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References

Adobe Systems Inc. (1985). *PostScript Language Reference Manual.* Reading, MA: Addison-Wesley.

ALLEN, F. H., BELLARD, S., BRICE, M. D., CARTWRIGHT, B. A., DOUBLEDAY, A., HIGGS, H., HUMMELINK, T., HUMMELINK-PETERS, B. G., KENNARD, O., MOTHERWELL, W. D. S., RODGERS, J. R. & WATSON, D. G. (1979). *Acta Cryst.* B**35**, 2331–2339.

BERNSTEIN, F. C., KOETZLE, T. F., WILLIAMS, G. J. B., MEYER, E. F. JR, BRICE, M. D., RODGERS, J. R., KENNARD, O., SHIMANOUCHI, T. & TASUMI, M. (1977). *J. Mol. Biol.* **112**, 535–542.

BLUNDELL, T., CARNEY, D., GARDNER, S., HAYES, F., HOWLIN, B., HUBBARD, T., OVERINGTON, J., SINGH, D. A., SIBANDA, B. L. & SUTCLIFFE, M. (1988). *Eur. J. Biochem.* **172**, 513–520.

BRÄNDÉN, C. -I. & JONES, T. A. (1990). *Nature (London)*, **343**, 687–689.

BRÜNGER, A. T. (1988). *X-PLOR* Version 1.3. *Crystallographic Computing* 4, edited by N. W. ISAACS & M. R. TAYLOR, pp. 126–140. Oxford Univ. Press.

BRÜNGER, A. T. (1992). *Nature (London)*, **355**, 472–475.

ELANGO, N. & PARTHASARATHY, S. (1990). *Acta Cryst.* A**46**, 495–502.

ENGH, R. A. & HUBER, R. (1991). *Acta Cryst.* A**47**, 392–400.

HUBBARD, T. J. P. & BLUNDELL, T. L. (1987). *Protein Eng.* **1**, 159–171.

ISLAM, S. A., STERNBERG, M. J. E. & WEAVER, D. L. (1990). *Accuracy and Reliability of Macromolecular Crystal Structures*, edited by K. HENRICK, D. S. MOSS & I. J. TICKLE, pp. 53–62. Proceedings of the CCP4 Study Weekend, 26–27 January 1990, Daresbury Laboratory, Warrington, England.

IUPAC–IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (1970). *J. Mol. Biol.* **52**, 1–17.

JONES, T. A., ZOU, J. -Y., COWAN, S. W. & KJELDGAARD, M. (1991). *Acta Cryst.* A**47**, 110–119.

KABSCH, W. & SANDER, C. (1983). *Biopolymers*, **22**, 2577–2637.

KRAULIS, P. J. (1991). *J. Appl. Cryst.* **24**, 946–950.

LÜTHY, R., BOWIE, J. U. & EISENBERG, D. (1992). *Nature (London)*, **356**, 83–85.

LUZZATI, P. V. (1952). *Acta Cryst.* **5**, 802–810.

MORRIS, A. L., MACARTHUR, M. W., HUTCHINSON, E. G. & THORNTON, J. M. (1992). *Proteins*, **12**, 345–364.

RAMACHANDRAN, G. N., RAMAKRISHNAN, C. & SASISEKHARAN, V. (1963). *J. Mol. Biol.* **7**, 95–99.

READ, R. J. (1986). *Acta Cryst.* A**42**, 140–149.

WIERENGA, R. K., KALK, K. H. & HOL, W. G. J. (1987). *J. Mol. Biol.* **198**, 109–121.

WISTOW, G., TURNELL, B., SUMMERS, L., SLINGSBY, C., MOSS, D., MILLER, L., LINDLEY, P. & BLUNDELL, T. (1983). *J. Mol. Biol.* **170**, 175–202.

J. Appl. Cryst. (1993). **26**, 291–294

The FROG PC series: programs for electron-density and model investigations for proteins.

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Abstract

A set of computer programs, developed for IBM-compatible personal computers and aimed at crystallographic use, is described. The programs have user-friendly interfaces and allow the calculation of various Fourier syntheses, which can be vizualized and compared. The possibility of obtaining a synthesis and an atomic model together and performing the model image rotations and translations with respect to the synthesis also exists.

