

$n = 2, 1, -1$ or 0 respectively. A sum S_m ($m = 0 - 3$) may be required for l even for the formation of S'_{2m} , and l odd for S'_{2m+1} , or the reverse; in these two cases we store $n = 3$ or -3 respectively.

The arrays G, G', G'' are first cleared to zero and then filled with values of n . For each spacegroup, the values of g_i and the associated t_j are divided into p sets as described in Section 2. We number the sets $0 - (p - 1)$ and search for pairs $g_{i'}, g_{(i'+1)}$ ($i' = 0, 1, 2, 3$); these occur in sets p_1 and p_2 . For each term t_j in set p_1 we put $G(p_1, [j/2]) = 2$ or 1 according as $p_1 = p_2$ or $p_1 \neq p_2$. If $p_1 \neq p_2$ then for each t_j in the set p_2 , we store a value in $G(p_2, [j/2])$; if this element contains 0 or -1 , we store -1 , but if it contains the value 1 we store 3 or -3 according as j is odd or even.

In order to fill the matrix G' , for each set of g_i we evaluate $i' = [i/2]$ and form the values n_0 and n_1 according to the values of i' present in the set:

values of i' present	$2q, 2q + 1$	$2q$	$2q + 1$	—
values of n_q	2	1	-1	0

$$q = 0, 1.$$

Then for each t_j in the set, we put $G'(q, j) = n_q$ for $q = 0, 1$.

The vector G'' is filled as follows: the terms S''_0, S''_1 are required according to whether any of the terms S_0, S_3, S_5, S_6 and S'_1, S'_2, S'_4, S'_7 are present. The presence

Reference

MATTHEWMAN, J. H. (1963). "Note on the selective summation of Fourier series," *The Computer Journal*, Vol. 6, p. 248.

of these terms for h even and h odd is sought in the matrix G' and appropriate values are stored in G'' .

6. The calculating phase

The data is stored in the computer with the indices in the order h, k, l and with $h \geq 0$ for all spacegroups and $k \geq 0, l \geq 0$ for orthorhombic spacegroups. The calculation is most efficient when this data is stored in an order where h and l are the slowest and fastest changing indices.

The sums $S_0 - S_3$ are calculated for a fixed value of Z for each change in h, k ; these are then used to calculate $S'_0 - S'_7, S''_0$ and S''_1 for a fixed value of Y for each change in h ; then values of S'''_0, S'''_1 and $\rho(X, Y, Z)$ are calculated for each value of X . The latter is repeated for each value of Y and then the whole is repeated for each value of Z .

At each stage, sums of the type:

$$\sum_{r=1}^n y_r \cos(r\theta) \text{ and } \sum_{r=1}^n y_r \sin(r\theta)$$

are formed as described by Matthewman (1963); that is, for each pair of summations, only one sine and cosine need be calculated. One substitution is performed for each value of r and the method is particularly efficient when all values of y_r ($r = 1 - n$) are present.

7. The program

This program is written in Atlas Autocode and a complete specification may be obtained from the author.

Book Review

International Journal of Computer Mathematics. Vol. 1. No. 1, edited by Peter H. Friedlander, 1964; 89 pages. (New York: Gordon and Breach, 47s. 6d., single issue, 160s. per volume of 4 issues.)

This is the first issue of a Journal which sets out to be non-specialized, international in outlook and to cover a field midway between theoretical mathematics and actual engineering applications. It will cover broadly the newer mathematical developments of interest in the fields of Numerical Analysis, Operations Research, Automation, Econometrics, Mathematical Logic and Communication. Selected articles of unusual interest which have appeared in recent French, Soviet and German journals will be published complete in English. Original work in English will be accepted and in some cases in the author language accompanied by an English translation.

- (1) The criteria for acceptance of papers will be:
Does the paper contribute to the understanding of the trend of development in this field?

- (2) Is the paper of interest because it typifies the work of a certain school?
- (3) Does it contain an element of great importance to related fields?

This first volume contains 6 papers, an American paper and five Soviet translations (3 from *Automation and Remote Control* and 2 from the *Journal of Computer Mathematics and Mathematical Physics*). The papers were received for their original journals between May and December 1961, giving a time lag of nearly three years. At first sight this appears to be a long delay, but if the papers are fundamental and contain material not easily found in English Journals then a good translation might be worth waiting for. The six papers in Volume I are spread over the suggested field, and have been well translated and printed with care. Forthcoming papers will include a translation of a Soviet paper on the theory of self-teaching machines, a paper describing an application of Monte Carlo methods to shielding calculations, and a report on work in the field of artificial intelligence of computers.

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