Interactive Visualization and Automated Analysis of Neutron Scattering Experiments

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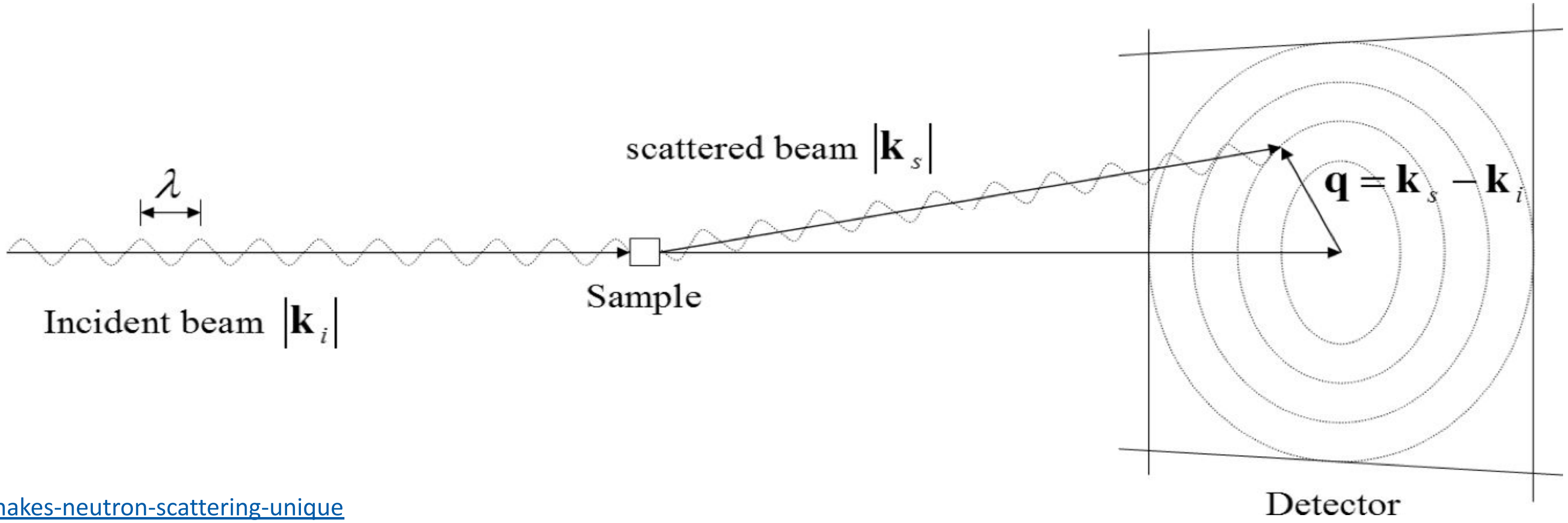
Boulder, Colorado USA | radiasoft.net

Neutron Scattering probes within Materials

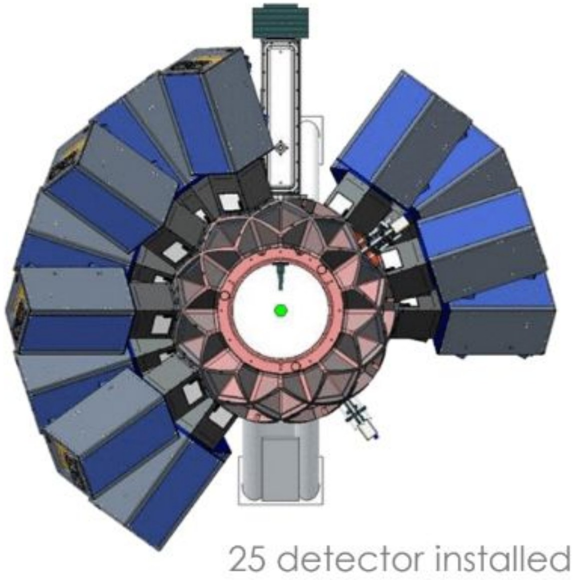
- Why do we shoot particles at things?
  - X-ray scattering probes low-Z materials and are scattered by electrons
  - Electron scattering is great for low-Z materials and is strongly interacting
- Neutrons are weakly scattering!
  - Neutrons will either pass straight through most materials or only single scatter off the atomic nuclei in the material
  - Neutrons can penetrate materials that stop X-rays or electrons
  - Beneficial for studying materials near absolute zero

