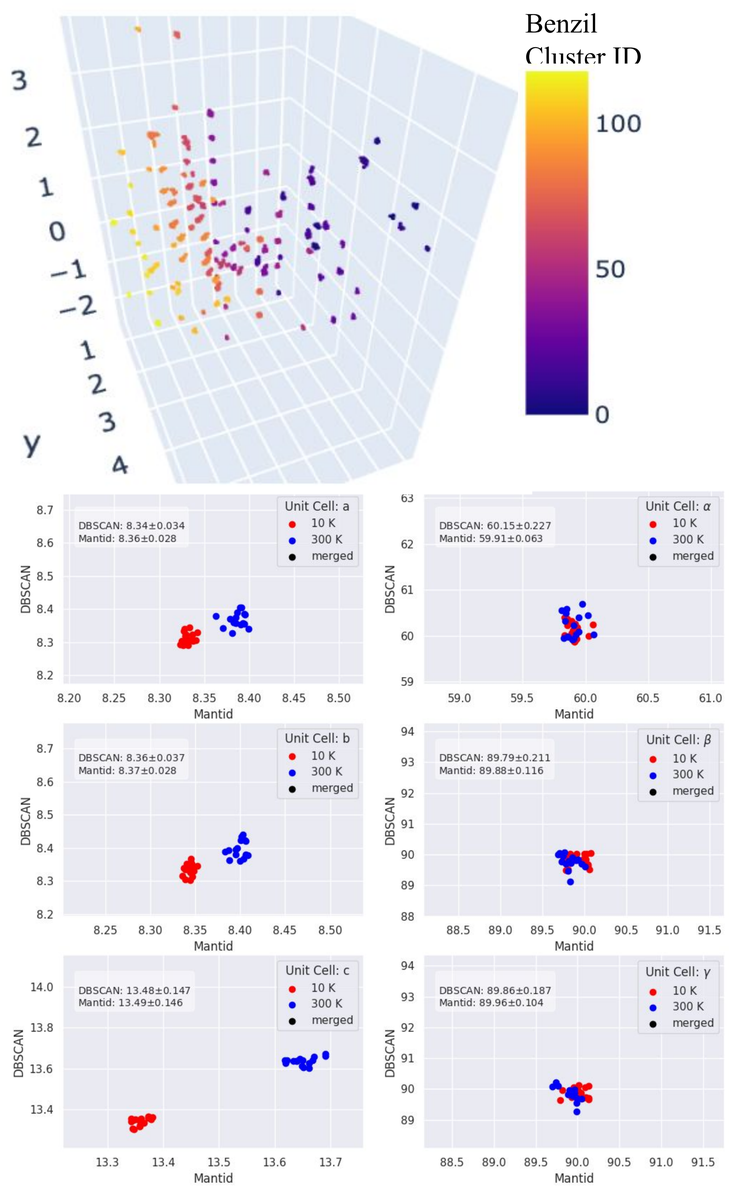
- TOPAZ instrument [1] at the Spallation Neutron Source at Oak Ridge National Laboratory
  - Typical analysis using Mantid [4]
  - Non-interactive large dataset analysis
  - Methods use 2D slices which can miss important features



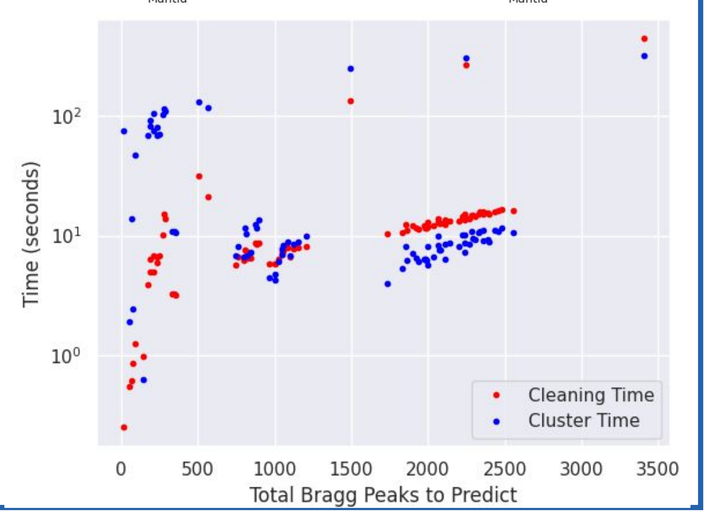


Bragg Peak Detection with Machine Learning





- Density based clustering algorithm with DBSCAN
  - Can identify oblong cluster and attribute data to noise
  - Sparse background can be easily removed
  - Automatic peak finding within datasets
- Calculate a signal-to-noise for identified peaks
  - Tunable cut to allow for optimized data cleaning
- Comparisons with Mantid
  - Compare peak locations with clean signal-to-noise
  - Complete analysis demonstration with 5 different crystal lattices at 10 K and 300 K
  - DBSCAN shows a higher number of peaks within reconstruction tolerance
  - Automatic scanning of signal-to-noise and intensity parameter space to optimize Bragg peak reconstruction
- Further work…
  - Normalization to merge datasets from different user runs
  - Development neural network to remove consistent background from detector devices



References

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