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Theoretical Division *Quarterly*

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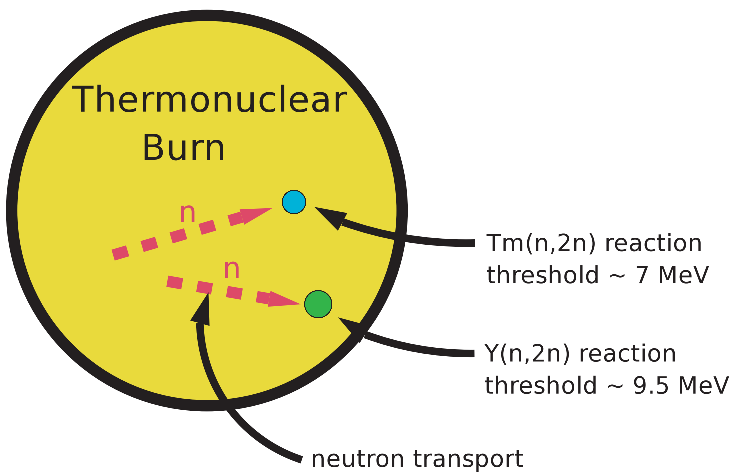

The Physics of Yttrium Equivalence for Radiochemical Detectors

Radiochemical detector systems provide the fundamental method for measurement of neutron properties in the thermonuclear environment. These measurements are important in the determination of fission and fusion yields, and therefore provide a basis for interpretation of Nevada Test Site (NTS) data.

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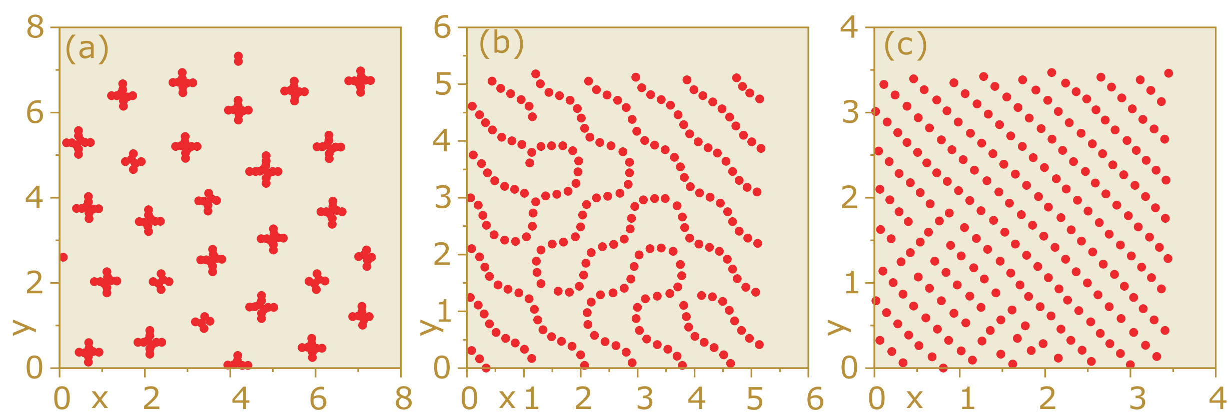

Fibrillar Templates and Soft Phases in Systems with Short-Range Dipolar and Long-Range Interactions

Our understanding of the transport properties of most single crystal materials is based on the assumption that the underlying charge structure is homogeneous. This assumption has recently been challenged due to the unusual and poorly understood behavior of a wide class of complex electronic materials, including high temperature superconductors. Recent theories for the mechanisms responsible for these phenomena suggest that the mobile charges are not homogeneously distributed throughout the media. Instead, charge-ordered states such as stripes or clumps may form.

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National Nuclear Security Administration

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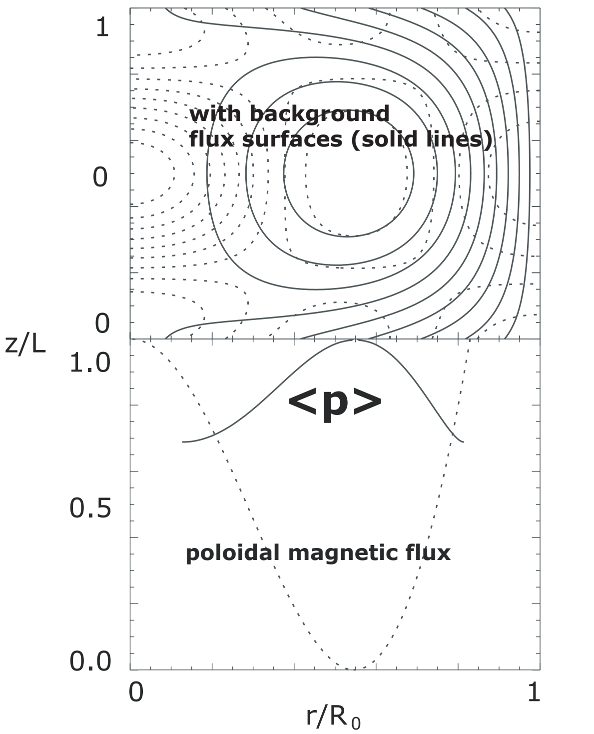

