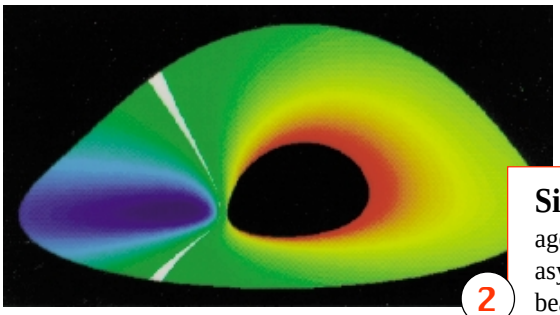
No.1

Theoretical Division

quarterly – fall 1997

CFDLIB Multiphase Flow Simulation Computer Code: An evaporating oil-gas-catalyst flow in a circulating fluidized bed flow loop, used in petroleum refining, was simulated with CFDLIB. Red: catalyst rich regions; blue: catalyst lean regions. CFDLIB is also being used to study multiphase flow problems in the chemical process industries and in the DOE weapons complex.

1



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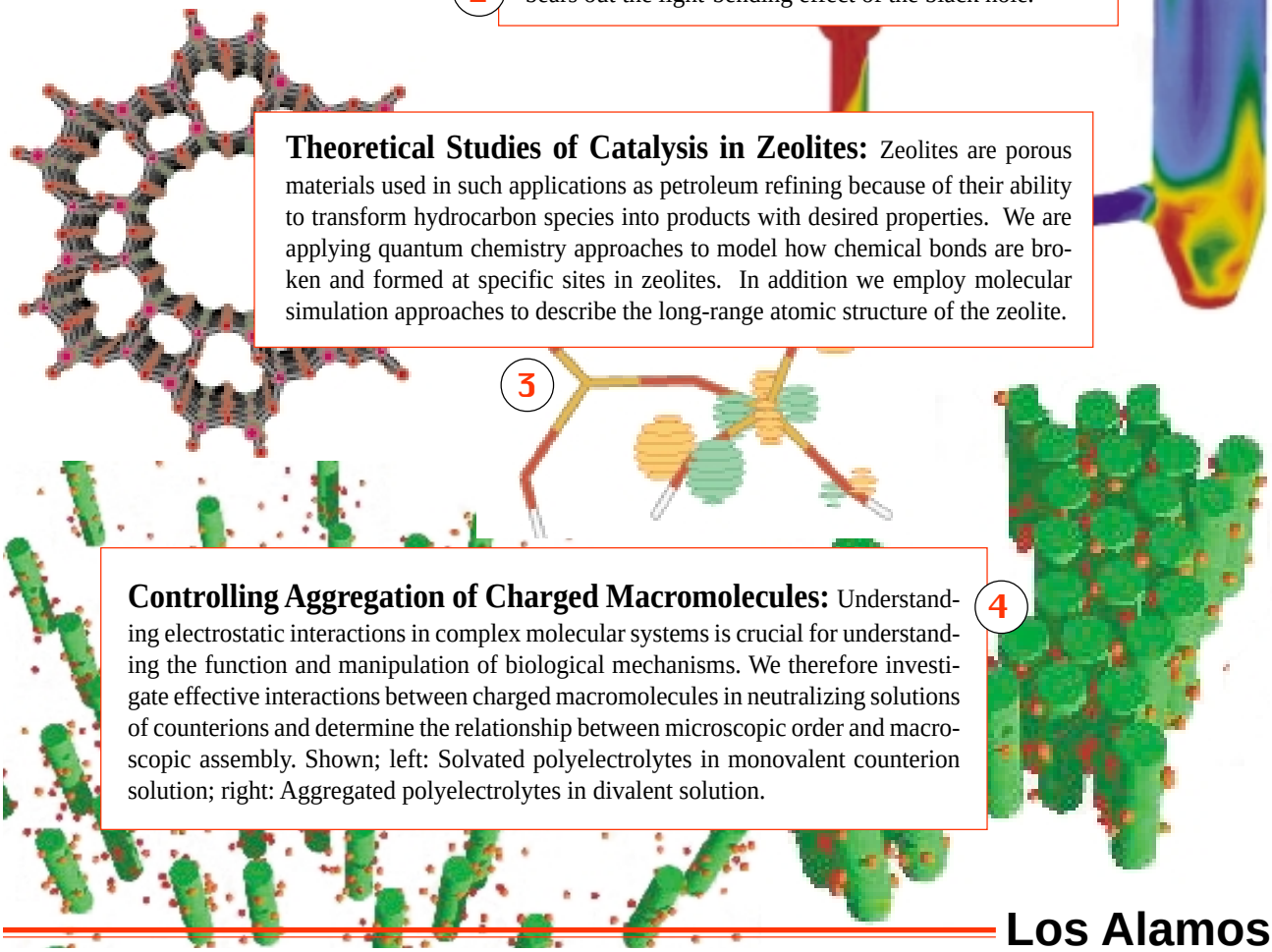
Signature of a Rotating Black Hole: X-ray image of a disk around a rotating black hole. The left-right asymmetry reveals rotation, the top-bottom asymmetry bears out the light-bending effect of the black hole.



