



Interactive Automated Bragg Peak Identification with 3D Neutron Scattering Data

Matthew Kilpatrick*, David Bruhwiler, Evan Carlin, Ben Gur, Robert Nagler (RadiaSoft 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

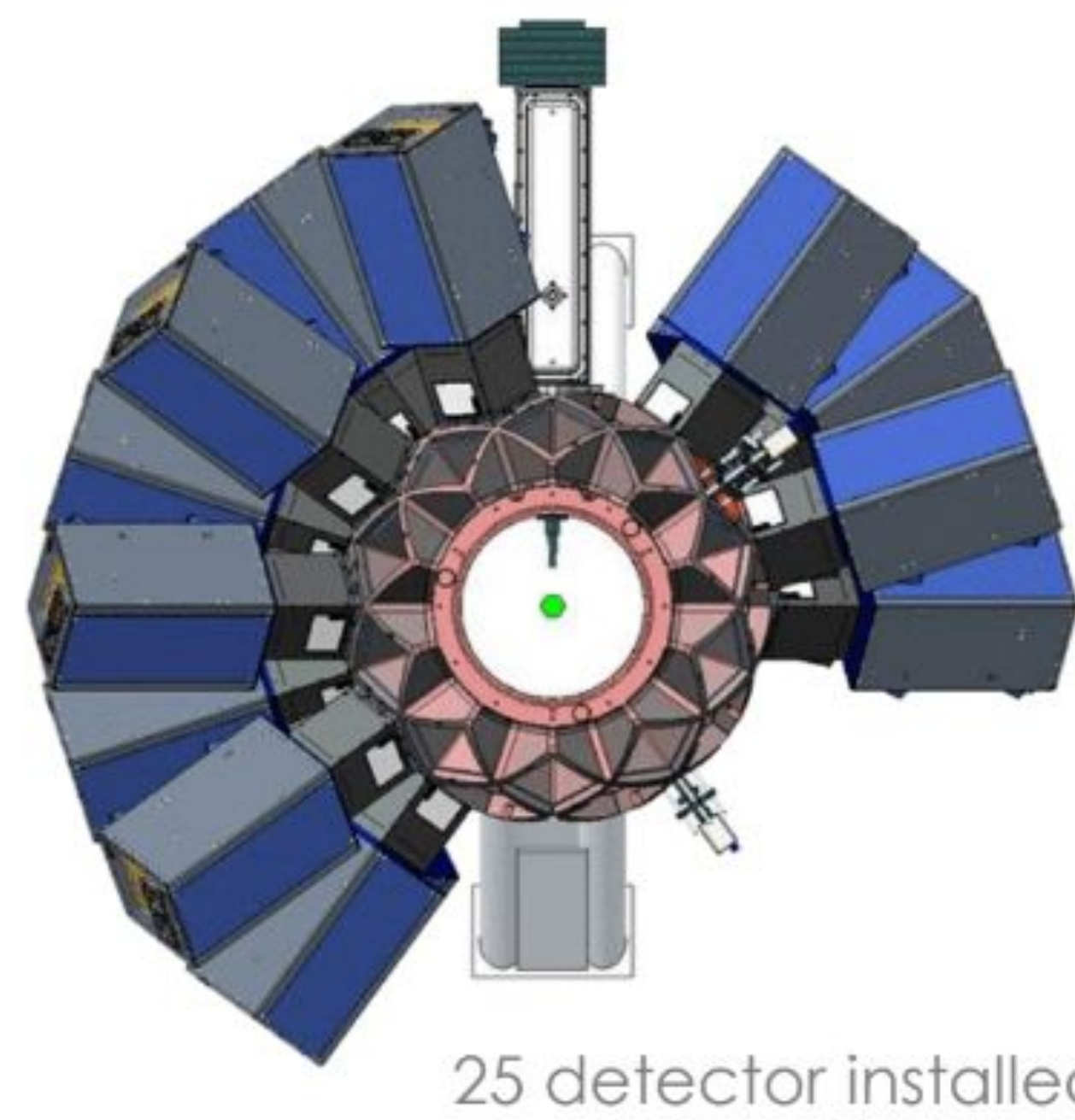


Summary

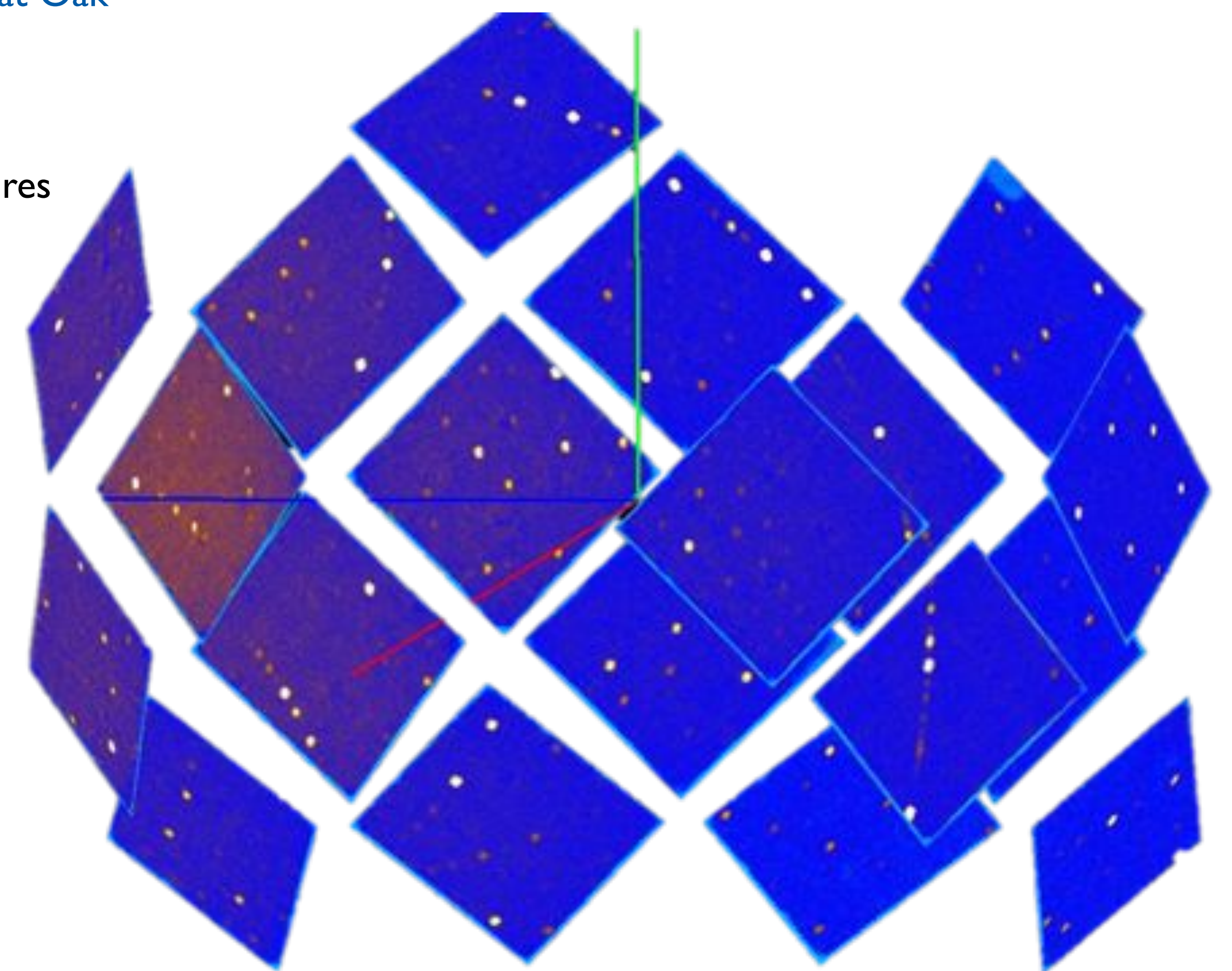
- **Fast, interactive 3D rendering of reciprocal space**
 - In your browser via NVIDIA's IndeX technology
- **Automated identification of Bragg peaks**
 - DBSCAN clustering distinguishes peaks from noise
 - More accurate and robust than Mantid algorithms
- **Mantid uses DBSCAN peaks for UB matrix & hkl 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**
- **Live Demo of Index visualization**
 - Interactive visualization of many crystal lattices
 - Intensity analysis to find Bragg peaks
 - Docker based deployment

