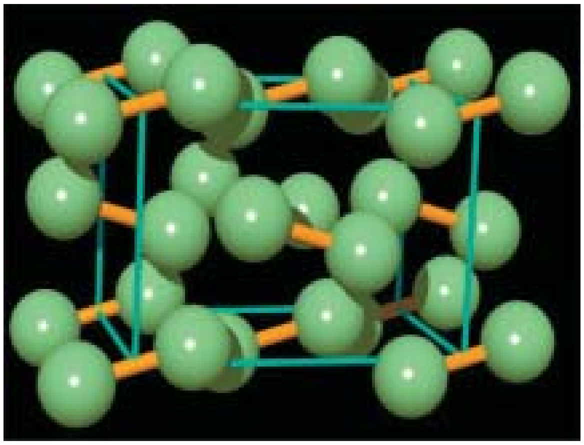
Theoretical Division Quarterly

Summer 2003



Structural Phase Transitions in Ga: Massive Parallel Implementation and Application of the Modified Embedded Atom Method

The Modified Embedded Atom Method applies to metals with greater covalent bonding than the conventional Embedded Atom Method, which is restricted to nearly-free-electron (simple fcc) metals.

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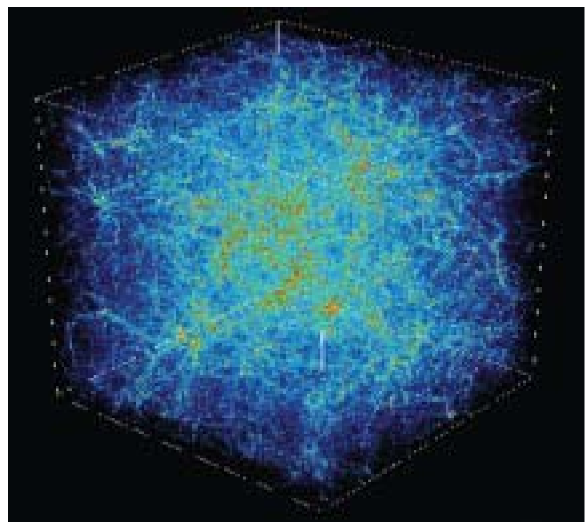
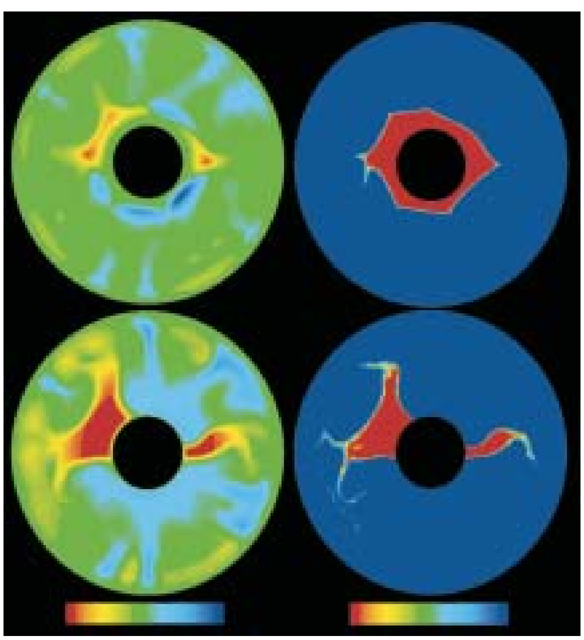
Cosmological N-Body Simulations

Cosmology is the study of the large-scale structure and evolution of the Universe. Observations of the Universe have revealed a wealth of structure in the form of galaxy clusters, filaments and voids. The image represents the density of dark matter in the Universe in a region about one billion light-years across showing many thousands of galaxy halos. The simulations used an advanced parallel treecode algorithm to solve the gravitational N-body problem in unprecedented detail.

Michael S. Warren, *mswarren@lanl.gov*





Early Lunar Mantle Overturn Causes a Transient Lunar Core Dynamo

The Moon presently has no internally generated magnetic field. However, paleomagnetic data combined with radiometric ages of Apollo samples record the existence of a magnetic field from ~3.9–3.6 Ga, suggesting the possibility of an ancient lunar dynamo. However, a dynamo during this time period has been difficult to explain, because previous thermal evolution models for the Moon have provided too little core heat flux. We show that a pulse of core heat flux following an overturn of an initially stratified lunar mantle can explain the existence and timing of an early lunar dynamo.

