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Introduction: Parallel Computing in Chemical Physics

This international workshop was held at Argonne National Laboratory, July 17–19, 1991. It was jointly organized by the Theoretical Chemistry Group, Argonne National Laboratory, and the Molecular Science Research Center, Pacific Northwest Laboratory. Funding was from the ANL Physical Research Theory Institute Discretionary Funds, and Battelle Pacific Northwest Laboratories.

Massively parallel computers have the potential for dramatically increasing the scope and accuracy of molecular simulations, allowing us to address problems which were heretofore intractable. The challenge is to develop the software which will take full advantage of this emerging capability. One can now point to calculations and results that would not have been feasible or affordable on conventional computing resources. Timely dissemination of such results and experience is extremely valuable given the rapid evolution we are witnessing in both software and hardware.

To emphasize the widening gulf between serial and parallel computer power consider the capability that several vendors project for their top-of-the-line products by 1995. These machines will comprise up to thousands of processors, several giga-words of memory, tera-bytes of disk space and sustain a *useful* computation rate in excess of one tera-FLOP/s. This technology is being driven by use of inexpensive commodity parts and is expected to cost no more than current supercomuters.

The objectives of the workshop were to encourage productive interaction between groups actively using highly-parallel machines in their research and to publish a collection of papers representing the direction and state of such research. The approximately forty participants represented a broad spectrum of chemical-physics (simulation of condensed phases, *ab initio* electronic structure, quantum dynamics, quantum Monte Carlo, molecular modeling) and included leading computer scientists specializing in parallel computing.

Of most widespread interest was discussion of requirements for future generations of parallel machines which varied quite markedly with application area. Much improved message-passing bandwidth and latency seem fundamental requirements for molecular dynamics, increased local memory and disk bandwidth for *ab initio* electronic structure and raw computer power for Monte Carlo simulations. A general consensus was that software tools and system support from all vendors were woefully inadequate but there was little agreement about appropriate programming paradigms. This is one of many open research questions which also include fundamental theoretical and algorithmic issues.

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