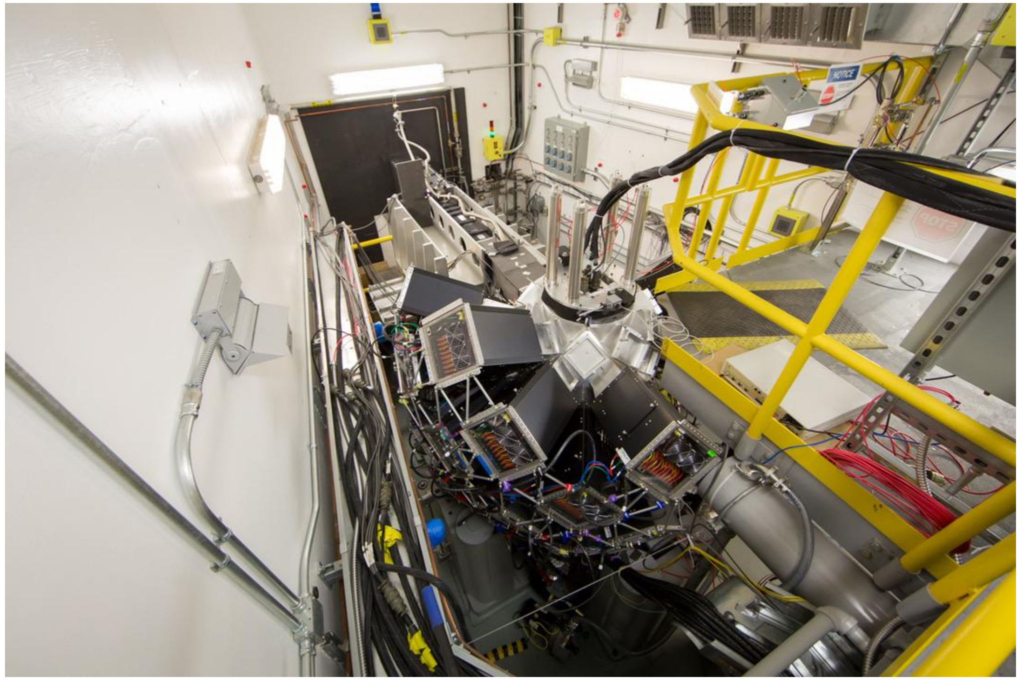


https://www.ornl.gov/blog/what-makes-neutron-scattering-unique

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

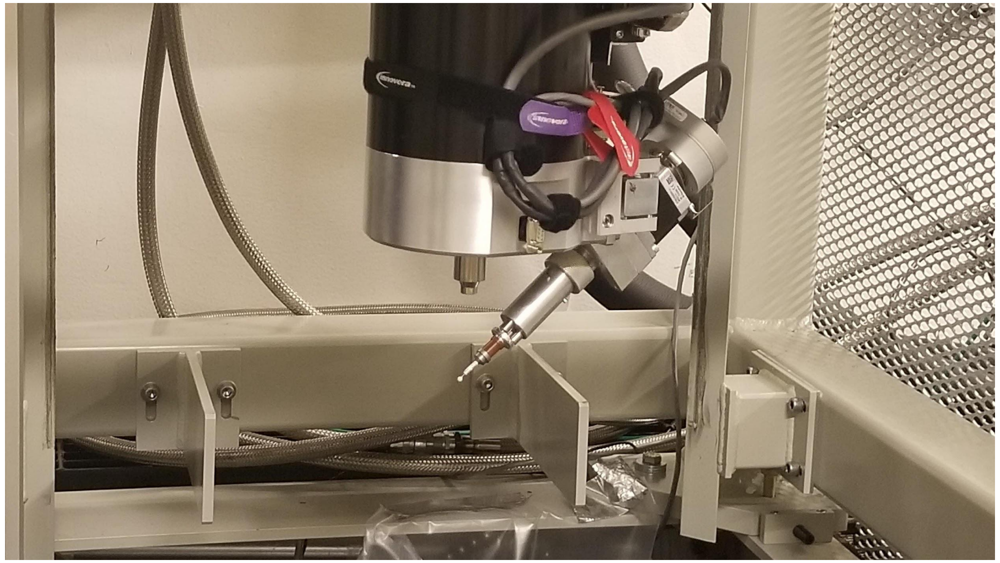


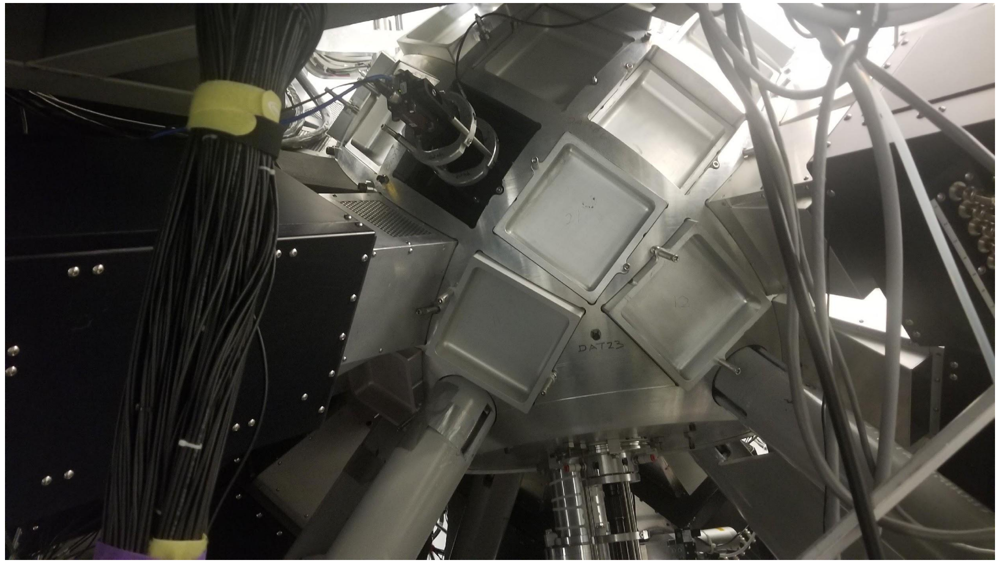


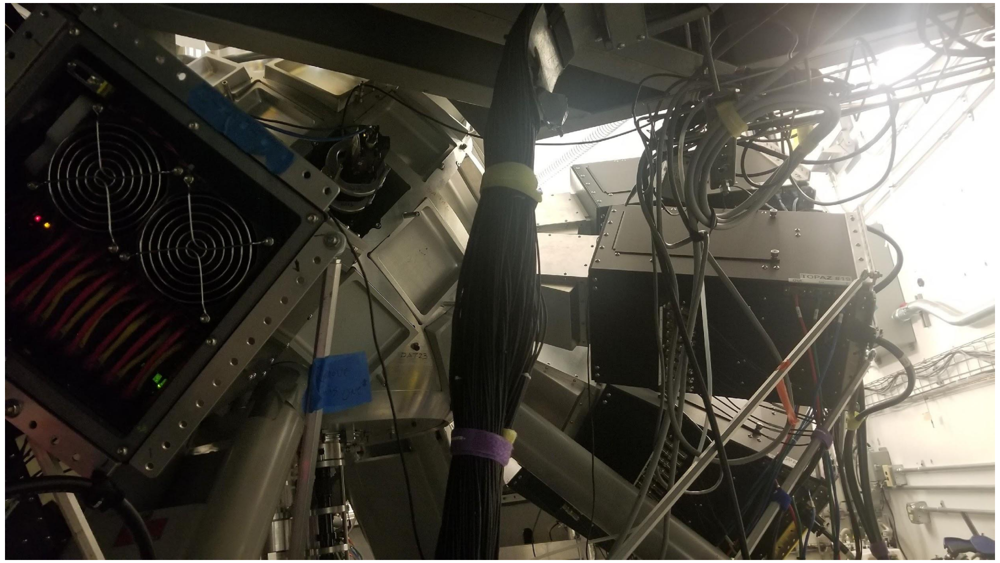
https://neutrons.ornl.gov/topaz

Oak Ridge National Laboratory

TOPAZ Single-crystal Diffractometer

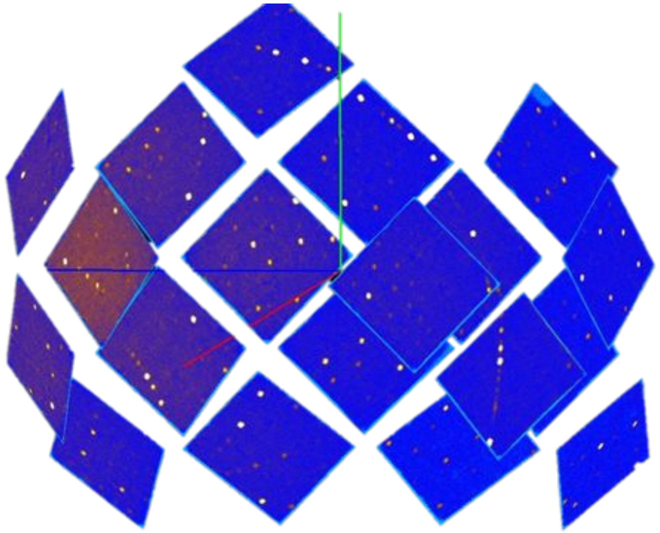






Analysis methods for TOPAZ data

- 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
  - Timescale: 1-2 hours

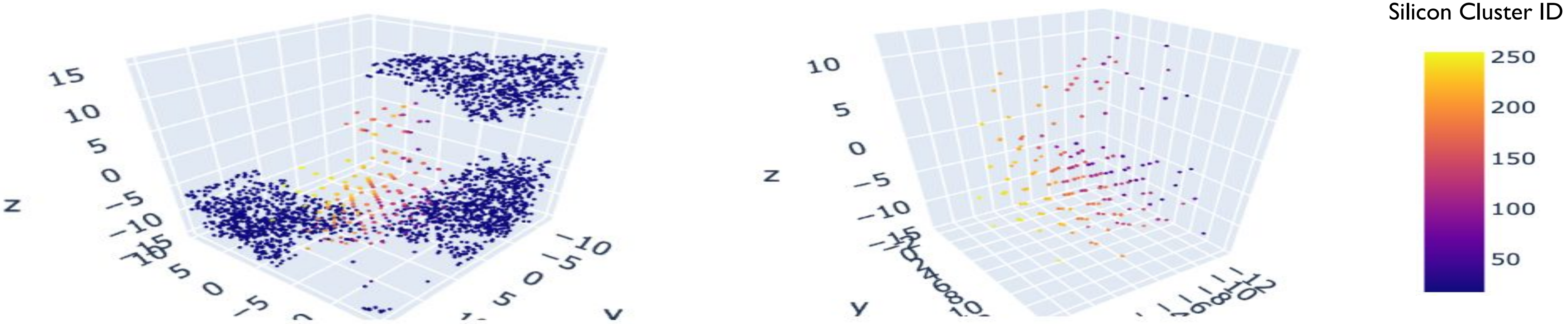


- Working collaboratively to leverage Mantid
  - Machine learning – DBSCAN, U-Nets
  - Automated Bragg peak identification
  - Automated background subtraction
- Also improving the interactivity of the data viz
