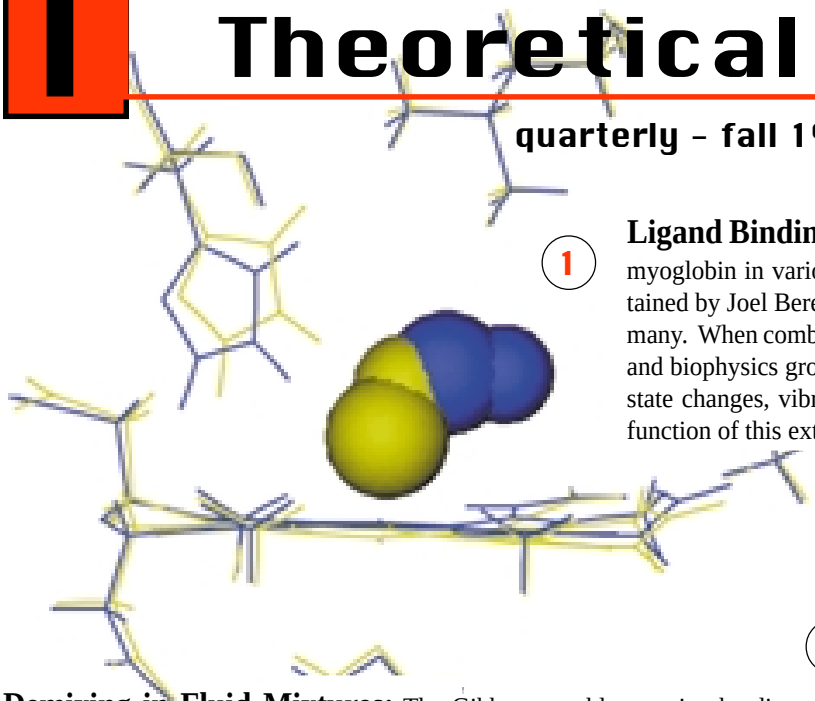
No. 9

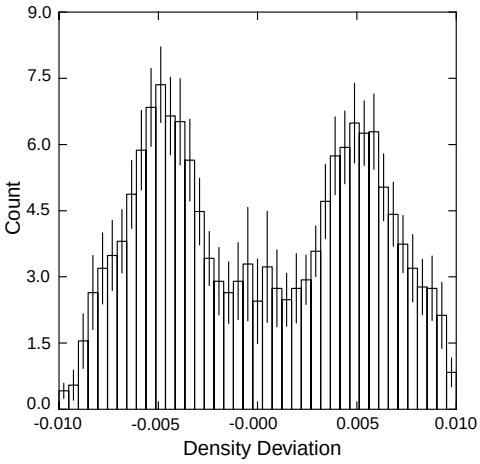
Theoretical Division

quarterly – fall 1999



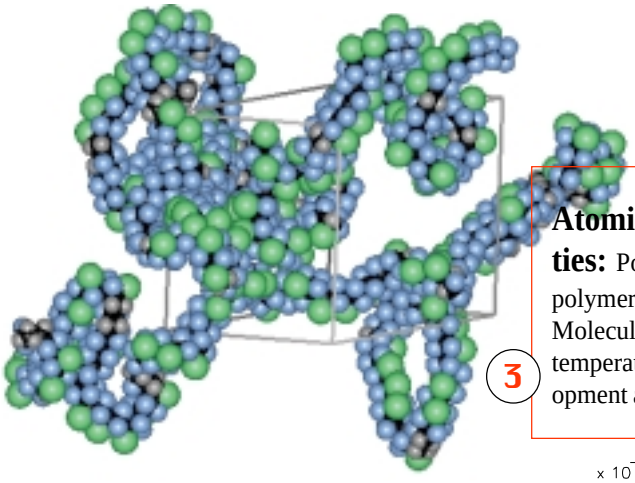
1

Ligand Binding to Myoglobin: Atomic resolution structures of myoglobin in various intermediate states of binding CO are being obtained by Joel Berendzen of Physics Division and collaborators in Germany. When combined with calculations from the theoretical chemistry and biophysics groups in Theoretical Division, the effects of electronic state changes, vibrational motion, and conformational changes on the function of this extensively studied protein can be evaluated.



