

FROM MARS TO MINERVA: THE ORIGINS OF SCIENTIFIC COMPUTING IN THE AEC LABS

In the 50 years since the ENIAC (Electronic Numerical Integrator and Computer) was publicly announced at the Moore School of Electrical Engineering at the University of Pennsylvania, computers have transformed the natural sciences and even become the subject of their own science. Designed to be a tool of Mars rather than Minerva, the ENIAC was finished too late to be of use for its intended purpose of calculating ballistic tables in World War II. It was initially applied instead to the "Los Alamos problem," a calculation of the behavior of Edward Teller's thermonuclear weapon design, known as the "Super." However, after the formation of the Atomic Energy Commission (AEC) in 1946, Los Alamos and the other AEC laboratories actively developed computers and applied them to a wide variety of physical problems in a fruitful partnership with industry and academia.

Although the Office of Naval Research, the Army Ordnance Command and the National Bureau of Standards also provided important Federal support for computer technology development in the early postwar era,¹ the AEC labs pioneered in modern scientific computing, applying computers to nuclear and high-energy physics, the genetic code and a wide variety of stochastic processes using the Monte Carlo technique. The AEC supported scientific computer development by IBM, Remington Rand and other manufacturers, and distributed grants to universities to facilitate scientific computing.

The need for greater computing power was clearly evident during the Manhattan Project.² When the Los Alamos facility opened in the spring of 1943, Donald "Moll" Flanders, a mathematical physicist from New York University, assigned wives of project scientists to work as "computers" solving computational problems with desk calculators. Military personnel of the Special Engineering Detachment (SED) later replaced these computers, and IBM electromechanical office machines replaced the desk calculators early in 1944.

The IBM machines proved crucial in calculating the behavior of imploding systems—calculations that were used in designing the plutonium bomb. Seth Neddermyer had proposed to minimize the danger of predetonation of a critical assembly by using implosion instead of gun assembly. In the fall of 1943, Los Alamos consultant John

Although the AEC laboratories are renowned for the development of nuclear weapons, their largess in promoting scientific computing also had a profound effect on scientific and technological development in the second half of the 20th century.

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von Neumann (see figure 1) had pointed out that implosion would also compress the critical mass and increase the efficiency of the fission reaction. However, with only the desk calculators at his disposal, von Neumann could not calculate the final behavior of the compressed mass. Frustrated, he suggested scale experiments instead.²

Rudolph Peierls, the first member of the British scientific contingent at Los Alamos, suggested applying a British algorithm for blast-wave calculations to the implosion problem. A single hydrodynamics problem in this implosion simulation required passing a deck of IBM punched cards representing the state of the implosion at one instant through a dozen IBM machines, then repeating the process for each step in the integration of a partial differential equation. The whole procedure required three months. By color-coding IBM cards, Richard Feynman and his SED personnel learned to run two or three decks through simultaneously but out of phase with each other. These calculations demanded rewiring the tabulator plugboards and each calculation had to be checked—and perhaps a third of the calculations had to be repeated. The parallel procedure was so alien to von Neumann, however, that he later rejected parallel methods in favor of serial processing.²

It was von Neumann, also a consultant to the concurrent ENIAC project, who suggested that Teller's design for a Super might provide a suitable test of the computer's capabilities. In the fall of 1944, Los Alamos physicists Nicholas Metropolis, Stanley Frankel and Anthony Turkevich ran a one-dimensional version of the Super calculation on the machine. It used 95% of the machine's capacity. The full calculations, which included hydrodynamic, energy transport and neutronic processes that could not be calculated on the ENIAC, could only be "programmed" in design codes until the computers needed to run them were ready six years later. Los Alamos programs provided a test for every other computer developed in the interim.²

His wartime experience with computing at Los Alamos made von Neumann the leading proponent of scientific computation. His disciples at Los Alamos and in other laboratories sponsored by the AEC fulfilled his prophecies and made the computer a valuable sci-

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JOHN VON NEUMANN became a leading proponent of the use of computers in science through his wartime work as a Los Alamos consultant. After the war, he left his mark on nearly all aspects of computational science, from machine architecture to computational techniques to the problems tackled. (All photos courtesy of Los Alamos National Laboratory.) **FIGURE 1**

tific instrument for physics research.

