02-Methods for Structure Determination and Analysis, Computing and Graphics

02.08 – Crystallographic Computing

OCM–02.08.01 HYPERTEXT FOR CRYSTALLOGRAPHY by R.Diamond*, Medical Research Council, Laboratory for Molecular Biology, Hills Road, Cambridge, CB2 2QE, England and A Mummery, Oxford University Press, Walton Street, Oxford, OX2 6DP, UK

"Hypertext" designates a system of text and related material, prepared in machine readable form so that its presentation on a computer screen includes within it 'links' which enable the reader to invoke supporting material, references, figures etc. as he wishes, using a mouse or similar device to control the process. One such system, 'Molecular Structures in Biology', will be described both from the users' point of view and in terms of its internal construction, which is based on a 'web' which is a file defining many 'nodes' which may themselves invoke software to provide a pop–up reference, or another text, or graphics software or a stored bit map image etc. The web itself is traversed by software known as the 'spider' which puts into execution actions specified by nodes of the web. Such techniques, coupled with the high storage capacity of CD–ROM (600 Mbytes), provide an efficient means of publishing high–volume numerically intensive data, especially data with a high degree of permanence, as in data banks, where its crystallographic application seems most likely to be fruitful. MSB itself is both a textbook and a reference work, containing over 500 coordinate sets from the Protein Data Bank, plus twelve chapters of text exploiting hypertext techniques, plus many references, over 1000 illustrations (as bit maps), and the capability for the user to create an unlimited number of others.

OCM–02.08.02 IF WE CAN DO IT, YOU CAN DO IT: WRITING A GUI INTERFACE FOR A CRYSTALLOGRAPHIC PROGRAM by Paul N. Swepston* and Beverly R. Vincent, Molecular Structure Corporation, 3200 Research Forest Drive Woodlands, TX 77381 USA

Many crystallographic programs are still based on card–image input. The user is required to use a text editor prepare are instruction file for program execution. While this can be a simple effective means of program control, it fails to take advantage of modern software developments.
Examples will be given of graphical user interfaces (GUI) that have been developed for crystallographic programs using the MOTIF tool kit. Actual examples of source code will be shown in order to demonstrate easy it is to develop a modern graphical interface.

OCM–02.08.03 PC - A CRYSTALLOGRAPHIC COMPUTING TOOL FOR EXPERTS AND NOVICES. By V.K. Pecharsky, Dept of Inorganic Chemistry, L'viv State University, L'viv, Ukraine.

The choice of type of computer(s) for daily use in the laboratory for the tasks of diffraction-data processing, crystal-structure solution, refinement and final representation faces every crystallographer. For work on inorganic crystal structures and on small organic molecular structures (up to 100-150 independent atoms in the unit cell, with ca.1000 free least-squares parameters), personal computers (PCs) can be used very effectively. PCs have many advantages, viz: they are open and friendly systems, they can easily be used by students, by regular scientific staff and by experts, and their capital cost is low. With proper software and suitable user interface, success is assured for everyone. PCs are excellent tools for crystallographic computing today and probably in the future.

We will illustrate our experience with PCs by describing the software package CSD (Crystal Structure Determination) for crystallographic computing on single-crystal and powder, X-ray and neutron diffraction data developed over the past few years. It will be shown that the average time spent by a crystallographer in the solution and refinement of a crystal structure is significantly less than the time necessary to collect the diffraction data. It does not usually exceed 1-4 hours, depending on the number of free least-squares parameters. Over two thirds of this time is spent on the final stages of refinement.

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OCM–02.08.04
THE PROFILE FITTING IN SINGLE-CRYSTAL X-RAY DIFFRACTOMETRY. By Ewa Gałdecka, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul.Okólna 2, 50-950 Wrocław, Poland.

The whole-profile fitting that playes a fundamental role in crystal-structure determination from powder samples (the Rietveld method) is rather occasionally used for processing the single-crystal intensities [Clegg (1981). *Acta Cryst.* A37, 22-28 and 437; Oatley & French (1982). *Acta Cryst.* A38, 537-549]. Usually, the traditional background-peak-background procedure is considered to be sufficient in the latter case. The purpose of the paper is to work out a suitable method for approximation the single-crystal diffraction profiles and to test the effect of the careful data processing on the precision and reliability of the crystal-structure determination. The subjects of detailed considerations are such problems as criteria of the goodness of fit, the choice of the basic approximating function (shape function), the proper number of independent adjustable parameters, the dependence of parameters of the profiles on the Bragg angle and direction cosines of the diffraction vectors, and - recently discussed by Schwarzenbach & Flack [*Acta Cryst.* (1991), A47, 134-137] and Lenstra, Geise & Vanhouteghem [*Acta Cryst.* (1991), A47, 597-604] - treatment of the background and 'negative' reflections. The basis for the considerations is the papers mentioned above and two papers by the author [Gałdecka (1993). *Acta Cryst.* A49, 106-115 and 116-126]. Results of the present work are currently being incorporated into a computer procedure which approximates the diffraction profile and calculates the integrated net intensities. The newest results of the crystal-structure determination that includes the profile fitting, as compared with those obtained using the common approach, will be presented.

OCM–02.08.05 THE USE OF ORTHONORMAL FUNCTIONS FOR THE REPRESENTATION OF 3-DIMENSIONAL INFORMATION
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