2

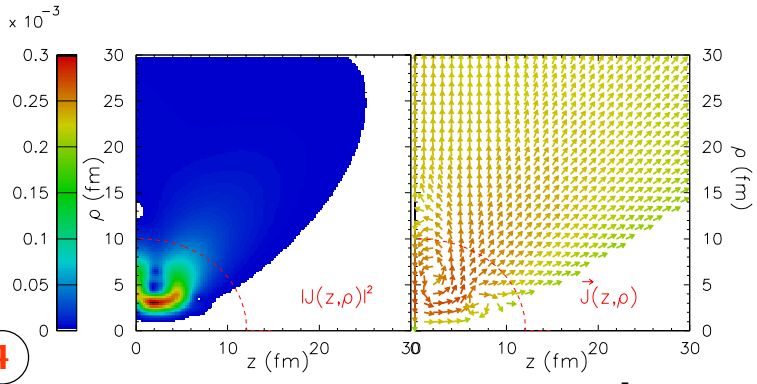
Demixing in Fluid Mixtures: The Gibbs ensemble permits the direct study of the demixing phase transition by considering a pair of noninteracting subsystems of arbitrary composition and density in mechanical and thermal contact, constrained by the overall state. The subsystem density distribution from Monte Carlo calculations for a hard-sphere mixture having a diameter ratio of five is shown. The bimodal distribution indicates demixing.



3

Atomistic Calculations of High Explosive Binder Properties: Poly(chlorotrifluoroethylene vinylidinefluoride), Kel-F 800, is a copolymer used as the binder in some plastic-bonded explosive formulations. Molecular dynamics methods are being used to compute the pressure- and temperature-dependent elastic coefficients of Kel-F 800 to aid in the development and parameterization of micromechanical models for such materials.

Multidimensional Quantum Tunneling: This is one of the key ingredients in the understanding of the proton decay of deformed nuclei. We investigated this phenomenon via the numerical solution of the two-dimensional time-dependent Schrödinger equation for initial proton metastable states. This approach provided important insights on the dynamics of the tunneling process. Figure shows vortices of the current density distribution inside an axially-deformed nucleus.



4

Comparison of CHAD Calculation with the analytic solution for the one-dimensional LeBlanc shock-tube problem. This problem was devised to test capabilities of hydrodynamic algorithms to handle very strong shocks. Initial conditions are described in Figure 2, below.

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Initial Conditions, *Figure 2*

Internal Energy = 1000	Internal Energy = 0.001
Density = 1	Density = 0.001
Pressure = 666.7	Pressure = 666.7e-09

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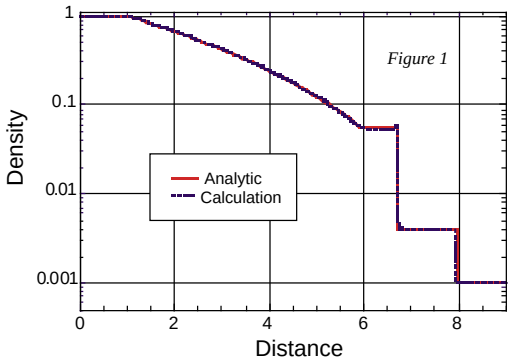