Monte Carlo and MANIAC

In 1947, von Neumann and Stan Ulam at Los Alamos formulated the Monte Carlo technique, a brute force approach to the calculation of stochastic problems that relied on computers to supply the force. In 1947, Enrico Fermi devised an analog computer, the FERMIAC, to simulate neutron diffusion and multiplication. (See figure 2.) This "Monte Carlo Trolley" generated individual histories of neutrons as they passed through various materials at different velocities and were absorbed, caused fission or scattered. John and Klari von Neumann and Metropolis applied the ENIAC to Monte Carlo techniques in February 1948. Ulam's lectures at Los Alamos and Los Angeles stimulated widespread interest in the technique.³ The demand for more computing power to use Monte Carlo techniques led Los Alamos to build its own computer, the MANIAC (Mathematical Analyzer, Numerical Integrator, and Computer). This computer, built by Metropolis, was based on von Neumann's design for a computer at the Institute for Advanced Study (IAS) in Princeton, New Jersey. At the suggestion of Los Alamos director Norris Bradbury the AEC also underwrote the completion of the IAS computer.

The MANIAC provided ample power for scientific and applied research. In the summer of 1952, Fermi programmed it to analyze results of pion-proton scattering experiments he had conducted at the University of Chicago. One single problem in this analysis, a system of six equations with six unknowns, had required weeks to solve by hand. The MANIAC could solve it in five minutes. The procedure could be generalized to solve more complicated systems of n equations with n unknowns. Fermi returned to Chicago full of enthusiasm for digital computing, gave a series of lectures on the subject, and urged that the university build its own computer. "Fermi, with his great common sense and intuition," Ulam recalled, "recognized immediately their importance for the study of problems in theoretical physics, astrophysics and classical physics."

In the summer of 1953, Fermi used the MANIAC to calculate the approach to equilibrium of a nonlinear vibrating string. With Ulam and John Pasta, he ran a test program that showed that, as expected, the initial vibrational energy gradually transferred to neighboring modes. However, rather than achieving equilibrium distribution among the modes, the energy concentrated in a single mode with a frequency close to that of the string's initial state after only a few thousand virtual oscillation periods—Poincaré's return theorem predicted that such a concentration would take a time on the order of the age of the universe. The unexpected result upset the classical view of the equipartition of energy and spawned interest

