Guest Editorial

The Future of Scientific Computing

by C. Gordon Bell

Forty-one years after the birth of ENIAC— the first electronic computer—computers are still in their infancy. We are on the verge of a true revolution, when we will see the computer itself "doing science." In the next decade advances in computer-assisted science should dwarf the past historical accomplishments of scientific computing. Ken Wilson, Cornell University's Nobel laureate, points out that computational science is now the third paradigm of science, supplementing theory and experimentation.

This powerful computational science has only recently emerged with the development of the large-scale supercomputer able to carry out over 1 billion floating-point operations per second. A single processor of a Cray X-MP carries out in 2 seconds that which took 7 minutes on a VAX-11/780 and 35 hours on a personal computer. With over 200 times the power of the VAX and 60,000 times the power of a personal computer, the emergence of a supercomputer offers a significant qualitative and structural change in the way science is carried out.

Computers In Science is choosing a propitious moment to begin its chronicle of computer-assisted science. Every field of science is changing—molecular chemistry, biology (computational molecular biology), materials structures, astrophysics (in effect a computational observatory), and every facet of large-scale engineering—all because of the enhanced capabilities of computing.

In the future the scientific computer will simulate new classes of phenomena such as the interaction of molecules and electrons. Add-on hardware such as the compact laser disc, which can store up to one-quarter megabyte of information, will soon hold textbooks about chemistry and physics that will permit the computer's database to "understand" these sciences, dramatically altering the textbooks of today. These "active" textbooks will be able to simulate the phenomena they describe. Rather than reading a static description of a chemical reaction, a student will be able to "see" a molecule, manipulate it, and call for experiments about it.

Four years ago the scientific community convinced Congress and the National Science Foundation (NSF) that scientific research was suffering from a lack of computing power. As a

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result, five national supercomputer centers were established at Cornell, Illinois, Pittsburgh, Princeton, and San Diego, raising the computing power available to scientists to roughly 40 Cray 1 equivalents (including a four-processor Cray X-MP and a Cray 1 at the National Center for Atmospheric Research). In addition, universities have now installed over 100 Cray 1 equivalents, including 40 IBM 3090/200s, various CDC Cyber 205s, and Cray X-MPs at Berkeley, Minnesota, Ohio State, and Texas. Minnesota has a Cray 2 and a commitment for the ETA-10.

In the coming decade computing power should increase 14 percent yearly, by roughly a factor of four, because of ongoing improvements in technology alone. Memory, for example, quadruples in size every three years for a constant price.

These technical improvements will come about largely because of microelectronic density and the innovation of more parallel computers employing vector and multiprocessor architecture, like larger supercomputers. Only recently, for example, in the world of personal computers, was the major impediment to improved programs lifted by the introduction of the Intel 80386 chip with its increased addressing power. Within a few years, even the new 32-bit chips will be considered a significant limit to physical and virtual addresses.

In every computer classification, supers to micros, directed to the scientific or engineering community, single-central-processor designs are making a transition to vector-based architectures with multiple processors sharing a common memory. This will lead to much more computing power in an increasingly smaller package. I would predict that the power of today's Cray X-MP (four processors, delivering a peak power of 1 billion floating-point operations per second, an average of 100 million floating-point operations per second—megaflops—and a main memory of 1 million 64-bit words) will be available in a workstation for under $100,000. Bill Joy of Sun Microsystems has predicted a 10-megaflop workstation by 1990, roughly three times the power of the first VAX-11/780, introduced almost 10 years ago. Contrast this with today's 0.5-megaflop workstations.

To make the most effective use of vector multiprocessors will require training, new programs, and new algorithms. Ideally, teams of scientists, mathematicians, and computer scientists will form to address the new challenges. Today's supercomputer users—about 6000, working on 1000 projects at 200 sites—are the pioneers in this new computing science.

More powerful computers will fuel a demand for faster access to that computational power, pushing the development of higher capacity networks. Today, while nearly every scientist has access to a computer network for file transfer, electronic mail, and the exchange of documents, tomorrow's networks must provide a four-order-of-magnitude improvement over those they use today. Computer networks of today are limited to 10 kilobits per second, or what can be transmitted over ordinary phone lines. Most campuses are installing campus area networks operating at aggregate speeds of 100 megabits (millions of bits) per second that require a wide-area network link of 10 megabits to 20 megabits per second in order to provide the same speed on a "global" basis.

The computer networks in use today are interconnected by only 56-kilobit links. These include the public nets (Dialup, Telenet, Tymnet), user-formed nets (BITNET, CSNET, HEPNET, SPAN), and government agency nets (ARPANET, MILNET, MFENET, and NSFnet).

An interagency Federal Co-ordinating Committee on Science, Engineering and Technology (FCCSET) is preparing a plan for Congress for a network that can provide scientists with wide-scale access to the nation's supercomputers. The second phase of this same plan would develop a national network that would link several thousand university, government, and industrial research sites at speeds up to 150 megabits per second. Such a network could be operational by 1992.

Only a lack of standards is slowing the full force of the computer revolution. The Federal Information Processing Standards (FIPS) for UNIX (POSIX P1009) is in progress and should be approved in the next few months, requiring all computers purchased by the government to provide a UNIX environment. Such a standard will go a long way to make programs transportable across a range of computers as well as to expedite network standards. Overall, the practice of scientists networking with one another will result in new collaborations, and perhaps even new forms of science.

We're on the verge of major changes in computers and their scientific role brought about by large, discontinuous increases in power, memory size, and network bandwidth. The only limit to this revolution is our own imagination, and the one remaining impediment is our own lethargy. Now is indeed a worthwhile time to launch *Computers In Science*.Ω