Figure: *left column, temperature; right column, radioactivity; top row, before dynamo; bottom row, during dynamo.*

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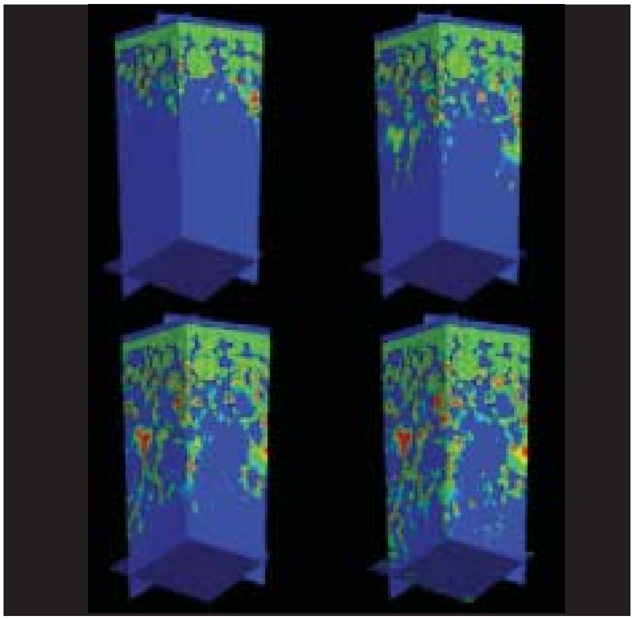

Direct Numerical Simulation of Weak Shocks in Granular Material and PBXs

Events on the scale of the constituent grains play a role in the mechanical response and chemical decomposition of Plastic Bonded Explosives (PBXs). Homogeneous continuum models provide good estimates of bulk material response. However, there is little connection to the underlying physics and hence they cannot be extrapolated with confidence. Numerical simulations are performed to gain insight into grain-scale material response in (dry) granular material as a first step toward simulations of PBXs. The University of Utah's ASCI Center's PIC code was used. Simulations run on 1000 processors predict the development of preferential load paths, or stress bridging, in the dynamic compaction of dense three-dimensional granular assemblies.

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Developments Towards a Complete Ductile Damage Model

Ductile damage occurs in plastically flowing materials. Void nucleation, growth, and coalescence are the three stages of ductile damage, of which coalescence is the least understood stage. The figure shows our recent Green's functions calculation of the plastic strains generated between two coalescing voids. It is seen that the plastic strain field is strongly distorted by the void-void interaction.

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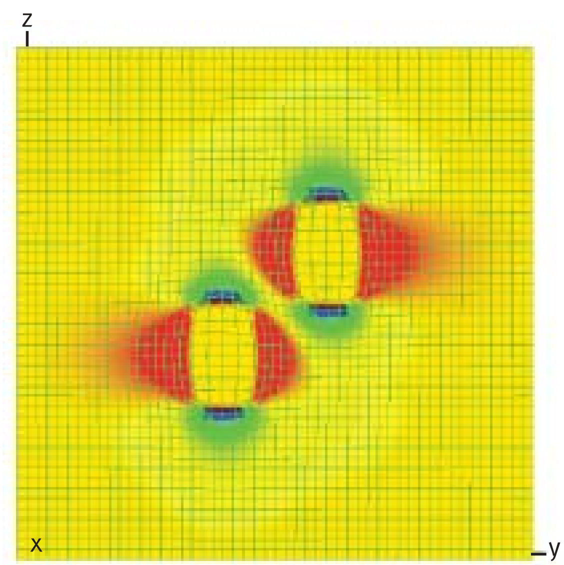