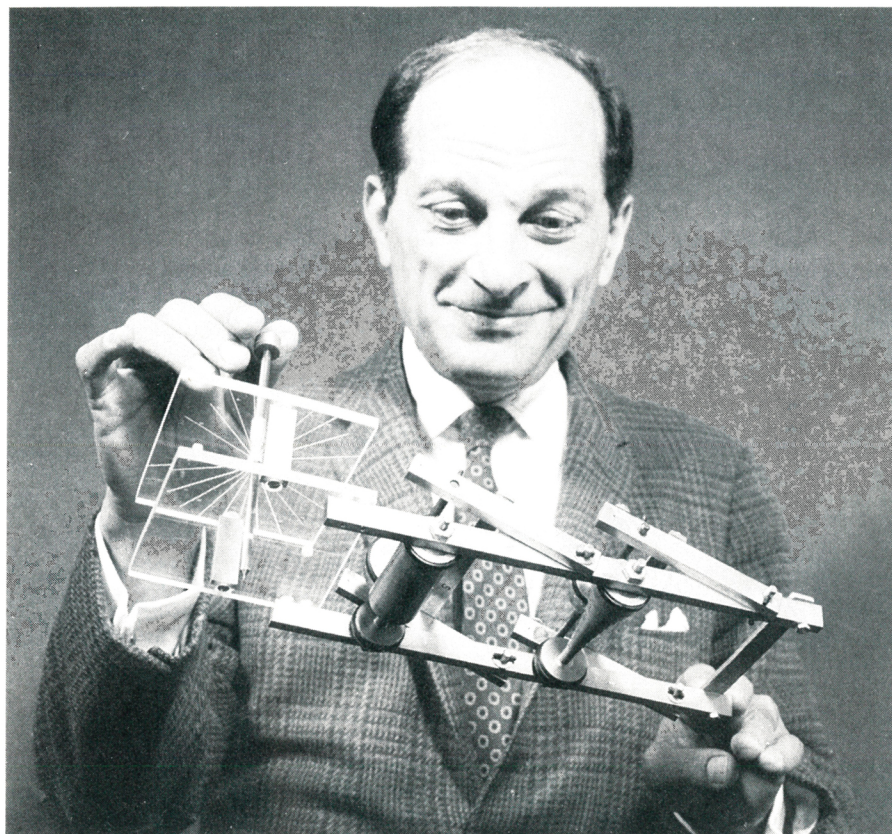


in nonlinear systems, which proved to be particularly fruitful ground for analysis by computers. Unfortunately, Fermi's premature death in 1954 cut short his activity along these lines.⁴

Other early uses of the MANIAC included Metropolis and Turkevich's calculation of the energy of "nuclear cascade" reactions, George Gamow and Verna Gardiner's code for DNA selection of amino acids, Metropolis and Paul Stein's discovery of the universal properties of iterative transformations, Ulam and Metropolis's studies of a subset of the prime numbers called lucky numbers, Marc Wells's "anticlerical chess" (bereft of bishops and bishops' pawns), the simulation of two-dimensional flow of two incompressible fluids and the development of the free-Lagrangian method for modeling turbulence. (See figure 3.)

The equations of state for matter under conditions of high density and pressure had a natural attraction and application at Los Alamos. Metropolis, Edward and Mici Teller and Marshall and Arianna Rosenbluth calculated the equations of state for hard spheres moving in two dimensions with the Monte Carlo technique using only a few lines of code. This "Metropolis method" has been used with many physical systems for which the forces between particles are known.³ For example, researchers at the AEC Computing and Applied Mathematics Center, founded at New York University in 1953 by Los Alamos physicist Robert Richtmyer, numerically followed a large number of particles over an immense number of collisions to provide the controlled equivalent of x-ray diffraction analyses, achieving excellent agreement with experiments.

Monte Carlo codes were also used to model various types of radiation transport using random-walk techniques. As time went on, cross-section libraries were developed and better mathematical techniques generated better distributions of random numbers. As a result of these developments Monte Carlo methods could be used



MONTE CARLO PIONEERS.

Stanislaw Ulam appears with the FERMIAC, or Monte Carlo Trolley, an analog computer invented by Fermi that generated the histories of individual neutrons as they passed through matter. Along with von Neumann, Ulam began using this brute force method to solve stochastic problems with programmable digital computers and helped to make the technique a standard method of computational physics. **FIGURE 2**

to account for processes such as thermalization of the energetic fission neutrons.⁵

Such examples of the application of the MANIAC to scientific problems could be multiplied indefinitely. Machines at other AEC labs extended computational physics to other realms. Flanders, who had moved to Argonne National Laboratory in Illinois from NYU in 1948, worked in partnership with ENIAC team member Jeffery Chuan Chu to build copies of the IAS machine at Argonne (the AVIDAC) and at Oak Ridge National Laboratory in Tennessee (the ORACLE). The AVIDAC used Monte Carlo techniques to track mesons through a nucleus, to calculate crystal lattice parameters, to forecast death rates of organisms due to radiation sickness, to parse diffusion kinetics for gases and to model behavior of nuclear reactors. The ORACLE found employment in plasma physics, reactor design and safety studies, chemical kinetics, health physics and elementary particle physics.⁶

The MANIAC II, built at Los Alamos in 1954, had five times the speed and ten times the memory of the original MANIAC, and incorporated floating-point techniques that became the hallmark of scientific computing. Metropolis also built the MANIAC III at the University of Chicago to study technical problems relating to the design and use of digital computers. The AEC also contributed to establishing scientific computing centers at the Rice Institute, the University of California, Los Angeles, and the University of Illinois (which produced the ILLIAC).

