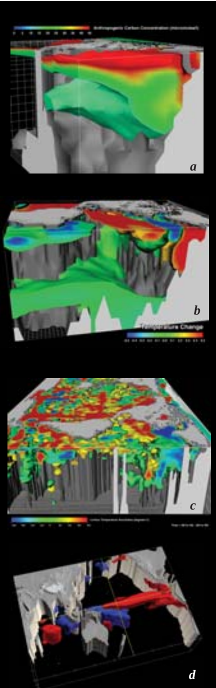
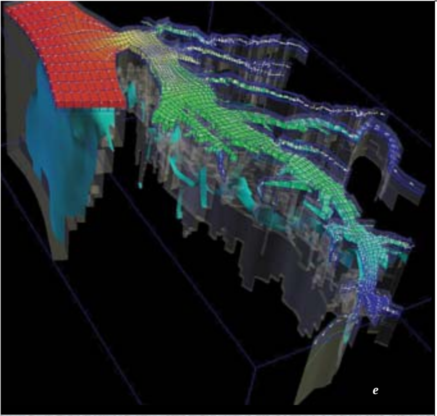
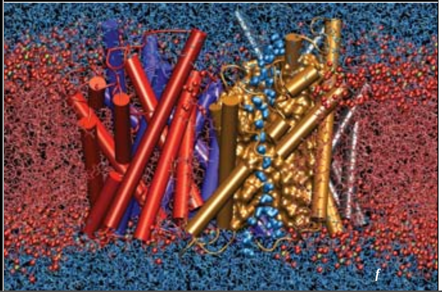
## Foundations for SCIENTIFIC LEADERSHIP

# NEW WAYS TO 'SEE' AND UNDERSTAND







Beyond the technologies that make high-performance computing and networking possible, no NITRD advances are more profoundly influencing scientific research and industrial innovation than computational modeling, simulation, and visualization. Modeling and simulation enable investigators to examine and experiment with very complex phenomena – such as the chemistry and kinetics of fire, or the mechanisms of viral infection – that exist far outside the boundaries of human vision. These phenomena can be infinitesimal (interactions of atomic particles), hazardous (biotoxins, radiation), multidimensional (combustion, neural signaling systems, air-traffic control), vast (the structures of galaxies), or a combination of factors at many scales (influences on global climate, stress factors in ship design).

Hard to perceive, such aspects of the physical world are even more difficult to explain because they typically represent the interplay of large numbers of disparate processes. Even if we understand individual processes, we cannot easily predict the results of their interactions. With high-performance modeling and simulation techniques, researchers can for the first time create "likenesses," or simulations, of enormously complicated and dynamic realities – such as the development of tornadoes – and make them visible in imagery.

### Trillions of calculations per second

Computational models break a phenomenon under study into very small pieces, each described by mathematics. The model is the scientist's approximation of how the physical process works as a whole. Very powerful computing platforms then perform the calculations – often many trillions of operations – specified in the model. The resulting simulation also is an approximation, but by comparing the results to observational data, researchers can evaluate how closely the model matches reality. If the data validate the model, it can then be used to predict behavior for which no data exist. Visualization software plays a key role, turning simulation data into three- or four-dimensional renderings of the results. In the case of tornadoes, for example, full-color imagery can highlight such invisible factors as air pressure and wind velocity, revealing relationships that would not be apparent in raw data or photographs.

Because they make complex systems visible and testable, modeling and simulation have become the tools of choice for designing, evaluating, and managing elaborate structures and systems, such as aircraft and avionics, automobiles, buildings, manufacturing machinery and processes, and power grids. Military planners use simulations to assess large-scale, multidimensional staging and battlefield scenarios with such variables as personnel, weaponry, vehicles, portable infrastructure, communications systems, and supply chains.

