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NDIP and NOVA: Workflows and Interfaces for Neutron Scattering

Neutron Scattering workflows are a core part of daily operations for SNS and HFIR scientists at Oak Ridge National Laboratory (ORNL). However, there can be challenges relating to the ease of access, use, and reproducibility of these workflows. We have developed the Neutron Data Interpretation Platform (NDIP) and the Neutrons Open Visualization and Analysis (NOVA) framework to tackle these challenges. NDIP and NOVA provide scientists with the tools to create web based user interfaces (UIs) and take advantage of computational resources, advanced visualization tools, and reproducible analysis pipelines.

NDIP is built around the open-source Galaxy project, a web-based scientific workflow engine and UI, built to enable scientists to easily manage data, create workflows, and simplify the reproduction of past results. Our efforts have integrated our own Galaxy instance, Calvera, with various computational resources including Frontier at ORNL and Perlmutter at NERSC. Calvera handles the authentication, the submission, and the reporting of results from these resources.

The NOVA framework was designed to enable scientists to develop custom UIs that take advantage of NDIP's capabilities to run workflows and tools. NOVA provides tools to create Model-View-ViewModel applications utilizing a variety of front-end technologies including Trame, Panel, and QT. Scientists can also use NOVA to launch jobs through NDIP, run workflows, retrieve their results, and display them in their interfaces.

Our poster will highlight the work done on both NDIP and NOVA, describe their capabilities, and show examples of how NDIP and NOVA have facilitated the development of Neutron Scattering workflows and interfaces.

Topical Area

AI and data science

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