

CCP4 NEWSLETTER ON PROTEIN CRYSTALLOGRAPHY

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Tcl/Tk-based programs. I. CONFOR : user-friendly converter for crystallographic data files

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1. Introduction.

Different crystallographic program packages do not always use the same formats of the crystallographic data files of structure factors, electron density maps or atomic models. However, the data interchange between them is important in order to optimise the process of structure determination, and corresponding service software has been developed in different laboratories for this purpose, for example by Heinemann (1992) for the atomic coordinates and by the Uppsala group (Kleywegt & Jones, 1996) for different data.

A major part of the current crystallographic software is based on the idea of macrolanguage and macrocommands and not on the modern principles of menus. The first reason for this "delay" is the significant computation time for many of the crystallographic programs which makes ineffective their run in interactive mode. The second reason is the variety of different types of computers with different graphic interfaces where the packages are used.

Tcl/Tk (Ousterhout, 1993) is an universal interpreting language in which scripts can be ran with no changes at different types of computers. These scripts allow to run any combination of command and executable files depending on their results and pressed keyboard buttons. The Tcl/Tk is both very powerful, convenient for use and easy to program.

A program to reformat the crystallographic data files can be taken as an example of the software, which could be used at any computer and which is short enough to be ran in the interactive mode. Moreover, during its run a user needs to make several choices : name and type of the files, etc.

These conditions allow to include such program in a list of ones for which an effective interface based on the Tcl/Tk language can be developed. Such series of programs is under development in the UPR de Biologie Structurale, and some first results are reported below.

2. Program description.

The program CONFOR allows to change the format for three types of crystallographic data: structure factors, electron density maps and atomic coordinates. The choice of the type of data is defined by a radiobutton on the screen menu (Fig.1), and the following choice of the file is carrying out by clicking in the list of the files like in Microsoft programs.

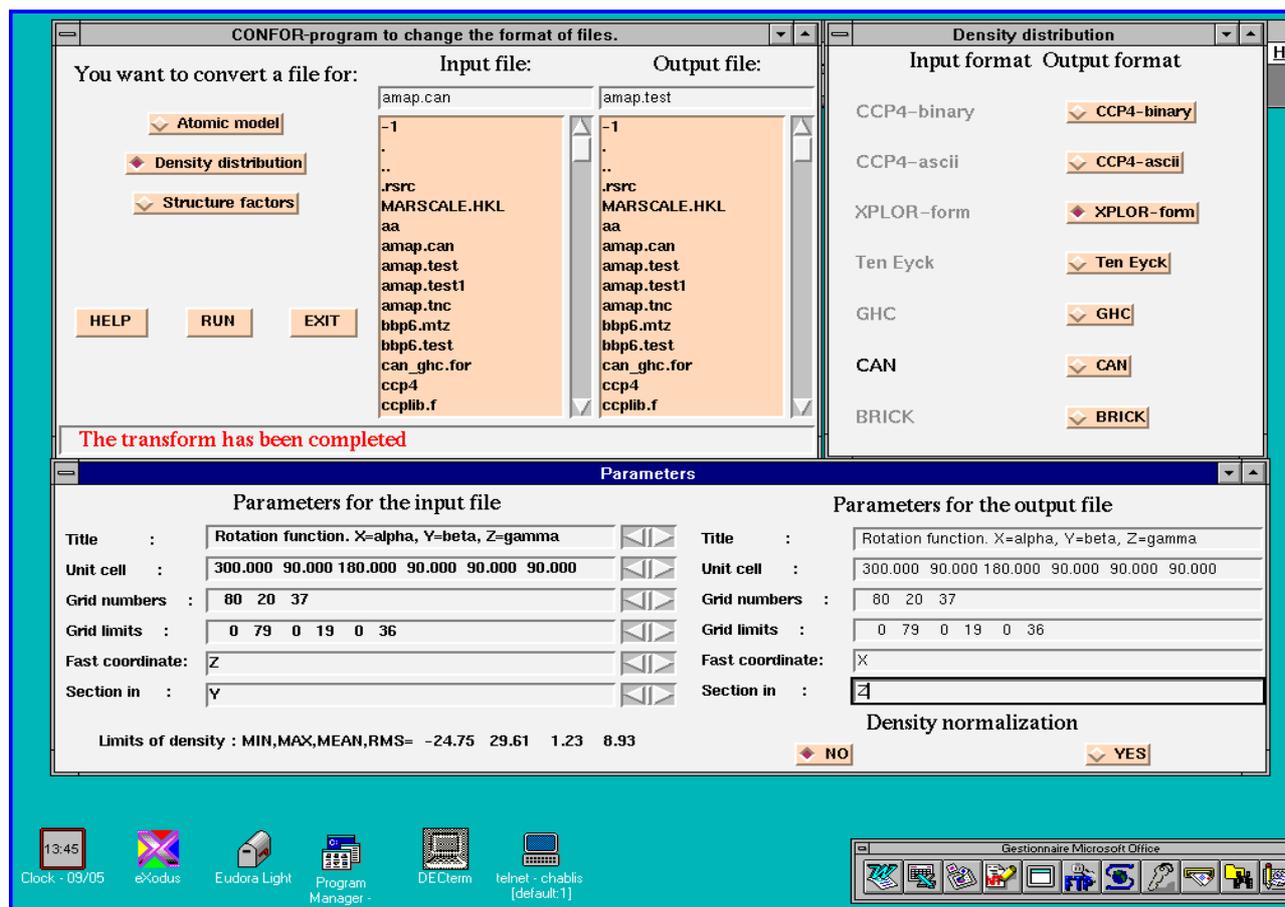


Fig.1. Example of the CONFOR application to change the format of the map file from CAN to X-PLOR with changing the map orientation. [Click on figure for full size image.]

For the map files, the program can normalise the function of the electron density distribution and change the orientation and the limits of the map. For the structure factors, the data values can be reassigned, e.g., for the X-PLOR format (Brünger, 1992) FPART amplitudes can be assigned to FCALC or to FOBS ones. The current version of the program does not yet allow to make any other data transformation, which is supposed to be included in the following versions.

The format of the input file is defined automatically, and the format of the output file and necessary data transformations are chosen from the menus.

The program calculates major statistical information for the data (limits of the model coordinates, minimal and maximal density values, etc).

Any number of files of any type of data can be processed during the same run of the program.

The current version of CONFOR recognises the following input/output formats:

- a) for the structure factors
 - X-PLOR (Brünger, 1992)
 - MARSCALE (Kabsch, 1988)
 - UF (Urzhumtsev et al., 1989, Vernoslova & Lunin, 1993)
- b) for the electron density maps
 - X-PLOR (Brünger, 1992)
 - CCP4-binary (CCP4, 1994)
 - CCP4-ascii (CCP4, 1994)
 - "bricks" (Jones, 1978; Jones et al., 1991)
 - Ten Eyck (1973)
 - GHC (Cohen, personal communication)
 - CAN (Vernoslova & Lunin, 1993)
- c) for the atomic models
 - PDB (Bernstein et al., 1977)
 - PROLSQ (Hendrickson & Konnert, 1980)

The subroutines for other formats, e.g., for the MTZ format of structure factors file, are under development.

The standard Tcl/Tk libraries are necessary to interpret the CONFOR script which calls the basic programs written on standard FORTRAN-77. The CCP4-formatted files are read/written using the CCP4 standard subroutines. The program is available by request from the authors. The corresponding e-mail address is sacha@igbmc.u-strasbg.fr.

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