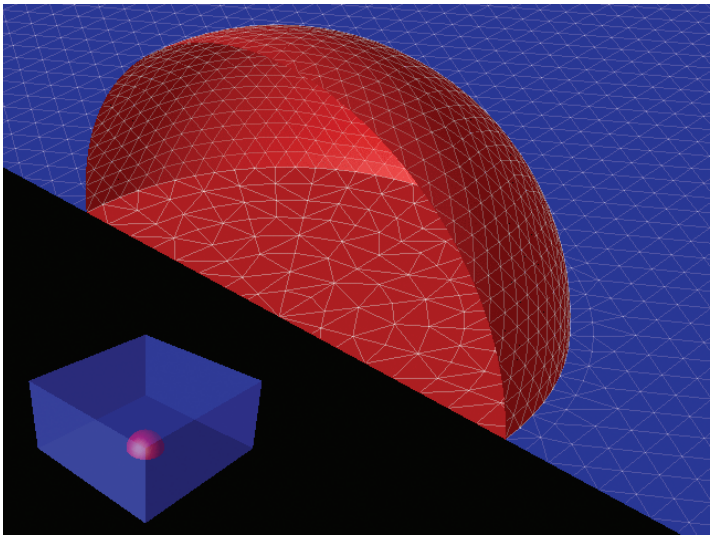
Los Alamos
NATIONAL LABORATORY

Theoretical Division *Quarterly*

Spring 2004

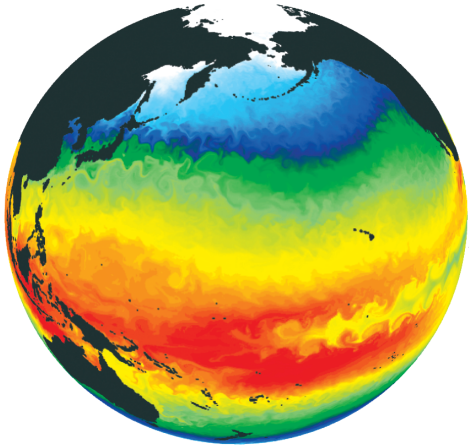
featuring work for the DOE /Office of Science



Mimetic Methods for Partial Differential Equations: Discrete Models for Maxwell's Equations in 3-D

We have developed high-quality algorithms for numerical modeling of electromagnetic problems. The new discrete models mimic many fundamental properties of the underlying physical problem, including the conservation laws, and the nondivergence of electric and magnetic fields. This new class of numerical methods will enable scientists to gain greater insights into electromagnetic systems, and solve new problems of interest to the DOE mission, and effectively use the inherent power of the current and future generations of scalable parallel supercomputers.

Mikhail J. Shashkov and J. Mac Hyman, T-7; and Neil Carlson, Independent Consultant; shashkov@lanl.gov



Climate, Ocean, and Sea-Ice Modeling

Over the last ten years, Los Alamos has built a strong program in computer modeling of the Earth's oceans, sea ice, and climate. In particular, our development of the Parallel Ocean Program (POP), and the CICE sea-ice model as well as the application of these models in fully-coupled climate model simulations have made Los Alamos nationally recognized for ocean, sea-ice, and climate-related research.

Philip W. Jones, John R. Baumgardner, John K. Dukowicz, Elizabeth C. Hunke, William H. Lipscomb, Mathew E. Maltrud, and Richard D. Smith, T-3; Robert Malone, Matthew Hecht, Sumner Dean, Scott Elliott, and Beth Wingate, CCS-2; and Rainer Bleck, and Shaoping Chu, EES-2; pwjones@lanl.gov

National Nuclear Security Administration

May 2004 LALP-04-107

Ocean Biogeochemistry

Computer models of the Earth's climate system have, until recently, primarily simulated the distribution of heat and water throughout the atmosphere, ocean, land, and sea ice. In order to more accurately simulate responses to carbon dioxide and other emissions from human activities, climate models are now including capabilities for simulating the distribution and interaction of the many chemical species that have a significant influence on climate.

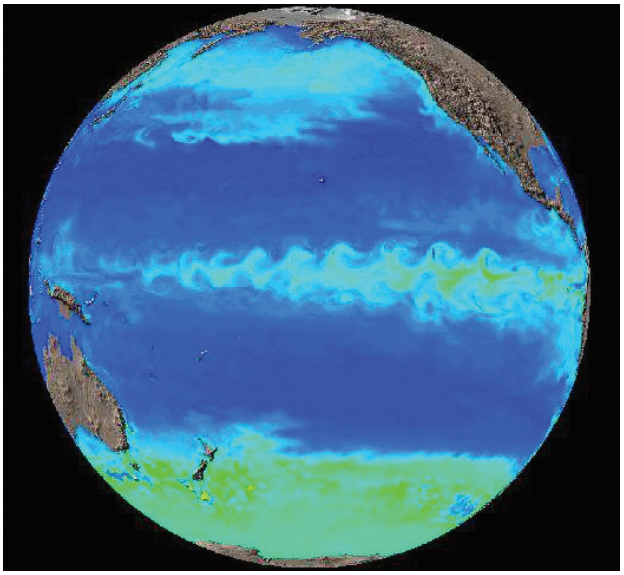


Figure: Phytoplankton concentration from a POP biogeochemistry simulation.