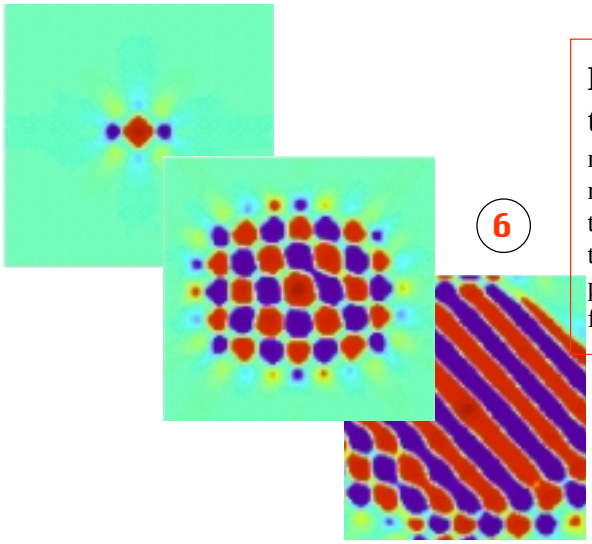

6

Modeling of Multiscale Functionality in Elastic Materials: Our approach to the inherent complexity and collective, multiscale phenomena (on materials where elasticity plays a crucial role) is to merge techniques from traditional materials science, statistical physics, and nonlinear condensed matter to relate materials' texture to local (e.g., electronic or magnetic) functionalities. Illustration partially shows the effect of a defect with a "Lorentzian" stress profile for a square-to-rectangle transition.

A Universe Made of Exotic Particles: Most of the universe appears to consist of exotic dark matter, which may take the form of weakly interacting massive particles (WIMPs). Analyzing WIMP models requires input from many areas of physics. Software created here is used by experimental groups around the world in their data-analysis efforts.

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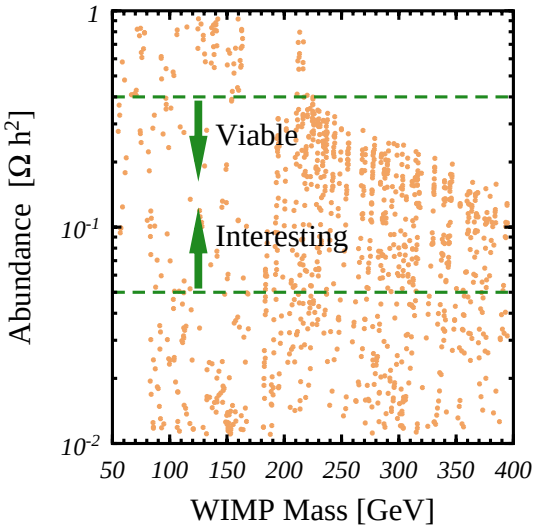
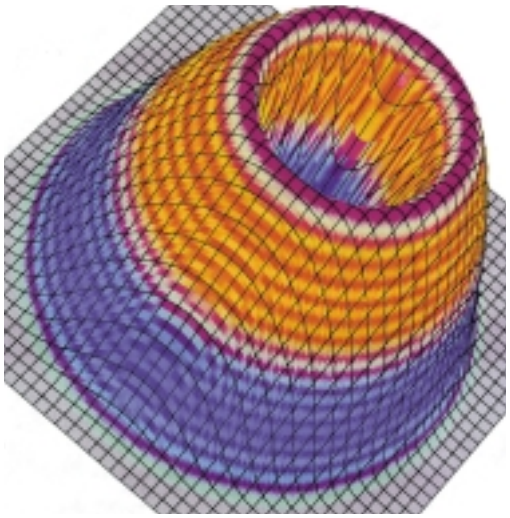
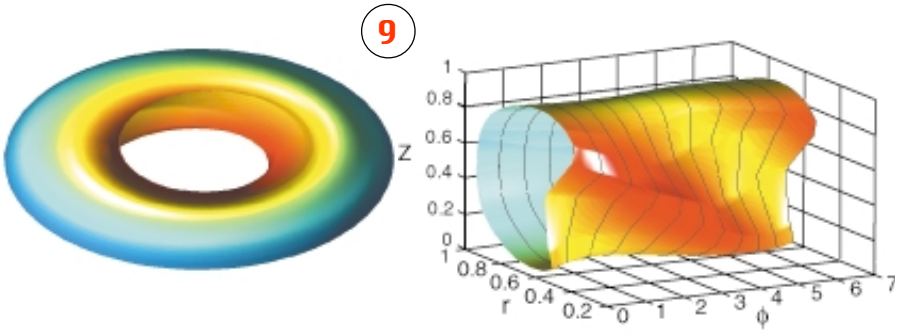




8

Superfluid Gas Mixtures: The ultra-cold atom trap systems provide ideal laboratories for creating and testing superfluid gas systems with novel properties. At T-4, we are exploring the physics of distinguishable boson superfluid mixtures, of mutually coherent condensates, and of the prospect for macroscopic quantum coherence in fermion-boson mixtures.