### NITRD modeling applications

But developing modeling and simulation capabilities for cutting-edge U.S. science and engineering remains one of the most technically difficult challenges in advanced computing. The more complex the phenomena to be modeled, the more demanding the software development issues. Current and FY 2004 NITRD research continues its focus on the advanced mathematical and computer-science underpinnings for scientific modeling and simulation. Recent NITRD achievements point to their increasingly critical role in sustaining U.S. technological preeminence.

Scientists at the National Center for Atmospheric Research (NCAR), with support from DOE/SC and NSF, in 2002 produced a high-resolution millennium-length global climate simulation. The 1,500-year simulation was generated using NCAR's Parallel Climate Model, which dynamically couples the major components of Earth's climate system, such as atmosphere, oceans, land, and sea ice. The simulation took 456 days to run on the IBM SP supercomputer at DOE/SC's National Energy Research Scientific Computing (NERSC) facility. Among the findings was the discovery that the familiar climate mode of El Niño can change its activity substantially over the centuries, even when not influenced by outside forcing. As a result, the scientists cautioned that interpretations of changes in

*NOAA Geophysical Fluid Dynamics Laboratory models: **a)** Atmospheric carbon (red) concentration. **b)** Atmospheric warming patterns. **c)** Temperature anomalies. **d)** El Niño/La Niña effects on water temperature.*

*AIR AND WATER AT EVERY SCALE* ***e)*** *Chesapeake Bay looking south, with major tributaries at right. Image shows computed salinity, (high levels red, freshwater dark blue). Rendered from a coupled hydrodynamic/water quality model developed by Army Corps of Engineers and EPA. The first fully 3-D, time-varying model of an estuarine environment, the model has enabled new understanding of multiple eutrophication factors, such as nitrogen from air pollution.*

***f)*** *In one of the largest molecular simulations yet achieved (106,000 atoms interacting over 5 million time steps), computational biophysicists at the University of Illinois have discovered a key mechanism enabling proteins called aquaporins, which make up the membranes surrounding cells, to transport large amounts of water – up to 250 liters daily in humans. For details, see page 51.*
***g)*** *Visualization of scientific data begins with exacting mathematics. Cubes test curvature-based transfer functions in a synthetic data set from a quartic polynomial implicit function, serving to debug/demonstrate correctness of convolution-based measurements and show their effectiveness in a volume rendering context. Cube at right is Gaussian curvature.*

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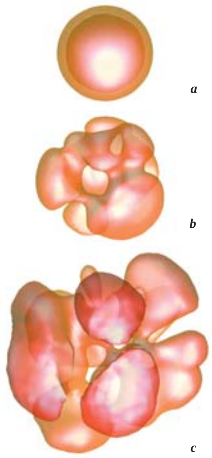
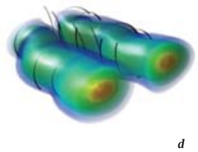
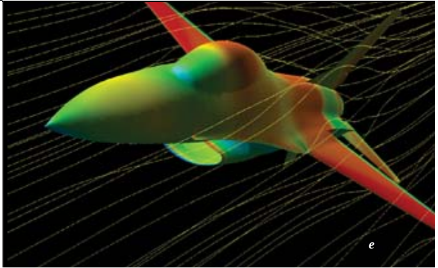
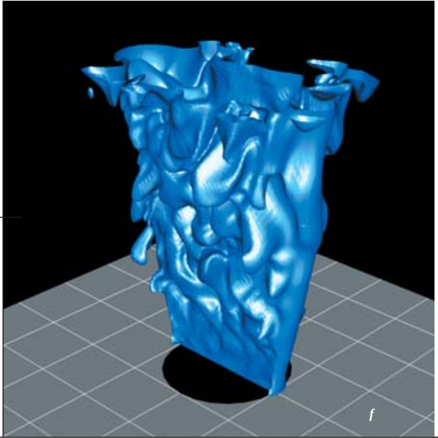


*Stages of a supernova explosion over 50 milliseconds: **a)** Initial implosion. **b)** In-falling gas approaches the core, where neutrinos heat and make the gas buoyant. **c)** Process causes enough convective energy transfer to create explosion.*