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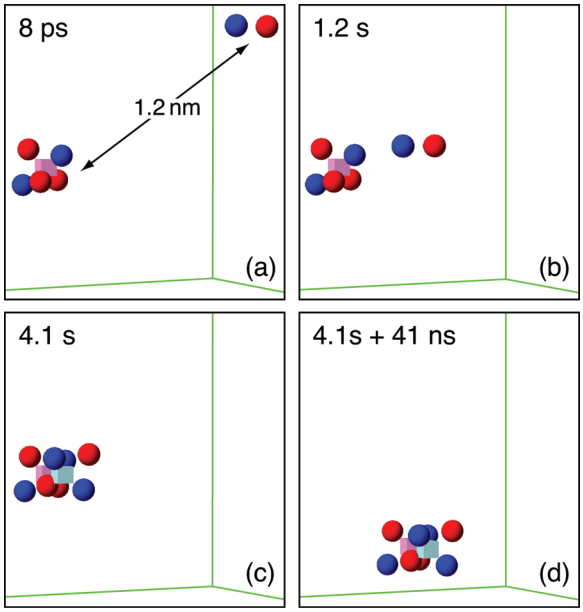
Radiation-Damage Annealing in MgO

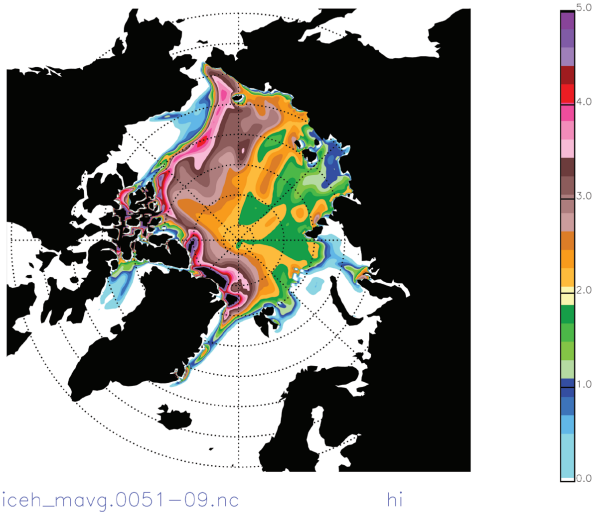
Combining molecular dynamics and temperature accelerated dynamics, an interesting picture emerges for the evolution of radiation damage in MgO. Point defects form during the cascades. Vacancies are immobile, but interstitials diffuse quickly, either recombining with vacancies or clustering. These clusters can be unexpectedly mobile, with the hexamer diffusing on the ns timescale. Clusters can thus aggregate with clusters from other cascades, increasing the overall damage accumulation rate.



Blas Pedro Uberuaga, T-12; Roger Smith, MST-8; Antony R. Cleave, Imperial College, UK; Graeme A. Henkelman, T-12; F. Montalenti, Universitá degli Studi di Milano-Bicocca, Italy; R. W. Grimes, Imperial College, UK; Kurt E. Sickafus, MST-8; and Arthur F. Voter, T-12; blas@lanl.gov

Sea Ice and Climate

For many years sea ice was represented fairly crudely in large-scale models. More sophisticated approaches were available, but were considered too complex and expensive for global climate simulations. Recently, however, sea-ice models have become more realistic as computing power has increased. CICE is a numerical model developed at Los Alamos to examine sea-ice physics using high-performance computers. It contains state-of-the-art methods for simulating ice dynamics, thermodynamics, and transport.