Introduction

Computer calculations are involved in all stages of X-ray structure determination. The present tendency is towards the use of efficient computers and supercomputers to perform laborious calculations and graphic stations to analyze and interpret results. At the same time, the constantly growing possibilities offered by personal computers (PCs) allow the performance of some investigative steps by means of relatively cheap and widely available equipment. This arouses interest in the development of crystallographic programs aimed at the facilities of personal computers.

This paper briefly describes some of the PC programs developed at the Institute of Mathematical Problems of Biology (Research Computing Center) of the Russian Academy of Sciences. A full description of the programs is available from the authors on request. The programs use IBM-compatible personal computers with VGA or EGA graphic-display adapters running MS-DOS version 3.3 or higher.

The program organizations have similar features. Each has a built-in window editor to set the parameters managing a program session. The current parameter values can be saved in a special file created by a program at the end of a session and used when starting a new program session. The programs have the means to control the external files, which allows the detection and correction of errors introduced when entering file names. A user can obtain the short prompt at any time.

1. *FAN* (scalar field analysis)

The *FAN* program is designed for the visual investigation of functions that depend on three variables (in crystallography, as a rule, electron-density Fourier synthesis or

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difference synthesis). The function to be studied is specified in the form of the set of function values calculated at the uniform grid points in the unit cell. *FAN* input files may be either formatted or be in a specially packed format, which is one of the output formats for the fast Fourier transform program, *FFT*, described below.

FAN displays a function by its isolines, obtained in two-dimensional sections parallel to one of three coordinate planes (according to the user's choice). It is based on an efficient subroutine, developed by the authors to calculate and display the isolines, which allows one to change isolines quickly (Figs. 1 and 2).

Two ways to set an isoline are possible in the program. The first one is to specify the absolute function value corresponding to this isoline. The second way is to set a part of the unit-cell volume, bounded by the corresponding isosurface. Either of them may be used.

FAN allows one:

(i) to display specified isolines in the chosen section;

(ii) to display isolines in a number of sections at one time;

(iii) to change easily the set of displayed sections by adding or deleting sections;

(iv) to change the scale of the displayed image, *e.g.* to 'magnify' or 'diminish' the desired fragment, and to move the window frame into any desired region of space;

(v) to vary easily the set and the color of displayed isolines;

(vi) to determine the relative coordinates of any point.

FAN allows one to extend, by periodicity, the visual investigation of a function to anywhere within the entire space of its existence and to deal with oblique-angled unit cells.

2. *CAN* (comparative analysis)

The *CAN* program allows one to display (together or separately) images of three objects: two electron-density syntheses (*e.g.* an ordinary one and a difference one) and the protein molecule atomic model (Fig. 2). We will call these syntheses the main one and the auxiliary one.

CAN possesses the same capabilities of processing syntheses that the *FAN* program has and in addition allows one to move the auxiliary synthesis with respect to the main one and to reflect it in coordinate planes and at the origin. When running *CAN*, the auxiliary synthesis may be changed for another one.

CAN allows one to display either all the atoms of a model or the C_α atoms only. In the course of study, the user may change the set of atoms he wishes to study and display the numbering of residues. *CAN* allows one to perform translations and rotations of the model as a rigid body with respect to coordinate axes, as well as to display (or delete from the screen) images of molecules obtained from the given molecule by symmetry transformations.

