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Simulating single-crystal inelastic scattering in full phase-space

To simulate inelastic neutron scattering in a single crystal, the algorithm needs to sample a high dimensional distribution. The numerical difficulties are twofold. To start with, the memory footprint of such distribution is typically challenging for mainstream computers to handle. Secondly, the energy and momentum resolutions of the sampled results may not optimised, if the distribution is not calculated with a suitable set of parameters.

In this talk, a toolchain to produce and sample the high dimensional scattering distribution is introduced. A self-adaptive integration method is used to calculate the cross section. In addition, a rejection sampling method [Cai, et. al, J. Comput, 2019] is implemented in a machine learning model. There are no tunable physical parameters in the overall process. This toolchain will also be discussed for the application of high-throughput computation.

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