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SHORT COMMUNICATIONS

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Acta Cryst. (1987). **A43**, 283-284

Comments on *From a partial to the complete crystal structure. II. The procedure and its applications*, by M. Camalli, C. Giocovazzo & R. Spagna (1985). By PAUL T. BEURSKENS, *Laboratory for Crystallography, Toernooiveld, 6525 ED Nijmegen, The Netherlands*

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Abstract

A recent paper by Camalli, Giocovazzo & Spagna [*Acta Cryst.* (1985). **A41**, 605-613] describes a method which is almost identical to the *DIRDIF* method for the application of direct methods to difference structure factors. The similarities and differences, incorrectly described in that paper, are discussed in the present paper.

Introduction

The application of direct methods to the solution of a heavy-atom superstructure problem (Beurskens & Noordik, 1971) led to the concept of the *DIRDIF* method, which

has been extensively developed over fifteen years of practical experience [see Beurskens (1985) and references therein]. It has been intuitively assumed that direct methods are applicable to a hypothetical structure consisting of the complete structure minus the known part of the structure. The program *DIRDIF* can expand a partial structure to the complete structure, if the partial structure comprises as little as ten percent of the total scattering power of the structure. Camalli, Giocovazzo & Spagna (1985) have now described a very similar method, justified in terms of the probabilistic formulae of Giocovazzo (1983). Unfortunately, they make several important errors in the comparison of their method with *DIRDIF*, a comparison which is made more difficult by differences in terminology.

Table 1. Comparison of symbols (see text)

<i>DIRDIF</i>	CGS	
p, r	p, q	Subscript referring to partial structure, remainder of the structure
N_p, N_r	p, q	Number of atoms
p^2, r^2	$\sum_p/\sum_N, \sum_q/\sum_N$	Relative scattering power ($p^2 + r^2 = 1$) (p, r substituted below)
$F_r(\mathbf{h})$	$(F_h - F_{p,h})$	Structure factor of the difference structure
$E(\mathbf{h})$	rE'_h	Normalized structure factor of the total structure
$E_p(\mathbf{h})$	$(r/p)E'_{p,h}$	Normalized structure factor of the partial (known) structure
$E_r(\mathbf{h})$	$(E'_h - E'_{p,h})$	Normalized structure factor of the difference structure
$ E_i(\mathbf{h}) $	$\ E'_h\ - \ E'_{p,h}\ $	Lowest possible modulus of E ,

Symbols and formulae

A concordance of the nomenclature of Camalli, Giacobozzo & Spagna (hereafter CGS) with that of Beurskens *et al.* (1983) (hereafter *DIRDIF*) is given in Table 1. The use of 'pseudo-normalized E 's' by CGS for something which is not normalized at all is unnecessarily confusing, and we use here the *DIRDIF* notation.

The vector equation $\mathbf{F} = \mathbf{F}_p + \mathbf{F}_r$ may be given in terms of normalized structure factors:

$$E(\mathbf{h}) = pE_p(\mathbf{h}) + rE_r(\mathbf{h}). \quad (1)$$

The tangent formula for the difference structure is

$$E_r(\mathbf{h}) = c \sum_{\mathbf{k}} E_r(\mathbf{k}) E_r(\mathbf{h} - \mathbf{k}) \quad (2)$$

where c is a positive scaling factor defined to satisfy (1). The reliability of the result is estimated as usual, using $c \approx N_r^{-1/2}$. CGS have derived a generalized Sayre equation [CGS, equation (8) multiplied by r]:

$$E(\mathbf{h}) \approx pE_p(\mathbf{h}) + rc \sum_{\mathbf{k}} E_r(\mathbf{k}) E_r(\mathbf{h} - \mathbf{k}) \quad (3)$$

with $c = N_r^{-1/2}$ which is, in fact, a combination of (1) and (2).

Comparison and comments

(a) The application of the tangent formula implies the application of (2) (*DIRDIF*) or (3) (CGS) using a limited number of terms. The reliabilities for the two formulae are calculated with the same value of c and should lead to identical results.

(b) For the initiation of the procedure, some reflections phased by the known fragment and some additional reflections are used. In *DIRDIF* the additional reflections are used only in case of enantiomorph or supersymmetry problems (Prick, Beurskens & Gould, 1983); symbolic addition techniques are used; one single solution is obtained. In CGS the additional reflections are always used, and multi-solution techniques are employed.

(c) CGS comment (CGS, pp. 606, 607):

(1) 'A phase is associated with each ($|F| - |F_p|$), which is refined cycle by cycle.' This is not true; it is the phase of $(F - F_p)$ which is refined cycle by cycle [see *DIRDIF*, p. 398, equation (8)].

(2) '... reliability is given by the parameter

$$K_{\mathbf{h},\mathbf{k}} = 2N_r^{-1/2} |E_1(\mathbf{h}) E_1(\mathbf{k}) E_1(\mathbf{h} - \mathbf{k})|.$$

This is also untrue; it is given by

$$K_{\mathbf{h},\mathbf{k}} = 2N_r^{-1/2} |E_r(\mathbf{h}) E_r(\mathbf{k}) E_r(\mathbf{h} - \mathbf{k})|$$

where E_r is calculated by equation (2) [see *DIRDIF*, p. 398, equation (9)].

(3) 'During phase refinement the values φ_r vary but moduli $K_{\mathbf{h},\mathbf{k}}$ remain fixed.' This is a serious misconception. It is fundamental to the *DIRDIF* concept that $E_r(\mathbf{h})$ values vary both in phase and in magnitude; see equation (2).

(d) CGS comment (CGS p. 608) that the *DIRDIF* scaling method 'is particularly useful when ... all the N_p atoms are expected to have a nearly equal temperature factor.' In fact, individual temperature factors are used whenever reliable estimates are available, and an additional overall temperature factor is determined.

(e) The two methods use the same formulae [*i.e.* equations (1)+(2) or (3)] except for some differences in the assignments of weights (see *DIRDIF*, p. 399). The most interesting difference in this respect is the adjustment of c , equations (1) and (2). In the first cycle this c (*DIRDIF*) is larger than $N_p^{-1/2}$ (CGS): this enhances the difference between φ and φ_p , and thus speeds up the refinement. In practice, complete convergence is usually achieved by *DIRDIF* in four cycles.

(f) Finally, the main practical difference is in the selection of reflections which participate in the summations in equations (2) or (3). Although all reflections are used in the final *DIRDIF* Fourier synthesis, only reflections with $|E_r|$ greater than some threshold are subjected to the phase refinement procedure. The selection criteria are not defined by CGS. For instance, strong reflections with $|F| \approx |F_p|$ (*i.e.* $|E_r| \approx 0$) are not used in (2) but, presumably, are used in (3). It is not expected that these differences lead to significant differences in the final Fourier maps.

Despite these misunderstandings, Camalli, Giacobozzo & Spagna have shown that the *DIRDIF* method is justified by the probabilistic formulae obtained by Giacobozzo (1983).

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