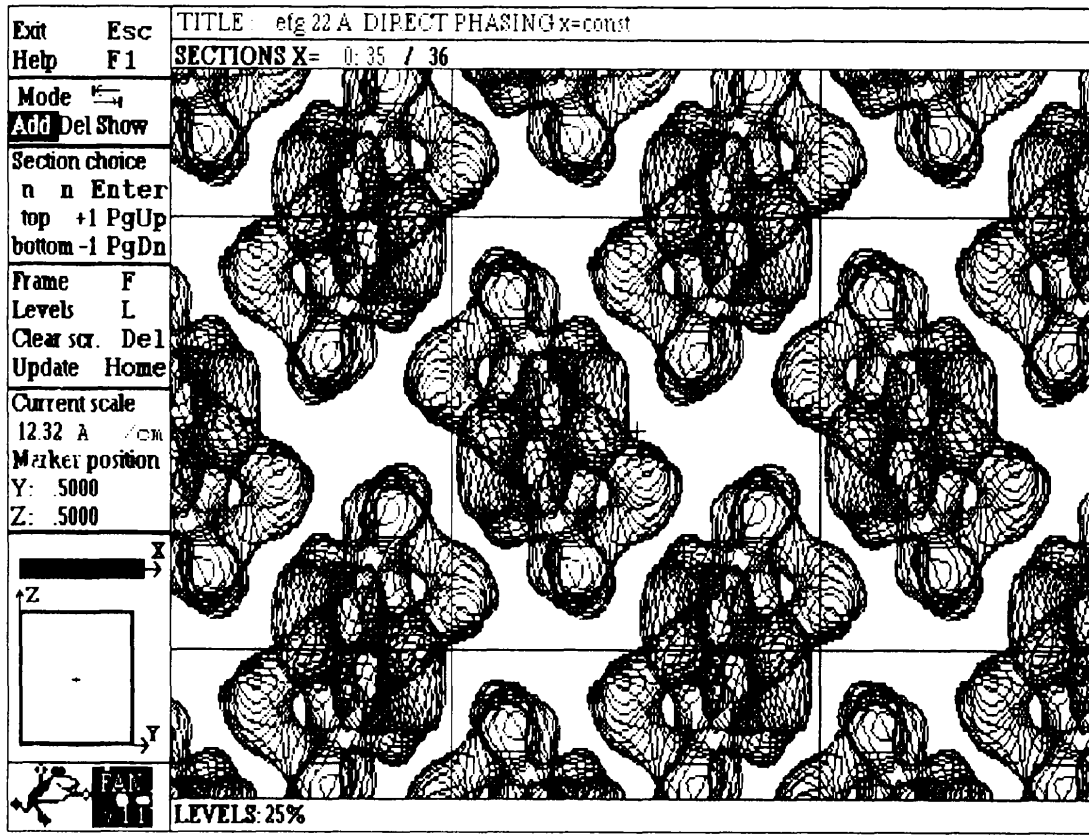

Fig. 1. The superimposed-sections image in *FAN*. (It takes about 60 s to calculate and display this picture with an IBM PC-AT 386/387 computer.)

3. *FANS* (scalar field analysis stereo)

FANS possesses the same capability of processing electron-density syntheses and the atomic model that the *FAN* and *CAN* programs have, but it displays a stereoscopic picture of a desired region of space analogous to that in the 'Richards box' (Richards, 1968).

4. *FFT* (fast Fourier transform)

The *FFT* program (Fig. 3) is designed to calculate various Fourier syntheses and uses the fast-Fourier-transform algorithm as formulated by Ten Eyck (1973).

The input data file contains for each of the reflections its indices and some additional information, *e.g.* the modulus and various variants of phase values for the native protein and its derivatives, the figure-of-merit of phase determination, individual weights *etc.* The calculated Fourier synthesis may be output either in a formatted form or in one of the specially packed formats used by the *FAN*, *CAN* and *FANS* programs.

FFT may process any space group and allows one to calculate syntheses of a general form. However, for the sake of convenience, the following types of synthesis are specified as separate:

(i) the Fourier synthesis is calculated with coefficients

$$W_s(CF_s)\exp(i\varphi_s);$$

(ii) the Patterson synthesis is calculated with coefficients

$$W_s(CF_s)^2;$$

(iii) the difference Fourier synthesis is calculated with coefficients

$$W_s(C_1F_s^1 - C_2F_s^2)\exp(i\varphi_s);$$

(iv) the difference Patterson synthesis is calculated with coefficients

$$W_s(C_1F_s^1 - C_2F_s^2)^2;$$

(v) the general-form synthesis is calculated with coefficients

$$\sum_j^N W_s^j(C_jF_s^j)\exp(i\varphi_s^j).$$

The subscript s represents the values determined for each of the reflections and taken from the input file; C_j are the values specified by the user when starting the program.

