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The Teraflop Supercomputer

BY GEOFFREY FOX

y the year 2000, the inexorable advances in computer technology will lead to supercomputers with sustained performance of a teraflop (1012 floating point operations per second) on a wide variety of scientific and engineering computations. This assertion may not be accepted by all and, in any case, glosses over much important detail. Some applications will realize this performance several years before the year 2000, others not until later. What will be the architecture of our teraflop supercomputer? Probably several designs optimized for different applications will be needed. However, surely this machine will be a massively parallel computer.

Many have speculated on the emergence of computation and simulation as a third approach to science joining the traditional experimental and theoretical methodologies. However at the moment, computation is at best a very junior partner and is more usually regarded as a rather tiresome tool to help theory or experiment. The teraflop supercomputer and its associated gigaflop workstation on your desk could change this. The year 2000 could see computation recognized as a respectable and essential approach to science. In physics, we will see convincing ab initio calculations of gauge theories, the design of new materials by computer, the compelling studies of phase transitions in a range of condensed matter systems and accurate studies of full globular clusters.

High performance hardware is inevitable, but this is not sufficient for our computational revolution. We need productive software for parallel advanced architecture computers. Currently, this is not available but the computer science community has recognized the problem. We expect increasing research on languages, software tools and programming environments which should lead to major improvements by the year 2000. It will be harder to find scientists trained and willing to use powerful parallel supercomputers. This is a major challenge to universities at both the undergraduate and graduate Masters and Ph.D. level. Whose responsibility is it? Computer science or the application science (e.g., physics) department? On the other hand, maybe it is an intermediate discipline such as applied mathematics? Currently, there is no agreement that the science of using computers is even worthy of academic status. Physicists view it as part of computer science and computer scientists as part of physics. As discussed at the recent supercomputer conference at Reno, a few universities are starting new educational initiatives in this area which many call computational science. These fledgling efforts must be coordinated and expanded if

computation is to realize its potential. We must teach physicists the nature and power of new computers. Their new algorithms should be developed to exploit parallelism and they should recognize the new areas opened up by computation. We must teach computer science about the requirements of scientific computing. Often this is to explain not its difficulty but rather how easy, or rather, special it is; computer science would do well to specialize its often abstract work on the important, but limited structures and concepts needed by science. I hope the federal government will play a major role in encouraging the partnership between existing fields and the establishment of new academic fields. Universities are traditionally rigid and resistive to change.

The growing interest in complex systems presumes computers that can simulate systems whose complicated interactions defy conventional theoretical analysis. The computer could lead to new insights into such areas as chemical and biological evolution, the structure of the cortex, as well as systems produced by mankind ranging from economics to the complex satellite network needed by the Strategic Defense Initiative. We have coined the term physical computation to describe the use of physical analogies and computer simulation to describe such systems. New physically based methods include cellular automata, nonlinear dynamical systems, simulated annealing, neural networks, and genetic optimization methods.

The computer will make these new approaches possible. Further educational initiatives will be needed in these new applications of computers, just as in the area of computational science, i.e., the methodology of using computers, described above. Academic programs that include such areas as complex systems and neural networks are needed. Where should these be—biology, physics or computer science? Universities must establish new interdisciplinary programs.

Computation is inevitable, but it will both need and create major changes. This will be much harder than building the teraflop supercomputer. The United States has a university system that is the envy of the world. It was built up to support the academic prejudices of twenty years ago. Now, the universities must change in an environment of constant or declining support and faculty levels. In spite of this more difficult scenario, universities must take the lead in these changes.

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