02-Methods for Structure Determination and Analysis, Computing and Graphics

The further development of the EDIb based approach is to consider the set of conditional histograms calculated from the points in the unit cell satisfying some additional restrictions. Such additional constraints may imply position of a point with respect to the molecular region or the values of some other functions connected with the object under investigation.

PS-02.01.08 ELECTRON DENSITY SQUARING METHOD AND NON-CRYSTALLOGRAPHIC SYMMETRY. By A.F. Mishnev, Latvian Institute of Organic Chemistry, Riga, Latvia.

Non-crystallographic symmetry imposes restraints on phases of the structure factors. Linear relationships among structure factors due to identical molecules in different crystallographic environments have been obtained by Main & Rossman (Acta Cryst. 1966, 21, 67-172). For a structure containing like atoms the electron density squaring method (Sayre, Acta Cryst. 1952, 5, 40-65) may be introduced in the analysis of Main & Rossman, that results in quadratic equations for the structure factors. In the presence of non-crystallographic symmetry the structure factor of the "squared" crystal takes the form

\[ G_{n} = \sum_{\mathbf{h} \in \Gamma} | \rho (\mathbf{h}) \rho^{*} (\mathbf{h}) | \exp \left[ 2 \pi i \mathbf{C} \mathbf{p} + \mathbf{d}_{0} \right] \exp \left( 2 \pi i \mathbf{h} \cdot \mathbf{d}_{0} \right). \]  

The "squared" structure factor may be expressed by \( G_{n} = g_{n} \rho_{n} f_{c} \).

\[ f_{c} \rho_{n} = \frac{e_{n}}{k^{2}} \sum_{\mathbf{h} \in \Gamma} x_{\mathbf{h}} f_{\mathbf{h}} \cdot S_{\mathbf{h} \mathbf{m} \mathbf{n}} \]  

where \( S_{\mathbf{h} \mathbf{m} \mathbf{n}} \) are functions of molecular envelope, rotation and translation parameters. When the two crystals are identical equation (2) reduces to the Sayre's equation. Numerical test calculations of equations (2) using simulated crystal data will be presented.

PS-02.01.09 DIRECT PHASING FOR MACROMOLECULES BY ENTRAPMENT MAXIMISATION AND LIKELIHOOD RANKING. By M. Brucigne, Department of Molecular Biology, Biomedical Centre, Box 390, 75124 Uppsala, Sweden; and LURE, Bâtiment 209D, 51405 Orsay, France.


The main components of the method as implemented in the computer program BUSTER [Brucigno (1993). Acta Cryst. A49, 37-60] are: (1) a tree-directed search through a space of trial phase sets; (2) the saddlepoint method for calculating joint probabilities of structure factors, using entropy maximisation; (3) likelihood-based scores to rank trial phase sets and prune the search tree; (4) a new method for optimising the choice of reflection so as to maximise the sensitivity of the likelihood to their phases; (5) efficient schemes, based on error-correcting codes, for sampling trial phase sets; (6) a statistical analysis of the scores for automatically selecting reliable phase indications by multidimensional Fourier techniques coupled with tests of statistical significance. This program has been successfully tested on two small structures and has been applied to data from two new proteinase.

The mathematical techniques now available in BUSTER bring closer a number of major enhancements of standard macromolecular phasing methods proposed earlier [Brucigno (1988). Acta Cryst. A44, 517-545] as an extension of the initial theory. In the molecular replacement method, for instance, the detection and placement of a known fragment described in a reference orientation and position by a density map with transform F can be accomplished by calculating the log-likelihood gain:

\[ \log \left( \frac{P(\mathbf{f} | \mathbf{h})}{P(\mathbf{f} | \mathbf{h})} \right) = \log \left( \frac{P(\mathbf{f} | \mathbf{h})}{P(\mathbf{f} | \mathbf{h})} \right) \]

where (\( P(\mathbf{f} | \mathbf{h}) \)) denotes the null hypothesis that all atoms are uniformly distributed in the asymmetric unit while (\( P(\mathbf{f} | \mathbf{h}) \)) the alternative hypothesis that the known fragment is placed in the asymmetric unit with orientation R at position t and the rest of the atoms are distributed at random. A drastic simplification of LLG yields a sum of (1) a Patterson correlation (PC) based rotation function in which a sum of point-group symmetry-related copies of the self-Patterson of the rotated fragment is correlated with the originally removed self-Patteron of the whole structure; and (2) a PC-based translation function, expressed as a Fourier series with argument t itself. This function is already an improvement on the PC functions used in XPLOR [Brünger (1990). Acta Cryst. A46, 46-57], yet it is in general a poor approximation to LLG. It will be shown how the systematic use of LLG and of its relations to Bayesian statistical methods yields a new procedure for the detection and accurate placement of a known molecular fragment and of its recycling into the phasing process which overcomes every single limitation of the current methodology [Brucigno (1993). In The Molecular Replacement Method, ed. by W. Wolf, E.J. Dodson & S. Gover, Warrington: SIRC Daresbury Laboratory, in press].

PS-02.01.10 FOURIER-TRANSFORM-BASED METHODS FOR PHASE EXTENSION AND REFINEMENT AND PERHAPS THE SOLUTION OF MACROMOLECULES. By L. Refaat, C. Tate and M.M. Woolfson, Department of Physics, University of York, UK.

The Sayre equation is known to be effective for phase extension and refinement, either alone (Sayre, D., 1972, Acta Cryst. A28, 210-212) or in conjunction with other constraints, as in the SQUASH procedure [Main, P., 1970, Acta Cryst. A46, 372-377].

A method is described by which the coefficients of a set of linear equations are derived, solely from FFT operations, leading to phase