

Fast & furious factors: reduced redundancy in DiSCaMB

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Computing structure factors for macromolecules has traditionally relied on applying the Fast Fourier Transform (FFT) to the dynamic electron density derived from spherical electron density contributions. Recent advances in quantum crystallography, however, enable the use of more sophisticated aspherical electron density models in structure refinement – improving the accuracy of atomic positions even in large biomolecules, in particular for hydrogen.

DiSCaMB [1] is a high performance C++ library developed to efficiently compute structure factors from these aspherical models. Among them, the Hansen-Coppens multipole model [2] – parametrized using data from the MATTS data bank [3,4] – has gained prominence in recent years. In this approach, the structure factors are computed by directly summing the Fourier transform contributions of multipolar electron density terms.

However, the vast number of atoms in macromolecular systems poses significant challenges in reflection computations. In this work we introduce symmetry-aware algorithms that leverage space group operations to eliminate redundancy and substantially accelerate the computations. We benchmark their performance using representative model macromolecules to assess benefits for refinement workflows.

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