Chandrasekhar Equilibria of Compact Toroids with Alfvénic Flows

The figure plots a pressure-confining, ideal MHD-stable, analytic Chandrasekhar FRC equilibrium with a vertical guide field. Favorable confinement property of nested closed flux surfaces and the unusual ideal magneto-hydrodynamic stability of such compact toroids are of interest for both magnetic trapping of high-energy electrons in astrophysics and confinement of high-temperature plasmas in the laboratory. We have also clarified the similarity and important distinctions between Chandrasekhar compact toroid equilibria and those predicted by relaxation theories. This work was supported by DOE OFES.

Figure: A Chandrasekhar FRC equilibrium with vertical background field. Top: dashed line are pressure contours. Down: flux-surface-averaged pressure and poloidal flux are normalized to their peak value, respectively.

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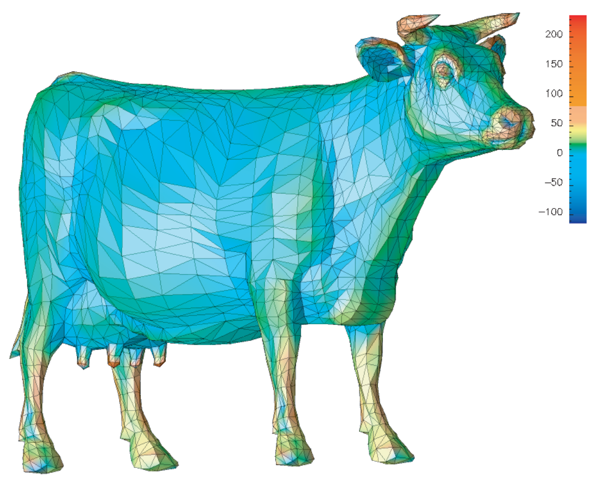

Curvature Estimation for Unstructured Triangulations of Surfaces

In this study, a comparative analysis and convergence study were done of several curvature estimation methods suggested in the literature and a new, improved method was proposed as an extension of one of those methods. The new method robustly estimates normals, principal curvatures, mean curvatures, and Gaussian curvatures at vertices of general unstructured triangulations. The method has been tested on complex meshes and has provided very good results shown in the example.

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Fundamental Detonation Behavior from Molecular Dynamics Simulations

While most aspects of detonation behavior of plastic-bonded explosives (PBXs) are well-understood and modeled at an empirical level, there are essentially no aspects of their behavior that can be predicted quantitatively from basic physical models. Examples include changes due to large temperature variations, curvature effects, changes in manufacturing processes, and aging phenomena. Improving our predictive capabilities in this regard is one of the primary goals of the ASC Materials and Physics Program.

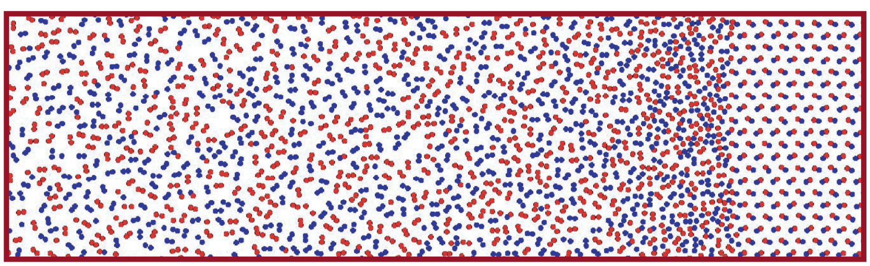

Figure: shows a snapshot from a propagating detonation in a model AB diatomic system.