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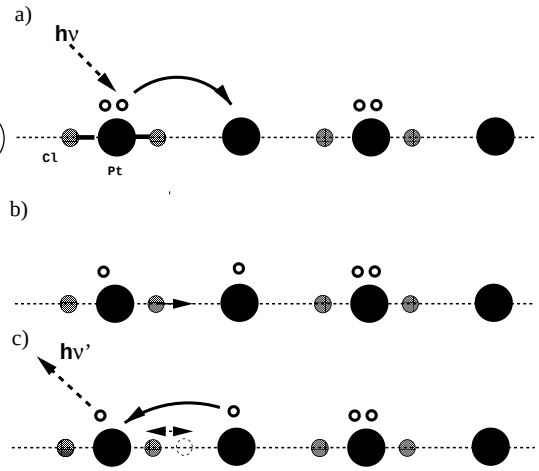
Magnetic Flux Surface Formation in 3D MHD Simulations of Spheromaks: Computations of z-pinches with embedded axial magnetic field produce sustained spheromaks as the nonlinear saturation of an magnetohydrodynamic instability. Weakly driven cases yield flux surfaces threaded by a helical current column. Two views of a surface, with color indicating radial position, illustrate the helical distortion on the inboard side.

Intrinsic Localized Modes in the Charge-Transfer-Solid PtCl: We report an analysis of intrinsic localized modes in a quasi-one-dimensional charge-transfer-solid [Pt(en)2][Pt(en)2 Cl2](ClO2)2 (PtCl). We discuss strongly nonlinear features of resonant Raman scattering (RRS) measurements arising from quantum intrinsic localized (multiphonon) modes (ILMs) and ILM-plus-phonon states. We show that RRS data display clear signs of a nonthermalization of lattice degrees-of-freedom, manifested by a nonequilibrium density of ILMs.



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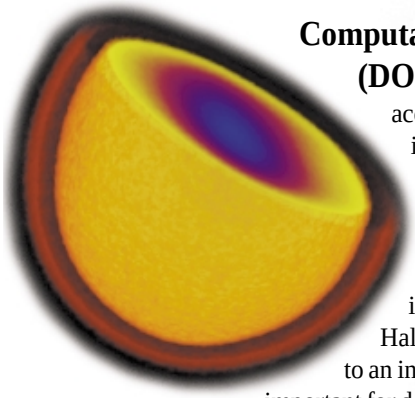
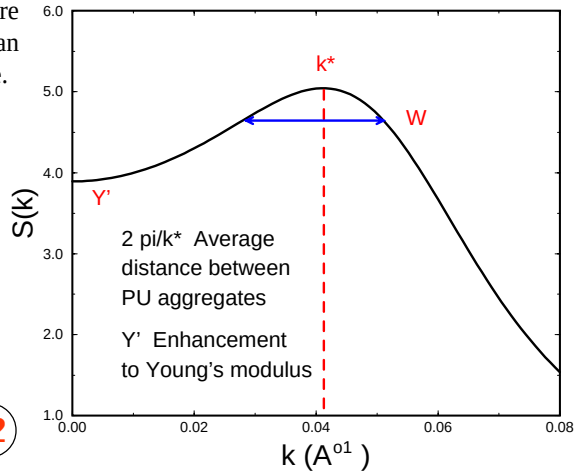


Computational Accelerator Physics (DOE Grand Challenge): Particle accelerators are playing an increasingly important role in basic and applied science and are enabling new accelerator-driven technologies. Figure: A particle bunch at the end of a simulation of the APT superconducting linac, based on the code IMPACT. Halo (diffuse outer region in red) is due to an initial rms mismatch. Such studies are important for determining how large a mismatch can be tolerated without having particles strike the beam pipe.