An alliance with industry

Partnerships between industry and academia dedicated to improving calculators were carried forward into computer development at the AEC labs. In the 1930s, Wallace Eckert had formed Columbia University's Thomas J. Watson Astronomical Computing Bureau, where he had worked on adapting IBM business tabulators and account-

ing devices for use in astronomy. After the war, he formed the Watson Scientific Computing Laboratory at Columbia and helped develop the Selective Sequence Electronic Calculator (SSEC) in 1947. Robert Richtmyer, leader of the theoretical physics division at Los Alamos was among the SSEC's earliest users, and his weapon design calculation was the largest problem ever run on that machine.⁷

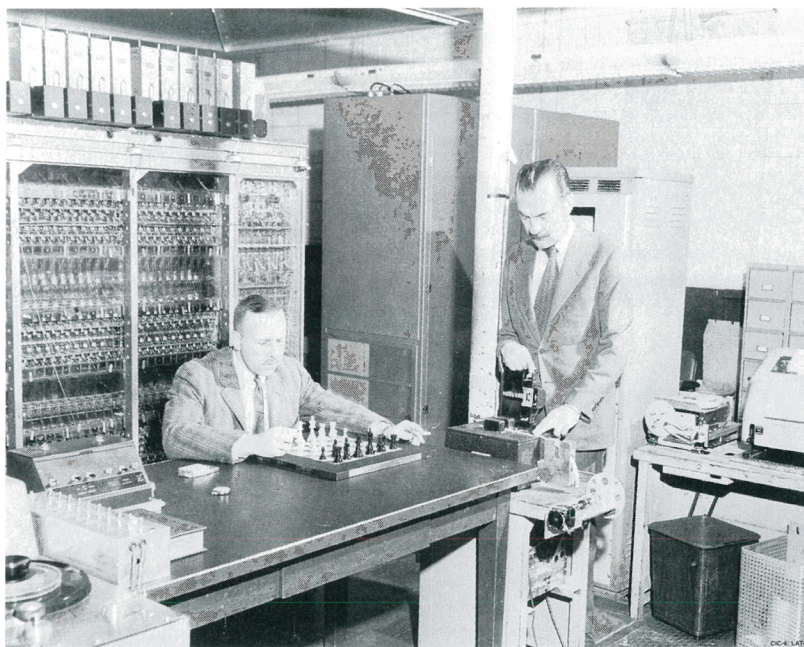
The IBM strategy for expanding scientific computing was formulated by Cuthbert Hurd, who was hired by Thomas Watson from Oak Ridge in 1949. At Oak Ridge, Hurd had been involved in modeling advanced gaseous diffusion processes, a computation-intensive problem because of the thousands of separation stages involved. Hurd, who organized the first open conference on Monte Carlo methods and the IBM Scientific Computation seminars, convinced IBM to enter the field.

At the outbreak of the Korean War Hurd persuaded Thomas Watson Jr to build a "Defense Calculator." The first production machine, the IBM 701, was assembled late in December 1952. The second was shipped to Los Alamos in March 1953. One month later, in symbolic recognition of the contributions of Los Alamos, the AEC and the IAS, IAS director J. Robert Oppenheimer spoke at the unveiling of the 701 at IBM headquarters in New York. A Los Alamos test calculation of neutron scattering was run. The Los Alamos machine had already been operating for four days.

Between April 1953 and June 1956, some 250 staff members ran more than 700 individual problems on two IBM 701 and three 704 computers at Los Alamos. Forty-six individuals were employed as programmers and operators, and IBM supplied a maintenance staff of 15.⁸

Von Neumann consulted with IBM in the construction of the 704. As a member of the AEC's General Advisory Committee and of the AEC, itself (starting in 1954), he also sought to stimulate the development of more ad-

A MANIACAL GAME OF CHESS. The Los Alamos computer MANIAC was applied to a broad variety of tasks, ranging from number theory to weapons physics. Marc Wells developed a simplified version of chess that MANIAC could play (in this case with Paul Stein). Played on a 36-square board, this "anti-clerical chess" had no bishops or bishops' pawns, but all other pieces moved according to the traditional rules of the game. **FIGURE 3**



vanced computers in the laboratories. "It seems to me that high-speed computers are just as vital to the AEC development programs as . . . high-speed particle accelerators," he argued in a GAC meeting and recommended a \$1 million annual budget for their acquisition. He summoned Pasta, who later became head of the National Science Foundation's computer program, to Washington to lead the computing program of the AEC.⁹

In 1955, at the AEC's lab at Livermore, California, Teller commissioned Remington Rand UNIVAC to build the Livermore Automatic Research Computer (LARC), one of the first machines to use transistors rather than vacuum tubes. Livermore programmers worked closely with Remington Rand in the development of the LARC.

