

3D Visualization and Analysis of Neutron Scattering Data in the Control Room

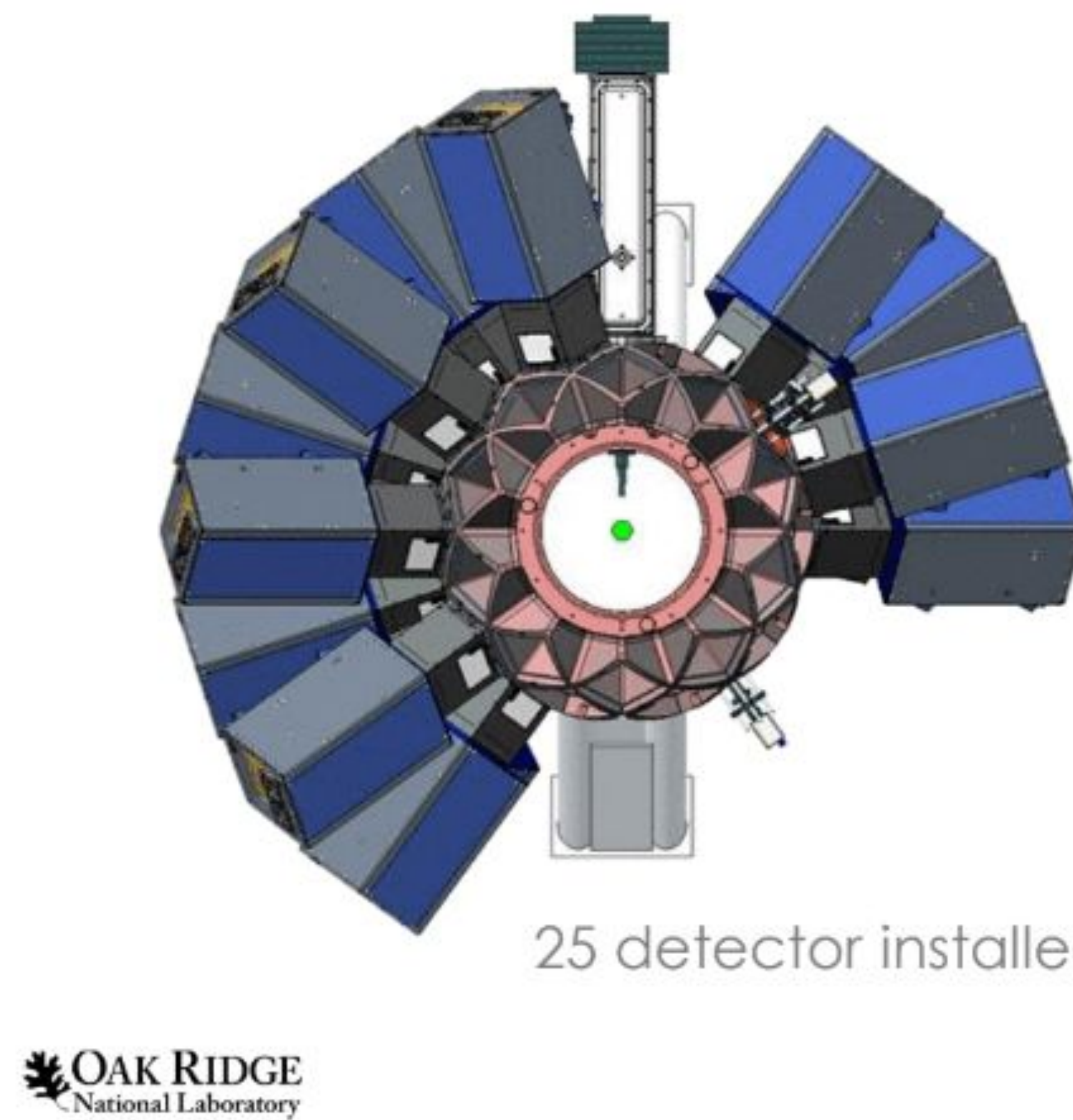
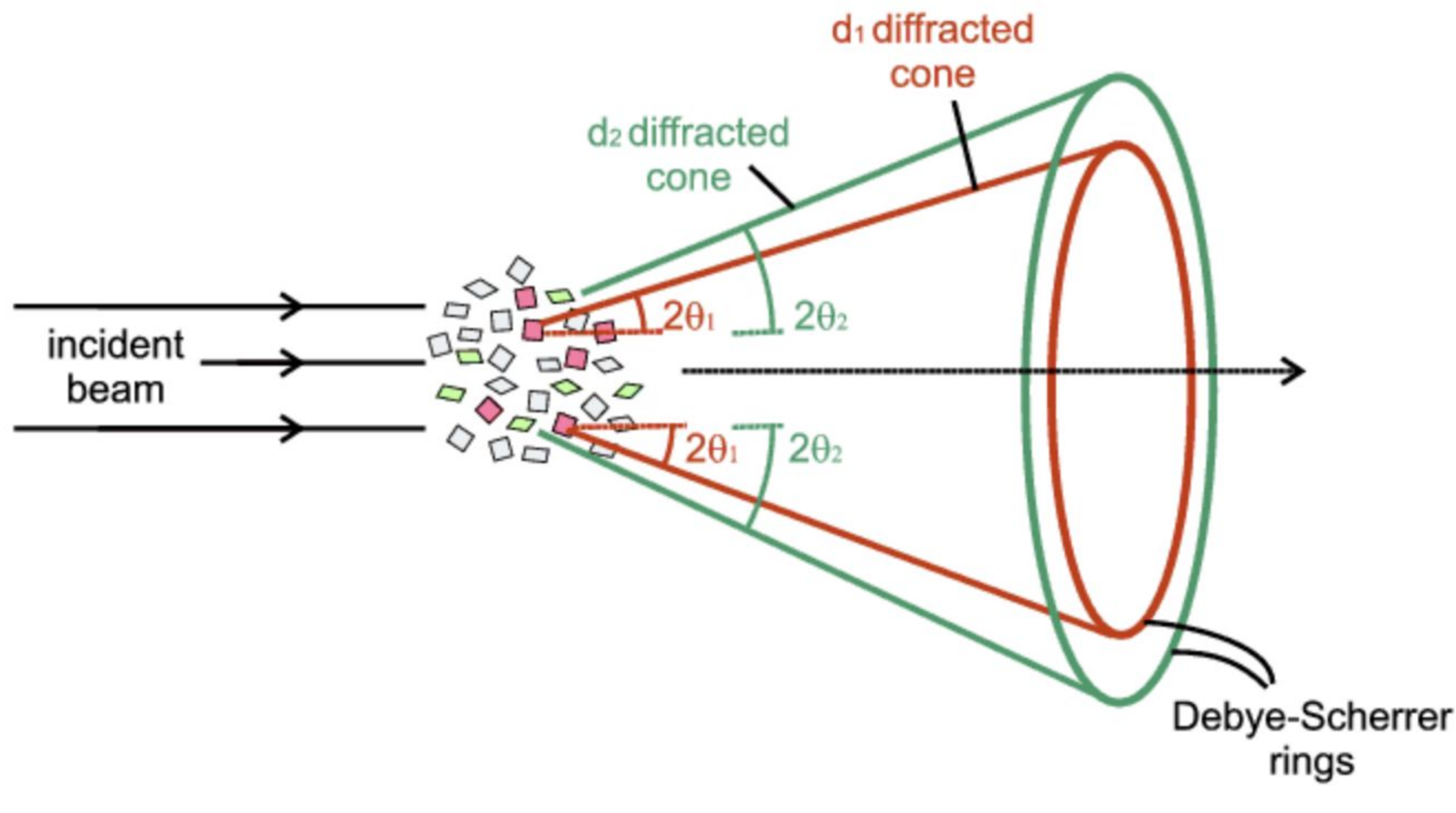
Matthew Kilpatrick*, David Bruhwiler, Evan Carlin, Ben Gur, Robert Nagler (RadiSoft LLC, Boulder, USA);
Christina Hoffmann, Zachary Morgan, Andrei T Savici, Matthew Tucker, Bogdan Vacaliuc (ORNL, Oak Ridge, USA);
Alexander Kuhn, Jörg Mensmann, Peter Messmer, Marc Nienhaus, Steffen Roemer, Dragos Tatulea (NVIDIA, Berlin, Germany)
*kilpatrick@radiasoft.net