Additional flexibility of the program is provided by the possibility of setting various values of the scalar coefficients C_j and of determining various input-file positions to obtain the values W_s, F_s and φ_s, according to the resolution zone the particular reflection belongs to. To be more precise, the resolution interval (d_{min}, d_{max}) specified for the synthesis calculation may be divided into subintervals, each having its own formula for calculation of the synthesis coefficients.

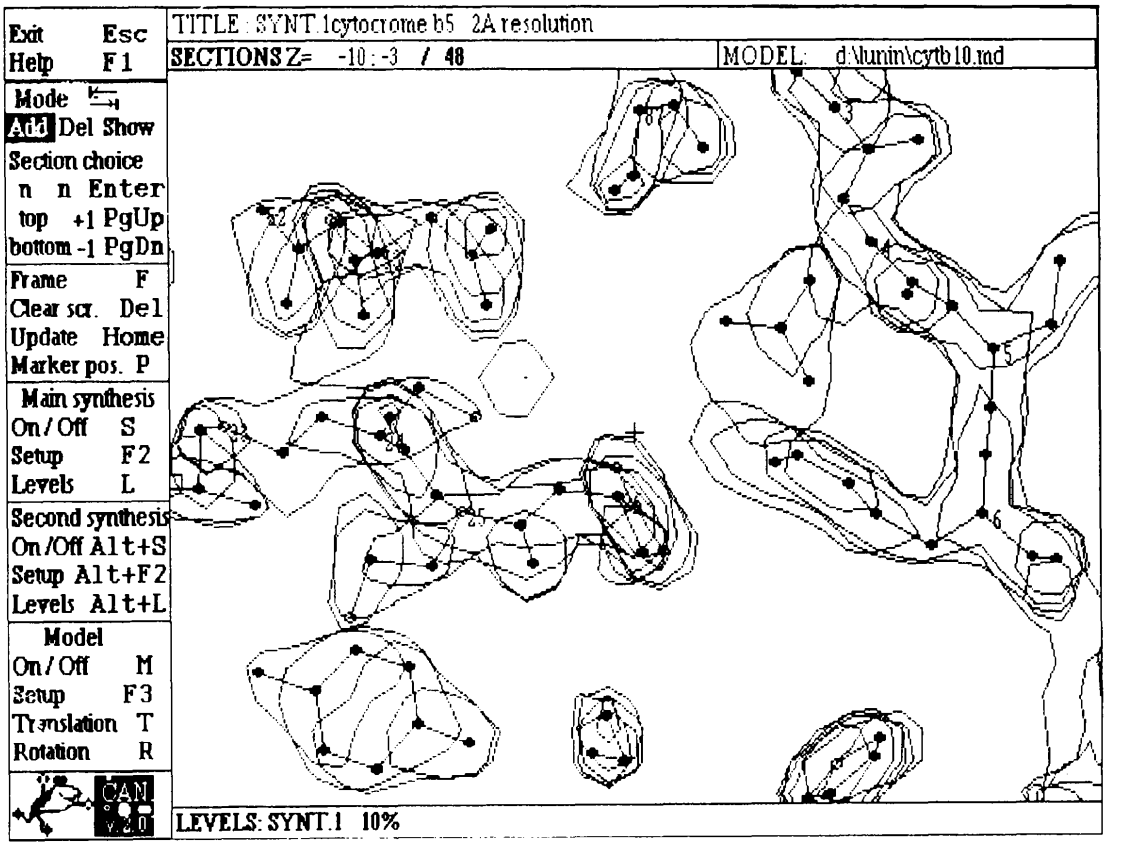

Fig. 2. The model superimposed on the synthesis in *CAN*. (It takes about 3 s to calculated and display this image with an IBM PC-AT 386/387 computer.)

