Contribution ID: **12** Type: **Oral (16mins + 4 mins)**

# Interactive Visualization and Automated Analysis of Neutron Scattering Experiments

*Thursday, March 7, 2024 12:10 PM (20 minutes)*

Neutron scattering experiments have undergone significant technological development through large area detectors with concurrent enhancements in neutron transport and electronic functionality. Data collected for neutron events include detector pixel location in 3D, time and associated metadata, such as, sample orientation, neutron wavelength, and environmental conditions. RadiaSoft and Oak Ridge National Laboratory personnel are considering single-crystal diffraction data from the TOPAZ instrument. We are leveraging a new method for rapid, interactive analysis of neutron data using NVIDIA's IndeX 3D volumetric visualization framework. We have implemented machine learning techniques to automatically identify Bragg peaks and separate them from diffuse backgrounds and analyze the crystalline lattice parameters for further analysis. A novel CNN architecture has been developed to identify anomalous background from detector instrumentation for dynamical cleaning of measurements. The implementation of automatic peak identification into IndeX allows scientists to visualize and analyze data in real-time. These methods can be applied in real-time during detector operation to improve experimental operations and scientific analysis. Our methods include a robust comparison with current analysis techniques which show improvement in a variety of aspects. These improvements will be incorporated into IndeX for visualization to allow scientists an interactive tool for crystal analysis.

## Primary Keyword

MLOps

## Secondary Keyword

anomaly detection

## Tertiary Keyword

ML-based optimization

**Primary author:** KILPATRICK, Matthew (RadiaSoft LLC)

**Co-authors:** KUHN, Alexander (NVIDIA); SAVICI, Andrei (Oak Ridge National Laboratory); VACALIUC, Bogdan (Oak Ridge National Laboratory); HOFFMAN, Christina (Oak Ridge National Laboratory); Dr BRUHWILER, David (RadiaSoft LLC); TATULEA, Dragos (NVIDIA); CARLIN, Evan (RadiaSoft LLC); KHALSA, Gurhar (RadiaSoft LLC); MENSMANN, Jorg (NVIDIA); NIENHAUS, Marc (NVIDIA); TUCKER, Matthew (Oak Ridge National Laboratory); MESSMER, Peter (NVIDIA); ROEMER, Steffen (NVIDIA); MORGAN, Zachary (Oak Ridge National Laboratory)

**Presenter:** KILPATRICK, Matthew (RadiaSoft LLC)

**Session Classification:** Analysis & Diagnostics

**Track Classification:** Analysis & Diagnostics