Los Alamos Science

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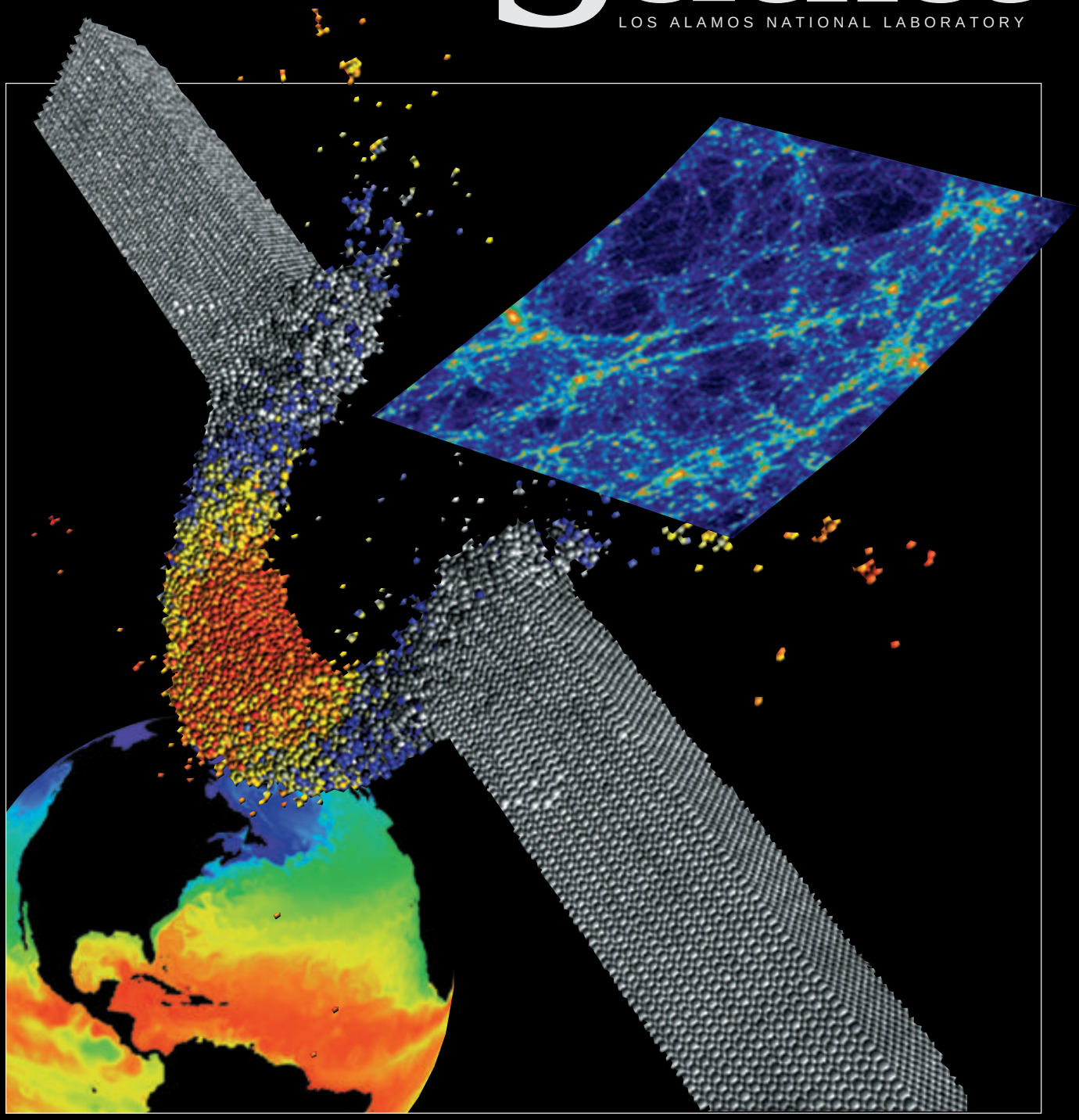

Number 22 1994

High-Performance Computing

Laboratory scientists have made enormous progress in performing large-scale numerical simulations on massively parallel computers. The images on the cover are frames taken from three such simulations. At the upper right is an image from a simulation of the formation of large-scale structure in an expanding universe. The simulation involves millions of particles representing both luminous and cold dark matter and is being used to compare observations with the predictions of cosmological models. The center image is from a molecular-dynamics simulation and shows a solid undergoing fracture. Multi-million-atom simulations such as this will be used to study the physics of materials. At the lower left is a frame from the simulation of global circulation patterns in the ocean. Simulations of ocean circulation are being combined with those describing atmospheric motions to model the long-term dynamics of climate.

