Optimizing experiments and creating unlimited realistic data for AI using HOGBEN

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We present our work on a software package called HOGBEN. It allows users to plan a neutron reflectivity experiment, enabling them to gain the most information about their system possible in their limited beam time.

The basis of our approach requires us to know how many neutron counts we will measure from a sample per unit time. This requires us to model our particular sample, in the correct conditions, on a specific instrument, in a given instrument configuration. We must therefore modify the traditional workflow of simulating a sample as a whole, and instead take account of exactly what will be measured from our sample at a given angle for a given time. This is fortunately easy to do with the assumption of Poisson error bars (no background subtraction), and is extremely fast. Our schema uses the Fisher information metric to estimate the parameter uncertainties we will measure in our experiment, which can then be optimized to give the most information (lowest uncertainties) possible for our experiment. We are also developing the ability to suggest changes to the sample structures which would result in better experimental outcomes, e.g. reference layers. Our code is based on the *refnx* so models and code can be easily re-used or transferred.

Using our approach rather than "rules of thumb" can give very significant gains, equivalent to measuring samples for several times longer (the gains are both sample and instrument dependent). The code developed also has the benefit of creating extremely "realistic" data, which we have thus-far been unable to differentiate from real data. Since we are able to create a dataset like this in sub-millisecond timescales, our approach can also be used to train machine learning algorithms on realistic data, with a known ground truth.

 References:
[1] *Determining the maximum information gain and optimizing experimental design in neutron reflectometry using the Fisher information* https://doi.org/10.1107/S160057672100563X
[2] HOGBEN Codebase https://github.com/jfkcooper/HOGBEN or 'pip install hogben'
[3] REFNX https://refnx.readthedocs.io/