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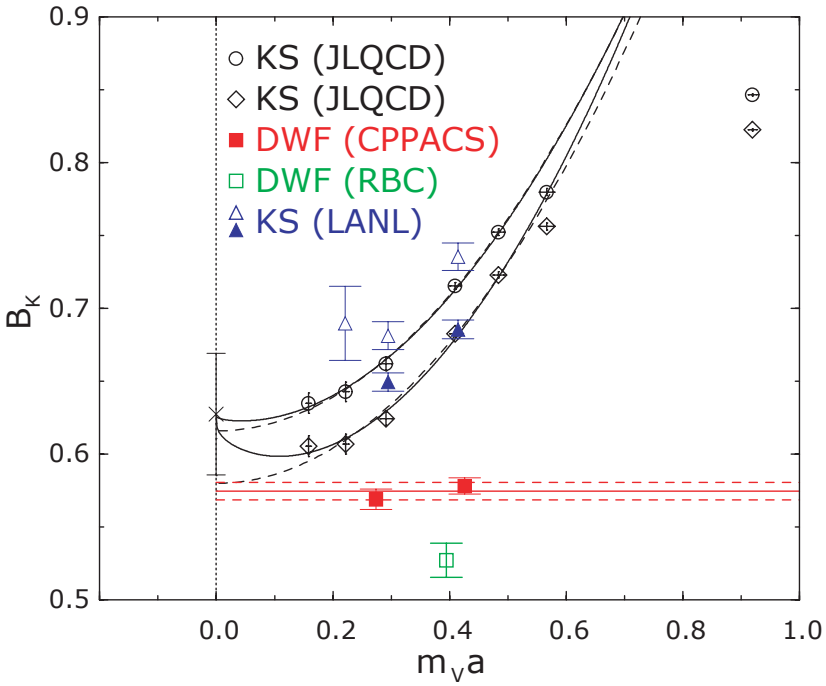

Lattice QCD at Los Alamos

Lattice Quantum Chromo Dynamics (QCD) calculations at Los Alamos have two goals—to validate a fundamental theory of nature and to push the envelope of high-performance computing. The LANL lattice QCD collaboration has pioneered the calculations of the kaon bag parameter B_K, which measures the QCD corrections to violations of charge conjugation and parity (CP) in the weak decays of kaons. Estimates in the quenched approximation, shown in the figure, are used by the particle physics community. Their current work is aimed at eliminating the largest remaining uncertainty due to the quenched approximation.

Figure: Results of lattice QCD calculations of the kaon bag parameter B_K.

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Inelastic Collisions Between Solitons in Optical Fibers

Collisions between optical pulses (solitons) from different frequency channels play an important role in multichannel fiber optics communication systems. We provide an accurate description of these collisions, including the effect of radiation emission. A schematic description of a collision is shown in the figure. We find that the radiation emitted in the collisions leads to random walk of the pulses, and consequently, to loss of information.

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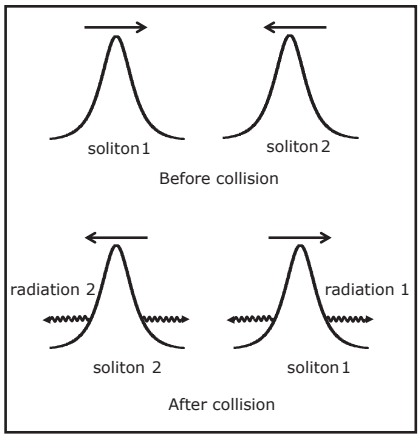

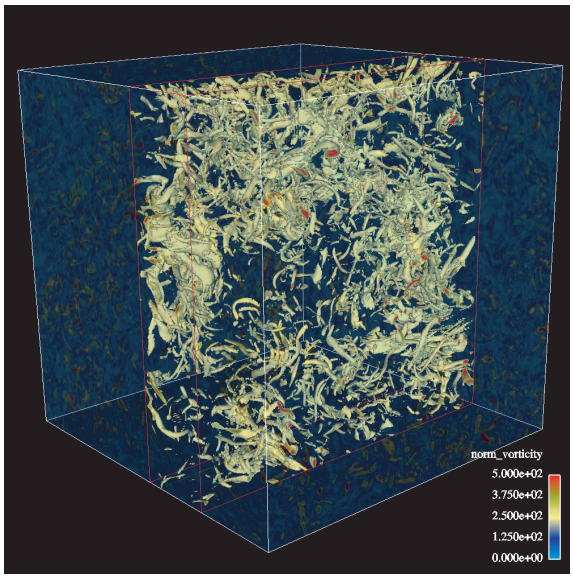

Capturing Small Scales in Nonlinear Models: Highly Resolved Simulation of a Turbulence Experiment

We performed a highly resolved simulation of the Navier-Stokes equations for decaying isotropic turbulence using 2048^3 grid points. The simulation emulates a recent wind-tunnel experiment performed at Johns Hopkins University and is the only existing computational effort of this magnitude (1 CPU-century) which directly parallels current experimental work.The data generated will provide to the turbulence research community crucial comparisons between numerical solutions, mathematical analysis, and experiments.

Figure: Visualization of the vorticity surfaces in a 256^3 sub-domain of the total 2048^3 simulation.