Editor
Necia Grant Cooper

Managing Editor
Nadine Shea

Science Writers
Gerald A. Friedman
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Technical Illustration
Andrea J. Kron

Cartoons
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Photography
John A. Flower
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Computer Art
James M. Cruz
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Production
Nadine Shea

Other Contributors
Kay P. Coddens
AnnMarie Dyson
Susanne M. Kornke
Cheri Tiedman-Isham
CIC-9 Photography

Printing
Guadalupe D. Archuleta

Address Mail to:
Los Alamos Science
Mail Stop M708
Los Alamos National Laboratory
Los Alamos, NM 87545

lascience@lanl.gov

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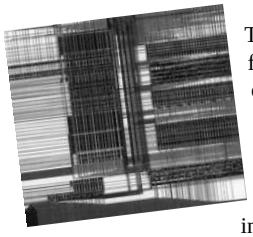
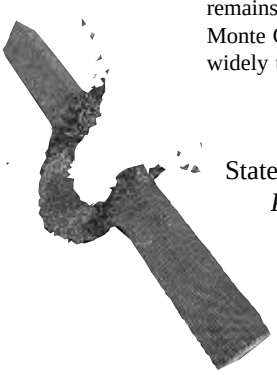


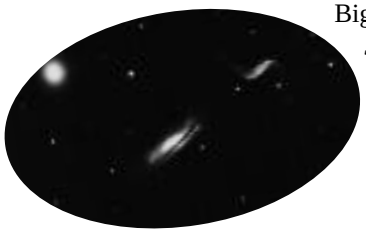
The Laboratory has been in the forefront of large-scale scientific computing since before the invention of electronic computers It is now a leader in the shift to parallel computing, in the development of collaborative relationships with industry, and in the development of data-management tools for use on the nation's future information highways.

All electronic computers are composed of simple elements that perform simple operations. This article explains the way those elements work together and describes the differences between serial, vector, and parallel supercomputers.

The Monte Carlo method, invented at the Laboratory in the 1940s, remains one of the most versatile numerical techniques. MCNP, a Monte Carlo particle transport code is one of the Laboratory's most widely used products.



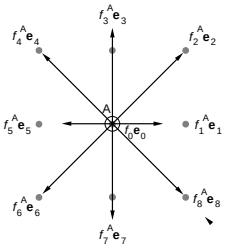
Realizing the performance capabilities of the massively parallel CM-5 supercomputer for real problems is a major challenge to computational scientists. This article describes how molecular-dynamics methods for materials science were optimized for the CM-5.



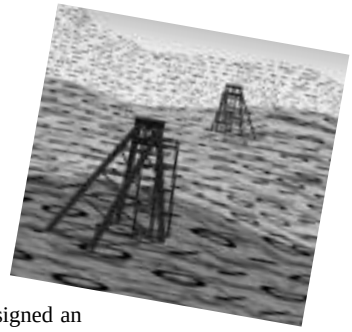
Stars make up galaxies, which make up galaxy clusters, which make up still larger structures. Theories of how these structures originated are being tested against observations through the use of "experimental cosmology"—numerical simulations on massively parallel computers that accurately follow the motions of tens of millions of massive particles under various sets of assumptions.

HIGH-PERFORMANCE COMPUTING

The lattice-Boltzmann method uses a simple set of kinetic rules to describe the motion of particles on a lattice. It yields informative and computationally efficient simulations of fluid flow, particularly for complex processes such as the flow of oil and water through porous rock—a process of great interest to the oil industry.



Researchers from Mobil Corporation and the Laboratory are collaborating on lattice-Boltzmann simulations to predict basic parameters that determine reservoir flow performance.



Extracting meaningful information from large datasets is a formidable task. The work can be efficiently divided between humans and computers, with each assigned an appropriate portion. Analysis is facilitated by using a powerful clustering algorithm along with a well-designed user interface.

In response to the National Information Infrastructure initiative, the Laboratory is collaborating with developers of local telecommunities—computer networks that provide services and facilitate communications.

A Laboratory scientist originated and implemented the idea of making a continually updated database of preprints accessible to users around the world. Such databases have become a very popular medium for scientific communication.