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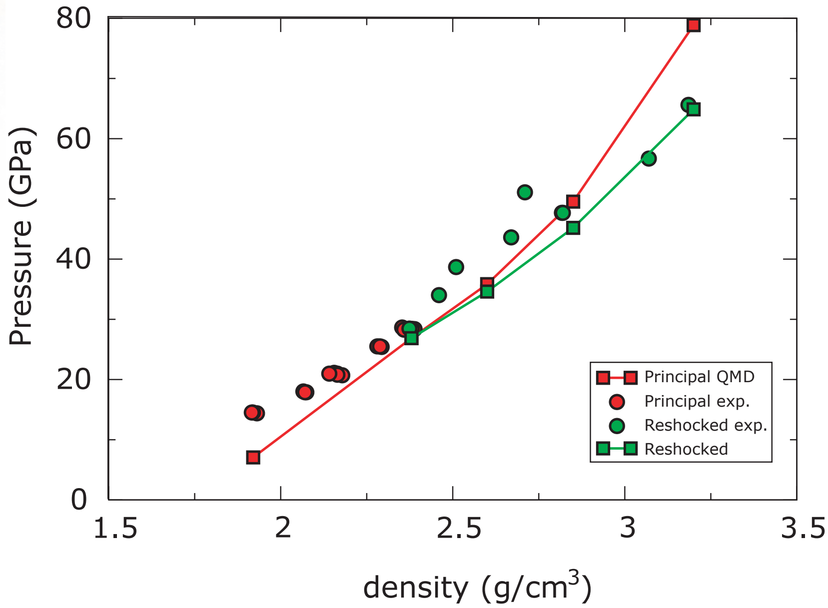

Quantum Molecular Dynamics Simulations of Shocked Nitrogen Oxide

We report here on the study of the EOS and dissociation of NO along the principal and second shock Hugoniots using Quantum Molecular Dynamics (QMD). While NO presents a natural extension to study the EOS of multicomponents systems, it also serves as a prototype for the study of explosive compounds and their associated reactive chemistry. Furthermore, the determination of reactive potentials, necessary for the study of technologically relevant and more complex systems such as H-C-N-O, also requires first a calibration to the NO system.

Figure: Principal and reshocked NO Hugoniots.

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T-13: Complex Systems

Quantum computers have considerable potential to contribute to national security. In the future such computers could be used to assist real time decision making, to enable fast searches of large unsorted databases, and to support more powerful cryptography. Within the framework of the National Security Agency Quantum Computer project on self-assembled quantum computers, a T-13 team carried out modeling and simulations of wave function collapse in a single electron spin measurement that used magnetic resonance force microscopy. These results enabled us to identify an optimized range of parameters for measuring a state with a single quantum bit (qubit) of information based on a single electron spin. The results were reported at the ARDA Quantum Computing Program Review, held this summer.

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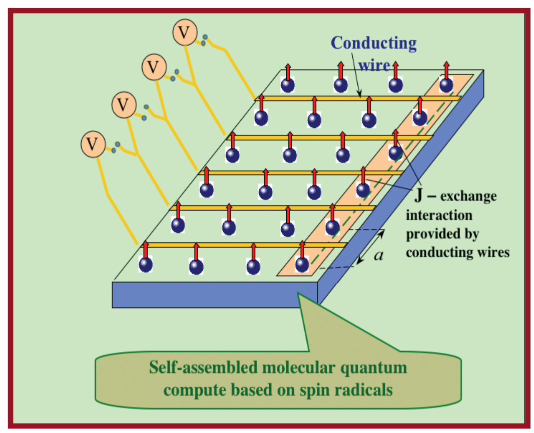

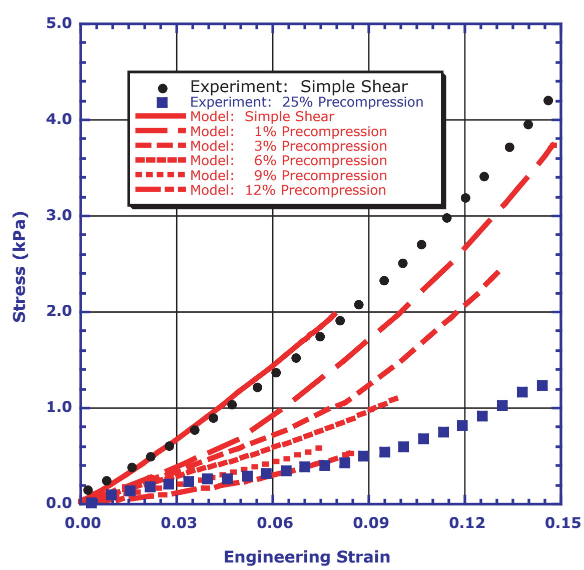

Modeling the Dynamic Response of Disordered Cellular Materials

The purpose of this project is to develop a constitutive law and a general modeling approach for describing the mechanical response of cellular materials to highly dynamic, large-strain, and high-rate loading conditions. The programmatic relevance of this project derives from the implementation and use of this modeling approach within large-scale codes for simulating the behavior of cushioning materials.

