Automated Analysis and Denoising of Neutron Scattering Data

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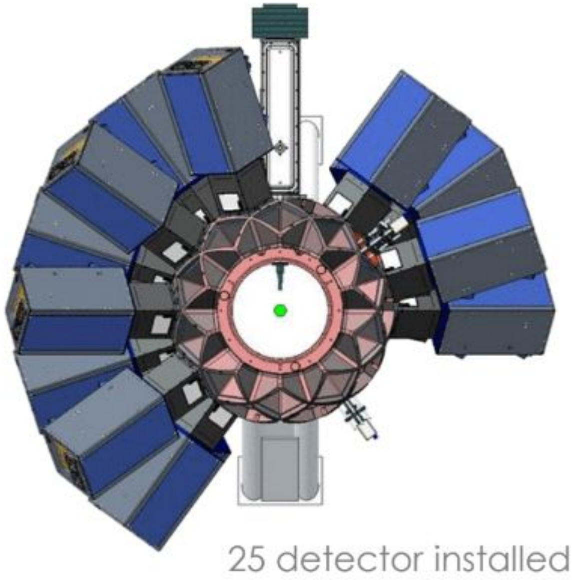
TOPAZ Single-crystal Diffractometer

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



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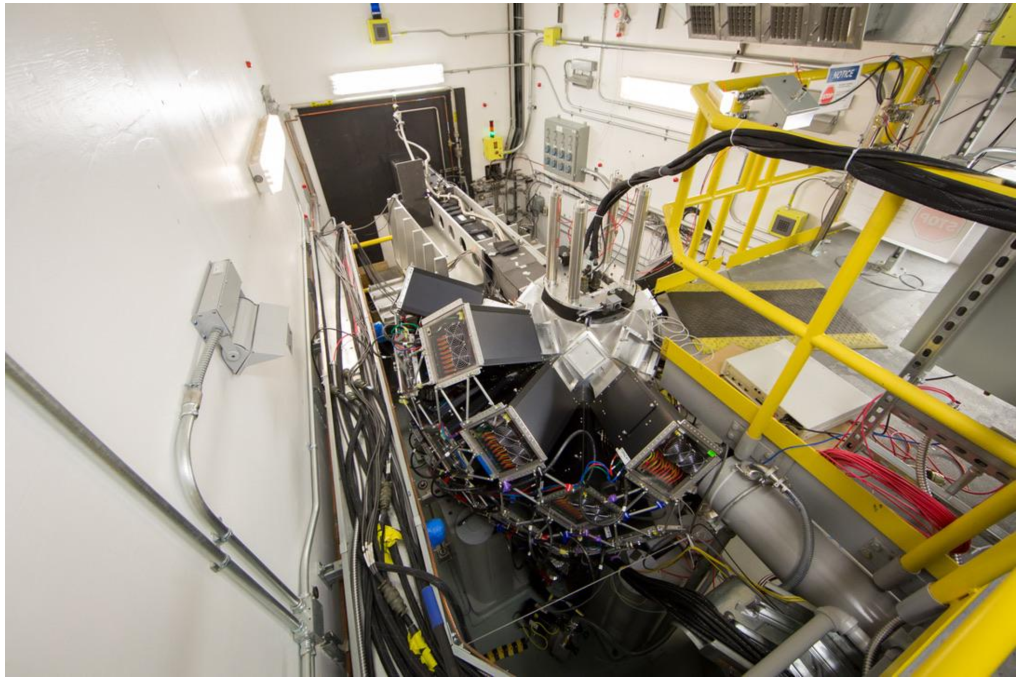
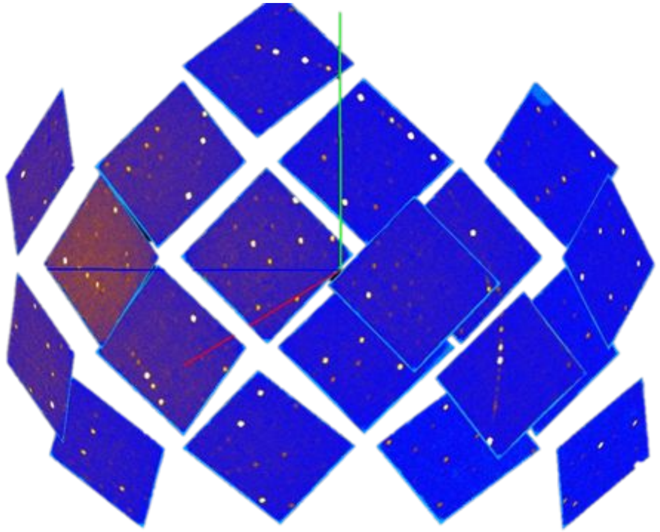
https://neutrons.ornl.gov/topaz