Background

- TOPAZ instrument [1] at the Spallation Neutron Source at Oak Ridge National Laboratory

- Aluminum casing used to cool samples during experiments
- Randomly oriented crystals cause spherical peaks in measured data
- Each pair of planes creates structured background



TOPAZ Cryogoniometer

Sample mount

IVC Shield will thread on and off, one to two turns

Sample

Sapphire Window (Optional)

Sapphire Window

OVC O-ring allows OVC to slide on and off. Vacuum will hold it in position

Structured Background Removal and Visualization



- Structured Background at TOPAZ

- Spherical background (rings) caused by detector setup
- Due to differences between runs the distribution cannot be predicted
- Typically centered around origin in reciprocal space

- Identify Accurate Ground Truths

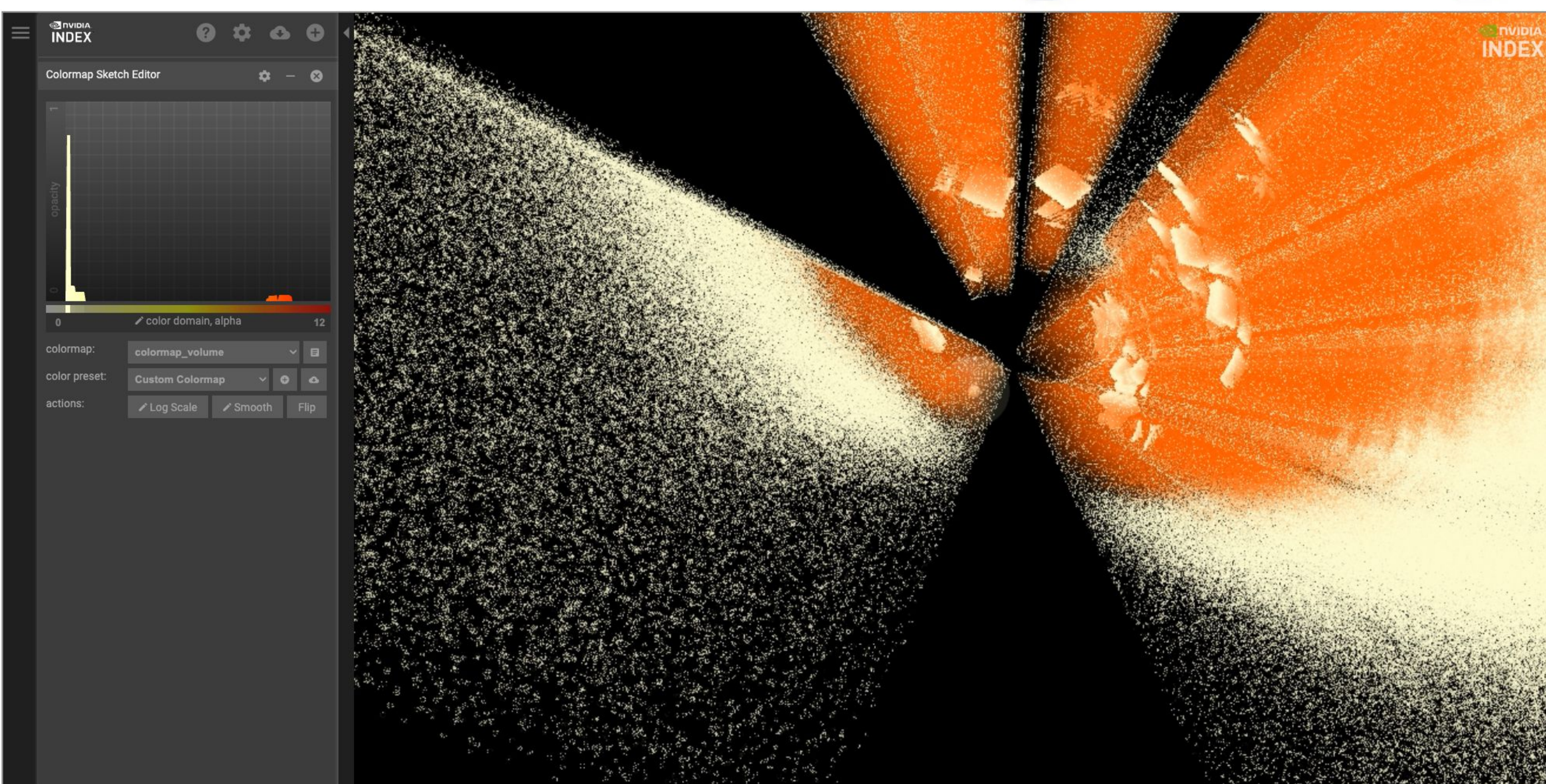