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



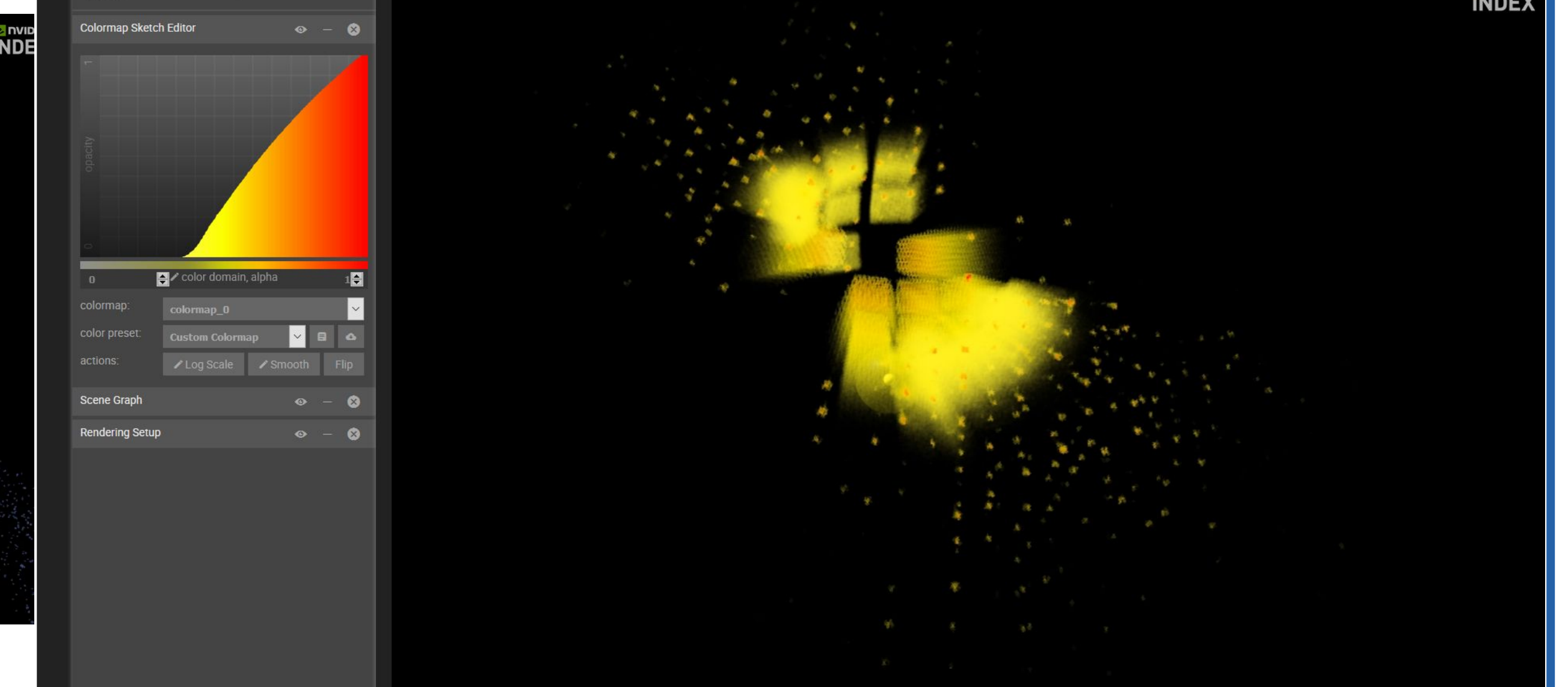
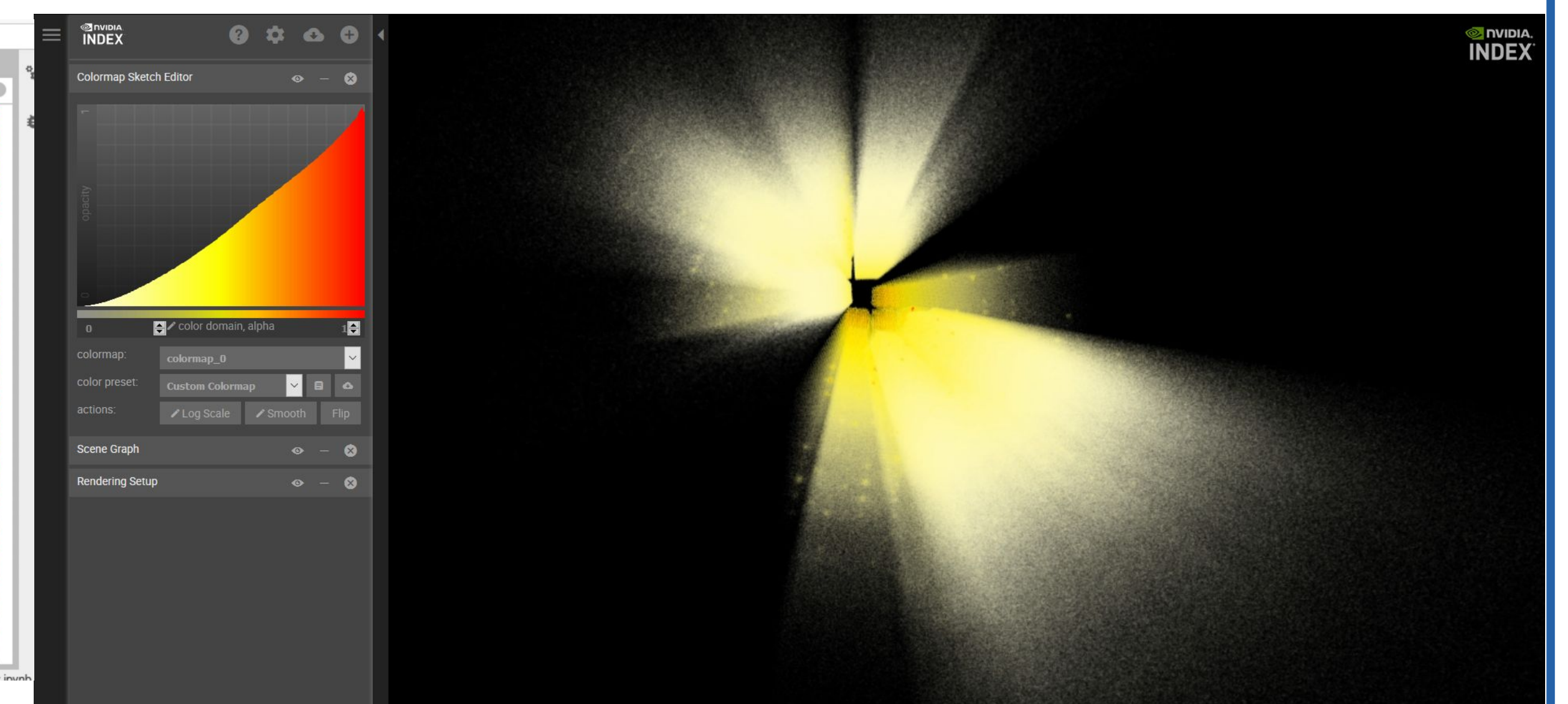