  - Close collaboration with the NVIDIA IndeX development team (Berlin)
- Working towards combination of 3D viz and automated analysis

https://www.mantidproject.org/

Analysis of Scattering Data for a Single Silicon Crystal

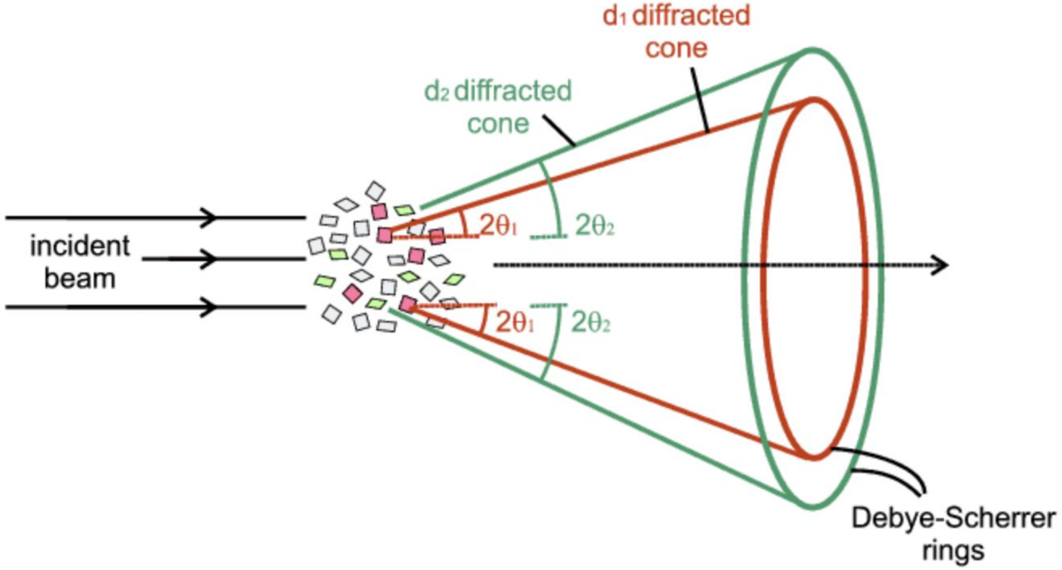
- Preprocessing the data
  - Measurements of the particles in momentum space
  - Looking for pockets of constructive interference
  - Measurements projected onto a 3D mesh
- DBSCAN is a density based clustering algorithm
  - Can identify oblong clusters and attribute data to noise if it doesn't match anything
  - Sparse background can be removed easily
  - Provides real time identification of Bragg peaks
  - Agrees with Mantid reconstruction of Bragg peaks

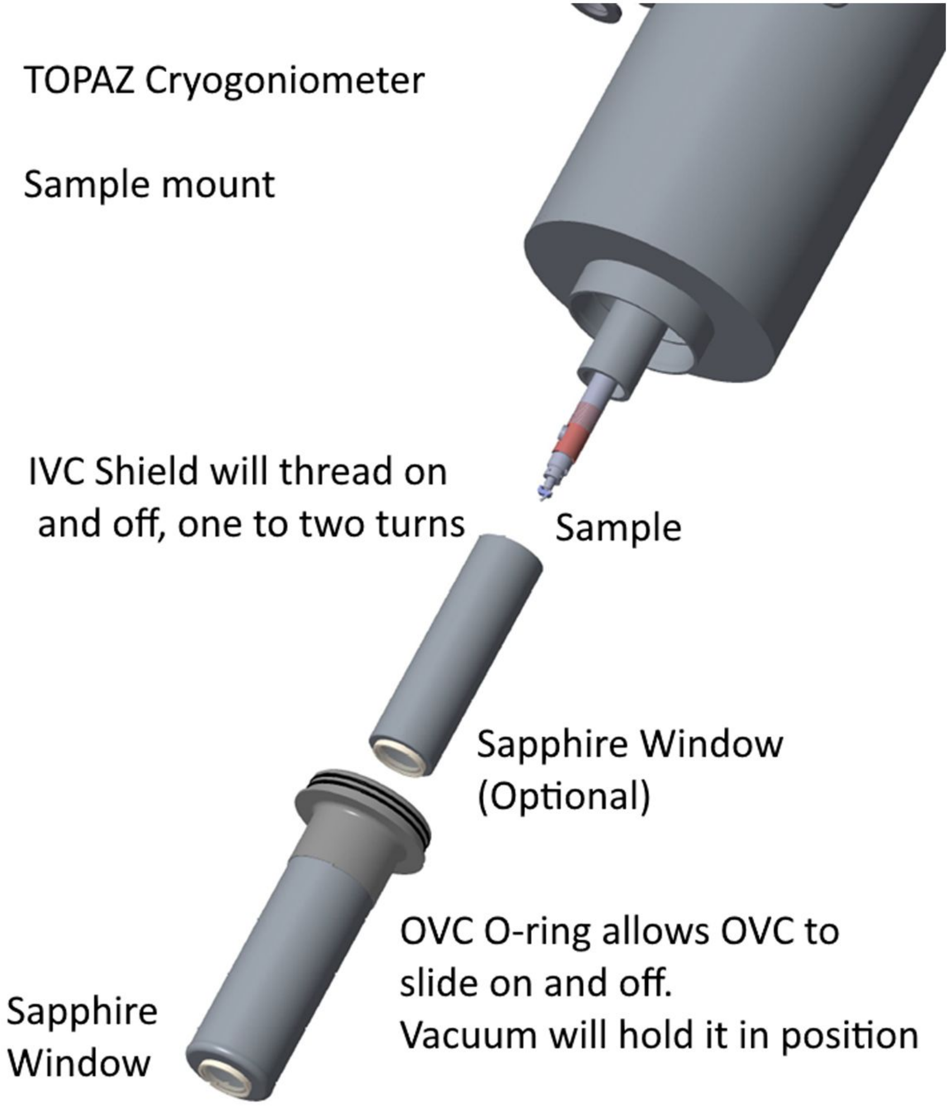


https://scikit-learn.org/stable/modules/generated/sklearn.cluster.DBSCAN.html#sklearn.cluster.DBSCAN

