CRYSTALLOGRAPHIC FORTRAN MODULES LIBRARY (CFML): A SIMPLE TOOLBOX FOR COMPUTING PROGRAMS

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We have developed a set of Fortran 95 modules that may be used (in the Fortran 95 sense) in crystallographic and diffraction computing programs. Modern array syntax and new features of Fortran 95 (and soon Fortran 2k) are used through the modules. We take advantage of all object oriented programming (OOP) techniques already available in Fortran (user-defined types, encapsulation, overload of procedures and functions). The lacking features (e.g. inheritance and class methods) will be easily implemented as soon as they become available in the forthcoming new standard. We aim to preserve the efficiency, the simplicity and the adequacy of modern Fortran for numerical calculations. All aspects of symmetry and handling of reflections are treated in dedicated modules. Main programs using the adequate modules may perform more or less complicated calculations with only few lines of code.
The present library contains procedures for generating space groups from their Hermann-Mauguin or Hall symbols for whatever setting. More generic space groups with non-conventional lattice centering vectors can also be built using user defined generators. Reflection handling modules may be used for generating reflections in selected regions of reciprocal space and for calculating structure factors. The documentation is written in the source code. A document, in HTML format, containing the description of all modules and procedures can be generated using a program based itself on CFML. The source code will be put in a Web site in order to be accessible for people wishing to use/develop the modules in a collaborative team.

Keywords: COMPUTER PROGRAMS, SYMMETRY, CRYSTALLOGRAPHIC CALCULATIONS

THE ULTIMATE FAST FOURIER TRANSFORM FOR CRYSTALLOGRAPHY

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So far, there has been no general space-group efficient implementation of Fast Fourier Transform (FFT). Such algorithms should operate only on the asymmetric unit and should have comparable speed to P1 FFT transform of the same amount of data. This problem has already been partially solved by Ten Eyck about 30 years ago [1]. Subsequently, it has attracted lots of attention and more than 20 research papers have been devoted to this issue. In particular, a general approach has been proposed by Bricogne [2], but without a clear picture how to design algorithms for a large number of space groups.
We have developed a different approach to crystallographic FFT, that results in easy-to-implement algorithms for all 230 space groups. Implementation already exists for over a hundred cases (including previously unsolved) and other will be programmed soon.
The algorithms described are significantly faster than existing ones. Their use will allow to perform more Fourier cycles, eventually resulting in more accurate solutions of the phasing problem.
References
[1] Ten Eyck, L. F.: Crystallographic Fast Fourier Transforms, Acta Cryst A29, 183-191 (1973).
[2] Bricogne, G.: Fourier Transforms in Crystallography, International Tables for Crystallography, Part B, 1996. This work is supported by NIH grant GM 53163.

Keywords: **ALGORITHM, FFT, SYMMETRY**

DERIVING PROTEIN FLEXIBILITY FROM CRYSTAL STRUCTURES - NEW TOOLS FOR AN OLD PROBLEM

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Understanding macromolecular function often relies on the comparison of different structural models of a molecule. In such a comparative analysis, the identification of the part of the molecule that is conformationally invariant with respect to a set of conformers is a critical step, as the corresponding subset of atoms constitutes the reference for subsequent analysis for example by least-squares superposition.
A method is presented that categorizes atoms in a molecule as either conformationally invariant or flexible by automatic analysis of an ensemble of conformers (e.g. crystal structures from different crystal forms or molecules related by non-crystallographic symmetry). Different levels of coordinate precision, both for different models and for individual atoms, are taken explicitly into account via a modified form of Cruickshank's DPI [1]. and are propagated into error-scaled difference distance matrices [2]. All pairwise error-scaled difference distance matrices are then analyzed simultaneously using a genetic algorithm [3].
The algorithm has been tested on several well-known examples (e.g. Aspartase Aminotransferase, Epimerase, Immunoglobulins) and has been found to converge rapidly to reasonable results using a standard set of parameters. Furthermore, a criterion is suggested for testing the identity of two three-dimensional models within experimental error without any explicit superposition.
References
[1] Cruickshank (1999), Acta Cryst. D55, 583-601.
[2] Schneider (2000), Acta Cryst. D56, 715-721.
[3] Schneider (2002), Acta Cryst. D58, 195-208.

Keywords: **LEAST-SQUARES SUPERPOSITION GENETIC ALGORITHM STRUCTURE COMPARISON**

FURTHER ENHANCEMENT OF SYSTER AND SYSTERPLOT, A TOOL TO EVALUATE SYSTEMATIC ERRORS

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Detailed insight into the differences between F_o and F_c and the underlying reflection data as a function of measuring order, Θ, F_o or position in reciprocal space can be very helpful during the validation of a structural model. It can show drifts and trends that may point to systematic errors related to instrumental malfunctioning, data reduction problems, wrong absorption correction or errors in the structural model. Therefore we continue to develop two programs, called SYSTER and SYSTERPLOT, which together are able to show drifts and trends of F_o vs F_c with respect to a large variety of variables. SYSTER collects the data, which can be visualized by SYSTERPLOT. Not only has the latest version of SYSTER been made more flexible, which means that it is up to the user to decide which parameters and functions are to be used in SYSTERPLOT, but also has their functionality been extended. Now the programs can be used to show and evaluate diffraction data outside the Bragg reflections, e.g. satellite or superstructure reflections, or even 'unconventional special-purpose' powder diffraction data, e.g. to evaluate preferred orientation. And SYSTER is no longer dependent on SHELXL output, which means that it is less dependent on the local computational environment. The programs are written in FORTRAN for speed and flexibility but use Visual Basic for the GUI. They are available as Windows 95/98/ME/NT applications, a UNIX version with an OpenGL GUI is being contemplated. The executables are available, free of charge, from
http://www-xtal.sci.kun.nl/documents/software/syster.html
http://www.crystallography.nl/documents/software/syster.html

Keywords: **SYSTEMATIC ERRORS DATA EVALUATION ERROR VISUALIZATION**