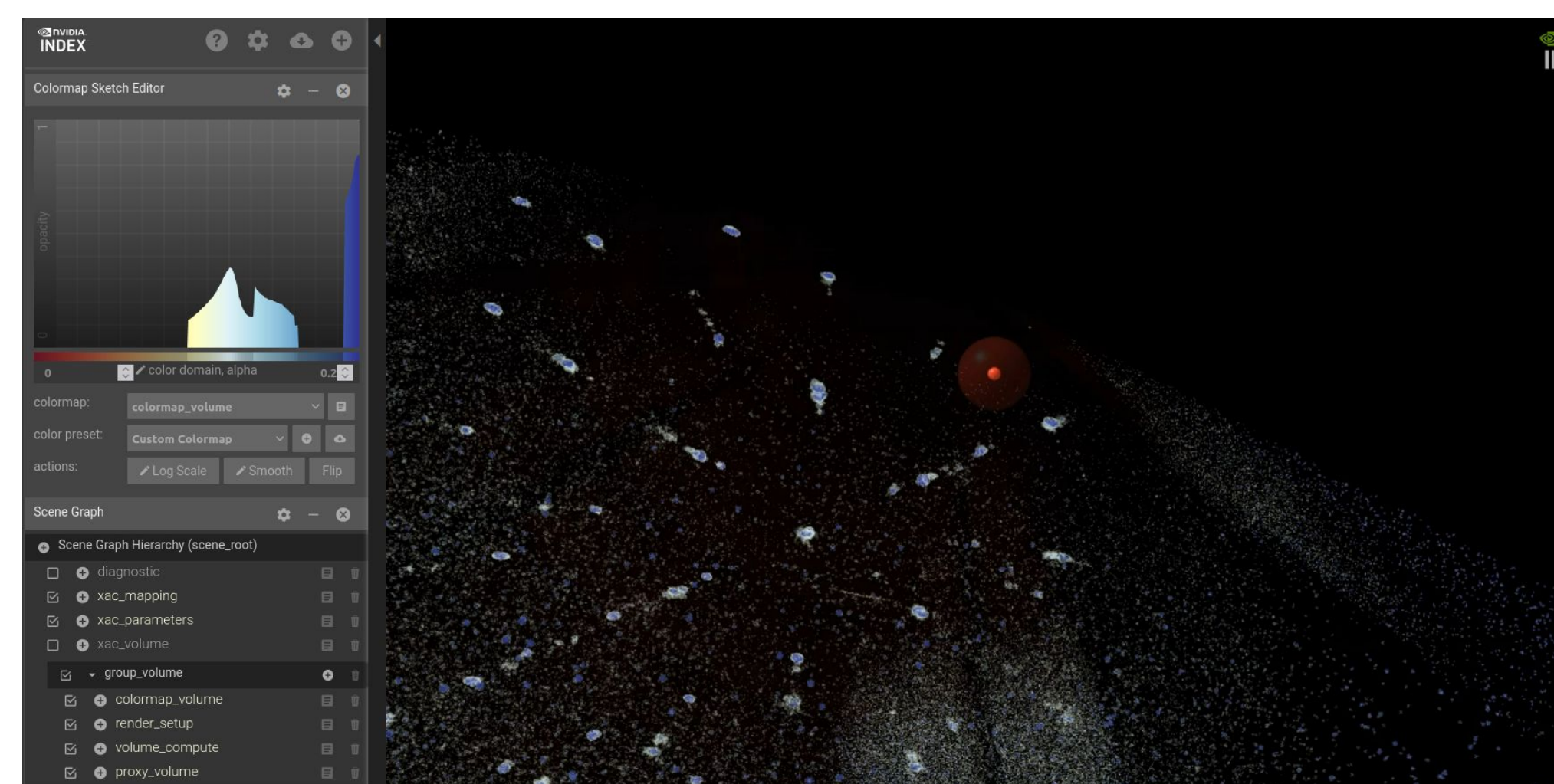