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



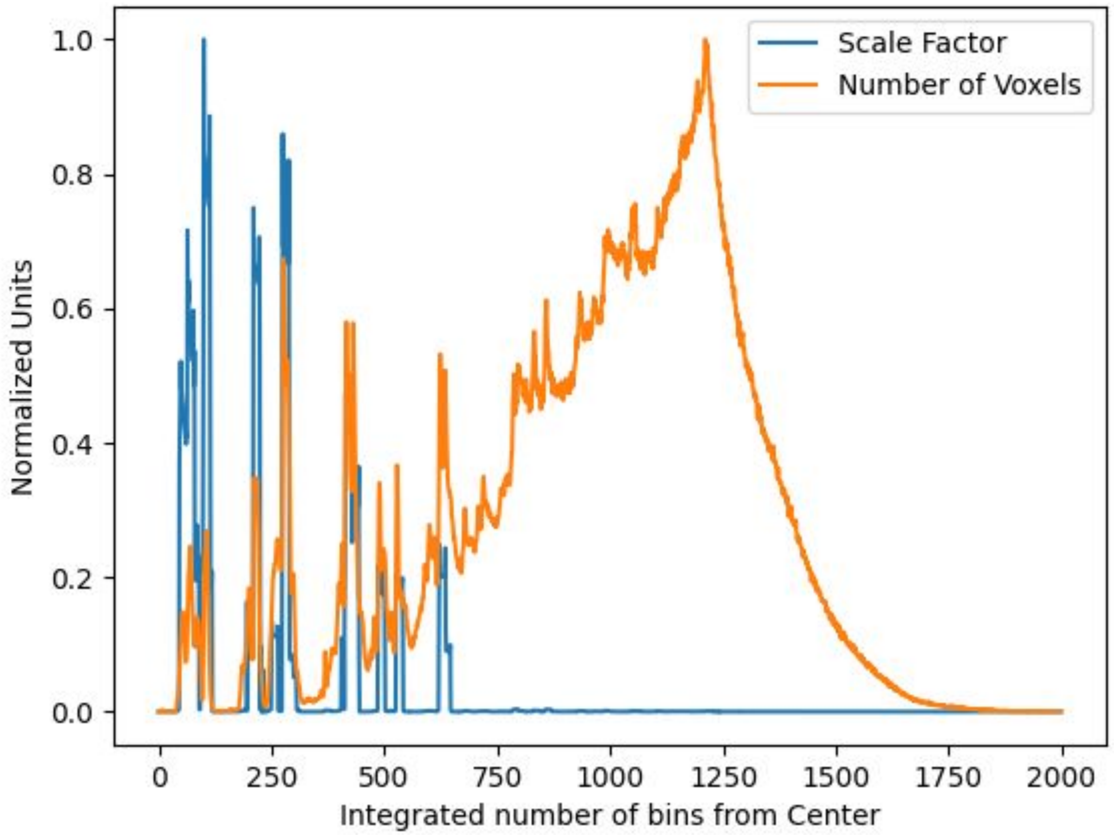


Identify Accurate Ground Truths

- 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

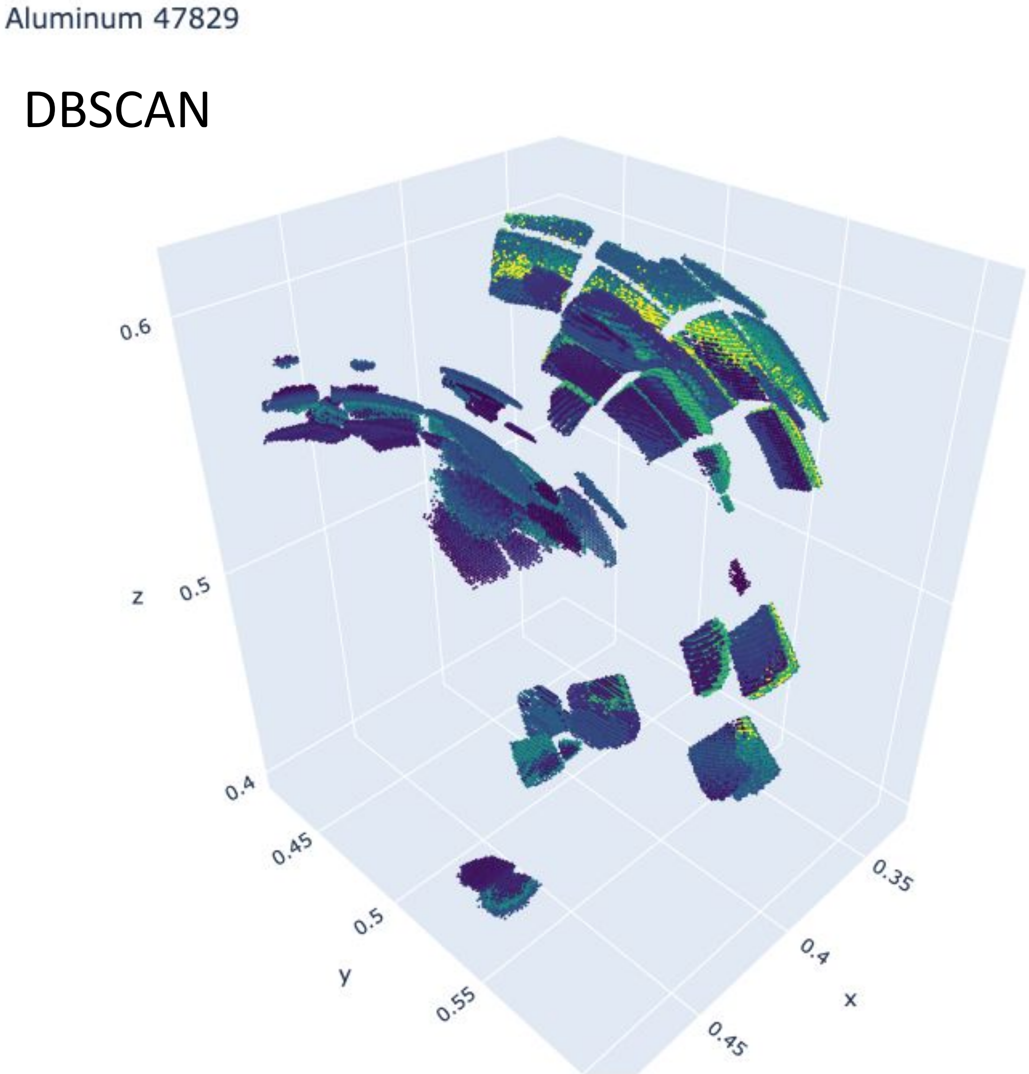
$$SF_i = max(\sum_{i}^{N+i} \nabla w_i)$$

