

A Decade of Processing Multi-Modal Data at Xfels

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As XFELs began to come online over 10 years ago, protein crystallographers quickly realized that the best usage of their powerful, pulsed photon beams was studying the dynamics of molecules in sophisticated, multi-modal experiments. Samples injected in a variety of means were exposed to laser pumps, oxygen chambers, ligands, and substrates, and changes were measured optically using cameras, in the electron density after processing, and using simultaneous emission spectroscopy. These experiments challenged existing data processing methods and new approaches were developed to integrate information from a variety of sources.

In this talk, a brief tour of some of the important developments in data processing using cctbx.xfel that were critical to handle these data will be presented. Further, recent focus has been on indexing difficult cases with multiple lattices, multiple isoforms, and (pseudo)-merohedral twinning. Rather than being rare situations, these use-cases are sufficiently common that advanced algorithms and methods are needed to treat them. As an example, a combination of a new filtering technique using the DBSCAN clustering algorithm and the Brehm-Diederichs method to fully correct the indexing of a monoclinic, pseudo-tetragonal crystal form with two independent mis-indexing operators will be shown.