Daresbury Laboratory

JOINT CCP4 AND ESF-EACBM NEWSLETTER ON PROTEIN CRYSTALLOGRAPHY

An informal Newsletter associated with the SERC Collaborative Computational Project No.4 on Protein Crystallography and the ESF Network of the European Association of the Crystallography of Biological Macromolecules.

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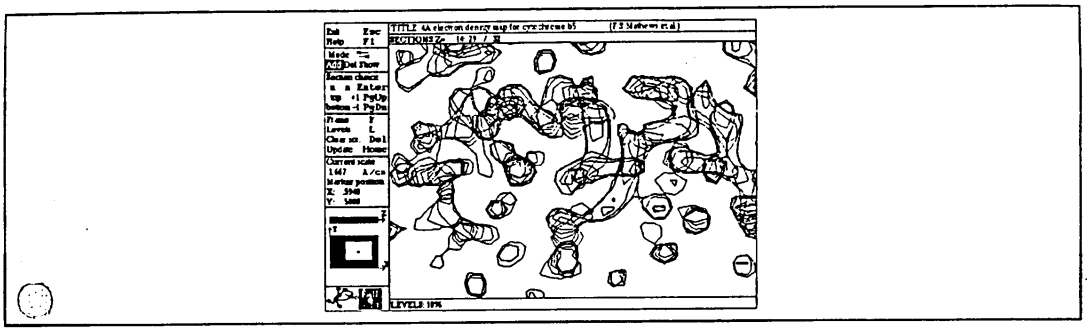
FAN
Scalar Field Analysis

FAN is a utility program especially useful in crystallography research. FAN was developed at the USSR Academy of Sciences especially for studying lattice functions which depend on three variables such as scalar fields and three dimensional distributions. FAN is the first microcomputer program of its type to let you display functions by isolines in two-dimensional sections of real physical space. Using FAN you can interactively explore the structure of your function by changing perspective or scale. FAN also lets you map functions in space by periodicity and display functions defined in oblique coordinate systems.



FAN works by letting users graphically explore fucntions. In the FAN graphical interface you can

⇒ change the set of displayed isoline sections,
⇒ change the scale values and viewing frame position,
⇒ control the colors of the displayed isoline sections,
⇒ view function sections in any orientation,
⇒ remove, replace or add single isoline sections,
⇒ magnify or reduce of function images.

FAN has built-in algorithms to process very large data sets and it can convert ASCII and binary data files to its own compact file structure.

FAN was written by Drs. E.Vernoslova and V. Lunin, of the Research Computing Center, Academy of Sciences of the USSR.

IBM PC or compatible;
DOS 3.3+; 512K RAM;
Hercules/ /EGA/VGA;
Math coprocessor.

Cost: $99
Site license: $195

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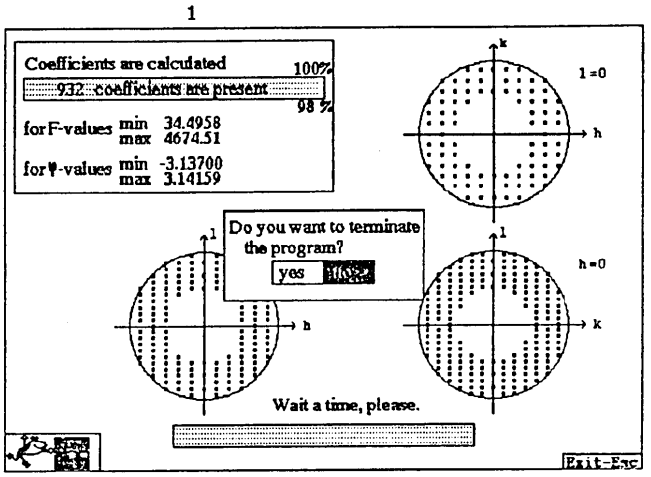
Available from: Exeter Software, 100 North Country Road, Setauket, New York 11733, USA.
Phone: (800)-842-5892 or (516)-751-4350. FAX: (516)-751-3435.

F F T

Discrete Three-Dimensional Fourier Transform

FFT (Fast Fourier Transform) is a convenient tool for calculating discrete three-dimensional Fourier transform in crystallography. FFT enables you to calculate Fourier and Patterson syntheses, difference Fourier and difference Patterson syntheses in a several formats. Program has a user-friendly interactive regime for input of all necessary parameters. FFT can calculate synthesis in any space crystallographic group, in any crystallographic axes orientation. The missing of structure factors is under control when synthesis is calculated.



Requirements: IBM PC or PS/2 compatible, DOS 3+, 512K RAM, and EGA,VGA or Hercules monochrome graphics monitor.

FFT was written by E.A.Vernoslova of the Pushchino Computing Center of the Academy of Sciences, USSR, and is one of the FROG-series of crystallographic IBM PC compatible programs.

C A N

Comparative Analysis of Three-Dimensional Functions

CAN is a microcomputer program especially useful in crystallography research, designed for visual investigation independently or at a time images of three objects:

- two lattice scalar function depending on three space variables;
- a protein molecule's atomic model.

The analyzing function is performed in the form of the set of function values calculated at the points of a grid in three dimensional space. The atomic model is determined by a set of atoms coordinates and displayed as s sceleton model's projection into the screen, where atoms are presented by globules and chemical bonds - by segments.

CAN makes it possible:

- to display at the screen the picture of the specified isolines in the one chosen section or in a number of sections;
- easy change the set of displayed sections (add/delete/replace);
- to change the scale of the picture (to "magnify" / "diminish" desired fragment) and move the frame into the desired region;
- easy vary the set and colours of displayed isolines (to change isoline levels for any values);
- to determine relative coordinates of any point of the screen;
- to depict a function by sections along any of coordinate axes;
- to display the skeleton model at the screen;
- to move and to rotate the model's image as a rigid body with respect to the analyzed main function.

Requirements: IBM PC or PS/2 compatible, DOS 3+, 512K RAM, EGA or VGA grahpics monitor.

CAN was written by E.Vernoslova and V.Lunin ,Reseach Computing Center, Academy of Sciences, Pushchino, Moscow Region, RUSSIA, and is one in FROG-series of crystallographic IBM PC compatible programs.