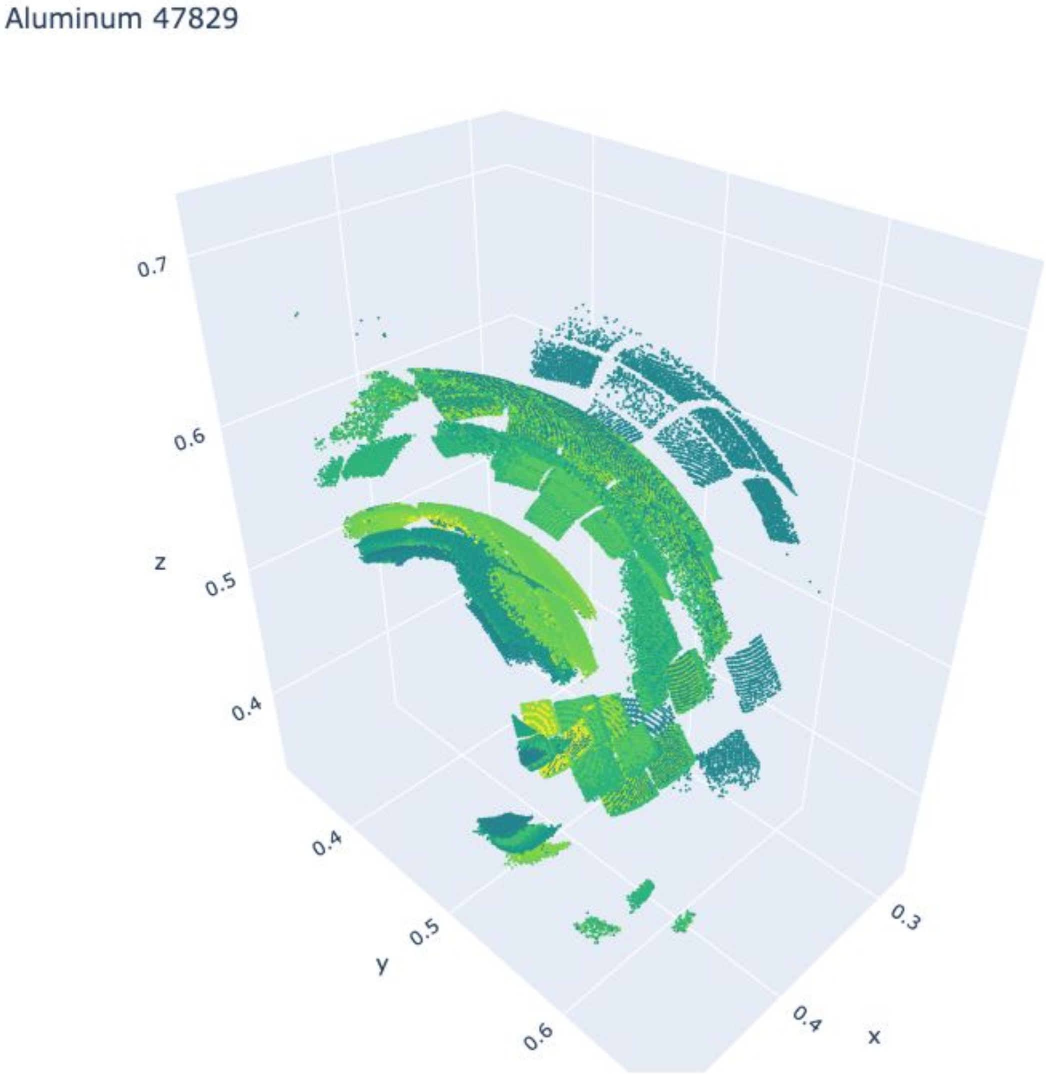
- How do these two methods compare?