Theoretical Studies of Catalysis in Zeolites: Zeolites are porous materials used in such applications as petroleum refining because of their ability to transform hydrocarbon species into products with desired properties. We are applying quantum chemistry approaches to model how chemical bonds are broken and formed at specific sites in zeolites. In addition we employ molecular simulation approaches to describe the long-range atomic structure of the zeolite.

3

Controlling Aggregation of Charged Macromolecules: Understanding electrostatic interactions in complex molecular systems is crucial for understanding the function and manipulation of biological mechanisms. We therefore investigate effective interactions between charged macromolecules in neutralizing solutions of counterions and determine the relationship between microscopic order and macroscopic assembly. Shown; left: Solvated polyelectrolytes in monovalent counterion solution; right: Aggregated polyelectrolytes in divalent solution.

4

Los Alamos

Modeling Metallic Microstructure Using Gradient-Weighted Moving Finite Elements: Shown is our current model results for the time-evolution (annealing) of 3D metallic grains. GWMFE is an efficient implicit method for mean-curvature-driven motion on the adaptive unstructured grids of the LANL Grid Toolbox (LaGriT). We are in the process of incorporating microtextural information to simulate faceting and residual stress.

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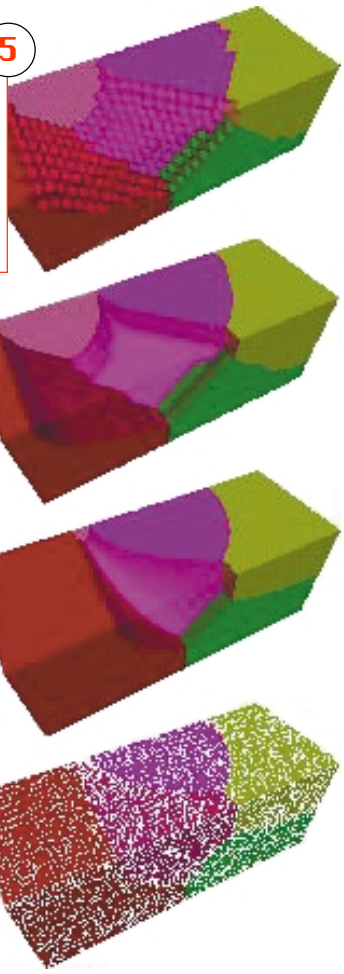

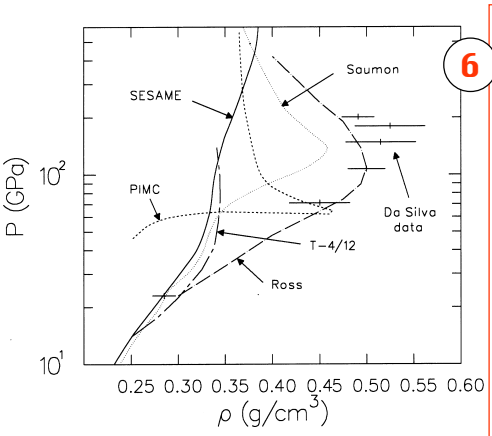

6

Is Fluid H_2 Anomalous at High Temperature?

New laser data, with a markedly large compressibility for H_2 along the shock Hugoniot, are in strong disagreement with past theory as represented by SESAME. More recent models give a wide range of behaviors. However, simple arguments, high-temperature expansions, and data on other materials convincingly support the SESAME Hugoniot and imply that the H_2 data are incorrect.

Carbon Dioxide Disposal: We are developing an economical, environmentally safe, and permanent method for CO_2-disposal from fossil fuel power plants based on combining CO_2 chemically in an exothermic reaction with abundant raw materials to form stable carbonate minerals.