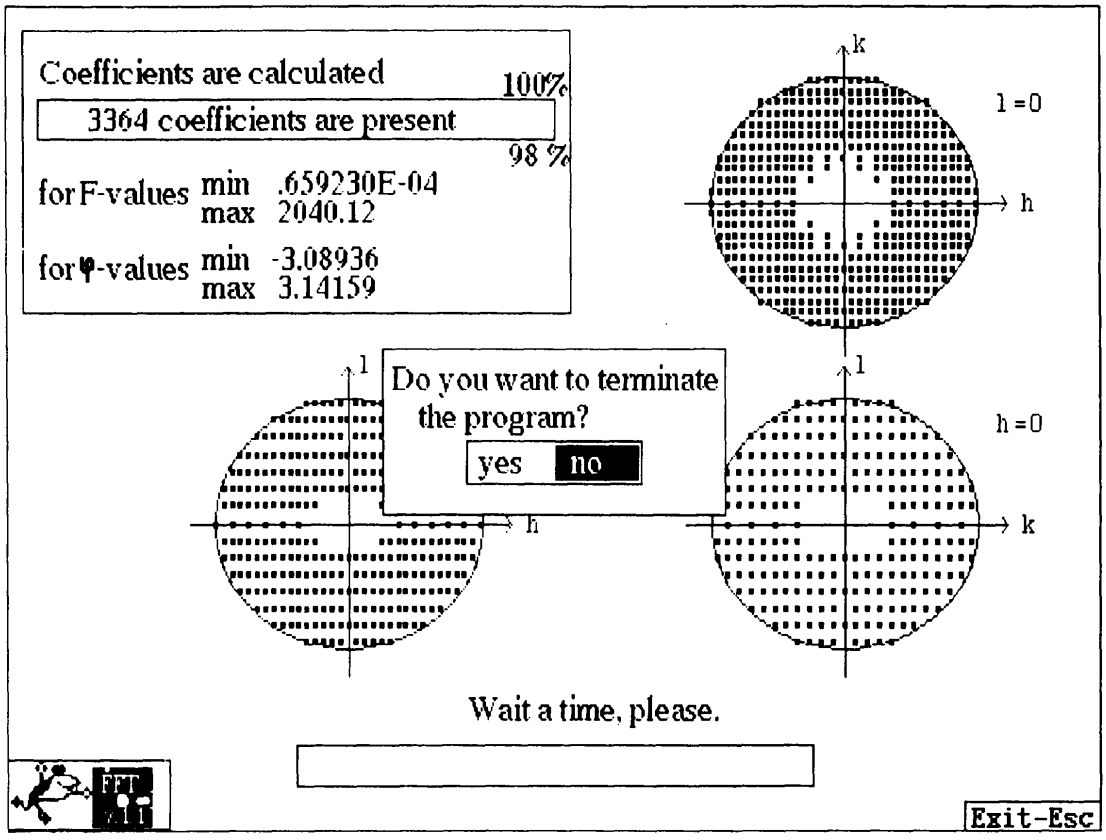

Fig. 3. The *FFT* program. (It takes about 2 min 45 s to calculate an 80 × 60 × 40 grid synthesis with an IBM PC-AT 386/387 computer.)

Concluding remarks

The programs described have been used for some years in the Research Computing Center, in the Protein Research Institute and in the Institute of Molecular Biology of the Russian Academy of Sciences. They are now used in the Laboratoire de Cristallographie Biologique (Institut de Biologie Moléculaire et Cellulaire, Strasbourg, France).

The *FAN* program is distributed by Applied Biomathematics (Exeter Software, 100 North Country Road, Setauket, New York 11733, USA). The programs *CAN*, *FANS* and *FFT* are available by sending a self-addressed envelope containing a $5\frac{1}{4}$ in diskette to the authors.

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References

Chirgadze, Yu. N., Brazhnikov, E. V., Nikonov, S. V., Fomenkova, N. P., Garber, M. B., Urzhumtsev, A. G., Lunin, V. Yu., Chirgadze, N. Yu. & Nekrasov, Yu. V. (1991). *Dokl. Acad. Nauk SSSR*, **320**, 488–491.

Mathews, F. S., Levine, M. & Argos, P. (1971). *Nature (London) New Biol.* **233**, 15–18.

Richards, F. M. (1968). *J. Mol. Biol.* **37**, 225–230.

Ten Eyck, L. F. (1973). *Acta Cryst.* A**29**, 183–191.