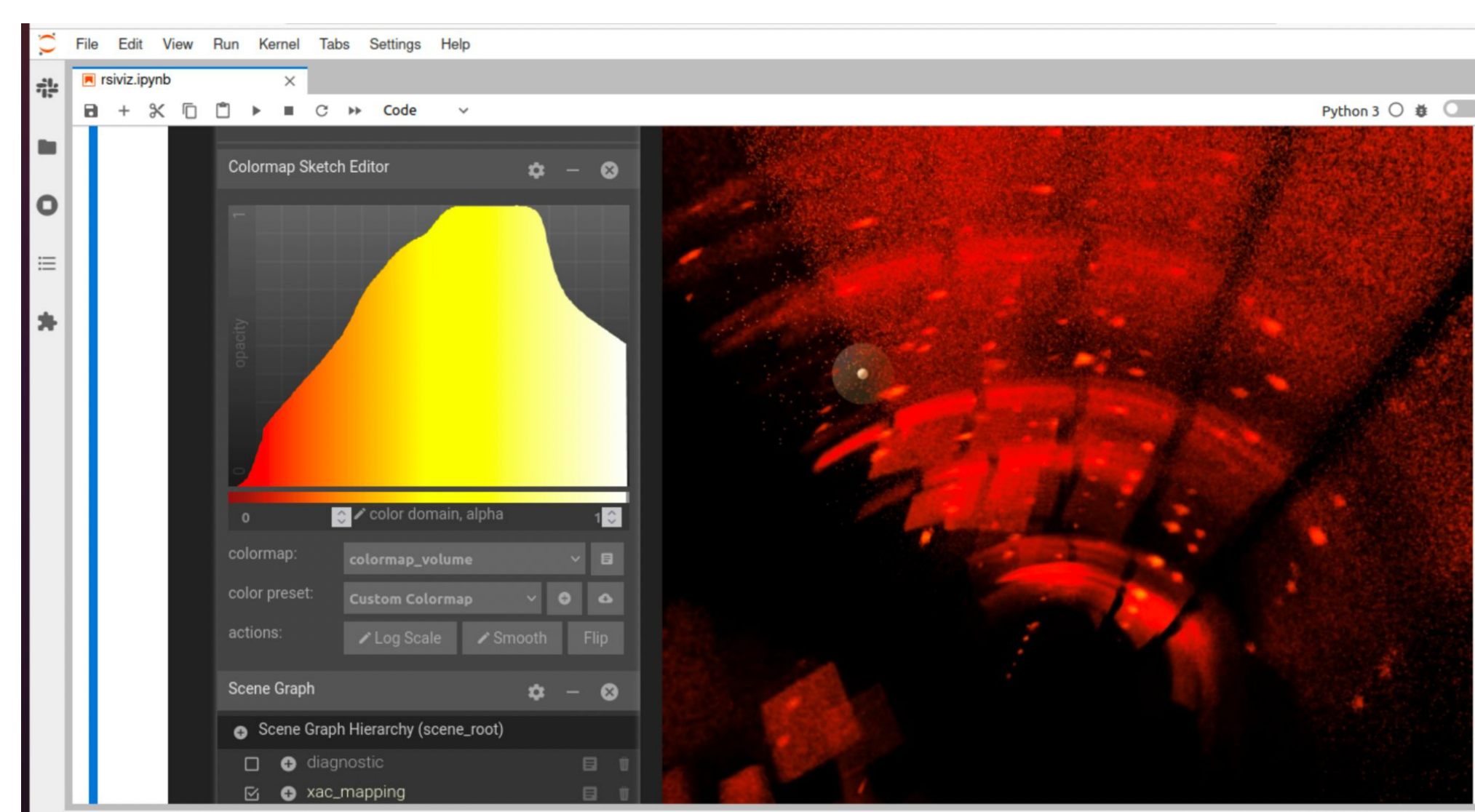
25 detector installed