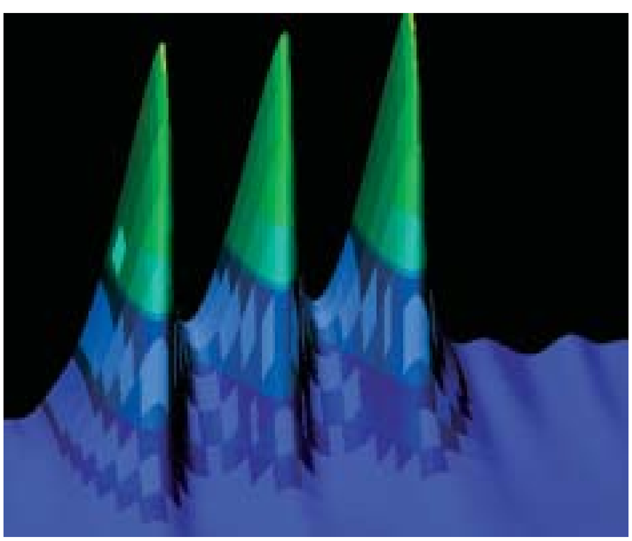

Bright Solitons in Bose-Einstein Condensates

Bose-Einstein condensates (BEC) provide a highly productive laboratory for the study of many fascinating quantum mechanical nonlinear phenomena such a vortices and solitons. The figure shows the production and interaction of three bright solitons. Such self-contained, coherent structures may have valuable applications to the construction of effective atom-optics systems.

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High-Explosive Safety

Friction experiments performed by Dyer & Taylor of the UK employed a sliding surface in contact with a sample of high explosives under pressure using a system of weights. When grit particles were present at the glass/high-explosive interface, frictional heating often resulted in explosions after only a millisecond. Numerical calculations of the process confirm that the presence of grit particles can indeed result in temperatures capable of initiating detonation.

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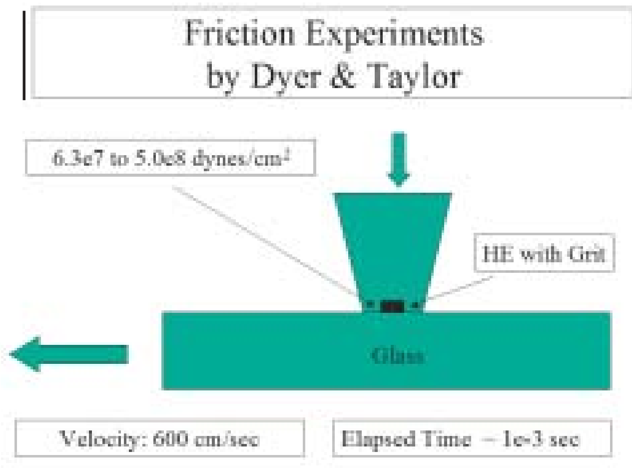

An Atomic Description of the Folding/Unfolding of Protein A

We studied the folding mechanism of a small three-helix bundle protein at atomic resolution, including effects of explicit solvation, over a broad range of temperatures spanning the folded and unfolded states. We decompose the free-energy landscape into its enthalpic and entropic components by fitting all free-energy surfaces at all sampled temperatures. We also explore the interplay between folding and water dewetting.

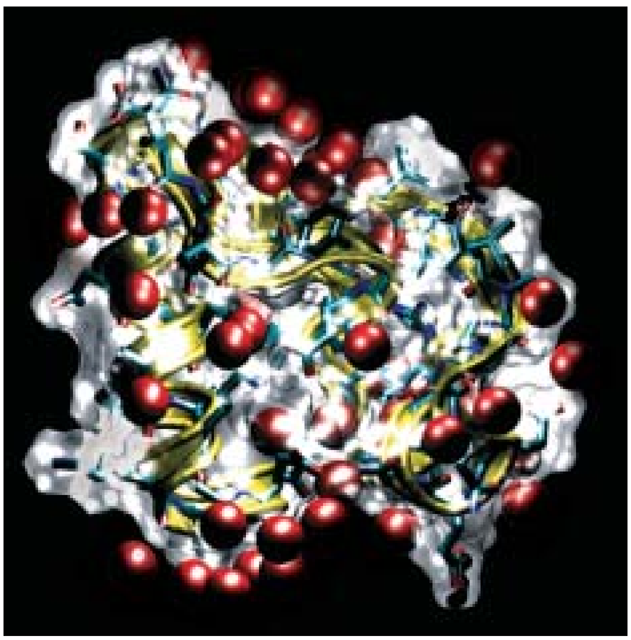

Figure: *Illustration of water molecules coordinated to carbonyl oxygens in the protein backbone. The protein configuration belongs to the folding transition state of the protein. Some water molecules are in the interior of the protein.*

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Temperature Effects on Charge Transport in DNA

Charge transfer in DNA is of great biological importance because of the role it plays in damage occurring under conditions of oxidative stress.

