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Euphonic: efficient inelastic neutron scattering simulations and more from force constants

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Chopper spectrometers produce large 4-dimensional inelastic neutron scattering (INS) datasets, allowing investigations of vibrational and magnetic properties of materials over large regions of momentum-energy (**Q**-E) space. While software (e.g. Horace) exist to enable visualisation and analysis of such data, computational challenges remain for the simulation and fitting of vibrational spectra, which requires the calculation of phonon frequencies and displacements at millions of **Q**-points to simulate a single 2D slice of data. Here we present Euphonic, a Python package designed to efficiently interpolate phonons and calculate INS intensities directly from force constants. Currently supported are CASTEP and Phonopy force constants, with the potential for more to be added in the future. Euphonic has a focus on performance, with key components written in C and OpenMP. The performance scaling of Euphonic means that, for example, instrument resolution convolved simulations of phonon spectra are now tractable for the first time. Euphonic is also useful as a library to the wider scientific community - providing both a Python API and command line tools. Euphonic has been developed following software best practice, is open source and can be obtained via Github, PyPI and the conda-forge Conda channel. This talk will give an overview of: the main features and benefits of Euphonic; development following the 1.0 release in August 2022; and development priorities going forward.

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