IBM also bid for the Livermore job, but could not deliver the computer as quickly as Livermore wanted. IBM then offered to build an advanced scientific computer called STRETCH for Los Alamos. (See figure 4.) STRETCH was designed to be significantly faster than either LARC or the IBM 704. IBM project manager Steven Dunwell later testified that IBM wanted "support for early development work from an organization which could afford the new technology," and he did not "recollect having considered that any others were in a position to do it at that time."¹⁰

Los Alamos scientists Mark Wells, Jack Worlton, Bob Frank, Roger Lazarus and Bengt Carlson helped design the new machine. Los Alamos mathematician Harwood Kolsky joined IBM to build a computer simulator to find a reasonable balance between complexity and cost in STRETCH's design. The IBM/Los Alamos group was also responsible for the instruction set and related features. According to Dunwell, "The STRETCH project involved exploring the unknown and redesigning almost every aspect of earlier IBM computer systems." It contributed to many of the technical innovations in the IBM 360 series.

Although STRETCH failed to achieve the target of calculating Monte Carlo code 240 times faster than the IBM 704, its memory could handle all the data for a two-dimensional weapons design code, allowing the weapons tested in Operation Dominic in 1962 to be redesigned and retested during the series. STRETCH was adopted

by the British and French atomic energy commissions, the MITRE Corp, Dahlgren Naval Proving Ground, the National Security Agency, and the US Weather Bureau.

STRETCH was applied to a variety of scientific problems. The particle-in-cell method, developed at Los Alamos, used the large storage and high speed of the machine to advantage in modeling multidimensional dynamics of several compressible fluids or high-velocity impacts, and incompressible fluid dynamics. In this method, a continuous system was divided into cells and then the cells were replaced with particles that had the average properties (velocity, momentum and so on) of the cell and were located at the cell center. The method, which combined the features of Eulerian and Lagrangian calculations of fluid dynamics, and other methods developed by Los Alamos theoretical division's group T-3 in the 1960s gave the group a reputation as a "recreational fluid dynamics group." Carlson's group used STRETCH to elaborate neutron and other radiation transport codes into the Los Alamos Radiation Transport Code System, which was applied in accelerator and nuclear reactor design, electronics shielding, criticality safety, materials science, medical physics and astrophysics.¹¹

High-energy physics

Computers transformed high-energy physics data analysis for large detectors such as Luis Alvarez's liquid hydrogen bubble chamber at the Lawrence Radiation Laboratory (LRL) at Berkeley, California. Such detectors produced millions of particle interactions per year. Alvarez, who had worked at Los Alamos as a consultant, recognized the need for an automatic system to interpret these events as early as 1955. (See the article by Joel Butler and David Quarrie on page 50.) Part of the solution was mechanical: Hugh Bradner and Jack Franck designed the "Frankenstein" track-measuring device, which became operational in 1956. Such machines reduced the measuring time for bubble chamber events to approximately ten minutes per event by 1966 and, by 1970, a technician could measure approximately 50 000 events per year.¹²

Alvarez believed that the digitized output of such machines could be analyzed by computers much more



THE STRETCH COMPUTER was designed by IBM to calculate Monte Carlo codes 240 times faster than previous computers, such as LARC and the IBM 704. Although it never achieved such speed, STRETCH's architects did pioneer novel techniques of computer design, including simulating possible designs with a special computer, and STRETCH incorporated features later included in the IBM 360. STRETCH computers were used in a wide variety of applications in France and the UK as well as in the US.

FIGURE 4

quickly than by traditional manual means: "The Lawrence Radiation Laboratory didn't even have an IBM 650 at this time, but I had seen the MANIAC at Los Alamos and felt that computer calculation was the answer to many of the problems we would face."¹³ To program the calculations, Alvarez hired Frank Solmitz, who had been trained by Fermi at Chicago. Solmitz wrote the code for the IBM 650 computer to evaluate the digitized output of Franckenstein. The code listed the momenta and directions of the tracks for each vertex, and calculated errors in those measurements. A physicist would plot the tracks' angular coordinates on a stereographic projection of a unit sphere known as a Wolff-plot. If the vertex had three tracks, the physicist had to move the points on the sphere to make them coplanar and simultaneously vary the momentum values to make the momentum vector triangle close and to ensure energy conservation. This time-consuming iterative procedure meant that even an experienced physicist could solve only a few Wolff-plot problems per day.