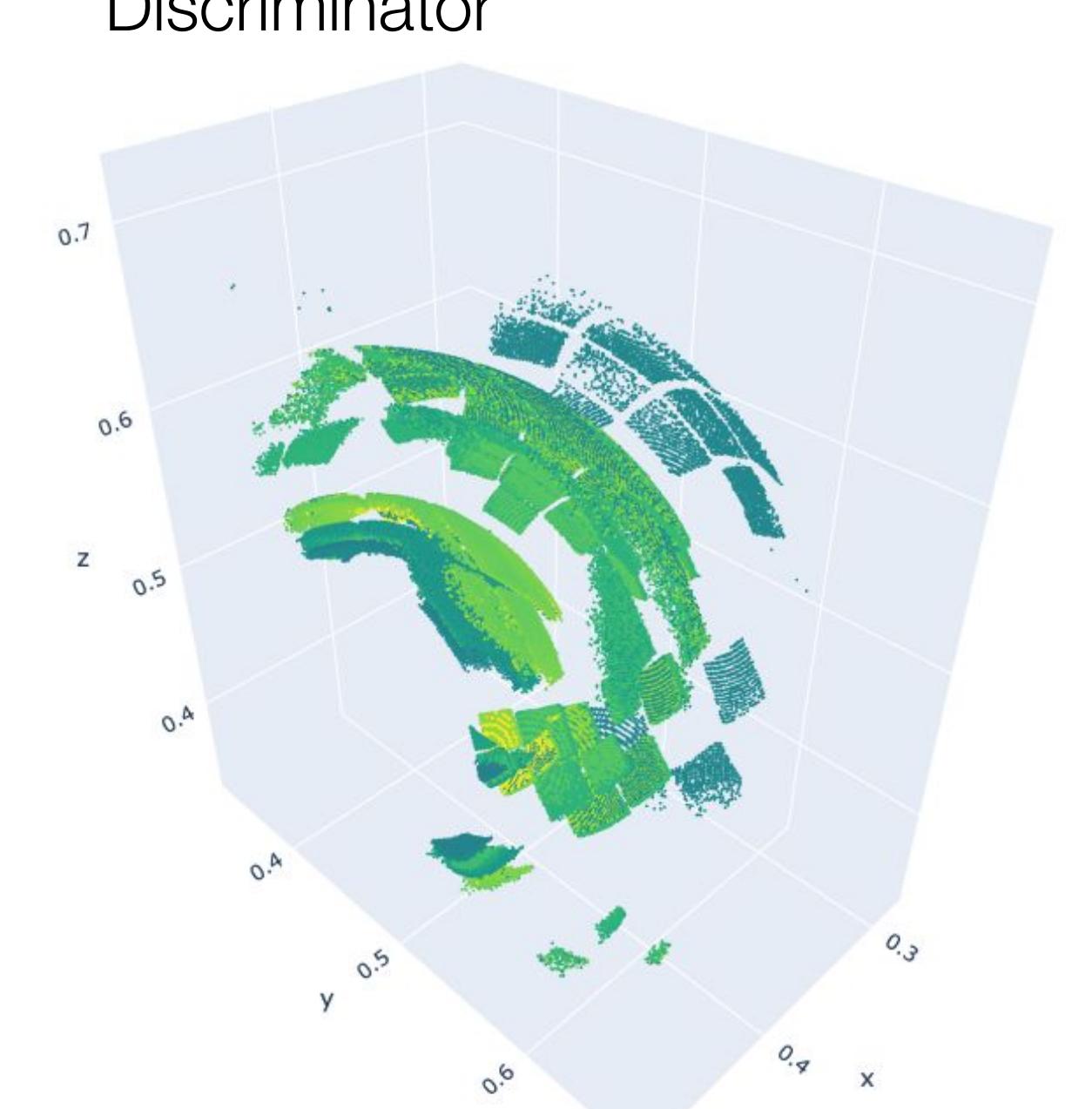
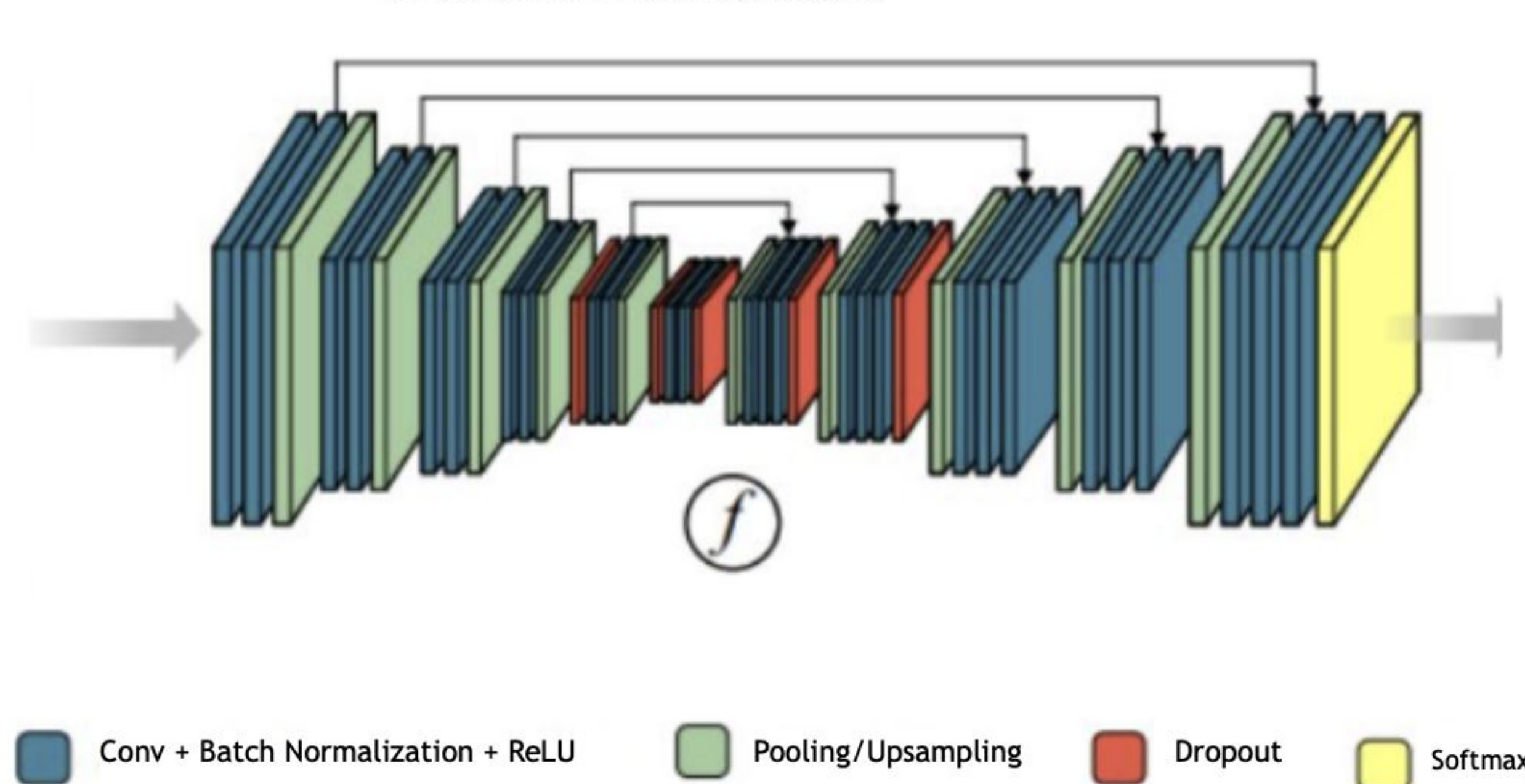
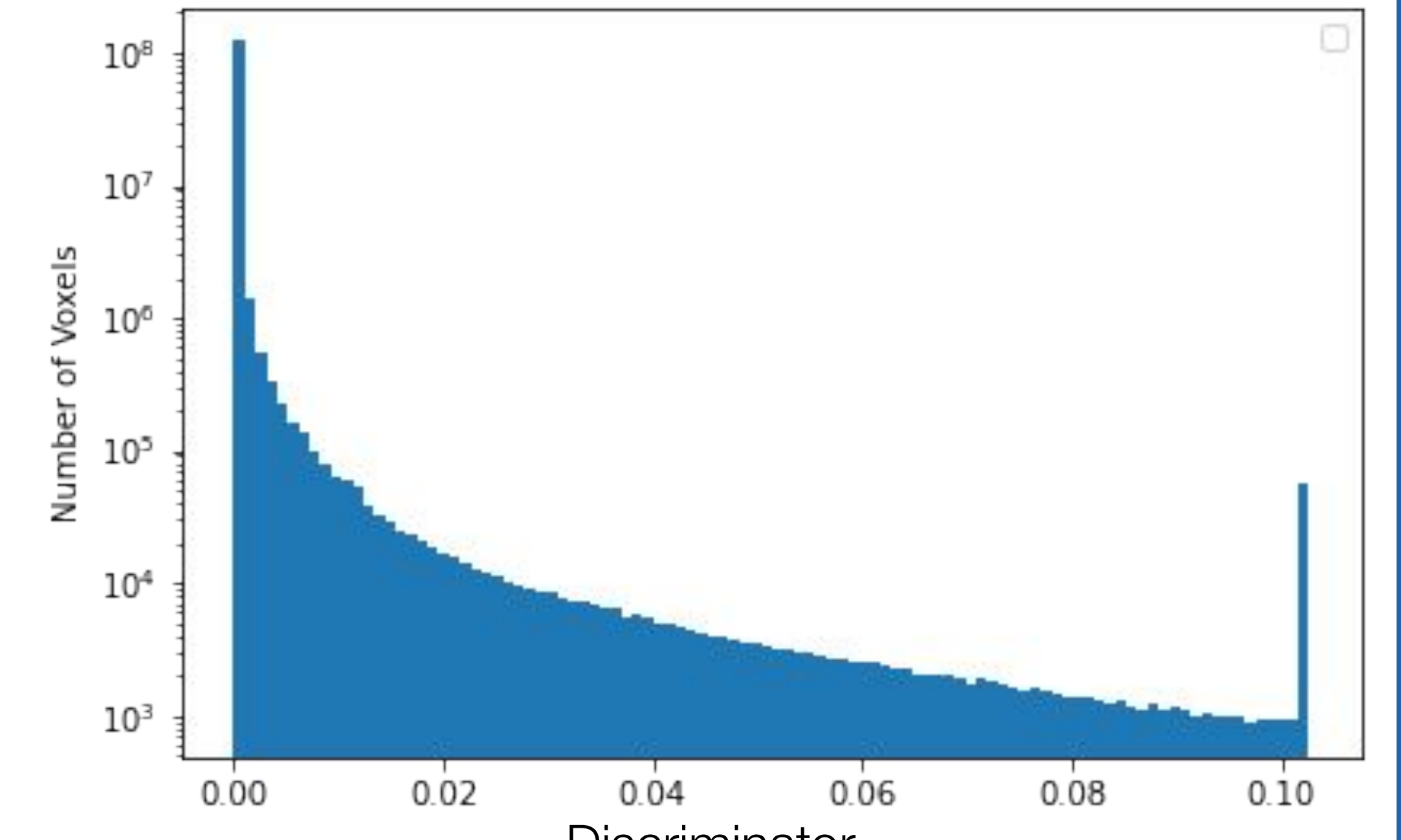
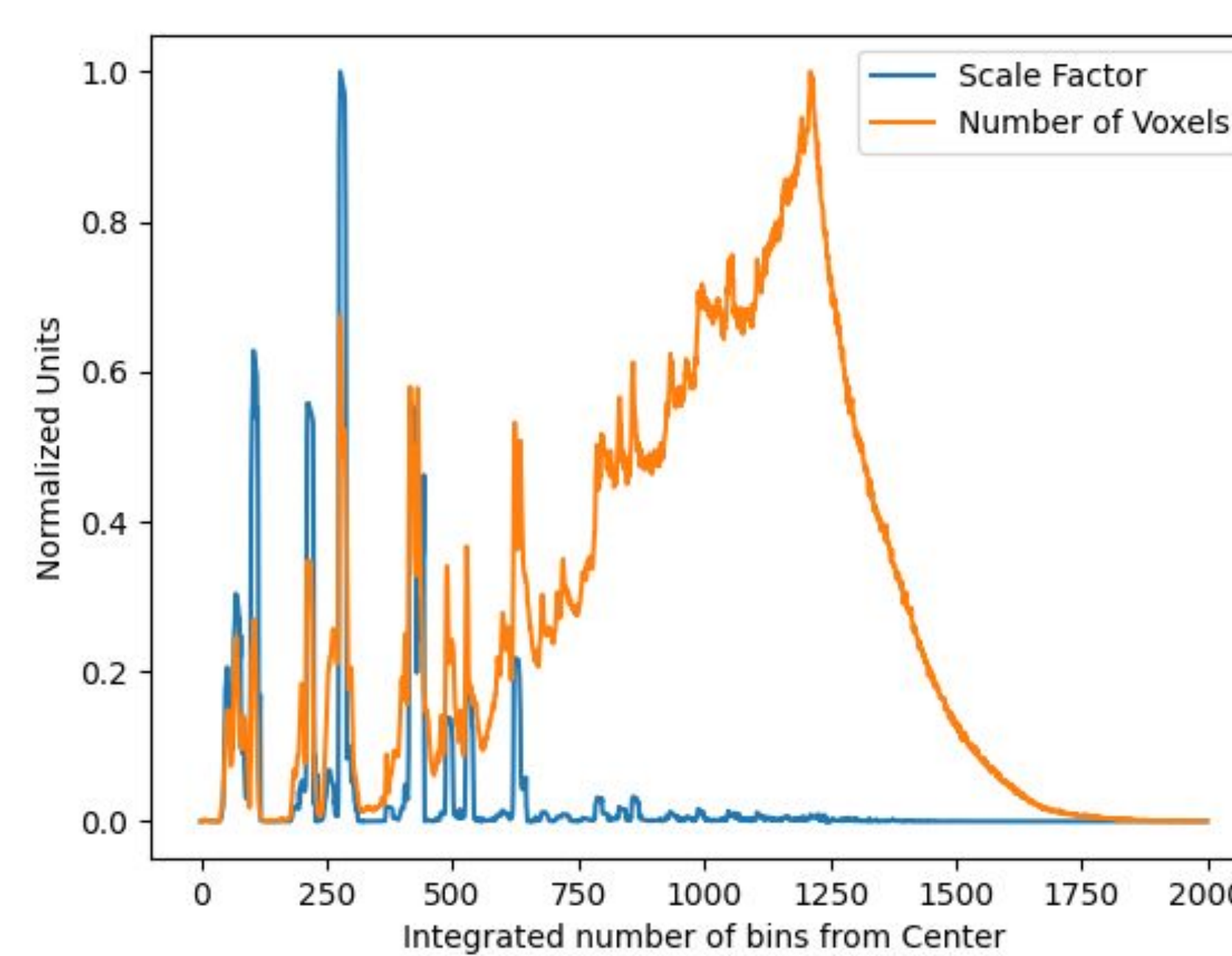
- Aluminum rings are monochromatic in neutron intensity
- Variance in distribution means we have no ground truth label for datasets

