Contribution ID: **44** Type: **Poster**

McStas Union simulations of a 15 T magnet and background prediction with Machine Learning

Tuesday 9 April 2024 18:30 (20 minutes)

Neutron scattering allows for quite complicated sample environments with control over the sample conditions, such as temperature, as well as for the presence of strong magnetic fields. The presence of magnets in scattering experiments necessitates a significant amount of material in the structure. The coils of the magnets, outside the direct beam, add more material into the structure and could influence the experiments, since neutrons would scatter multiple times before reaching the detector. Additionally, they exert large magnetic forces on the structure that need to be withstood, requiring more material to safeguard the structural integrity of the system.

In an attempt to investigate the effect of the sample environment on the resulting background scattering, simulations of elastic neutron scattering data in the presence of multiple scattering from the sample environment were carried out. A model of the 15 T magnet for the BIFROST spectrometer at ESS was constructed with the Union tool in McStas, a neutron ray-trace simulation package. The contribution of the sample environment towards background was studied and analysed.

Furthermore, the model was parameterised to cover different experiment setups with a number simulation parameters, generating a substantial amount of simulation results. A comprehensive database of 24000 simulation results was constructed, analysed and utilised for the training, optimisation and testing of Machine Learning models that were able to predict the background of simulated experiments.

This novel approach can serve as an introduction to a new method of background recognition, paving the way for the development of automated background prediction tools that can be used within a wide range of instruments, with combinations of simulated and experimental data in the future.

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Session Classification: Posters

Track Classification: MLC