Pyhyperscattering: A Collaborative Framework for Highly Multidimensional Scattering Dataset Loading, Reduction, Analysis, And Display

Dr Peter A Beaucage[1]

[1]*NIST Center for Neutron Research*

peter.beaucage@nist.gov

The continued march of progress in synchrotron and neutron instrument performance has resulted in the proliferation of data-intensive, multidimensional scattering experiments as a 'new normal' for materials characterization. in situ studies such as thermal annealing, formerly stand-alone experiments, are now routinely supporting components of studies, and new spectroscopic scattering techniques such as resonant soft x-ray scattering (RSoXS) have made the acquisition of hyperspectral scattering data a routine probe for highly complex, multicomponent systems.

We report the development of PyHyperScattering, an extremely versatile Python library built on the xarray package which aims to provide a uniform toolbox for loading, reduction, fitting, and downline processing of scattering data collected as a function of time, wavelength, temperature, shear rate, or any other arbitrary additional axis. The resulting library allows the single-line expression of complex queries such as "the (100) diffraction intensity as a 2D function of temperature and angle about the beamstop" and the routine inline generation of both figures and programmatic data.

PyHyperScattering has been and will continue to be developed using an open-source and open-development model on GitHub, with several substantial features added via the pull request process and a roadmap for future developments that aim to increase its performance and utility. We expect that PyHyperScattering will form the foundation of a wide variety of bespoke analysis frameworks across numerous varieties of data-intensive scattering experiments.