Analysis methods for TOPAZ data

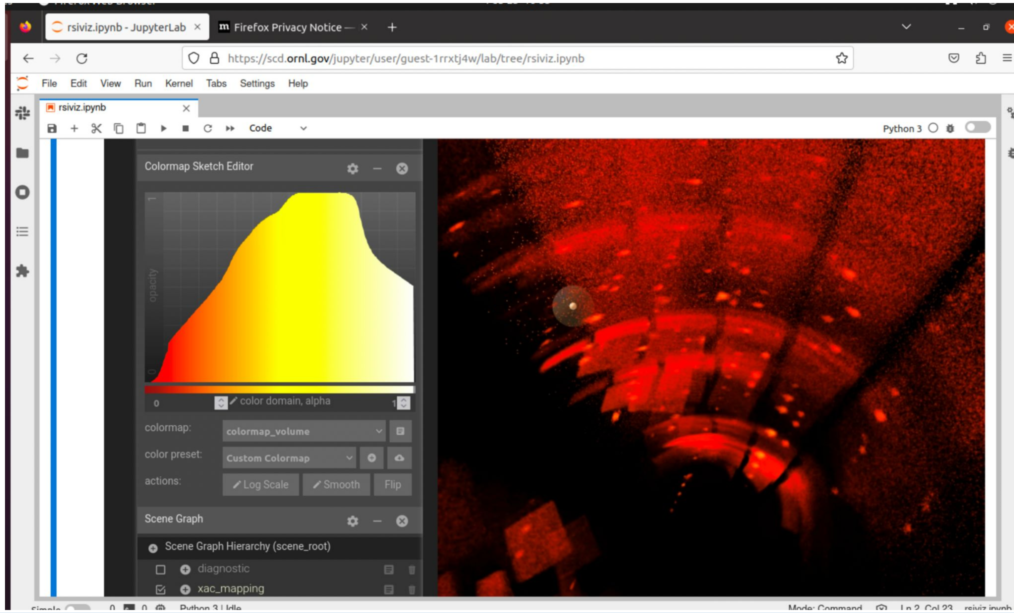


- Mantid, https://www.mantidproject.org
  - Open source community-developed application
  - Algorithms use raw data processed within 2D slices of the 3D data

- 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

- Using ML & leveraging Mantid to automate analysis & viz
  - DBSCAN used to automate & improve Bragg peak identification
  - 3D UNet used to automate detection of aluminum signature

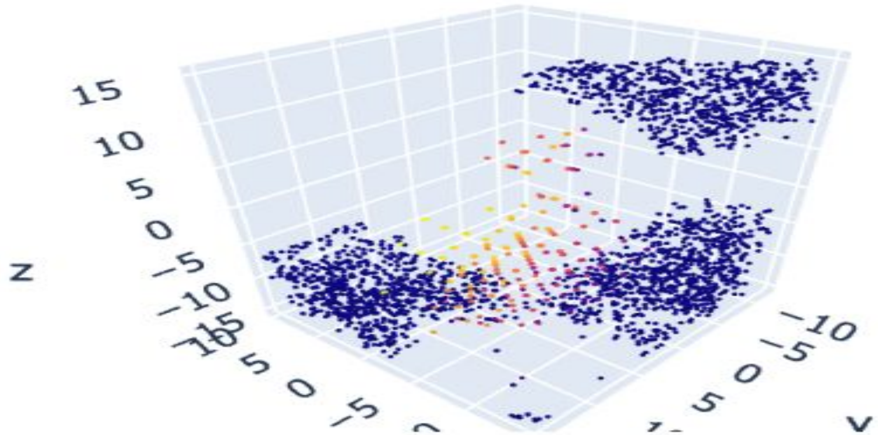
- We are improving interactivity of the data viz
  - collaboration with NVIDIA Omniverse/IndeX development team
  - working towards combination of 3D viz and automated analysis
  - IndeX 3D Scientific Data Viz, https://developer.nvidia.com/index
  - Enables 3D browser-based viz of streaming data (deployed)

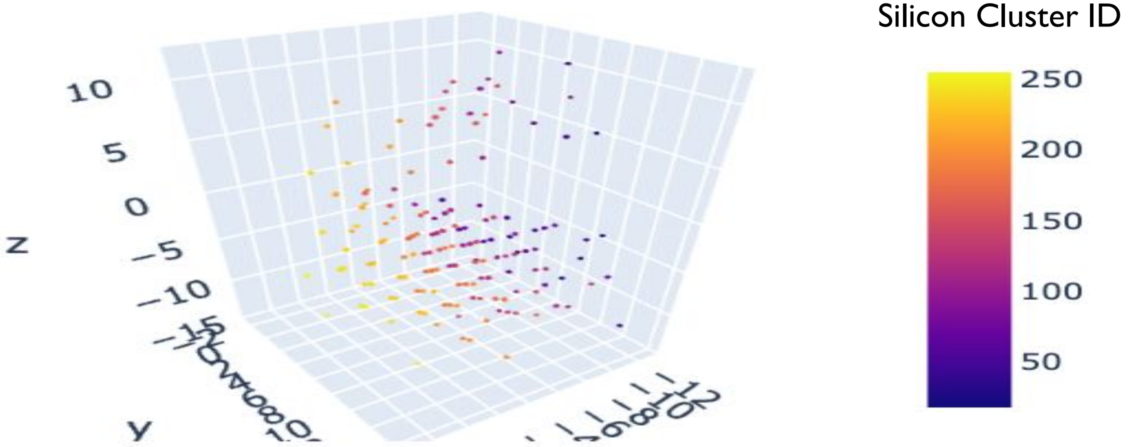


Previous work: analysis of scattering data for a Silicon crystal

- Preprocessing the data
  - Data is transformed to q-space in the usual manner
  - We consider a 3D histogram of neutron counts in q-space
  - Typically use 1,000 cubed histograms these are voxels to NVIDIA Omniverse / IndeX
  - 5,000 cubed voxels will be practical on a single, modern GPU with latest version of IndeX software

- DBSCAN (a density based clustering algorithm) is used for Bragg peak detection & analysis
  - Bragg peaks are automatically identified as oblong clusters (Mantid requires user input)
  - Mantid takes peaks and calculates UB matrix & Miller indices
  - DBSCAN / Mantid approach is 10x faster, more accurate & requires no user input
  - Timescale: 10-20 min