Between 1957 and 1959, Solmitz and Horace Taft wrote the first fitting routine for such problems and overcame the bottleneck. The routine used a least-squares analysis to give an overall fit to several interconnected vertices. A highly constrained fit could be obtained only if the particle responsible for each track was properly identified. If the degree of constraint was low, more than one hypothesis (set of track identifications) might give a fit, and the physicist still had to rely upon his judgment in making the identification.

To remove much of the remaining drudgery from the bubble chamber physicist's life, Arthur Rosenfeld and Solmitz wrote SUMX, which allowed physicists to use logical tests to select events, based on effective masses of particles, momentum transfer or other parameters. A physicist simply instructed the computer to plot all histograms of any possible significance, and then flipped the pages to see which ones had interesting figures. Gerry Lynch wrote GAME, which evaluated the statistical significance of such figures by plotting many histograms containing the same number of events as the original histogram from the real experiment (as determined by a smooth curve through the experimental data). Physicists would leaf through the histograms and vote on the

apparent significance of the statistical fluctuations that appeared. Alvarez recalled that "the first time this was tried, the experimenter . . . didn't know that his own histogram was in the pile, and didn't pick it out as convincing; he picked out two of the computer generated histograms as looking significant, and pronounced all others—including his own—as of no significance."¹³ FAKE, also written by Lynch, generated simulated measurements of bubble chamber events to determine how frequently the analysis programs arrived at an incorrect answer and to distinguish between similar events. Like GAME, FAKE was widely used by bubble chamber groups all over the world. It gave rise to the Monte Carlo simulation subroutines that make possible the calculation of systematic errors in particle physics experiments.¹⁴

Computer-aided discovery

When the bubble chamber system began operation, the Franckensteins were kept busy around the clock measuring large numbers of strange particle events. A kinematics program, KICK, helped physicists discover that combinations of particles that were common in many events reconstructed to a particle-like state with a unique mass of 1385 MeV and an isotopic spin of 1. The discovery of this first "strange resonance," dubbed the Y_1^* (1385), began a hunt for more short-lived particles. The group found two other strange resonances, including the K^* (890), the first example of a "boson resonance," which had a lifetime (as determined by the width of its mass distribution) on the order of 10^{-23} second, approximately 10^{13} times shorter than the bubble chamber had been designed to detect.

On the basis of high-energy electron scattering experiments by Robert Hofstadter, theorists had predicted the existence of two spin-1 (vector) mesons, the ρ and the ω . Bogdan Maglich used KICK to obtain a sample of proton-antiproton annihilations that had the topology predicted by the theorists and then plotted a reconstructed-mass histogram for his candidates. SUMX was just beginning to work and still had bugs in it, so the preparation of the histogram was a very tedious and time-consuming chore, but as it slowly emerged, Maglich saw bumps appear in the side of his phase-space distri-

bution. One peak signaled the discovery of the ω meson.¹³

In his review of the use of computers in high-energy physics in 1963, C. N. Yang pointed out that without the use of a computer, the ω meson probably would not have been discovered in 1961. He concluded that computers were "obviously an absolutely indispensable tool in experimental high-energy physics. With the large amount of data which must be selected out of larger backgrounds, it is impossible to do without the computing machine."¹⁵

As the bubble chamber system improved, the numbers of tracks measured increased rapidly. In the mid-1960s the Franckenstein gave way to the Spiral Reader, which could measure over a million particle interactions a year. The Lawrence Radiation Laboratory developed a hunger for new computers to process the data, and the AEC fed this hunger to the tune of \$30 million between 1959 and 1969, the year Luis Alvarez received his Nobel Prize in Physics for the discovery of new particles with the bubble chamber and its computerized data analysis system. The techniques pioneered at the LRL were adopted at major high-energy physics laboratories worldwide. Physicists at CERN carefully followed developments at LRL during the period, and an early collaboration with Brookhaven and the LRL resulted in a machine for digitizing bubble chamber tracks, the Hough-Powell device, or "flying spot digitizer," as well as computers to handle data analysis. Argonne developed CHLOE, a film data analysis system to handle the million bits of photographic information expected from the Zero Gradient Synchrotron each second. It included a scanner that sent the digital coordinates of scanned points to an ASI210 computer and displayed output on a cathode-ray tube.

