

## W0251

**Algebraic Direct Methods from Few-Atoms to Few-Macromolecules.** D.Y. Guo, Robert H. Blessing, Hauptman-Woodward Medical Research Institute, 73 High St., Buffalo, NY 14203, and Dept. of Structural Biology, State Univ. of New York at Buffalo.

Algebraic direct methods for few-atoms structures (Hauptman *et al.* (2002). *Acta Cryst.* A58, 361-369) are generalized for few-macromolecules structures, with perhaps thousands of independent protein atoms inside, and liquid-like solvent molecules outside, the macromolecular envelopes. At  $d_{\min} \sim 15 \text{ \AA}$  envelope resolution, macromolecular structures can be approximated by constant density inside, and zero density outside, the macromolecular envelope, and under that approximation, we introduce an algebraic direct phasing technique based on iteratively populating  $m$  points of a three-dimensional uniform density grid. The structure factor,

$$F_h = \sum_j g_{h,j} \exp [2\pi i h^T (t_j + R_j r_c)] \quad (j = 1, n_{\text{sym}}),$$

is a function of the  $m$ -point grid centroid  $r_c$  and the  $m$ -point, uniform-grid-density macromolecular scattering factor,

$$g_{h,j} = m^{-1/2} \sum_k \exp [2\pi i h^T R_j (r_k - r_c)] \quad (k = 1, m_{\text{grid}}).$$

The analysis leads to a minimal function for structure invariant structure factor triples. Test calculations for glyceraldehyde-3-phosphate dehydrogenase (PDB 4gpd) with 47 reflections measured to 20 Å resolution yield a molecular envelope image with  $\sim 65^\circ$  average phase error.

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