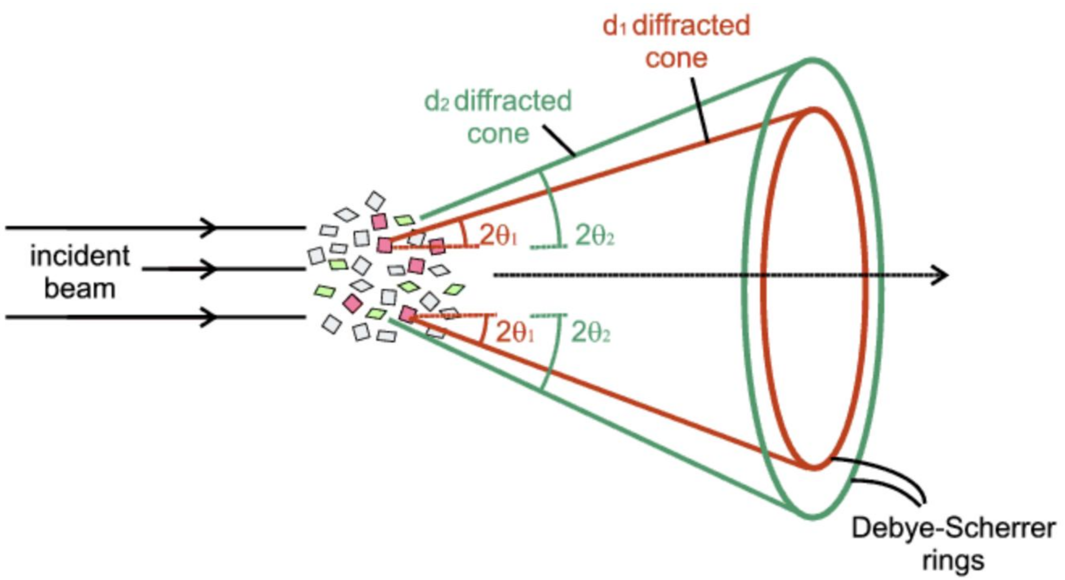


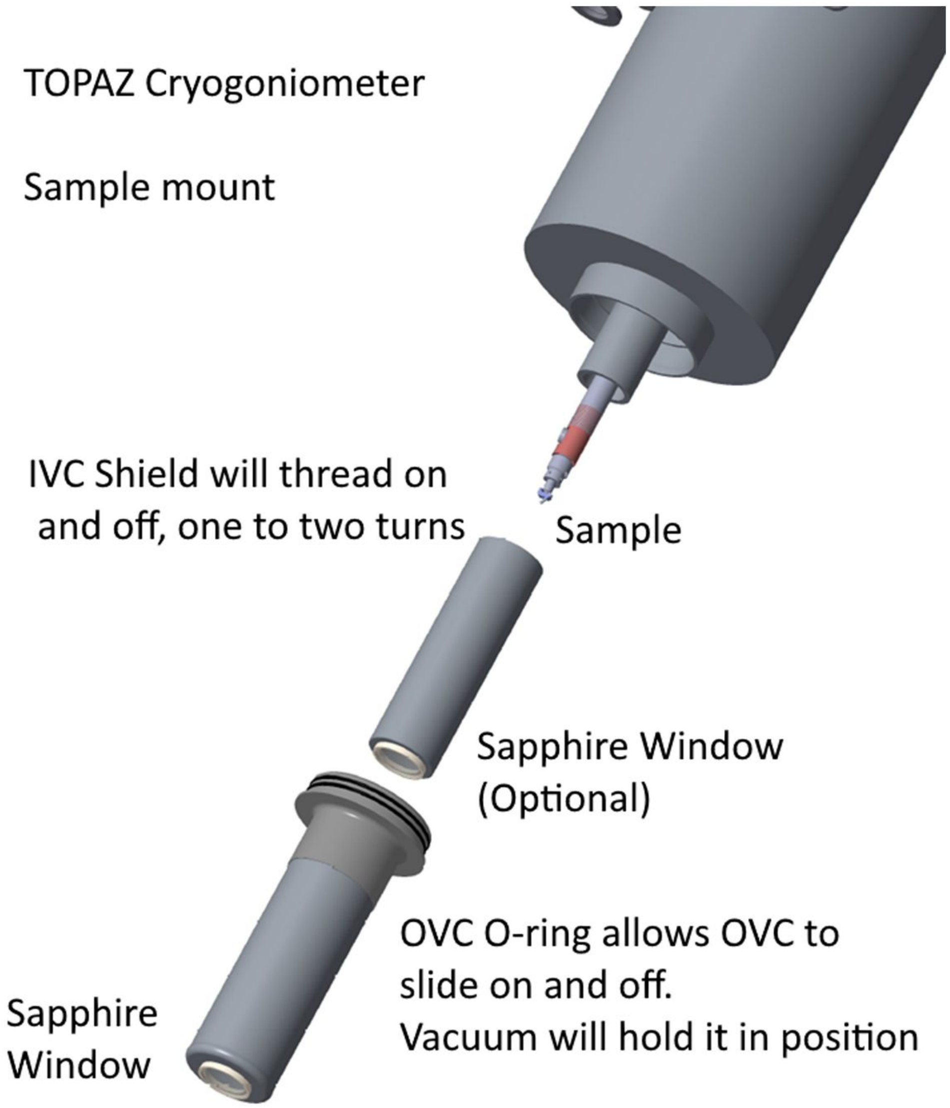


https://scikit-learn.org/stable/modules/generated/sklearn.cluster.DBSCAN.html#sklearn.cluster.DBSCAN

Background Removal Processes

- Sample mounting
  - Crystal sample can be tested at low temperatures
  - Aluminum cylinders have a randomly oriented crystal structure
  - These rings will scatter neutrons into a sphere or ring
- Scattered neutrons
  - Each plane orientation will create rings within reciprocal space
  - Translates into a sphere in 3D representation



