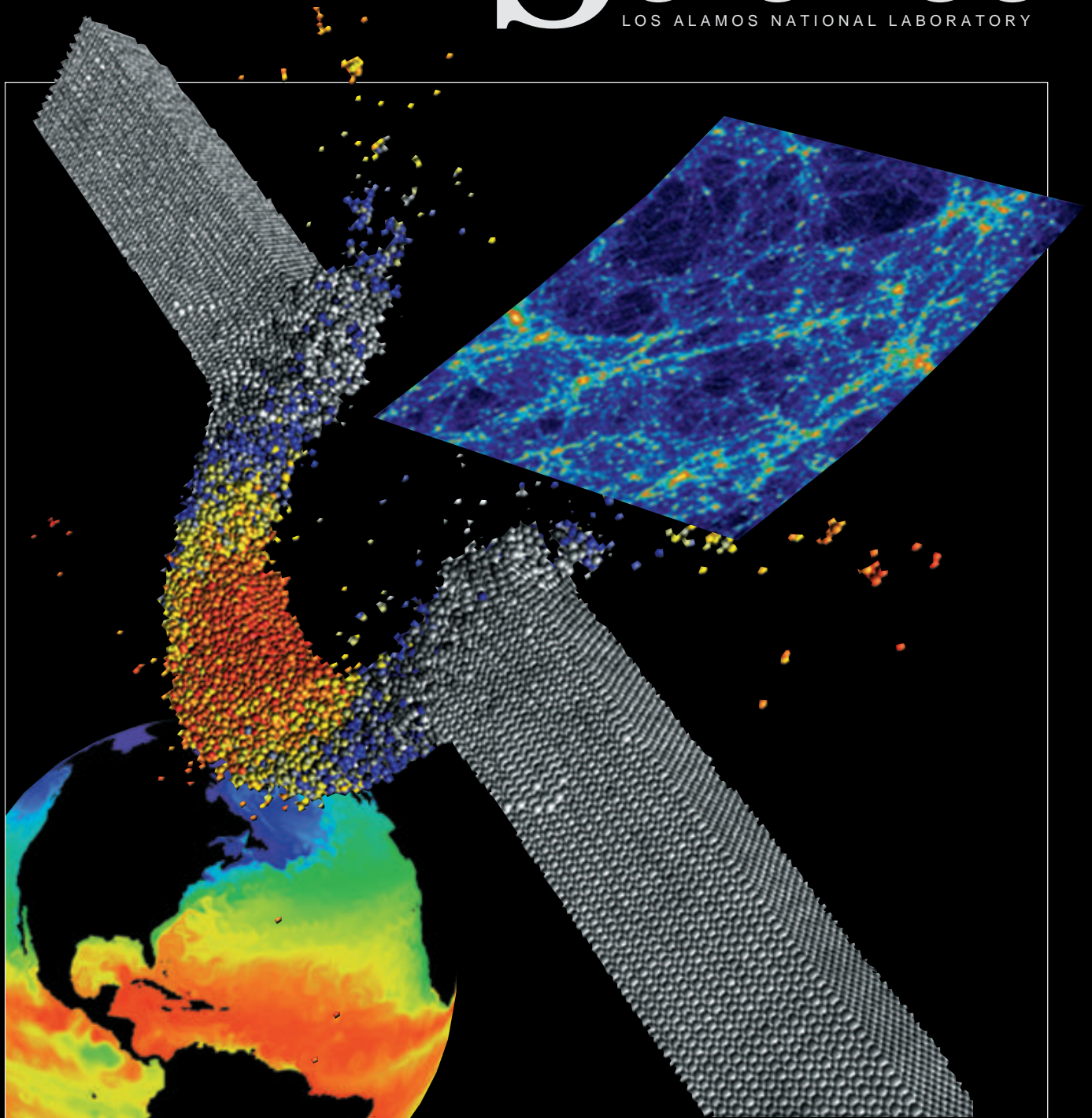


Los Alamos Science

LOS ALAMOS NATIONAL LABORATORY



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.

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Windows on Computing: New Initiatives at Los Alamos 1
David W. Forslund, Charles A. Slocomb, and Ira A. Agins

History of Computers at Los Alamos 2

Collaborations with Industry on Parallel Computing 12
Bruce R. Wienke

How Computers Work: An Introduction to Serial, Vector, and Parallel Computers 14
Gerald A. Friedman, Douglas D. Lemon, and Tony T. Warnock

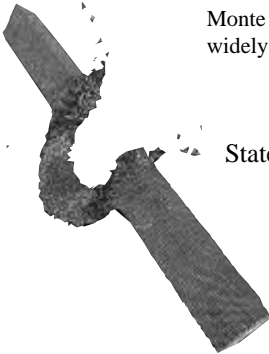


All electronic computers are composed of simple elements that perform simple operations. This article explains the way those elements work together and describes the differences between serial, vector, and parallel supercomputers.

HIPPI – The First Standard for High-Performance Networking 26
Stephen C. Tenbrink and Donald E. Tolmie

A Monte Carlo Code for Particle Transport – An Algorithm for All Seasons 30
John S. Hendricks

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.



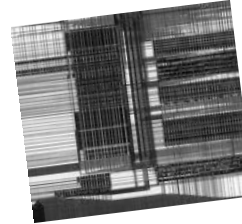
State-of-the-Art Parallel Computing – Molecular Dynamics on the Connection Machine 44
Peter S. Lomdahl and David M. Beazley

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.

Experimental Cosmology and the Puzzle of Large-Scale Structure 58
Wojciech H. Zurek and Michael S. Warren

Big Bang Cosmology and the Microwave Background 82
Salman Habib and Raymond J. Laflamme

A Fast Tree Code for Many-Body Problems 88
Michael S. Warren and John K. Salmon



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.

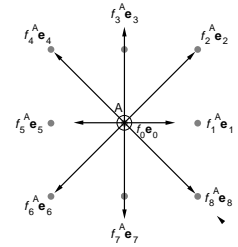


Stars make up galaxies, which make up galaxy clusters, which make up still larger structures. Theories of how these structures originated are being tested against observations through the use of "experimental cosmology"—numerical simulations on massively parallel computers that accurately follow the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

Lattice-Boltzmann Fluid Dynamics – A Versatile Tool for Multiphase and Other Complicated Flows 98

Shiyi Chen, Gary D. Doolen, and Kenneth G. Eggert

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.



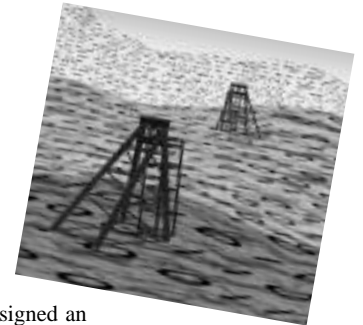
Equations of the Lattice-Boltzmann Method 110



Toward Improved Prediction of Reservoir Flow Performance —
Simulating Oil and Water Flows at the Pore Scale 112

John J. Buckles, Randy D. Hazlett, Shiyi Chen, Kenneth G. Eggert, Daryl W. Grunau, and Wendy E. Soll

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



Concept Extraction – A Data Mining Technique 122

Vance Faber, Judith G. Hochberg, Patrick M. Kelly, Timothy R. Thomas, and James M. White

Clustering and the Continuous *k*-Means Algorithm 138

Vance Faber

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.



The Digital Village Initiative 150

John D. MacCuish, Susan M. Mniszewski, Gregory E. Shannon, and Bonnie C. Yantis

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

@xxx.lanl.gov — First Steps Toward Electronic Research Communication 156

Paul H. Ginsparg

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.