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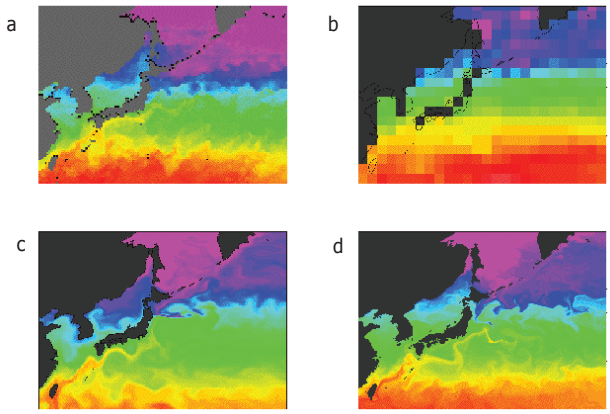
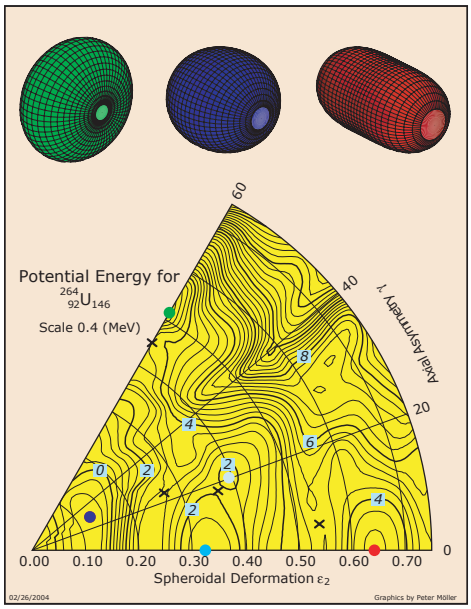
Eddy-Resolving Ocean Modeling



This figure shows the sea surface temperature in the warm Kuroshio current region from a) satellite observations and Parallel Ocean Program (POP) global ocean circulation simulations, b) coarse 2-degree resolution, c) eddy-permitting 0.28-degree resolution, and d) eddy-resolving 0.1-degree resolution. Although the eddy-permitting case shows substantial improvement compared to coarse resolution (typical for fully coupled climate models), only the eddy-resolving simulation can capture the detail and full extension of the Kuroshio current that is necessary for simulating realistic heat and salt transports towards the north.

Mathew E. Maltrud and Richard D. Smith, T-3; Matthew Hecht, CCS-2; and Julie McClean, Naval Postgraduate School; maltrud@lanl.gov



Fission Barriers at the End of the r-Process

A large number of the elements on Earth heavier than iron have been formed in stars in the rapid-neutron-capture process, or r-process. To model the r-process in the heavy-element region it is necessary to know various reaction Q-values, β-decay half-lives, branching probabilities to β-delayed fission and neutron-emission, and fission barriers for thousands of neutron-rich isotopes of nuclei. We model all these quantities within a global, comprehensive nuclear-structure theory developed at LANL. The calculated fission potential-energy surface for ^{264}U in the inner barrier region is complex with five minima (round dots) and four saddles (crossed lines). For more elongated nuclear shapes near division into two fragments we calculate the potential energy in terms of five different shape-degrees of freedom for about four million different shapes on computer clusters, using up to 100 CPUs for several days. Some results have appeared in Nature.

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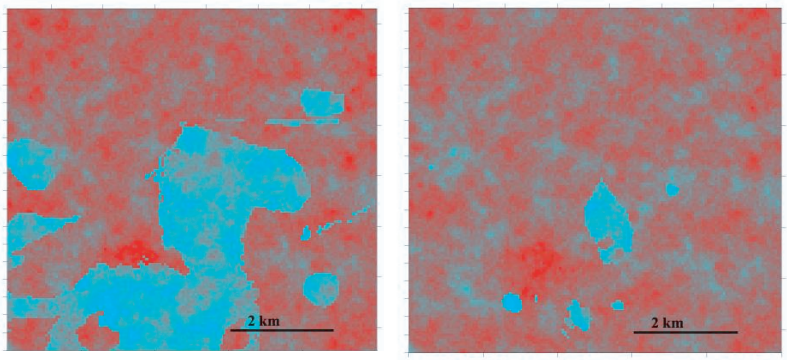

Stochastic Partial Differential Equations: Predictive Modeling–Coping with Uncertainty

Shown are porous media composed of two heterogeneous materials, one of high (turquoise) and the other of low (red) conductivity. The material distributions are reconstructed from a sparse geophysical data set. The left figure shows the boundary configuration corresponding to 74% probability of low-conductivity occurrence. The right figure provides a more conservative estimate of the boundary configuration (87% probability of low-probability occurrence).

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Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36. This document was produced for the Theoretical Division, Mail Stop B210, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, 505.667.4401, http://www.tdo.lanl.gov/. This scientific work is being performed primarily in Theoretical Division. Publication: Shirley Veenis, IM-1/T–DO