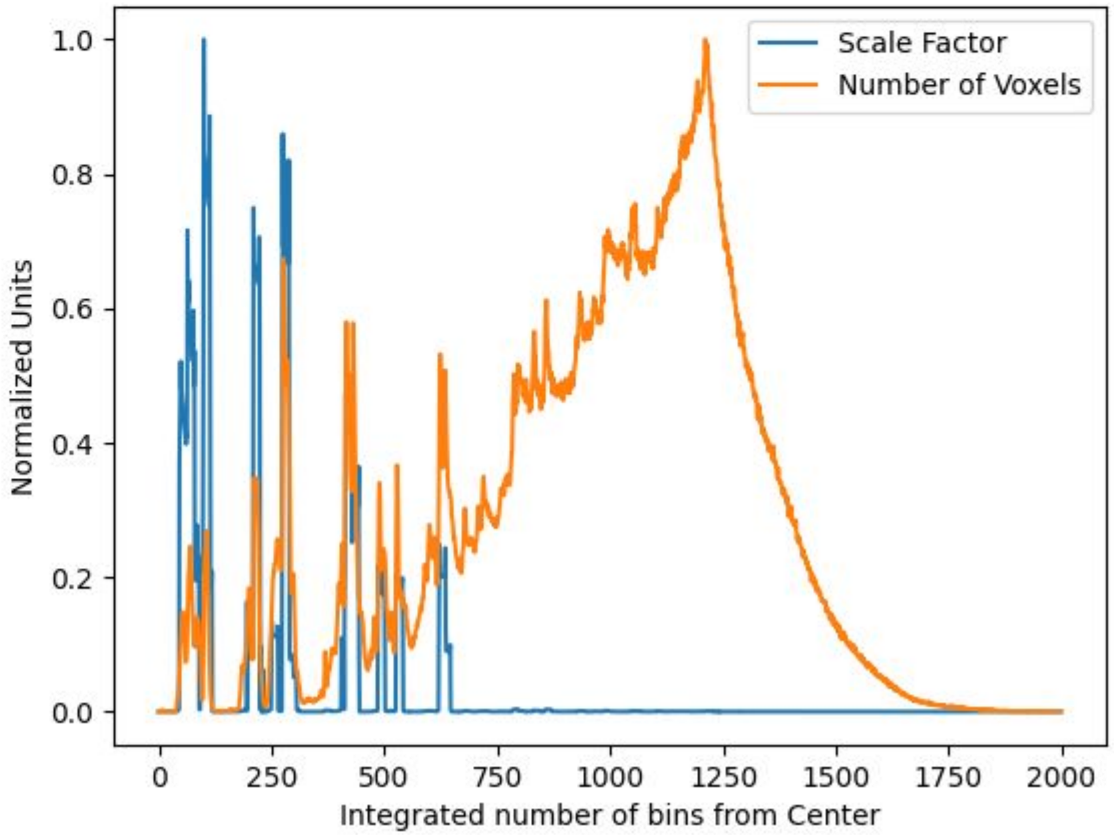


Identify Accurate Ground Truths

- Properties of Aluminum Rings
  - Monochromatic in neutron intensity
  - Concentrated at a fixed radius
  - Varies from sample to sample
- Define a scale factor
  - Simple clustering
    - Tune DBSCAN parameters to get rings
  - Gradient based definitial for clustering
    - Normalized by the mean number of voxels

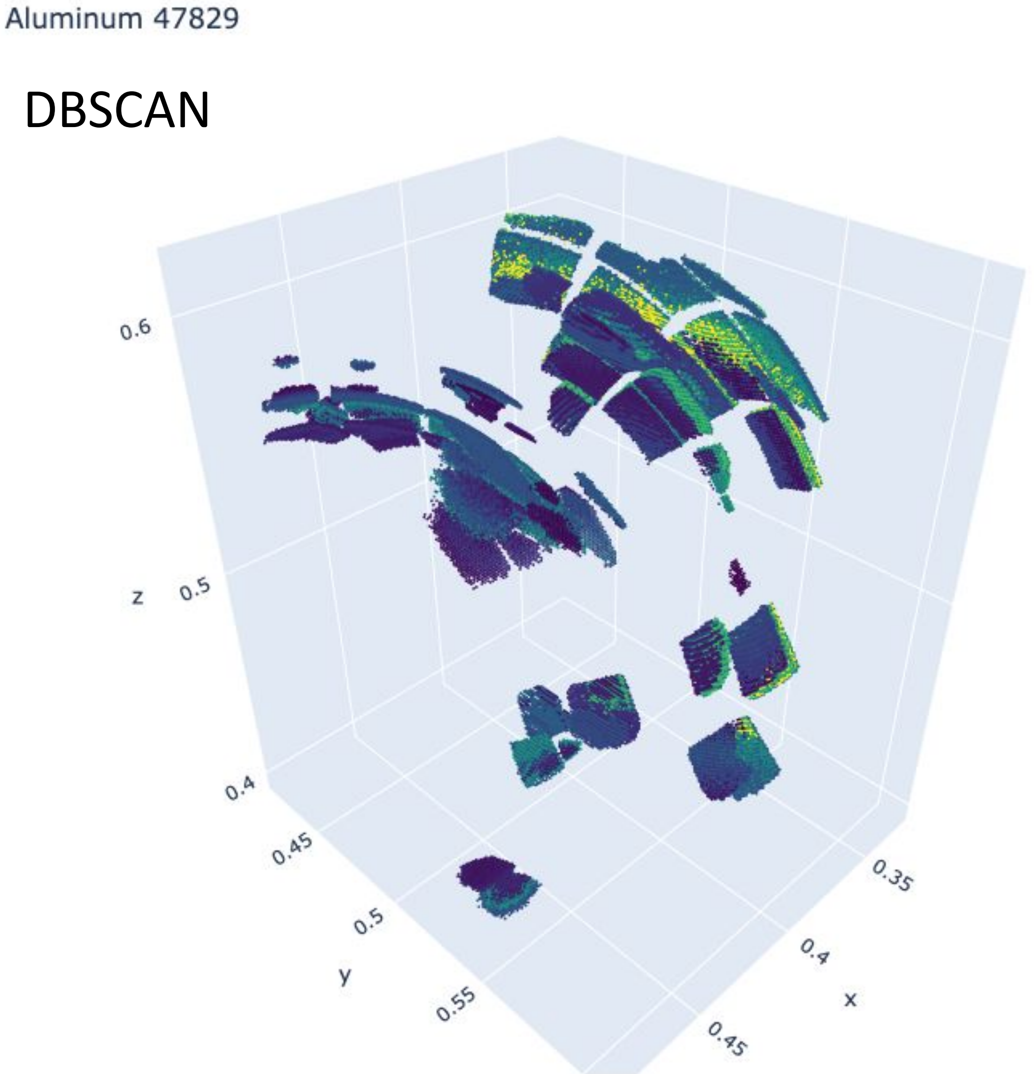
$$S_{rings}(R_w) = \frac{max(\nabla_w R) \cdot \bar{R}}{1 + r}$$

