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SF2CNS: general purpose program to calculate *CNS*-formatted maps easily

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1. The crystallographic problem

Macromolecular crystallographers operate with very complicated objects. The available computer tools give a good space representation of the crystal content and are powerful, fast and simple to use. For this reason, macromolecular crystallography graphics programs, such as *O* (Jones *et al.*, 1991), are very attractive for a variety of structural research. These programs work with atomic models and electron density maps, prepared in a number of widely distributed formats. In particular, the *X-PLOR*/*CNS* format (Brünger *et al.*, 1998) for electron density maps is accepted by many graphics programs. Unfortunately, very few crystallographic suites allow one to calculate *CNS*-formatted maps directly from structure factors.

2. Method of solution

The general-purpose program *SF2CNS* calculates the Fourier syntheses in the *CNS* format starting directly from structure factors written in various formats, without the need for any format converter or the use of *CNS* (Brünger *et al.*, 1998) itself, thus avoiding running auxiliary *CNS* steps and commands. *SF2CNS* accepts files in the *CNS* format, in any other fixed format, files written in a free format and unformatted files. It is requested that all file records have a similar structure and that each record corresponds to a single structure factor.

SF2CNS calculates Fourier syntheses with the coefficients of a general type

$$k_1 w_1(\mathbf{s}) F_1(\mathbf{s}) \exp[i\varphi_1^{(s)}] - k_2 w_2(\mathbf{s}) F_2(\mathbf{s}) \exp[i\varphi_2^{(s)}]. \quad (1)$$

In particular, this includes the cases of the coefficients

$$w_1(\mathbf{s}) F_1(\mathbf{s}) \exp[i\varphi_1^{(s)}] \quad (2)$$

or

$$[2w_1(\mathbf{s}) F_1(\mathbf{s}) - w_2(\mathbf{s}) F_2(\mathbf{s})] \exp[i\varphi_1^{(s)}] \quad (3)$$

or

$$w_1(\mathbf{s})\{F_1(\mathbf{s}) \exp[i\varphi_1^{(s)}] - F_2(\mathbf{s}) \exp[i\varphi_2^{(s)}]\}, \quad (4)$$

widely used in crystallography. The coefficients (3) are typical for macromolecules, and 'deformation maps' calculated with (4) are often used to study small molecules. The values of w_1, w_2, F_1, F_2, φ_1 and φ_2, being individual for each reflection, are taken from the input file of the structure factors, while k_1 and k_2 are defined in control data. The phase values can be in degrees, in radians or written in the trigonometric form, *i.e.* as cosine and sine values.

The program allows one to calculate the Fourier synthesis in any parallelepiped with edges parallel to the coordinate axes. This region can be a unit cell or its part, can be extended over several unit cells, or partially cover several unit cells. The density values can be either calculated on the absolute scale or normalized and calculated in terms of sigma. The program can be used for any space group, and the calculated synthesis can be converted to its enantiomer if requested.

The goal to create a general-purpose program that is as simple as possible and offers a large variety of schemes for Fourier coefficients forced us to leave the preparation of the weighting coefficients w_1 and w_2 to external programs. For the same reason, when different kinds of coefficients are used for different types of structure factors (Read, 1986) or in different resolution zones (Vernoslova & Lunin, 1993), the user should prepare corresponding values in file records in order to use the scheme (1). Similarly, the limits of a 'box' in which the synthesis is going to be calculated are defined by the user outside of *SF2CNS*. If the 'box' surrounds an available atomic model, a simple complementary program *SF2BOX* can be used to define its limits for any conventional orthogonalization agreement and for any 'margins' around the model, without the need to generate the additional topology file required by *CNS*.

3. Software and hardware environment

The program *SF2CNS* is written in standard Fortran 77 and can be run on any computer. The program uses a modified version of the Fast Fourier Transform subroutines originally written by Ten Eyck (1973). The Fortran program *SF2BOX* is available together with *SF2CNS*.

4. Documentation and availability

The program is self-descriptive and contains several examples of control data at its header. The program is available from the authors upon request.

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