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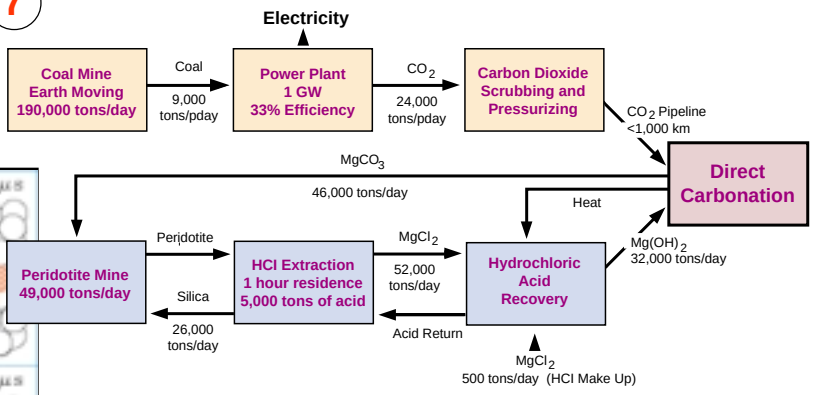
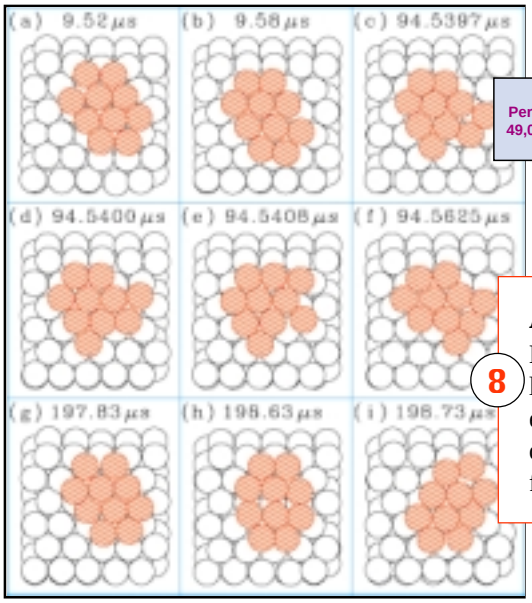
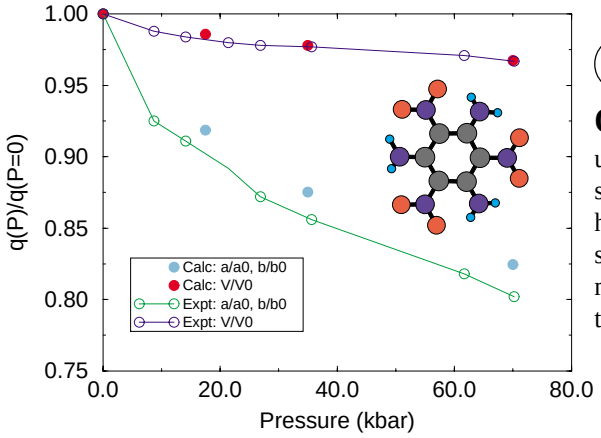




8

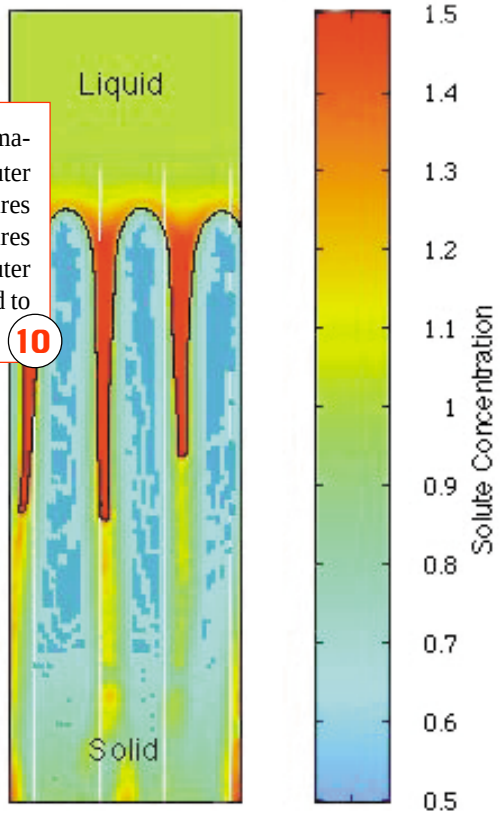
Atomistic Simulations on the Microsecond Time Scale: Even on the world's fastest computers, molecular dynamics simulations are limited to nanoseconds. For rare-event systems, a new acceleration method extends this to microseconds by stimulating transitions to occur more frequently. Here, a ten-atom Ag cluster on the Ag(111) surface is seen to diffuse by gliding (a-b), edge running (c-f), and a dislocation mechanism (g-i).



9

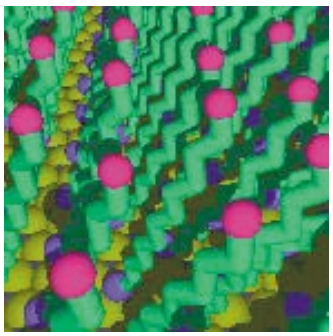
Computing Properties of Energetic Materials: We are using Monte Carlo methods in conjunction with an atomic-level description to compute the thermophysical and mechanical properties of high-explosive crystals over a wide range of temperatures and pressures. These properties can be used in the development of improved models for predicting the response of high explosives to the kinds of thermal or mechanical insults expected in various accident scenarios.