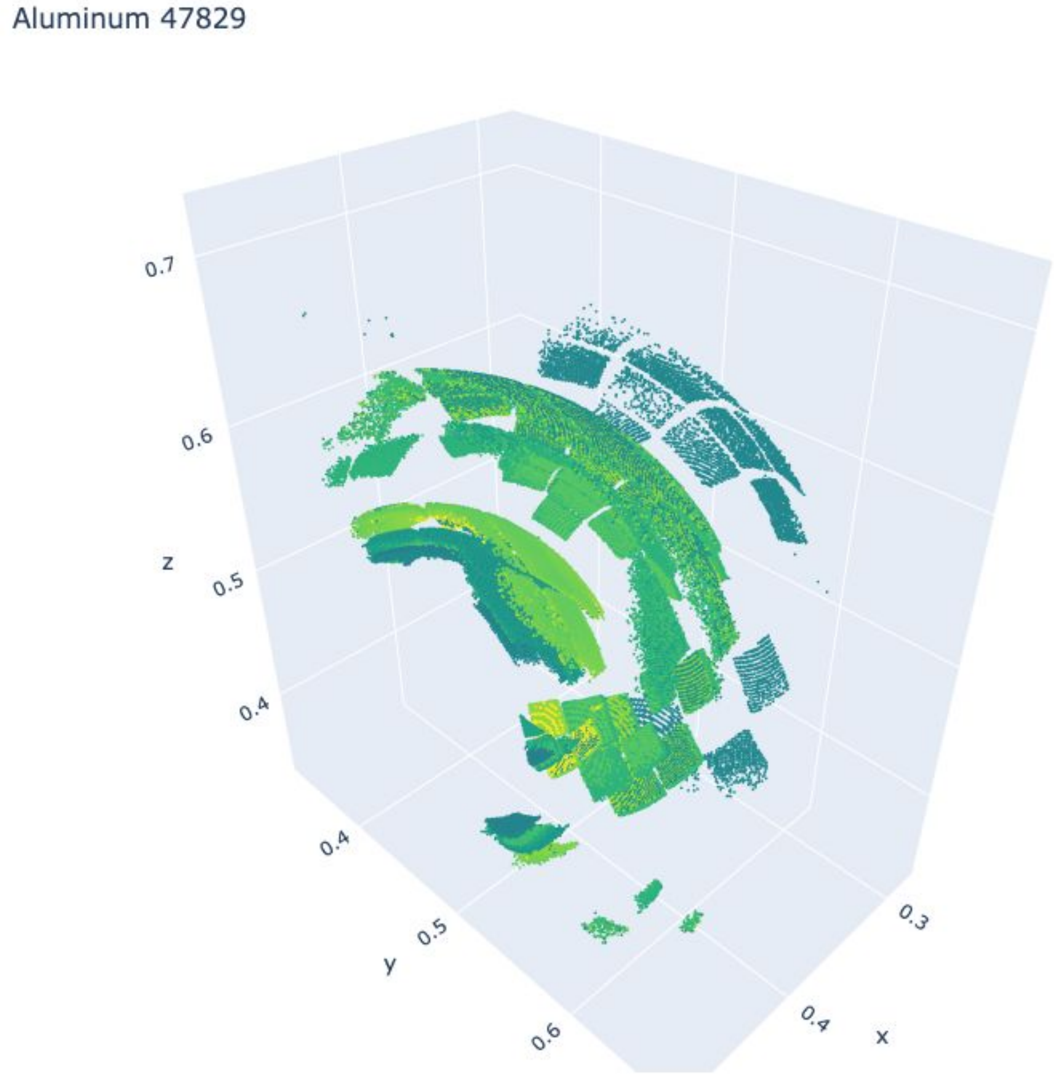
- How do these two methods compare?