Supercomputers and computational physics

The hundred-fold increase in computing power driven by the computational needs of the AEC weapons laboratories in the 1950s made possible many similar scientific appli-

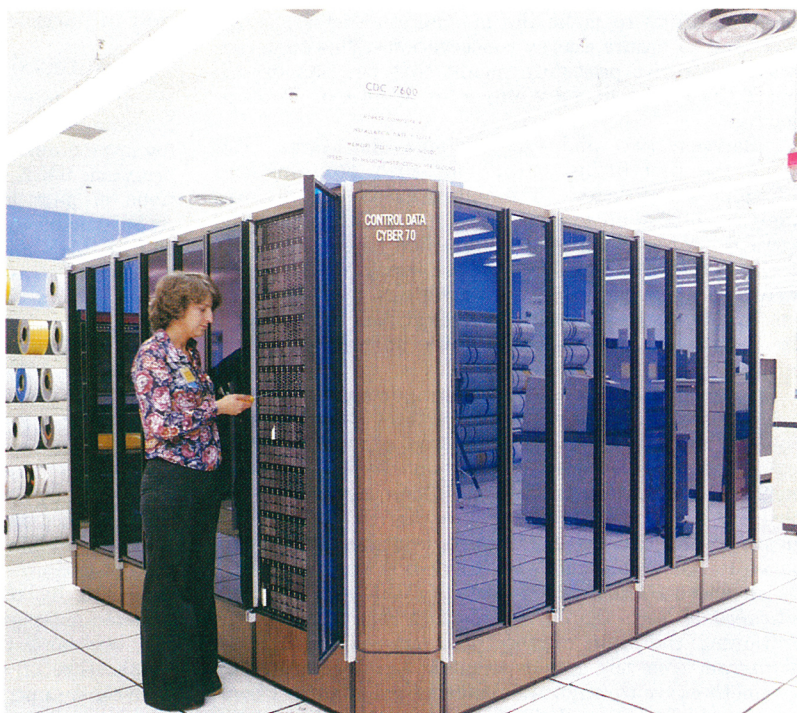
cations. One Los Alamos designer asked, "Why do we want all these computers, and why don't we ever have enough of them?"¹⁶ To meet the demand, the labs formed industrial alliances with the supercomputer manufacturers who came to dominate the industry in the 1960s and 1970s. Control Data Corporation (CDC), organized in 1957, made plans with Los Alamos, Livermore, the Lawrence Radiation Laboratory at Berkeley and Brookhaven to build a computer larger than STRETCH or LARC. The leader of Livermore's computer division, Sid Fernbach, ordered the first CDC 6600 in what turned out to be that machine's almost complete penetration of AEC laboratories, and the labs were the dominant consumers of computer horsepower. In the 1970s and into the 1980s the CDC 7600 became the mainstay supercomputer. (See figure 5.)