Figure: Shear stress versus shear strain for a low-density polyurethane foam, showing the softening effects of various levels of pre-compression.

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A Liquid Dynamics Theory

We believe that our recently developed Vibration-Transit Theory provides a physically realistic approach for the study of liquid dynamics. In monatomic liquids, the motion is comprised of normal mode vibrations in any of the large number of equivalent random valleys, interspersed with nearly instantaneous transits, which carry the system between neighboring valleys. The consequences for S(q,ω) are: a) when the system moves in a single random valley, the inelastic part of S(q,ω) is a sum over all vibrational modes of the inelastic cross section of each single mode, and b) in the liquid state the system undergoes transits at a rapid rate, causing the Rayleigh and Brillouin peaks to broaden but not shift. Our major finding, through comparison of theory with MD calculations, is that over the entire q range where the Brillouin peak is distinguishable, its location Ω(q) in the liquid is the same as it is in a single random valley.

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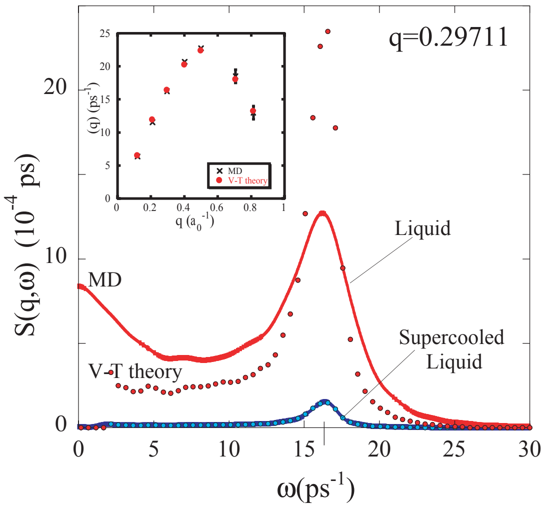
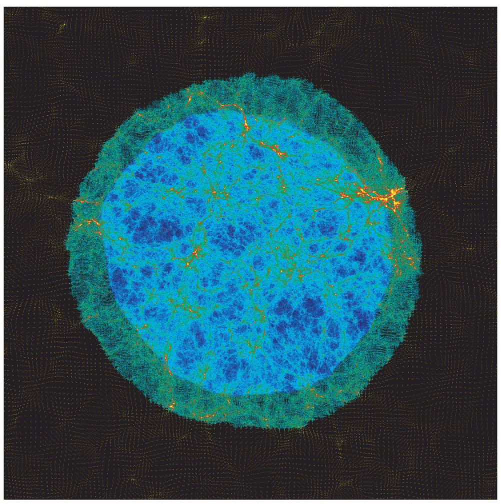


The Distribution of Dark Matter in the Universe on Scales of 10^{10} to 10^{15} $M_\odot$



The increasing sophistication in software and the use of large parallel computers have allowed us to perform a suite of N-body simulations using on the order of a billion particles. This allows us to study deeply nonlinear gravitational clustering, a regime that has not been well-studied, with other cosmological N-body simulations. Statistically, rather than basing results on just one or two large simulations, now one can investigate the role of the different numerical and physical effects on the statistics used to characterize the mass distribution of the universe.

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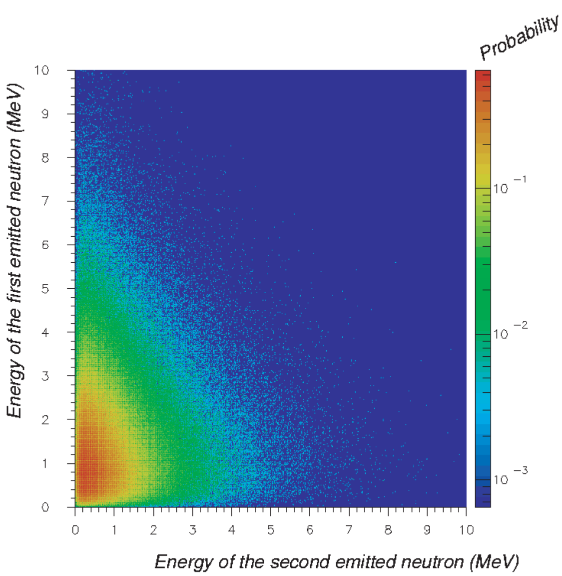

Correlated Neutron Emission in Fission: Initial Results

The research we have been doing relates to correlated prompt neutron emission in fission. It is motivated by needs in detecting correlated neutrons from a fission chain, for active and passive detection of special nuclear materials for nonproliferation applications.

Figure: Neutron energy correlations.

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