

SPECIAL ISSUE:

HIGH-PERFORMANCE COMPUTING AND PHYSICS

Concurrent computation and high-speed communication offer opportunities for simulations of more realistic physics.

Computers commonly process data and do simulations these days at rates of gigaflops (10^9 floating-point operations per second). In the next few years teraflop (10^{12} flops) computers will open an age in which we can study physics in new parameter domains, providing insights that may lead to new discoveries. These teraflop computers will be massively parallel, involving hundreds if not thousands of coupled processors tackling problems involving trillions of data points. To make effective use of these new resources will require new ideas about which problems should be solved, what numerical algorithms should be used to solve them, and what visualization and quantification methods should be used to enable scientists to comprehend and analyze the vast amounts of data that will be generated.

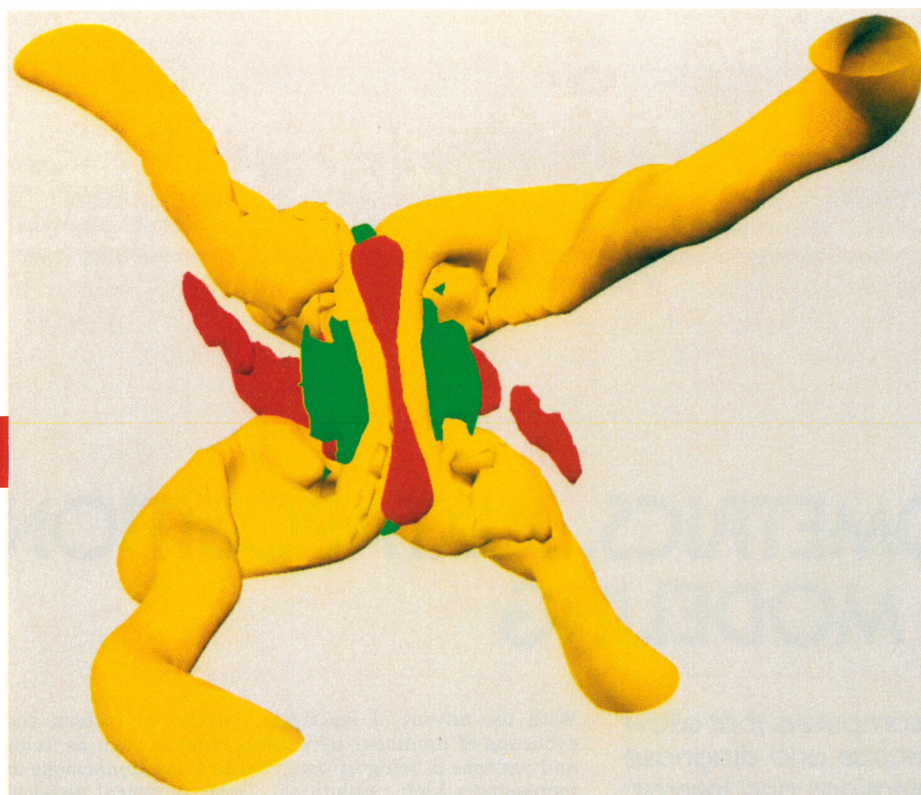
As supercomputers have evolved, so have the applications for which they have been used. In the 1940s researchers used the supercomputers of the time to help design the atomic bomb; in the 1950s supercomputers were employed for problems such as weather forecasting; in the late 1960s computational aerodynamics began making inroads on the problem of aircraft design. In the 1970s and 1980s seismological data processing and petroleum reservoir modeling, structural analysis of buildings and vehicles, circuit design and layout of electronic systems, econometric modeling, quantum field theory, drug design and a host of other fields joined in this computational revolution. It is now difficult to think of any area of science not affected by large-scale scientific computing and simulation.