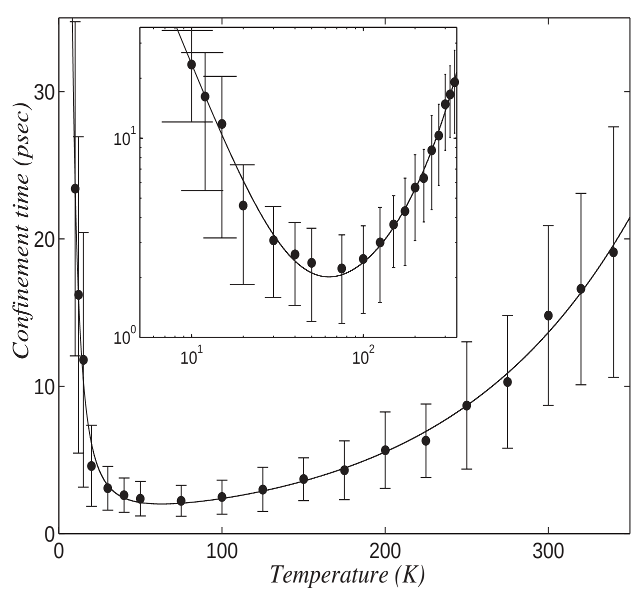

Figure: *Characteristic time, in which an initially localized charge remains confined, as a function of temperature (circles). Error bars represent statistical errors over 100 runs. The line represents a fit to a functional form comprised of a power law term for low temperatures and an exponential term at higher temperatures. The inset shows the same data in log-log scale to more clearly display the details at small temperatures.*

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Clustering in Granular Media

Energy dissipation plays a major role in the dynamics of granular media. Combining continuum theory, scaling analysis, and large-scale molecular dynamics simulations, we have shown that statistical characteristics of freely evolving granular gases are both universal and self-similar. Energy dissipation leads to the formation of complex large scale structure on multiple scales as shown in the figure, yet the laws governing these scales follow directly from conservation of mass and momentum.

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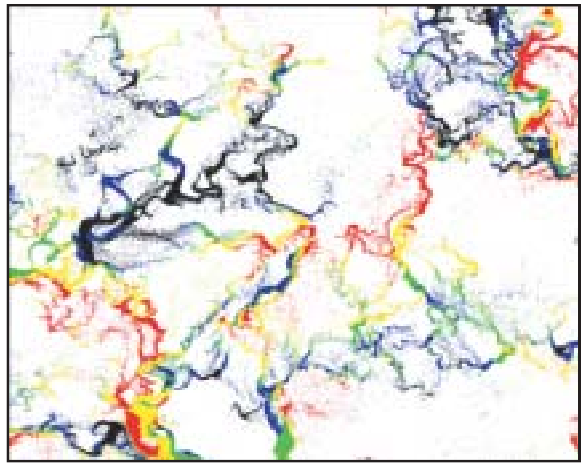

Boundary Effects on Chaotic Advection-Diffusion Chemical Reactions

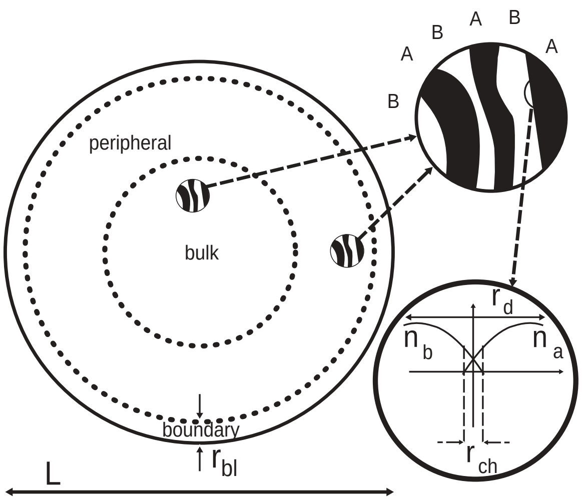

Figure: *Chemical reactor boundary is drawn by solid line on the main chart. Dotted lines separate bulk, peripheral, and boundary domains of the flow. Chart in the upper right corner shows schematically the stripe structure magnified from the bulk and/or peripheral domains. Black and white regions are the ones populated by A and B respectively. The chart in the lower right corner shows (under even stronger magnification) distribution of chemicals normal to their contact interface.*

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A Solution to a Cosmological Puzzle

In a recently published article in *General Relativity and Gravitation*, I found a new solution to Einstein's field equations. This solution goes smoothly between the observed behavior of the solar system and the expansion of the universe at cosmological distances. My solution depends on the concept of "dark energy." It finally provides an answer to the decades-old question of how to reconcile those two different behaviors!

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NNSA National Nuclear Security Administration

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