Aluminum Labels

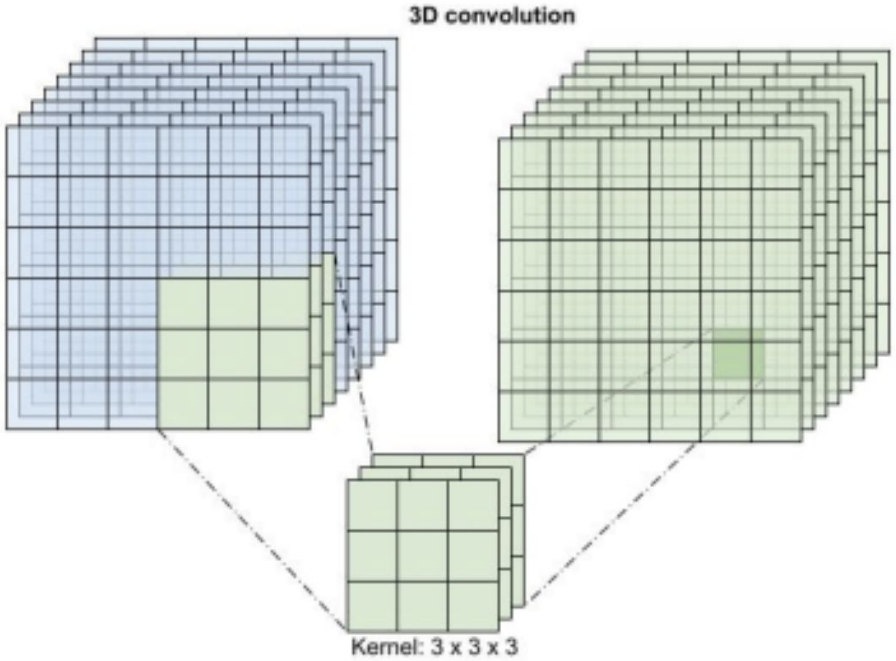
DBSCAN

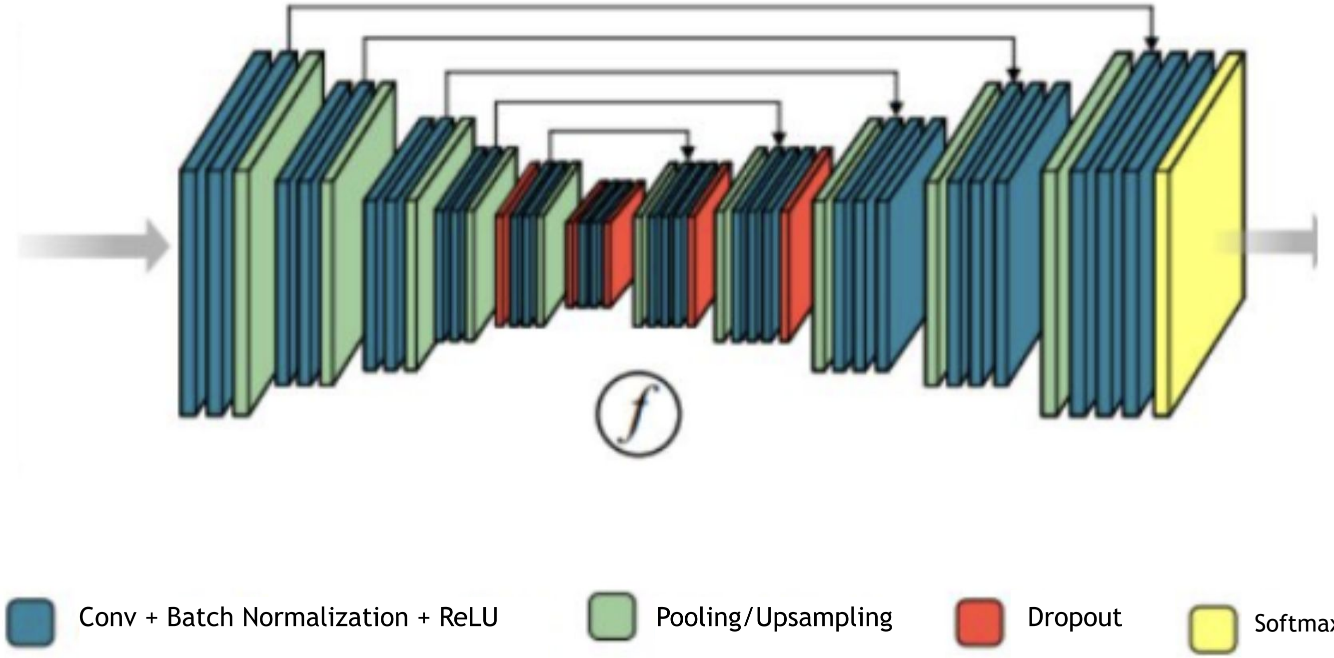




Identification of Aluminum Rings

- Building a neural network
  - Identify a 3D CNN to train and predict aluminum rings
  - General Unet mainly used for image segmentation
    - Fully connected
    - Contraction and expansion paths
    - 3D Unet used for learning dense volumetric segmentation from sparse annotations





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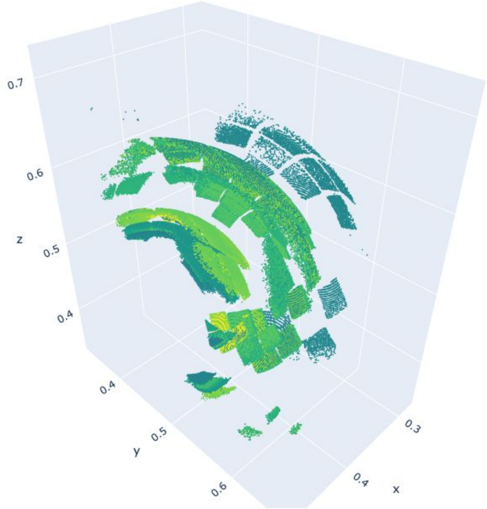
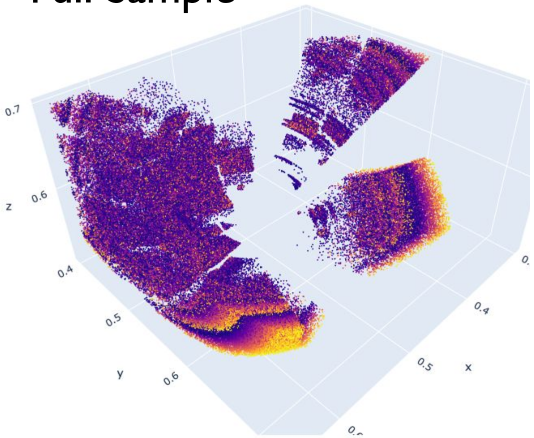
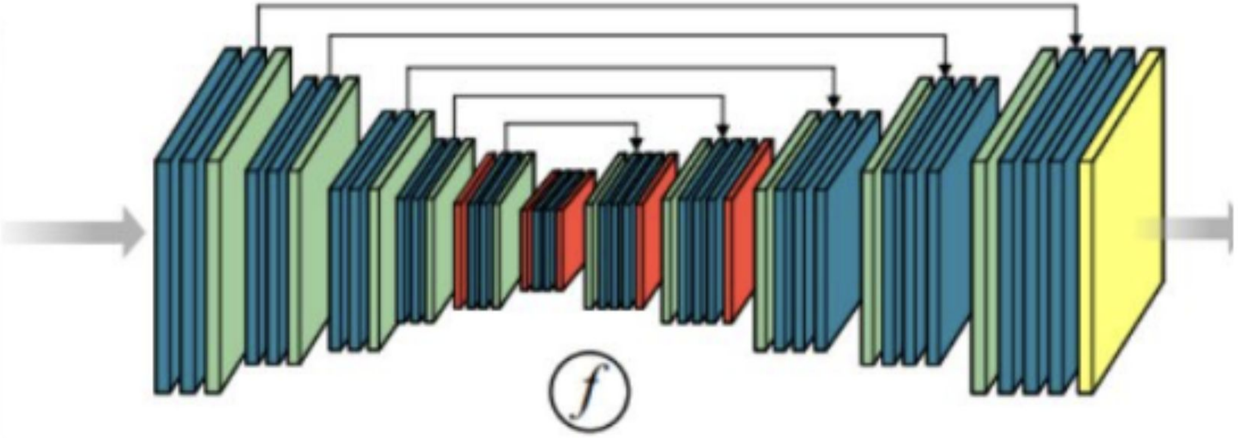
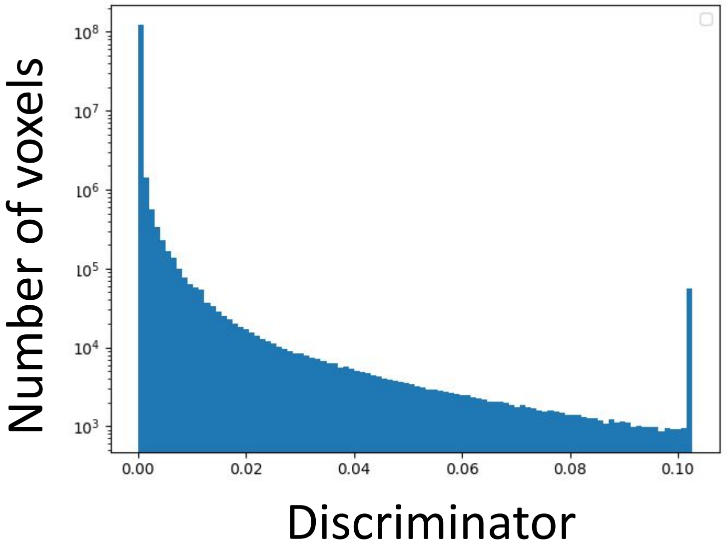
Labelled Rings



