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Exploiting symmetry with brille

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Modern time-of-flight neutron spectrometers routinely collect datasets covering volumetric reciprocal space. By taking advantage of multiplexing techniques or parametric studies datasets can exceed one billion independent observations. Software exists to facilitate collecting observations from volumetric datasets in arbitrary, user-defined, regions of reciprocal space; which can often be compared directly to theoretical models for the double differential cross section. Such comparisons benefit from existent software to account for instrumental resolution effects; however, the large number of observations makes the evaluation costs prohibitively high for typical physical models.

The open-source software package brille has been developed to facilitate faster evaluation of arbitrary physical models by exploiting the irreducible Brillouin zone symmetry of crystal samples. Typically, brille stores a cache of model eigenvalues and eigenvectors at the vertices of a conformal grid and later linearly interpolates between the cached values. Due to the possibility of atom-labelling permutations under application of a lattice symmetry operation, brille must typically be tailored to a model. Thus far brille can reliably interpolate the eigenvalues and eigenvectors of the grand dynamical matrix and has been used successfully to speed-up phonon calculation with Euphonic. Future developments will enable brille to handle second-quantized systems as well, with an eye towards speeding-up linear-spinwave calculations with SpinW.

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