Teraflop machines will initially be few in number and will be accessed via fast networks that can transmit gigabits per second in a style of working that Larry Smarr (director of the National Center for Supercomputing Applications in Urbana, Illinois) has called "metacomput-

ing." In metacomputing a gigabit/sec network of heterogeneous computational resources is linked by intelligent software flexibly configured to solve challenging problems. Metacomputing should make high-performance computing as easy as using a personal computer. Already, as part of the Federal government's High Performance Computing and Communications Initiative, the Corporation for National Research Initiatives, supported by NSF and the Defense Advanced Research Projects Agency, has launched five wide-area gigabit/sec network test-beds linking selected universities, supercomputer centers, national laboratories and industrial facilities. These test-beds will advance the technology and the understanding of needs for the proposed new National Research and Education Network.

The effective use of the fast networks will require innovative ideas on network architectures, switches and protocols and their smooth integration with multimedia environments for interactive and automatic image visualization and quantification. For example, one may "steer" ongoing simulations by varying parameters interactively.

The five articles in this issue of *PHYSICS TODAY* survey applications of massively parallel supercomputers to problems in classical physics. Norman Zabusky, Deborah Silver, Richard Pelz and their colleagues discuss in the article on page 24 a style of working in which the computer juxtaposes data sets from direct numerical simulations with different parameters and algorithms. The insights gained from interactive "visiometrics"—the process of visualizing and quantifying interactions among coherent space-time events—should lead to further understanding of underlying physical processes as well as to ideas for constructing models with reduced degrees of freedom. The figure on the opposite page juxtaposes vorticity and



Compressibility of the fluid medium slows down vortex reconnection in this simulation. The isosurfaces of vorticity are shown in yellow; the velocity divergence in red (negative) and green (positive). See the article on page 24 for further explanation. (Simulations by Thomas Scheidegger, Rutgers University.)

velocity divergence fields and thereby aids in the understanding of compressible vortex reconnection.

In the article on page 34 George Karniadakis and Steven Orszag survey the prospects for the solution of turbulent flow problems on teraflop computers. As John von Neumann said so eloquently in 1949, "a considerable mathematical effort towards a detailed understanding of the mechanism of turbulence is called for. . . . There might be some hope to 'break the deadlock' by extensive, but well-planned, computational efforts."¹ Turbulent fluid flows, with their complex space-time behavior, may serve as a prototype for other "grand challenge" physics problems in which theory coupled with computational simulations can lead to useful progress.

Theory is necessary for both the formulation of computations and the analysis of results. For example, a key issue for the turbulence problem, as well as for many of the other classical physics problems discussed in this issue, is the effect of computational resolution (discreteness) on the fidelity of observed simulated phenomena and thereby on the predictability of detailed events as well as on the statistical properties of chaotic solutions.

David Dritschel and Bernard Legras survey prospects for progress on problems of atmospheric and oceanic dynamics in the article on page 44; they emphasize ideas that are useful in the construction of models that lead to an understanding of the environment and climate. They present simulations with the Lagrangian contour dynamics-surgery algorithm and discuss the impact of high resolution on predictability.

In the article on page 54 Joshua Barnes and Lars Hernquist discuss computer models of colliding galaxies, with an emphasis on simulations based on collisionless particle dynamics as well as continuum gas dynamics.

They describe tree-based techniques for particle dynamics that enable large, efficient particle simulations, while for the continuum gas dynamics approach, they describe the method of smoothed particle hydrodynamics. They also cover a variety of challenging galactic dynamics problems.

John Dawson, Viktor Decyk, Richard Sydora and Paulett Liewer discuss applications of supercomputing to all areas of plasma science, including particle, fluid and hybrid models, in the article on page 64. In particular, they explore in depth gyrokinetic techniques that average over the rapid gyrations of particles and retain only slow particle drifts. They discuss the "numerical tokamak," a consortium project whose goal is to model transport processes in magnetically confined toroidal plasmas.

We see emerging the ability to juxtapose voluminous data sets from laboratory experiments, remote observations and model computer simulations. This ability will enable us to move more rapidly from the verbal description of observations of coherent and chaotic events to their quantification and finally to an understanding via appropriate asymptotic mathematical models. Ultimately such successes will help us to better control the outcome of engineering design, to better deliver drugs to and perform surgery on patients, and to better predict the course of natural phenomena such as weather, earthquakes, climate and astrophysical phenomena.

Reference

1. A. Taub, ed., *Collected Works of John von Neumann*, vol. 6, MacMillan, New York (1963), p. 469.

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