Full Sample







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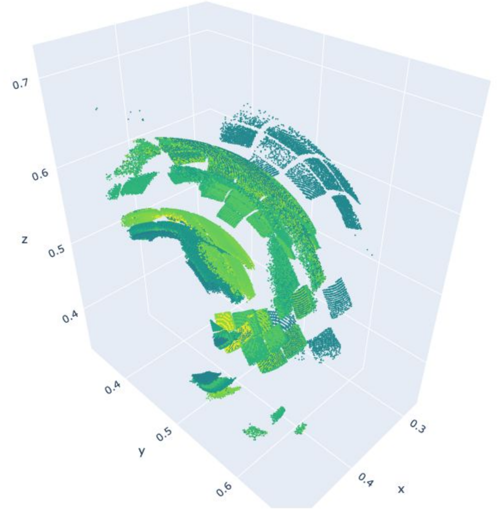

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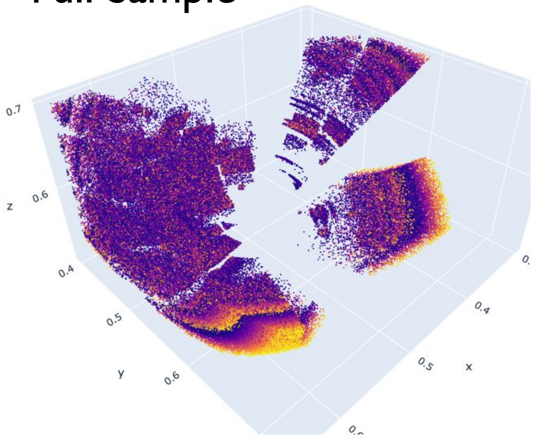
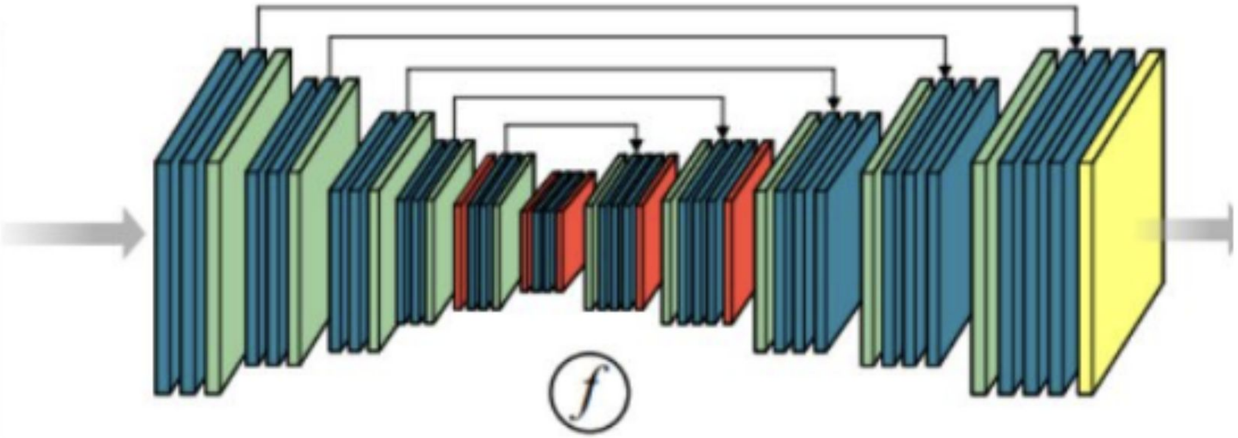
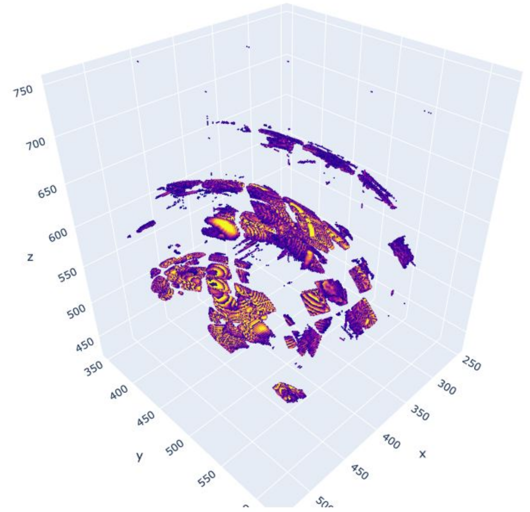