***d)** University of California-Davis researchers are experimenting with new ways to visualize multidimensional data sets. Image renders isosurfaces, vorticity, and velocity of wakes. **e)** Image of F-16 flying at Mach .9 shows levels of stress on surfaces from highest (red) to lowest (blue). A University of Colorado researcher's innovative model integrating fluid dynamics and structural stress data evaluates "flutter" – a dangerous vibration in high-speed flight – in aircraft designs.*



***f)** The physics and chemistry of combustion, one of the most complex processes in nature, remain a major scientific challenge. DOE/SC scientists have developed the first fully resolved 3-D simulation of turbulent methane combustion (image at left), winning the 2003 SIAM/ACM Prize in Computational Science and Engineering.*

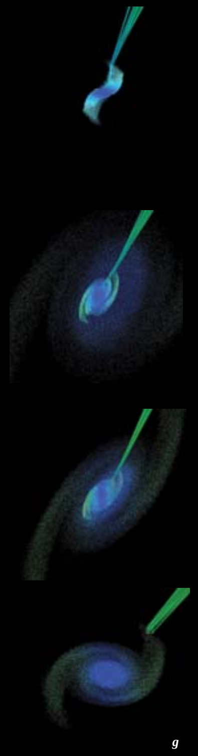
El Niño need to be evaluated with caution, and that physical mechanisms of these changes require further exploration.

The first 3-D simulations of the spectacular explosion marking the death of a massive star, called a supernova, were achieved by DOE/SC scientists in 2002. Such explosions, among the most violent events in nature, unleash power that can briefly outshine a galaxy of 100 billion stars. The work confirmed that the explosion process is critically dependent on convection, the mixing of the matter surrounding the iron core of the collapsing star. Understanding the nature of star deaths is considered a key to explaining the expansion of the universe. Supernova calculations are exceedingly computation-intensive because many processes, involving all four fundamental forces of physics, must be modeled for more than 100,000 time steps. Typical simulations (a million particles) took three months on the IBM SP at NERSC.

The Numerical Propulsion System Simulation (NPSS) developed by NASA scientists addresses one of the most costly and time-consuming elements of modern aviation manufacturing – testing the design, structure, and performance of jet engines. A first-of-its-kind tool for modeling and analyzing jet propulsion systems in a single package, NPSS can interact with and integrate externally generated data and design tools, and it allows geographically distributed teams to collaborate on simulations. This design advance was named one of the top 100 R&D achievements of 2002 by *R&D Magazine* and received the 2002 NorTech Innovation Award.

Researchers at the University of California-San Diego supported by NIH and NSF have developed a modeling technique that applies computational chemistry rather than "wet" laboratory methods to assess how well potential medications will work. Drug molecules bind to specific "receptor" proteins in the body, and pharmaceutical designers try to figure out where on the protein that binding will best occur. The computational model calculates the possible variations in a protein's shape and then tests the candidate drug's binding ability with all the variants, accounting for the molecular stretching and bending that can affect binding but are not captured in static models. This high-speed technique can be used with any drugs and proteins for which three-dimensional structural information exists – accelerating the search for alternatives to medications with severe side effects. Similar methods are helping immunologists identify the chemical triggers of immune response, a key step in the search for new vaccines.

A massively parallel structural dynamics software code named Salinas, developed by DOE/NNSA researchers for simulating the responses of structures to varying loads and stresses, earned a special 2002 Gordon Bell Award, the supercomputing field's top honor. The software supports the Federal nuclear stockpile stewardship program, which uses high-end computational capabilities to ensure the safety, security, and structural integrity of the Nation's nuclear weapons.



***g)** Acceleration of concentrated particle beams is a core technique in the search to understand the elemental forms and properties of matter. Simulation shows formation of a halo around a single particle, a sign of incorrect injection of beamline into cyclotron.*