Optimizing Neutron Reflectometry Experiments for Soft Matter Systems using HOGBEN

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Neutron Reflectometry (NR) measurements are both time-consuming and resource-intensive, making it vital to optimize the experimental approach in order to gain the greatest amount of relevant information about a system within a given time. However, determining how best to perform NR experiments is an unintuitive problem: which regions of a reflectivity profile contain the most information about a system? How long do you measure at each angle for? How many, and which, solvent contrasts are needed? These are questions HOGBEN was developed to help answer.

HOGBEN is a software tool designed to simulate and optimize Neutron Reflectometry experiments[1, 2]. Using a sample model defined in Refnx, and the neutron flux profile and set-up of a chosen NR instrument, it can be used to optimize the measurement angles, respective times at each angle, solvent contrast, and even the composition and thickness of reference layers within a substrate. By altering these, a significant increase in the amount of information gained within a given time for the parameters of interest can be acquired, which ultimately produces either a reduction in count time or an improvement in fit-uncertainties. Recently, experimental work has been performed using HOGBEN to demonstrate the improvement of information gained when measuring a simple bilayer system by up to 50% in comparison to a measurement at conventional measurement and angle times.

We present here an overview of the capability and applicability for HOGBEN to optimize neutron reflectometry measurements of soft-matter systems, and provide experimental confirmation of the information gain possible through such optimization.

Keywords:
Neutron Reflectometry, Fisher Information, Soft Matter, Simulation

References:

[1] Durant, J. H., Wilkins, L., & Cooper, J. F. K. (2022). *Optimizing experimental design in neutron reflectometry.* Journal of Applied Crystallography, 55(4), 769–781. [2] Durant, J. H., Wilkins, L., Butler, K., & Cooper, J. F. K. (2021). *Determining the maximum information gain and optimizing experimental design in neutron reflectometry using the Fisher information.* Journal of Applied Crystallography, 54(4), 1100–1110.

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