

A Front-End Framework with Embedded ML Tools for Automating Neutron Scattering Experiments

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The rscontrols framework developed at RadiaSoft was created to simplify controls automation for neutron scattering experiments using machine learning (ML), beginning with sample alignment. Written in Python, rscontrols uses virtual representations of equipment and controls to enable seamless integration of hardware, EPICS protocols, and analytical tools including deep networks and other ML models. Embedded UNet image segmentation models have already been deployed through rscontrols in live tests at ORNL in which we have successfully demonstrated automated sample alignment. Significant effort has been dedicated to live uncertainty quantification for generating reliability metrics and diagnostics, retaining the security of human feedback while reducing reliance on input for operations. In addition to image segmentation, a UNet encoder/decoder has been used along with a non-ML filter method for live neutron camera image denoising. Implementations of additional ML models are underway, including Bayesian optimization and reinforcement learning schemes to further automate controls and optimize the scientific value of scattering data. This will incorporate work from parallel efforts at RadiaSoft to perform detector-based fine-tuning using reciprocal space data and a 3D UNet.

Primary Keyword

AI-based controls

Secondary Keyword

uncertainty quantification for ML

Tertiary Keyword

MLOps

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