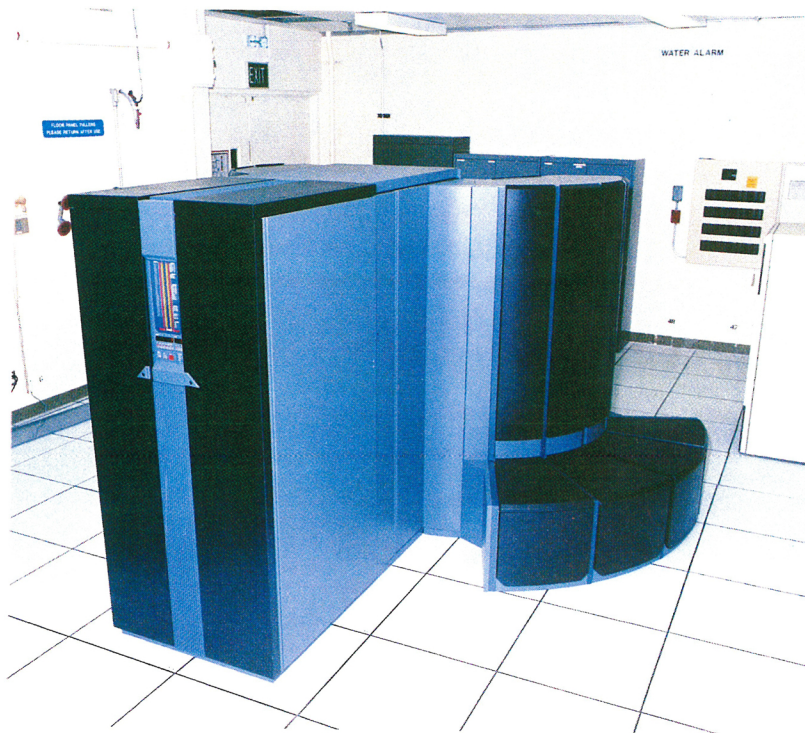
The ever-increasing applications of computers in physics gave rise to the new specialty of computational physics. Represented at first by annual collections of articles, and then, in 1966, by the *Journal of Computational Physics*, the field was rooted in the AEC labs whose scientists supplied most of the literature. As had Teller and Fermi earlier, AEC scientists continued to advocate the use of computers in physics. Richtmyer lamented in 1965 that "advances in computer technology have unfortunately not been paralleled by a corresponding advance in the art of scientific computing. . . . Contrary to popular belief, we are more often limited in what we can compute by the lack of sufficiently powerful mathematical methods than by the lack of sufficiently powerful computers."¹⁷

Such methods were forthcoming in the 1970s and 1980s, as scientists designed new computations and refined older ones to take advantage of the new capabilities of supercomputers. (See figure 6.) For the first time, rigorous attempts could be made to solve the three-body problem, chaotic processes could be simulated (as Mitchell Feigenbaum showed at Los Alamos), the electronic behavior of chemical reactions could be calculated and the

THE CDC 7600 SUPERCOMPUTER was the most advanced, and the last large, computer built with a ferrite-core memory and, during the 1970s, took over the duties of the CDC 6600 as the workhorse at the national labs. Like the 6600, the new computer was applied in fields ranging from weather prediction to nuclear weapons design.

FIGURE 5





NEW-GENERATION SUPERCOMPUTERS like this CRAY computer at Los Alamos helped computational physics to assume a place in the 1980s alongside theoretical and experimental physics as an indispensable tool for understanding the physical world. FIGURE 6

behavior of extremely complex systems could be investigated. In 1987, the American Institute of Physics announced a new magazine, *Computers in Physics*, edited by Robert R. Borchers, associate director for computation at Livermore; in 1993, the American Physical Society began publishing *Physical Review E*, in which a substantial portion of the articles are devoted to computational and nonlinear physics. (On the World Wide Web, see <http://www.aip.org/cip/> and <http://publish.aps.org/PRE/prehome.html>, respectively.)

The leadership of AEC laboratories in the development and application of scientific computing has left its legacies in many research programs here and abroad. The origins of this effort in nuclear weapons development have not prevented it from providing a useful tool in many other areas of science.

The development of scientific computers at Los Alamos and Livermore in the 1940s and 1950s presented many of the features of user-stimulated technological innovation: Physicists such as Fermi, Teller, Ulam and Metropolis used the AEC computers to do basic research and in the process helped to develop and improve those computers. This development also provides an example of successful cooperation between government and industry; the partnership between academia and the AEC led to the establishment of scientific computing centers at many universities. Manpower trained by AEC computer pioneers provided a means of transferring AEC computer technology to new laboratories and to industry. As with particle accelerators and other instruments of big science, the AEC labs' blend of programmatic and fundamental research with computers diffused beyond laboratory fences, allowing computational physics to join theory and experiment as an important tool of physics. (See the column by Leo P. Kadanoff, *PHYSICS TODAY*, July 1986, page 7.) The effects upon physics are only beginning to be felt as we enter the second half-century of the information age.

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