Modeling the Solidification of Materials: The integrity of any material used in high-technology applications such as airplane wings, computer chips, or nuclear weapons is determined by the microscopic solid structures formed during solidification. Our goal is to understand how these structures form and can be controlled to improve a material's properties. In this computer simulation of metal alloy solidification, the initially flat solid grows upward to form fingers and freezes into bands of high- and low-concentration solid.



10

Self-Assembled Monolayer of Dodecane-thiol on Gold (111): This is a snapshot from an all-atom molecular dynamics simulation to investigate the dynamical behaviour of self-assembled monolayers. The illustration shows the 2-dimensional hexagonal lattice of alkane-thiol molecules, with sulfur headgroups (blue), alkane backbones (green), gold (yellow), and methyl tail-groups (red).



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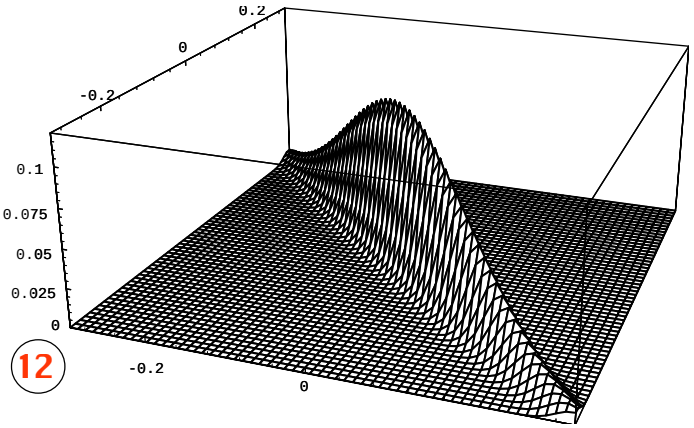
Dissipation and Decoherence in Quantum Mean Field Theory: The time-evolved Gaussian effective-density matrix for a particular fluctuation mode of a self-interacting scalar field theory, illustrating the strong suppression of off-diagonal components due to dephasing.



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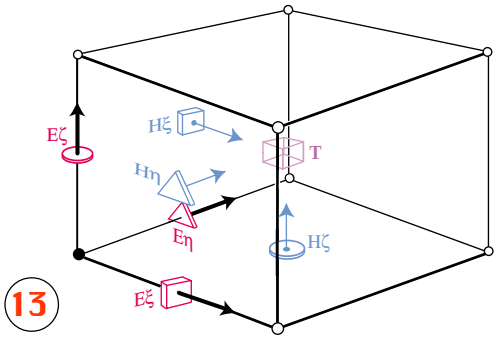
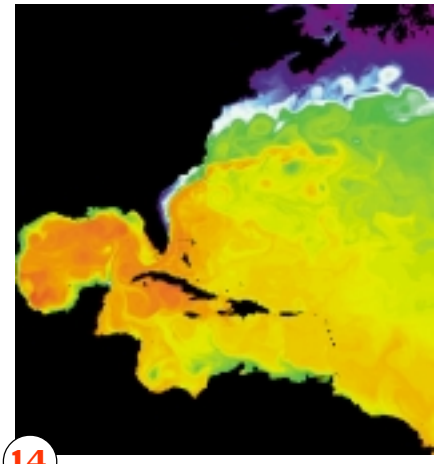


13

High-Quality Finite Difference Methods and Discrete Vector and Tensor Analysis: We have developed new mimetic finite difference methods for solving partial differential equations. These methods reproduce the fundamental properties of the differential operators and the underlying physical problem. The methods rely on defining scalar and vector quantities at locations that are naturally appropriate for the domains and ranges of the discrete operators.

Ocean Modeling: Numerical models of ocean circulation are useful in understanding the role of the sea in the full climate system. The Parallel Ocean Program (POP), a three-dimensional ocean circulation model, was developed at LANL for this purpose. A snapshot of the sea surface temperature from a high simulation of the North Atlantic shows very realistic features such as the Gulf Stream and its eddies.



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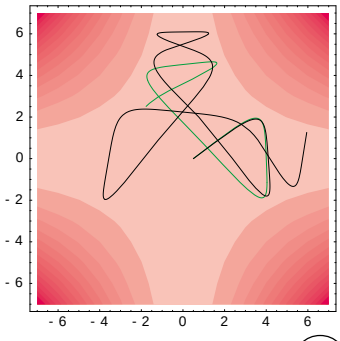

15

Old Quantum Mechanics Made New: Using just classical quantities, it is possible to compute quantum mechanical quantities. This is accomplished, despite the objections to Bohr's methods, by a better understanding of the geometry of classical flows and of the effects of chaos. The new methods are know as cycle expansions and code well in parallel computers.

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