11

Towards a Mesoscale Model for the Aging of Estane: Estane is a segmented copolymer composed of hard segments of urethane bonded covalently to soft strands of polyester and is one of the two main ingredients that compose the binder for insensitive high explosives. We are developing a model to understand the viscoelastic properties of estane and how they deteriorate due to various forms of attack.



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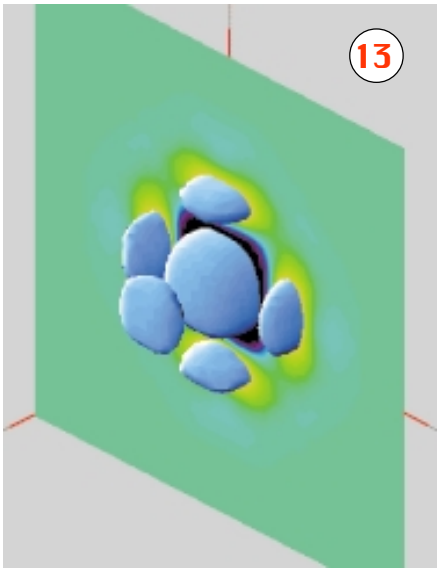
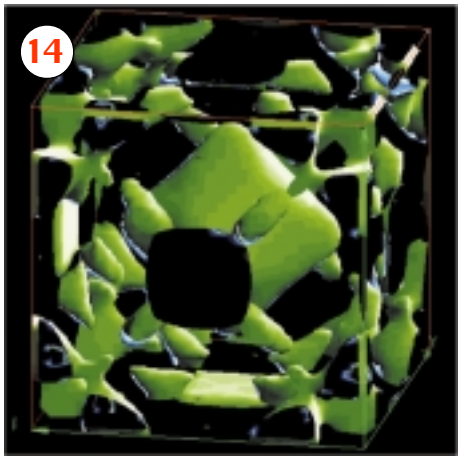
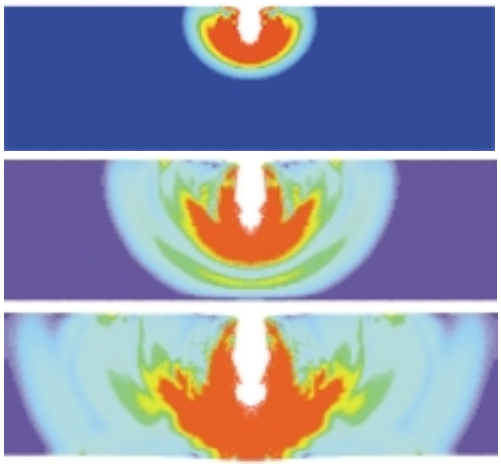


Non-Separable Multidimensional Wavelets: Wavelets are natural bases for problems which involve phenomena on distinct interacting length and time scales. These are ubiquitous in a large variety of fields of current scientific interests ranging from the interaction of vortices in turbulence, domain-wall patterns and dynamics in martensites and perovskites, to the atomistic domain where wavelets may serve as basis functions for electronic structure calculations.

The Electronic Structure of Actinide Elements and Alloys: The elements of the actinide series display a variety of interesting behavior unique in the periodic table. Elemental Pu and Pu and U compounds exhibit a broad range of correlated-electron behavior reflecting varying degrees of 5*f*-electron localization. This behavior can be described by adding correlations to *ab-initio* calculations. Figure: One sheet of the Pu_3Ga fermi surface.



Modeling Large Deformations, Damage, and Free-Surface Creation in Solid Materials: A simulation of the impact and penetration of a ballistic weapons casing fragment into a thick, laminated, composite plate. Figure shows deformed configurations of the composite plate at 25, 60, and 100 ms after impact. Stress-wave propagation through the composite material and creation of an impact crater resulting from fragment penetration are also shown (not shown are particles representing the fragments).



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