Aluminum Labels

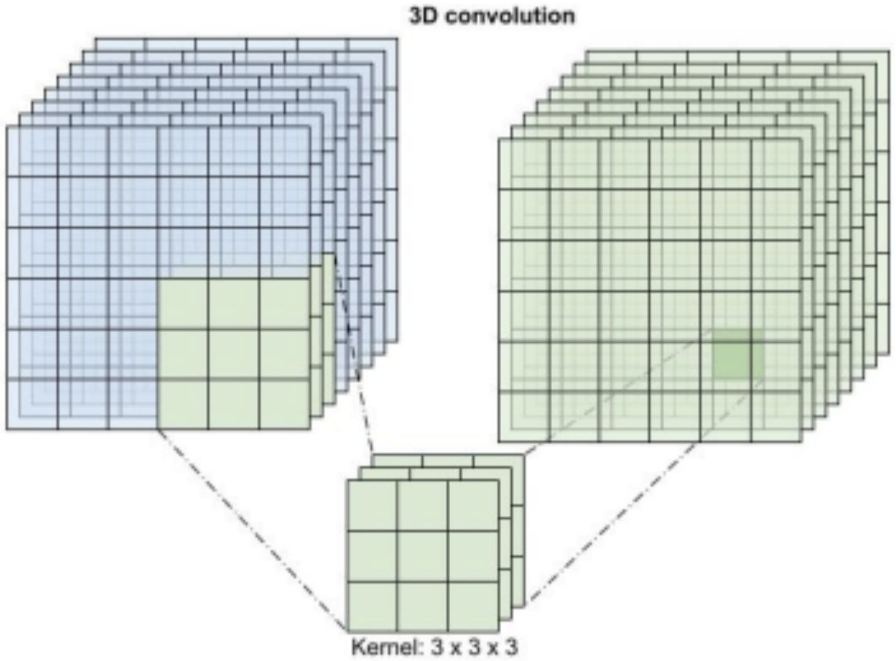
DBSCAN

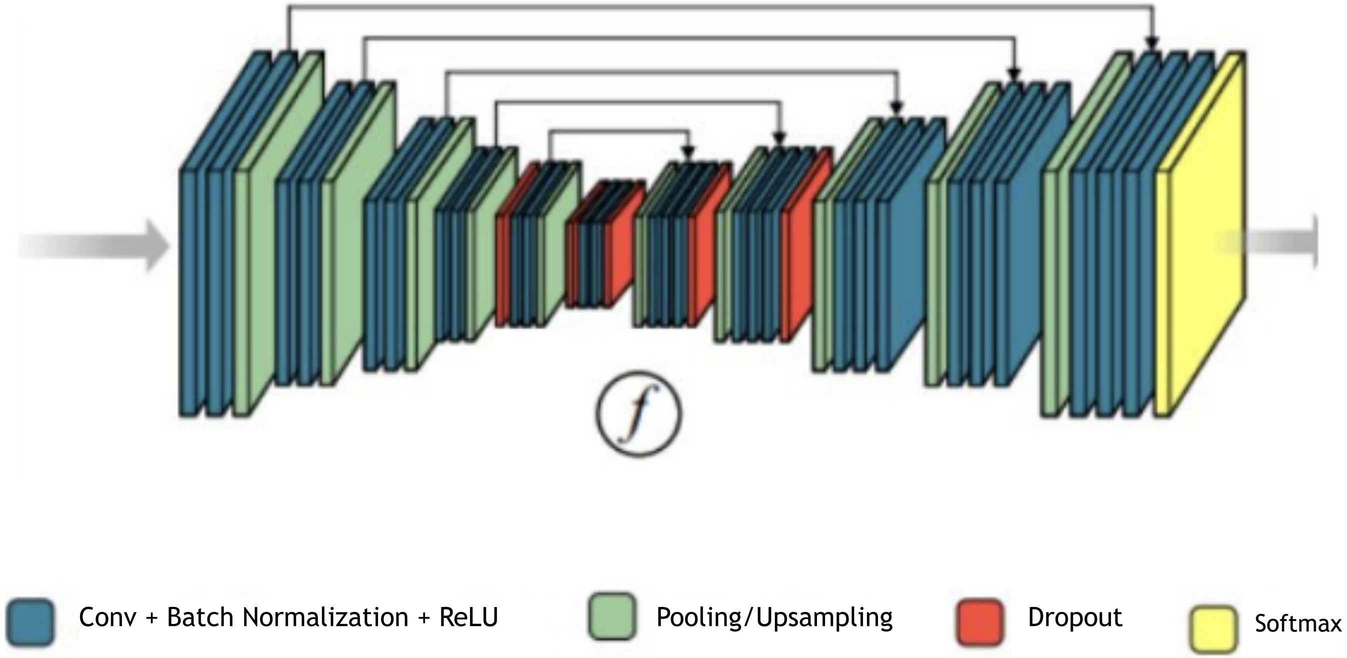




Identification of Aluminum Rings

- 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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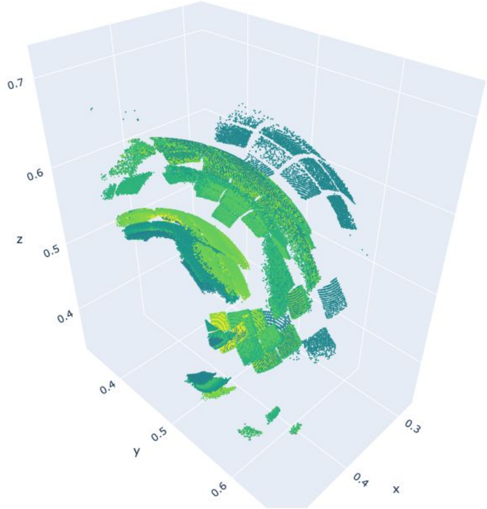
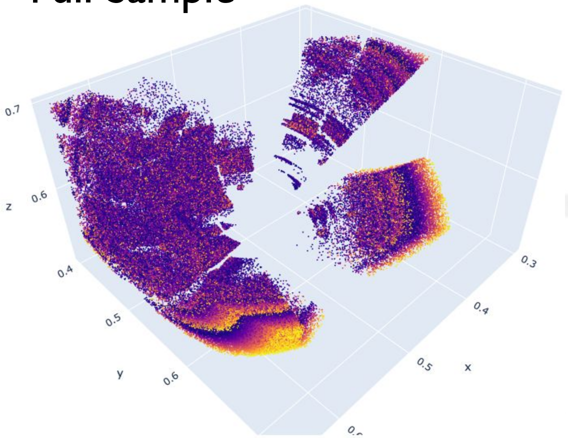
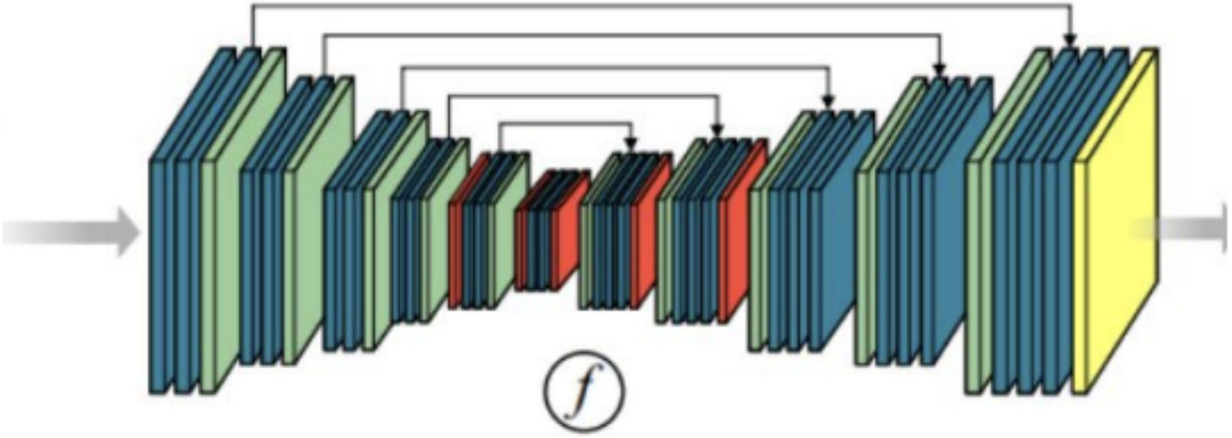
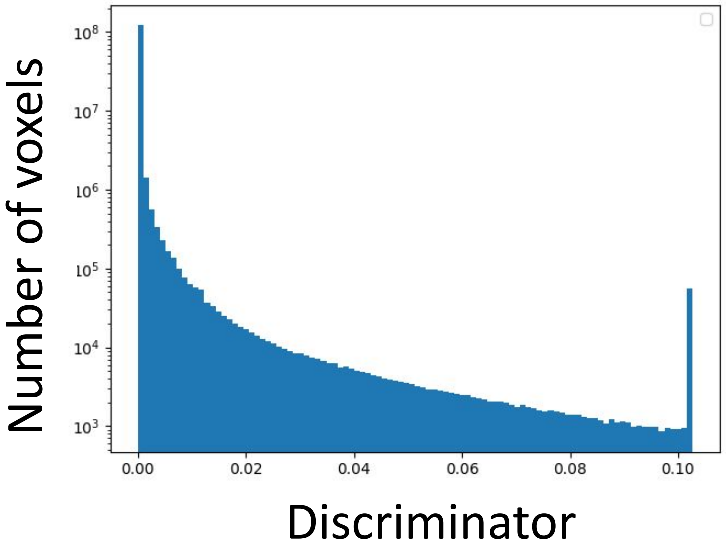
Labelled Rings



Full Sample







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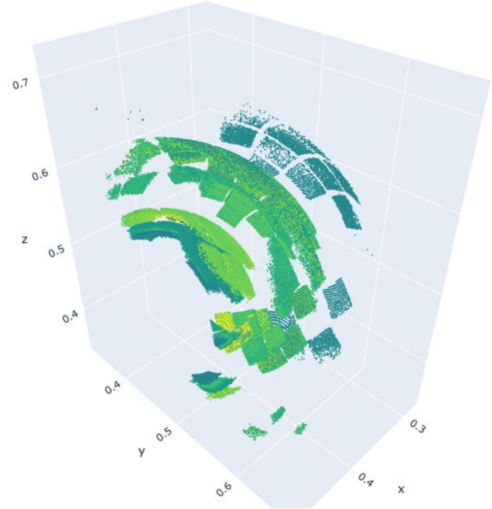

