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Optimizing Neutron Diffraction Experiments at the Spallation Neutron Source with Temporal Fusion Transformers: A Frontier for AI-Driven Real-Time Decision Making

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Neutron time-of-flight (TOF) data at the ORNL Spallation Neutron Source (SNS) contains multidimensional temporal information in diffraction and parameter spaces. The field's current state relies on sequential data reduction and analysis steps, often involving data transfer between different platforms and tools which introduces inefficiencies and hinders the seamless integration of different analysis techniques and workflows.
We are developing an integrated approach to reducing and analyzing single crystal neutron diffraction data recorded in event mode to overcome these challenges. The near-term goal is to enable real-time decision-making for TOPAZ beamline, a high-resolution single crystal TOF Laue diffractometer at SNS. This method harnesses an advanced AI/ML model tapping into the high-performance computing (HPC) resources at the Oak Ridge Leadership Computing Facility (OLCF), which seamlessly synchronizes neutron scattering experiments to enable live data analysis. Our model treats the neutron scattering data at the voxel level to accurately predict the neutron scattering pattern in a 4D temporal-spatial space.
The approach, anchored in a Markovian stochastic process, employs the Temporal Fusion Transformer (TFT) model to optimize experiment time. TFT is an attention-based deep neural network (DNN) model that combines long short-term memory (LSTM) encoding of time series and transformer attention layers, specifically designed to align with the multi-horizon forecasting job, providing greater accuracy and interpretability for predicting neutron scattering patterns at the voxel level in a temporal 4D space. We have developed a hierarchical parallelization approach on the OLCF Frontier supercomputer. Using a subset of the neutron TOF event dataset collected at TOPAZ, our TFT model trained on Frontier could help reduce over-counting by around 30% while achieving similar data quality using less neutron beamtime. The outcomes underscore that the integrated approach using AI/ML and HPC can significantly improve beamline efficiency by processing and analyzing live neutron scattering data in multidimensional scattering and parameter spaces, representing a significant step toward reshaping the landscape of neutron scattering research for real-time experiment steering and automation. Our work advances the Integrated Research Infrastructure (IRI) by bridging the gap between U.S. Department of Energy neutron facilities with the Office of Advanced Scientific Computing Research HPC facilities through the lens of AI/ML. This presentation invites us to join this journey, explore the possibilities, and envision the future of neutron science together.

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