Reciprocal Space Mapping for Macromolecular Crystallography

Steve P Meisburger[1], Nozomi Ando[2]
[1]Cornell High Energy Synchrotron Source, [2]Chemistry & Chemical Biology, Cornell University
spm82@cornell.edu

Diffuse scattering can provide insight into protein dynamics from macromolecular crystallography (MX) experiments. In conventional MX, the protein's average structure is determined by analyzing Bragg peak intensities. Diffuse scattering signals present in the same diffraction images contain a wealth of information about deviations from the average structure, including lattice disorder and protein breathing motions. We have shown that when diffraction data are measured carefully at room temperature, the diffuse scattering can be processed to obtain a three-dimensional reciprocal space map that is further analyzed to determine correlated motion. To make diffuse scattering techniques more widely available, we have created a python package mdx2 that is both convenient to use and simple to extend and modify. It is lightweight, relying on the scientific python ecosystem for numerical methods, dials and dxtbx for initial processing and data import, and NeXus format for data storage. Mdx2 can be run on the command line or imported as a package, for instance to encapsulate a complete workflow in a Jupyter notebook for reproducible computing and education. Finally, I will discuss our recent efforts to improve performance and scalability toward real-time data reduction at synchrotron beamlines.