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Book reviews

Computational Methods for Large Molecules and Localized States in Solids, Edited by F. Herman, A. D. McLean and R. K. Nesbet, 1973; 396 pages. (*Plenum*, 1973.)

This volume contains the proceedings of a symposium held on 15-17 May, 1972, at the IBM Research Laboratory, San Jose, California. To judge from the preface, the (unlisted) participants were nominally international, but in practice predominantly American. Certainly the active contributors were almost all, if not themselves American, then currently working in the USA at the time of the symposium. European work is thus rather under-represented; nevertheless one should recognise that most of the work in this field is indeed done where most of the big machines are—i.e. in the USA! Consequently the contributors to this volume do after all comprise a powerful assembly of the most active and creative workers in the field.

The leading motive of the symposium was the recent convergence of concepts and techniques between quantum chemistry and solid-state physics. Each of these deals with electron energies and wave-functions, satisfying the Schrödinger equation in the presence of an array of atomic nuclei. They have grown apart, over the last 40 years, because solid-state theory copes with infinite lattices by means which rest on their periodicity, while quantum chemistry handles a general atomic geometry at the expense of a restriction to structures of rather small size. Recently, however, solid-state theory has begun to grapple with non-periodic structures (amorphous solids, and localised defects) for which some 'chemical' techniques have been required, while also the simplifying devices developed in solid-state theory, to represent atomic potentials in a more compact way (e.g. the various pseudopotentials) have been tried out in quantum chemistry. The convergence of the two fields is thus a real and fruitful thing. This symposium was designed to help it forward.

Each day of the conference was devoted to a different topic: Scientific challenges, Computational methods, and Localized states and disordered solids. The first day (Scientific challenges) was entirely chemistry, and indeed something of a rag-bag; the general theme was to show the wide variety of problems currently under attack, picking especially those which were still at an early stage of development, computationally at least, if not also conceptually. As a result J. A. Pople's clear survey of computational success on small molecules rather stood out, and would perhaps have fitted better into the second day. So, in another way, did W. A. Little's contribution on 'Molecular Modelling': he was the only speaker dealing with minicomputers, which were all he required (plus a graphic display) for his interactive geometrical modelling programs.

For the would-be computer, day 2 provided the richest meat. Quantum chemistry (and its traditional methods, pushed to their limits) held sway in the morning, while the afternoon was begun with two techniques, originated by solid-state workers, but with molecular problems in mind. (K. H. Johnson: SCF-Xα scattered wave method; W. A. Harrison: orbital correction method.) These were followed by a panel discussion on computational methods. This runs to twenty pages of the book, and makes many useful points. (It goes far to make up for the lack of recorded discussion on any of the individual contributions.) Two extreme examples came up in the discussion, both emanating from the host laboratory. On the one hand was a 500-configuration calculation of the carbon atom, accurate to 3 milli-Hartrees of correlation energy. On the other was a 28-atom ab-initio minimal-basis calculation (on 2,4,7-trinitro-9-fluorenone) which involved 120 basis functions and 11 million integrals. After the discussion of this work K. H. Ruedenberg remarked 'The lesson to be learned is: If even IBM cannot afford hundreds of calculations of this size in one year, then one should think very carefully on which big molecules such a tremendous effort should be expended . . .' The participants could not finally answer this challenge, but they had much of interest to say about it.

Solid-state problems were represented on day 3. The clearest paper here was the excellent review of amorphous semiconductors by D. Weaire and M. F. Thorpe, but though rich in concepts this was poor in computational methods. It raises however (to the reviewer) the prospect of further computer experiments on the structure (especially the ring structure) of the random networks they were discussing, or indeed of any other models of amorphous solids. The paper by J. Keller on cluster scattering was by contrast rich in computable ideas (though one would need to go back to Keller's references to define them fully).

The book closes with a banquet address by G. S. Hammond, (centred on the role of 'cults' and fashions generally, in science) and lastly a useful summary of the conference by R. K. Nesbet.

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Management Systems, by Peter P. Schoderbeck, 1971; 561 pages. (*John Wiley & Sons Ltd*, £5·65.)

This book belongs to the Wiley Series in 'Management and Administration' and as such is aimed at the manager interested in computing rather than the computer specialist. I am therefore not completely convinced that the *Computer Journal* is the correct place for this book to be reviewed or that I am completely competent to judge this book in its entirety. However with those reservations in mind let us proceed . . . .

Management Systems attempts to encompass a wide range of material from the highly theoretical 'general systems concept' to the practicalities of PERT and the SABRE system. The book, a compendium of papers, is divided into three major parts: The system concept, Management information systems and Systems applications together with a short section entitled Prologue to the future. The three major parts are divided into sections each of which is composed of an editorial, a collection of papers and a bibliography.

Overall I found the book interesting although the first part (The system concept) was an uphill struggle possibly because of lack of the necessary theoretical background. I had hoped that Management information systems would provide some interesting practical papers but my hopes were dashed with the exception of one paper by Konvalinka and Trentin. When I finally reached the third part of the book (Systems applications) this proved to be the most rewarding. The five papers in the PERT section presented a balanced view of the subject and set a standard which the rest of the book should have achieved.

Each section contained a selection of papers which were chosen so that the subject was viewed from different angles by a variety of authors. For example the section on Industrial Dynamics contained three papers; the first two by J. Forrester and E. D. Roberts (both of MIT) extolling the virtues of ID and the third by Ansoff and Stevin trying to assess the subject impartially and in consequence challenging some of Forrester's assertions. Some of the papers selected seemed to me to be rather too dated to be relevant today although there are always exceptions: Stafford Beer's paper on 'What has Cybernetics to do with Operations Research' is still interesting although first published in 1959. However a section on Information technology and its impact on the organisation consisted of six papers, three of which were very neatly summarised in a fourth within this same section! Design, implementation and control of MIS—a promising title for a section I originally thought—contained no paper published later than 1964 and seemed particularly irrelevant

I cannot recommend this book for the shelf of the computer specialist or as a textbook for computer science. I enjoyed reading it but doubt whether it will prove useful except perhaps for the extensive bibliographies which provide pointers to other background readings in the management and computing area.

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