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Foreword

In this issue we are pleased to present the proceedings of the Symposium on Parallel Computing for Chemical Reactivity, held in Perugia, Italy, on August 31 and September 1, 1990. We are grateful to the Symposium organizer, Antonio Laganà, for serving as guest editor of this issue.

Donald G. Truhlar

Preface

Advances in accurate and high-level approximate theoretical formulations of molecular collisions and progress in computer technology are making possible extensive numerical studies of realistic systems starting from first principles. This is relevant to the understanding of reactive features of elementary chemical processes as well as to the modeling of the physicochemical subsystems of several modern technologies.

On the theoretical side, advances have been concerned with *ab initio* calculations of the potential energy and with the three-dimensional quantum treatment of the reactive dynamics. *Ab initio* methods have become powerful enough to allow a description of the reactive evolution of a molecular system converged to the level of chemical accuracy at least for light three-atom systems. Three-dimensional treatments of reactions have become so accurate that theoretical estimates of reactive properties can be used as a sensitive measure of the accuracy of a proposed potential energy surface. To this purpose, time-independent methods are already well established. Using this technique, several systems have been investigated in detail. Time-dependent techniques are also becoming quite popular for treating reactive processes.

On the computing side, the progress has become even more impressive since the advent of vector and parallel architectures. Two years ago we had another meeting on Supercomputer Algorithms for Reactivity, Dynamics and Kinetics of Small Molecules. That meeting, a NATO workshop, was mainly focussed on designing computer codes for treating reactive systems so as to take advantage of the vector features of large supercomputers. Now, only two years later, the evolution of parallel architectures has become dramatic enough to ask for another meeting. Peak speeds of Giga and Teraflops are presently achievable by distributing the program on concurrent processors when the computer code has been restructured (and sometimes fully redesigned) to efficiently load the available processors and not congest communication channels.

Therefore, while there is no doubt that the scientific community is well aware that parallelism is a winning trend in computing, a great effort has still to be paid to convince people to port their applications onto parallel architectures. This will have the immediate consequence of making feasible calculations that are otherwise impossible to perform. What is more, this will make theoretical chemistry

an area of development for parallel hardware and software. This will reinforce the role chemistry plays in fueling scientific and technological growth.

In this respect, the investigation of chemical reactivity has all the needed requisites for stressing the architectural features of parallel computers. Various theoretical approaches may have different critical needs regarding the size and organization of the memory, the number and connectivity of processors, the balance between processor and communication channels load. These issues are addressed to some extent in many of the enclosed contributions presented at the meeting. We hope, therefore, that the meeting, which was made possible by the generous support of the National Research Council (CNR) and IBM, and also this issue of *Theoretica Chimica Acta* will together serve as a little but useful step towards a better understanding not only of the role that parallel computing can play in chemical research, but also of the role that chemical research can play for the development of parallel computing.

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