- Clustering and Scale Factors

- Develop a scale factor to prioritize Aluminum rings centered around origin
- Scale factor is directly input in DBSCAN to provide a ground truth for training a 3D U-net

- 3D U-net Architecture

- Fully connected network used for learning dense volumetric segmentation
- Input datasets are 1000^3 which overloads a GPU easily
- Input datasets are sliced into 100^3 for training and evaluation
- Prediction provides discriminator for each voxel in a dataset
- Prediction time is approx. 1 second



- NVIDIA Omniverse 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 Omniverse

- Docker based deployment
- Interactively view many GB of neutron single-crystal diffraction data.
- TOPAZ regular 3D grid is easily integrated into the visualization
- Sparse representation is easily updated during streaming

- Real Time Analysis

- Data can be streamed from the experiment and visualized
- Voxels identified as background can be dynamically removed
- Bragg peak analysis is interactively displayed to the operator
- Interactive feedback provides an efficient analysis tool for optimized use and control of the TOPAZ detector

References

1. L. Coates et al., Rev. Sci. Instrum. 89, 092802 (2018). doi:10.1063/1.5030896
2. K. Bruhwiler et al., IPAC Proceedings, TUPAB413 (2021), <https://accelconf.web.cern.ch/ipac2021/papers/tupab413.pdf>
3. The IndeX home page, <https://developer.nvidia.com/nvidia-index>



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