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Computer Science and Crystallography

Information generated within one discipline often remains unknown in others for extended periods, despite the possibility of clear and sometimes urgent relevance, as illustrated by two important examples taken from the history of crystallography. The method of least squares has been known to mathematicians since Legendre's book was published in 1806, and had been regularly taught to classes in numerical data analysis by E. Whittaker and others since 1913 or earlier. Until E. W. Hughes introduced the method into crystallography in 1941, crystal-structure refinement was carried out exclusively by various Fourier techniques. Least-squares refinement remained uncommon as late as 1950, partly owing to computational difficulties but mostly to general unfamiliarity with the method. The now widely recognized importance of the method is easily verified by perusal of *Acta Crystallographica* Section B in which it is used in nearly every paper.

The second example comes from experimental crystallography. Until the late 1950's, the principal counter used in X-ray diffractometry was the Geiger–Müller tube. A scintillation counter in its modern form, using ZnS and a photomultiplier tube, was introduced into nuclear physics by S. C. Curran in 1944; NaI(Tl) and a photomultiplier tube was first used by R. Hofstadter in 1948. A decade or more elapsed before the scintillation counter was applied to crystallography, where its use is now nearly universal.

The Committee on Chemical Crystallography of the National Academy of Sciences – National Research Council has for some years been concerned with improving communications between crystallography and other disciplines. In 1973 it sponsored an interdisciplinary conference that resulted in the book *Critical Evaluation of Chemical and Physical Structural Information.** Realizing the probable importance to crystallography of the rapid progress currently being made in the field of computer science, the Committee on Chemical Crystallography arranged a one-day symposium on the 'Application of Current Advances in Computer Science to Crystallography' in conjunction with the 1976 winter meeting of the American Crystallographic Association in Clemson, South Carolina. The symposium was made possible by support from the National Science Foundation. Of many possible topics, the following four were selected as important for crystallographers.

– The design and application of algorithms for increasing computational efficiency.

– The application of artificial intelligence to experimental problems.

– The use of interactive computing in experimental measurement.

– The optimum use and selection of various sized computers.

Experts in these topics were invited to speak at the symposium and, since their talks were expected to interest a much wider audience than could come to Clemson, to submit manuscripts based on their talks and the ensuing discussion for publication in *Acta Crystallographica.* Each manuscript has been subjected to critical comment by at least two referees, one from the field of computer science and the other from an appropriate branch of crystallography.

The Committee on Chemical Crystallography [S. C. Abrahams (Chairman), J. Bregman, C. K. Johnson, G. G. Johnson Jr, K. Eriks and D. H. Templeton] hopes that the following four papers will be stimulating for crystallographers and will, indeed, help close the gap between some branches of computer science and crystallography.

S. C. Abrahams

Bell Laboratories
Murray Hill
New Jersey 07974
USA

* Available from the National Academy of Sciences, Printing and Publishing Office, 2101 Constitution Avenue, N.W., Washington, DC 20418, USA.