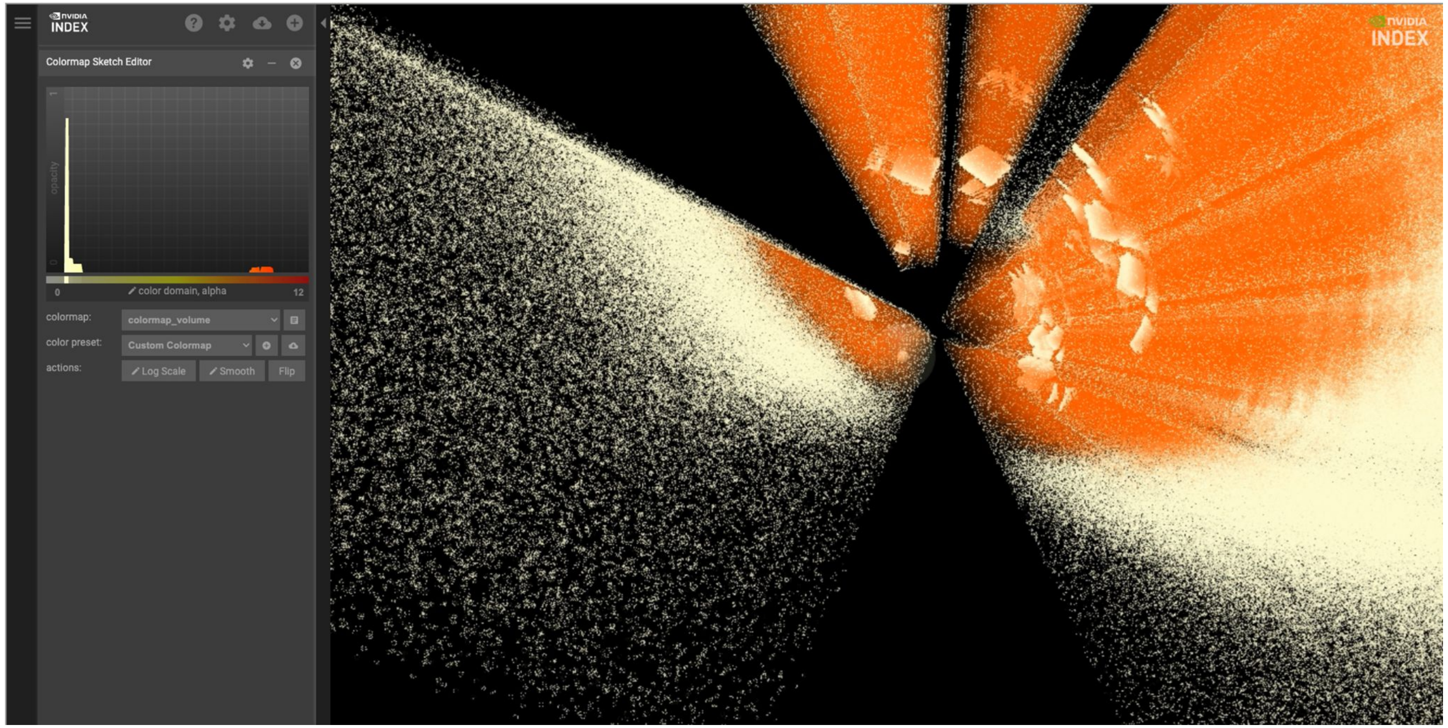


Predicted Rings



NVIDIA's Omniverse/IndeX: Browser-based 3D visualization

- Omniverse / IndeX is an interactive 3D volumetric visualization framework
  - rotate, pan, zoom into large 3D volumes
  - executes remotely on a GPU server
  - streams video to the user's browser
- TOPAZ event data is converted into a voxel database
  - voxels are a regular 3D grid
  - each is colored and/or made transparent based on the number of neutron events within it
  - colors & transparency can be dynamically edited
- The voxel database can be dense or sparse
  - large fraction of voxels are empty, so the sparse data format is very efficient
- Interactive response is robust to WiFi quality
  - even with a poor network connection, the typical delay after a mouse click is $<$ 0.25 s



Summary

- Our goal is to automate data analysis to enable scientific discovery
  - ML + leveraging Mantid
    - faster, better Bragg peak detection
    - deployed on-premises for TOPAZ
  - NVIDIA's Omniverse / IndeX technology
    - interactive 3D viz in your browser – in the control room, or at your home institution
    - an NVIDIA card is required, presently on the floor of the SNS experimental hall
    - deployed on-premises for TOPAZ
  - ML + NVIDIA/IndeX (the work presented here)
    - it is possible to automatically identify an unwanted aluminum signature
    - not yet deployed
  - ML + EPICS controls
    - has been used to automate sample alignment
    - demonstrated for TOPAZ & also at HIFR

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This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0021551.

- This lab-industry collaboration is facilitated by open-source software
  - RadiaSoft has an open source business model
  - Proprietary IndeX technology is free for scientific use, courtesy of NVIDIA
  - broad applications to other neutron beamlines