Phasing Methods for the Structure Completion Problem in Crystallography

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The problem of structure completion arises in protein crystallography in a number of ways: for instance, a partial model of the protein may have been constructed during model building and refinement, or molecular replacement may have been carried out with a probe similar to only a fragment of the target molecule. The problem of structure completion is intrinsic to surface crystallography, where both a known bulk structure and an unknown surface structure (to be determined) contribute to the measured diffraction pattern, and information is sought only about the surface structure. The diffraction data in the latter case are discretely localized in reciprocal-lattice planes parallel to the surface, but are continuous in the direction perpendicular to the surface due to the breaking of the periodicity in that direction.

In the present talk we will describe methods that are common to the structure completion problem in both bulk and surface crystallography. In particular, we will describe algorithms that depend on the phasing of the measured amplitudes by Fienup-type input-output feedback loops that oscillate between real and reciprocal space. It will be shown that the “maximum entropy” method of Collins may be recast as a similar input-output phasing algorithm.