PORTABILITY AND MACHINE SPECIFICITY: A DICHOTOMY FOR SOFTWARE PACKAGES

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Software packages are widely used in crystallography for reasons of convenience, economics and know-how. Rapid changes in computer technology, and the relative costs of computer time and manpower, have offset the advantages of developing efficient machinespecific software. Distributed packages place particular emphasis on the need for software portability. Unfortunately with existing packages portability has often been achieved at the cost of computational efficiency.

This is because portability and machine specificity have been treated as mutually exclusive properties. The FORTRAN language provides limited options for resolving this problem. In contrast the 'preprocessor' languages provide for both portability and machine specificity through the use of 'macros'. The application of the RATMAC preprocessor to the XTAL package (Hall, Munn & Stewart, Acta Cryst. A36, 979) will be outlined.

In conjuction with portability there is an increasing need for an integrated approach to the full spectrum of crystallographic problems. Crystal structure calculations on macromolecules and metals are similar in many respects except for the nature of the data. The XTAL approach to portable data management through the use of contiguous data storage, dynamic memory allocation and directory addressable archival files, will be discussed.


It is possible to write FORTRAN programs which are both transportable and efficient, provided that certain rules are obeyed. The author will describe his experience with a simple program for crystallographic data reduction, structure solution and refinement (SHELX), which has been installed on about 250 computers representing all major makes, in many cases without changing a single FORTRAN statement.

SHELX is entirely written in a very simple subset of FORTRAN, similar to PIGIN FORTRAN described by Stewart and Hall. Many problems affecting portability are avoided by NEVER using EQUIVALENCE, BACKSPACE, LOGICAL, double precision or complex variables, multiple dimension arrays, and subscripts other than 'I' or 'I+constant'. Subroutines are used sparingly and I/O is kept simple and buffered. A FORTRAN decoding routine enables free-format but machine-independent user input. Data are stored dynamically in a large one-dimensional array, which can easily be redimensioned to create small and large versions of the program. Sort-merge, direct methods and Fourier routines automatically make more use of scratch disc if less memory is available. Overlay may be used but is not essential: segmentation is also possible.

INDEXING ASYMMETRICAL LAUE PHOTOGRAPHS BY MINIDICOMPUTER. By H. V. Hart and E. A. Rietman, Department of Chemistry, University of North Carolina at Wilmington, Wilmington, N. C. 28406, U. S. A.

Recent computer solutions to the problem of indexing asymmetrical Laue photographs have been limited to maximum Miller indices of about 3 and a maximum number of reflections of about 10 and have required large amounts of time on a large computer. A more efficient algorithm has been programmed in BASIC for use with the Hewlett-Packard 2000/Access System, a 32 user time-shared minicomputer with 64K words of core memory. The programs will index asymmetrical or symmetrical (no photograph symmetry is used), transmission or back-reflection Laue patterns of any crystal. Computational steps are:

(1) Spot coordinates are reduced to film coordinates of the reflecting plane normals with the equations of Bernste (Acta Cryst. (1963), 19, 916), from which direction cosines of major zone axes are computed by a linear least-squares method. The reflecting plane normals in a zone are coplanar and therefore intersect the film on a straight line. The zone axis is the normal to the crystal plane which intersects the film plane in this straight line. Experimental interaxial angles are computed from the dot product of the zone axis direction cosines.

(2) Zone indices are determined (before Miller indices) by a trial-and-error search of interaxial angles computed from a master file of zone indices and orthogonal direction cosines prepared for each substance from its unit cell parameters.

(3) The zone law is used to determine the Miller indices of spots at the intersections of the major
18.1-02 IDENTIFICATION OF THE METRIC SYMMETRY OF A LATTICE BY FINDING ITS EVEN-ORDER SYMMETRY AXES.

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The present approach is based on the identification of even-order symmetry axes (EOSA) according to the following three points: (1) A row [h*] is an EOSA of a lattice if and only if there is a reciprocal row [p*] such that h* x p* = 0 with h* ≠ 1 or 2; (2) If the lattice is referred to its 3 shortest non-co-planar translations, the moduli of the Miller indices [h*] and [p*] cannot be larger than 2; (3) A lattice symmetry is uniquely determined by the number and distribution in space of its EOSA.

The first two points allow an exhaustive list of the EOSA in the lattice to be made. Comparison of this list with the lattice symmetry to be identified according to point 3. By this process, the lattice is placed in a conventional orientation and the selection of the edges of the conventional cell is guided by the coincidence of lattice rows with pre-determined symmetry axes. Some advantages over the traditional approach summarized in International Tables (1969) Vol. 1 pp. 530-535 are: The recognition of the lattice symmetry can be accomplished by one logical process rather than 44 branches; Pseudo symmetry in the primitive cell can be handled in a straightforward way; A Buerger reduced cell rather than the Niggli reduced cell is required; No metric considerations are built into the recognition of the lattice symmetry. Metric conventions in orthorhombic, monoclinic and triclinic are handled separately.

The program runs on PDPS-E, PDP11 and CDC 7400 computers and has been inserted as an overlay in the NRC Fortran diffractometer program.

18.1-03 INTELLIGENCE ARTIFICIELLE ET MESURES DE PIC

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On sait [1] que chaque observation permet l'affinement
immediat de toutes les variables descriptives du
phenomene physique qui lui a donne naissance. Cette
re-
marche conduit a la construction dun algorithme
generale [2] permettant a la fois le traitement des donnees
experimentales et le choix des conditions d'acquisition
suboptimales. L'emploi de cet algorithme evite de consa-
crer beaucoup de temps aux observations peu efficaces.

Pour optimiser il faut definir un critere qu'on
cherchera a rendre extremal. Le criterie choisi est le
gain d'information apporte par chaque observation sur une
combination lineaire des inconnues. On aboutit alors a l'algorithme suivant.

Ayant choisie la combinaison lineaire <c|> dont on
veut optimiser la mesure ayant les valeurs |<c|> a priori de
et la matrice d'erreur E relative a ces estimations.

1°) Pour chaque observation possible a) calculer son
esperance et l'esperance de son vecteur gradient a
par rapport aux inconnues estimees = E^p(y||z>)

b) calculer pour le temps d'observation y la quanti-
té

γ = qa + t<q|E|a> <c|>

c) determiner l' observation qui fait decroitre le
plus vite l'ecart type sur <|c|> c'est l'observation
qui presente le <c|> ou γ <c|> E||a>^" maximum.

2°) Effectuer cette observation.

3°) Calculer les nouvelles estimations |<c|> des in-
connues et leur matrice d'erreur E selon la formule de
réestimation lineaire [1]:

E = E - qa + t<qa|E|a> <c|> a

4°) Si la variation de |<c|> est deraisonnable ou
aboutit a des valeurs de |<c|> deraisonnables, effectuer
une réestimation non lineaire des inconnues [2]

5°) Si la precision obtenue n'est pas suffisante et
la duree totale acceptee pour l'ensemble des observa-
vons n'est pas epuisee revenue en 1°).

6°) Fin

Une application a la recherche, la determination et
l'affinement des caracteristiques intensite, position,
largeur, dissociometrie) de pic est presente.

3 Tournarie M. (1978), Cybernetica_21, _3, 227-262