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Methods of Information Processing for Neutron Scattering Data
PATRICK NAVE, Florida State University; Oak Ridge National Laboratory, LIN JIAO, Oak Ridge National Laboratory, MARTIN MOURIGAL, Georgia Institute of Technology, MATTHEW STONE, Oak Ridge National Laboratory — Inferring complex dispersion relations from resolution-limited neutron scattering measurements is a task which has been approached from a variety of perspectives from Monte Carlo (MC) scattering simulations to resolution function methods which convolve an approximate resolution function with a theoretical model dispersion. However, detailed MC simulations require a highly-accurate framework such as MCViNE, which is not available for all neutron scattering facilities and is also time consuming, while resolution function methods are faster yet more dependent on accurate analytical models of the instrument to construct a valid approximation. Our research investigates two methods for analyzing neutron scattering data in a more general context. The first is a numerical covariance method designed to be fast while retaining high enough accuracy to be useful and enough generality to be applicable to any time-of-flight direct geometry neutron spectrometer. The second is a theoretical method based in topological data analysis concepts. In particular, we explore the computation of invariant topological features which may be useful in algorithmically learning from large databases of scattering data and identifying resolution correlations across sets of instrument parameters.

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