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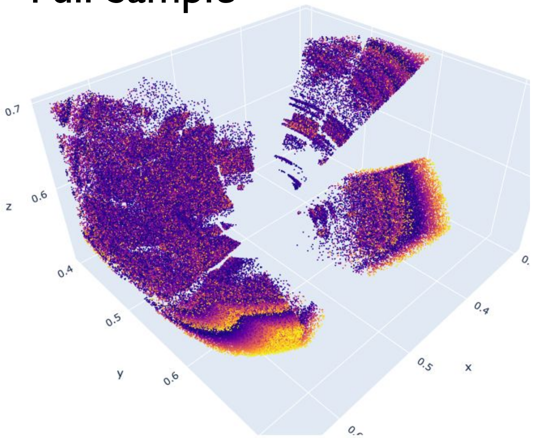
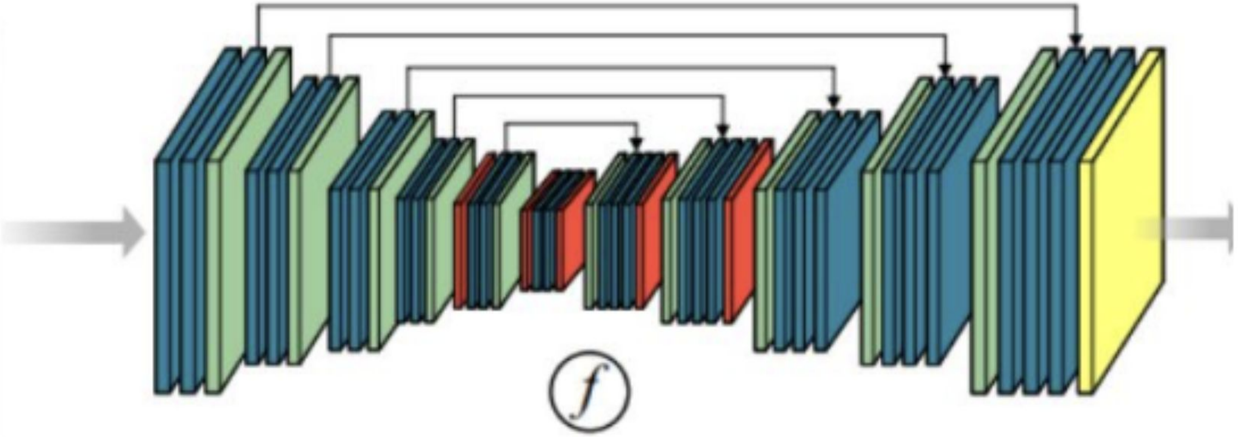
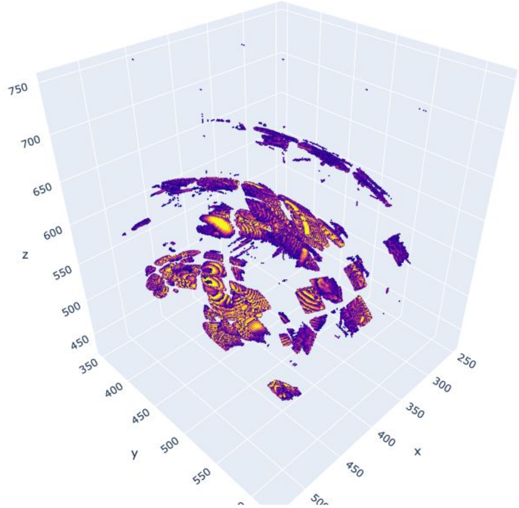
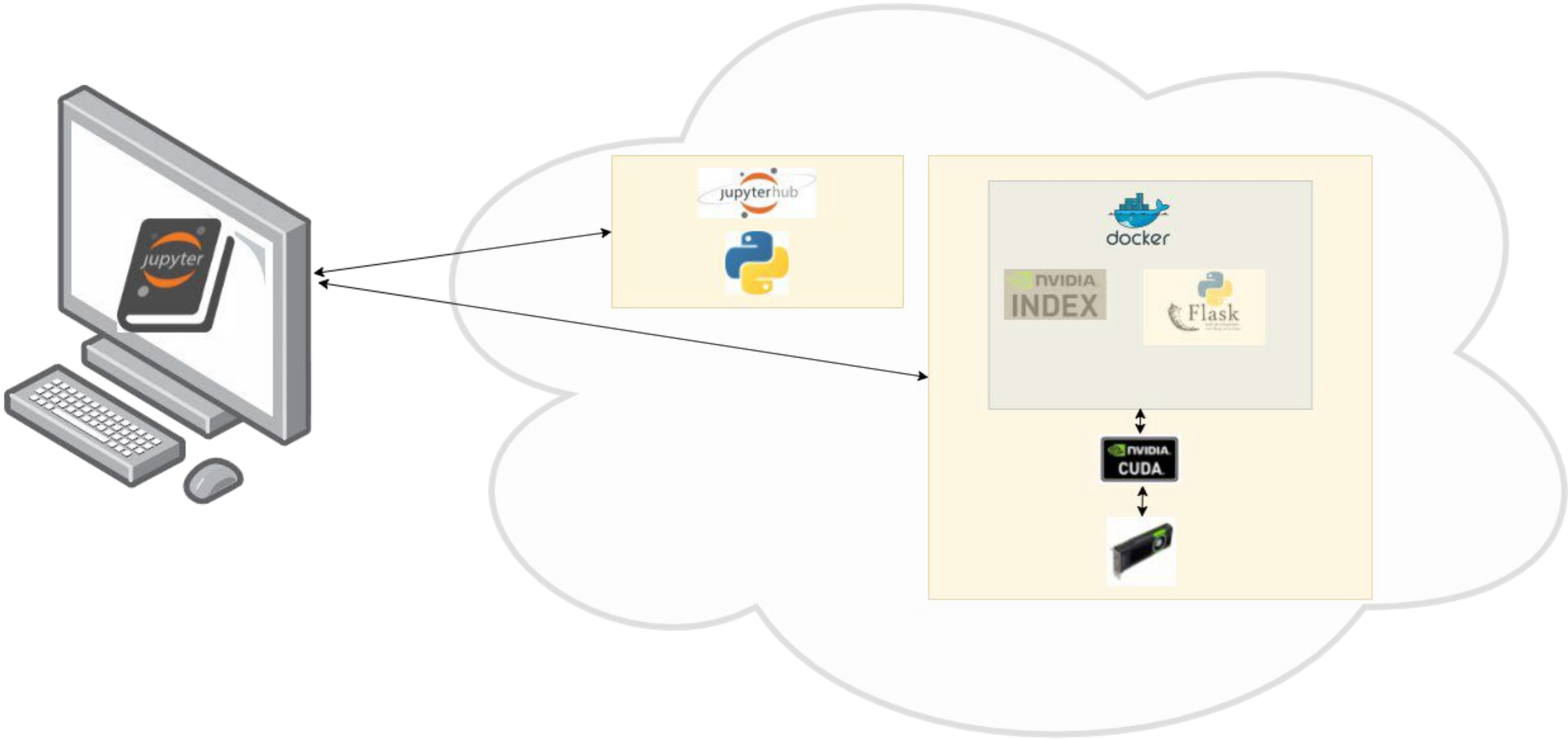