IndeX Visualization

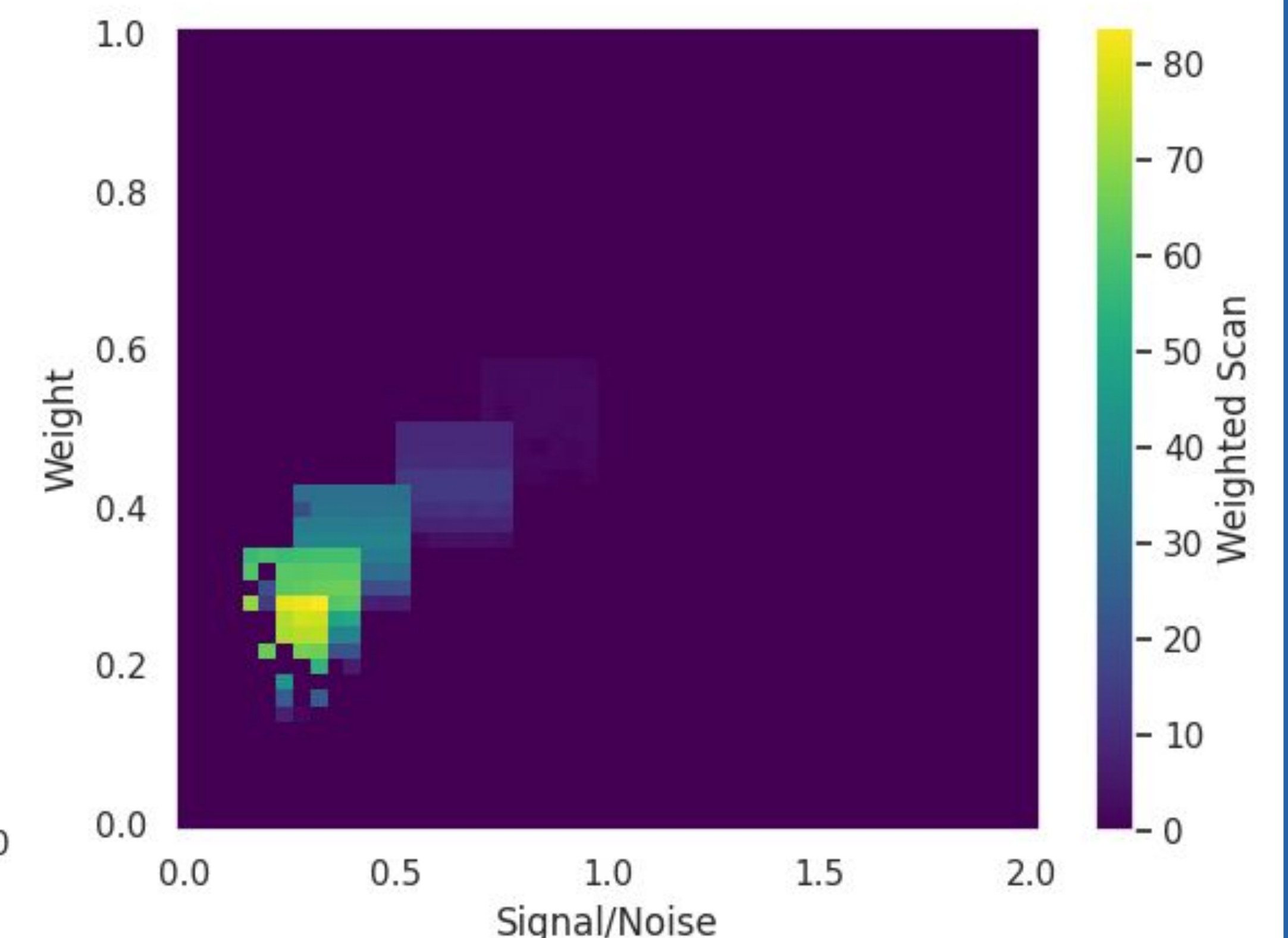
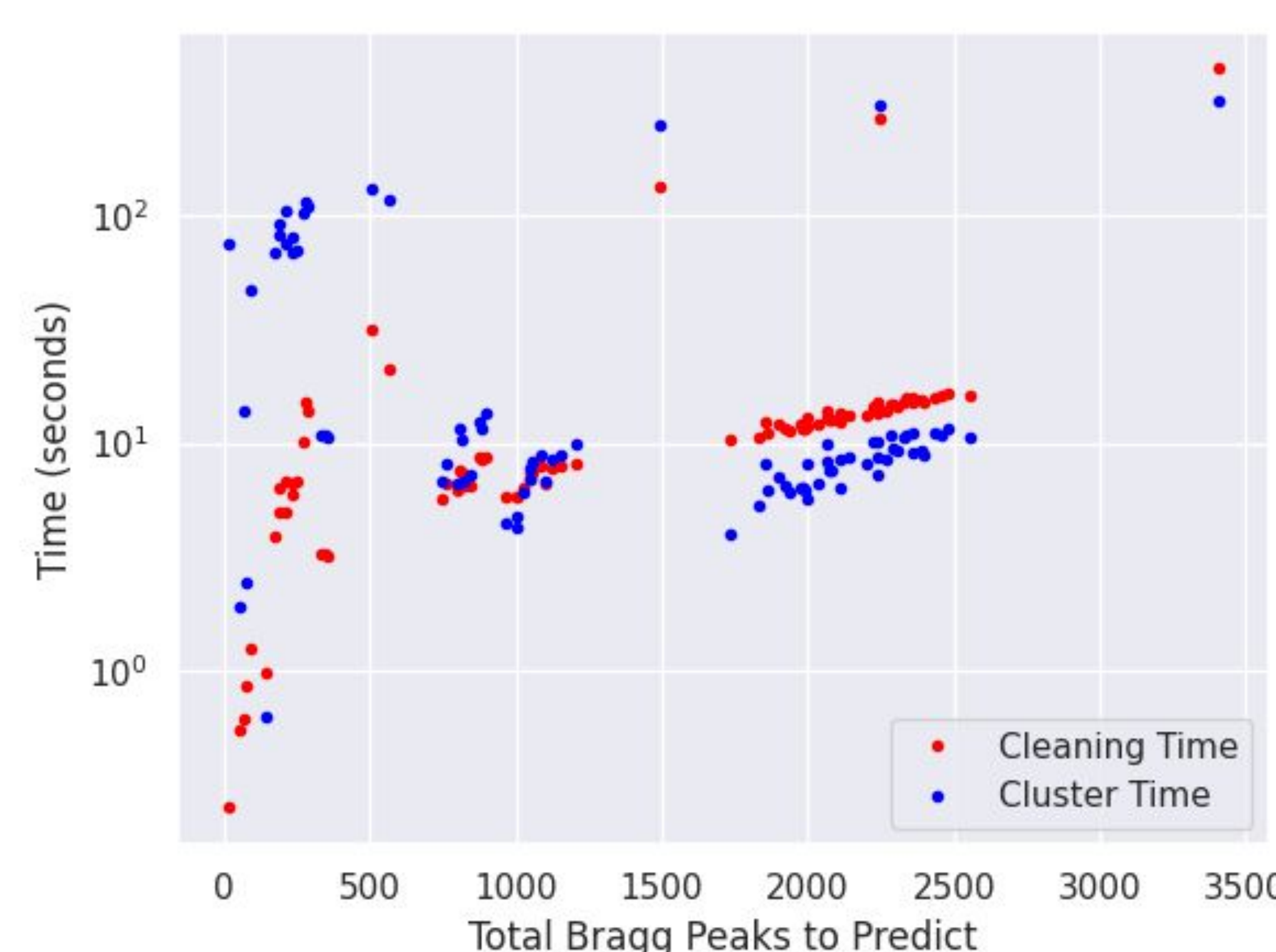


- **NVIDIA IndeX technology [3]**
 - 3D browser based volumetric interactive framework
 - Scientists can interact with massive data sets
 - Make real-time modifications
 - Navigate to the most pertinent parts of the data in real time
- **Our implementation of IndeX**
 - Docker based deployment Interactively 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
- **Live Demo!**
 - View five different crystal structures on IndeX
 - Full 3D capabilities
 - Color mapping customization for conference ready visualizations
- **Future Features**
 - Automatic UB matrix calculation and visualization
 - Streaming control and interactability



Automated Bragg Peak Detection

- **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

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>
4. Mantid (2013): Manipulation and Analysis Toolkit for Instrument Data.; Mantid Project. url: <http://dx.doi.org/10.5286/SOFTWARE/MANTID>.



Office of
Science

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

This research used resources at the Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.



Oak Ridge, TN. 06/5-8/2023



Boulder, CO USA | radiasoft.net