Predicted Rings

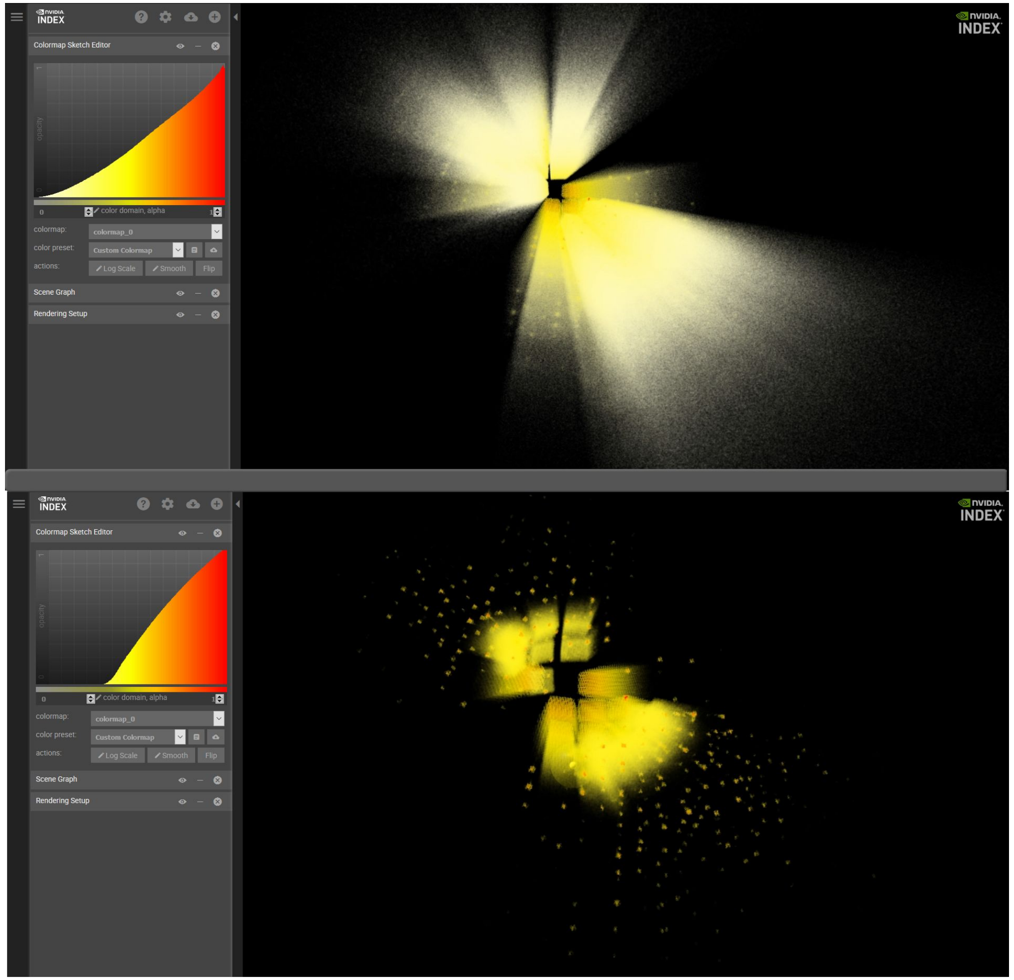


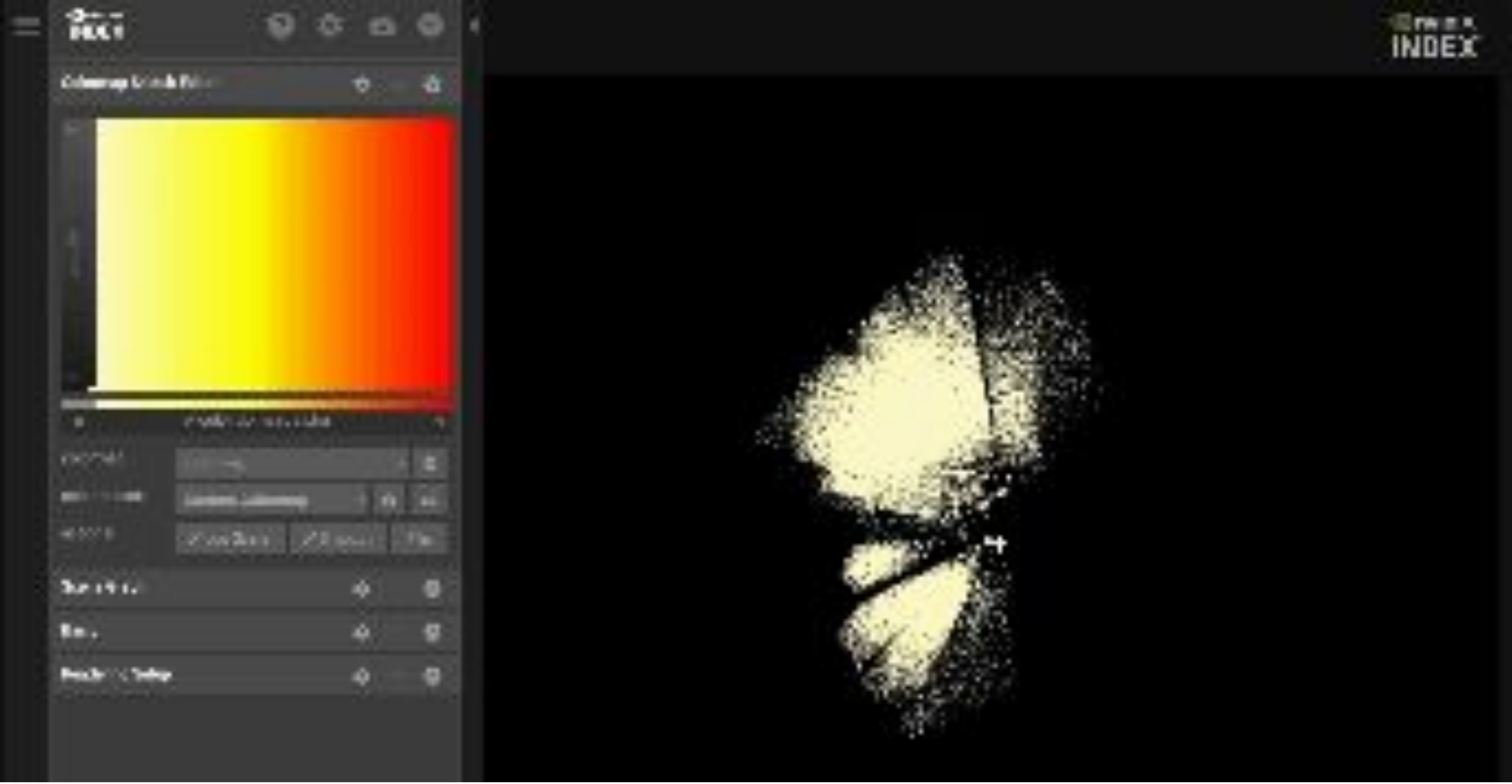
System Architecture, with JupyterHub Interface



NVIDIA's IndeX: Browser-based 3D visualization

- IndeX: 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

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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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  - C. Hoffman, B. Vacaliuc, J. Taylor, J. Kohl, Z. Morgan, A. Savici,
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