No. 3

Theoretical Division

quarterly - spring 1998

Topological Transitions: Gauge theories of strong and weak interactions have a multiple vacuum structure. Tunneling between vacua is responsible for important physical effects such as baryon number violation. The semiclassical tunneling rate is determined by solutions called periodic instantons. The figure shows a numerically obtained periodic instanton solution for the nonlinear sigma model. The calculation was performed on the CM-5 at the Advanced Computing Laboratory.

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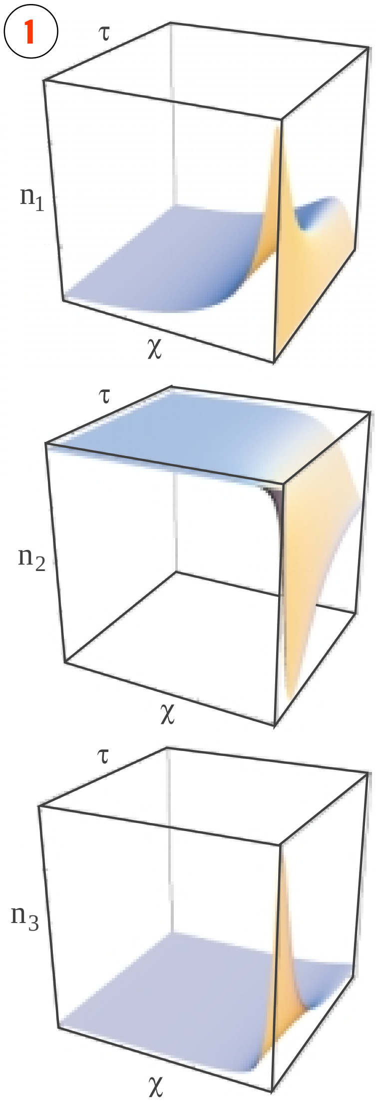

Shock Hydrodynamics and CHAD Code: CHAD is being used to simulate ASCI problems involving shock hydrodynamics. An essential requirement for ASCI predictions is to preserve symmetry for physically symmetric problems even on asymmetric meshes. The figure shows the mesh topology and density contours for the infinite-strength cylindrical shock problem of Noh on an asymmetric grid at a time of 0.6 units.

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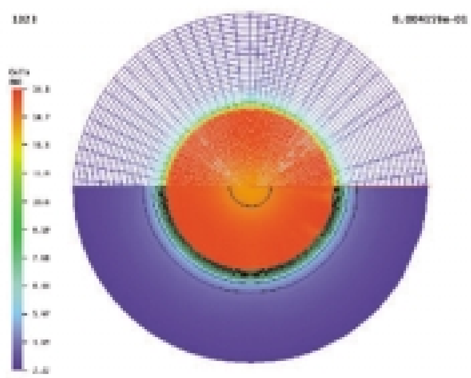

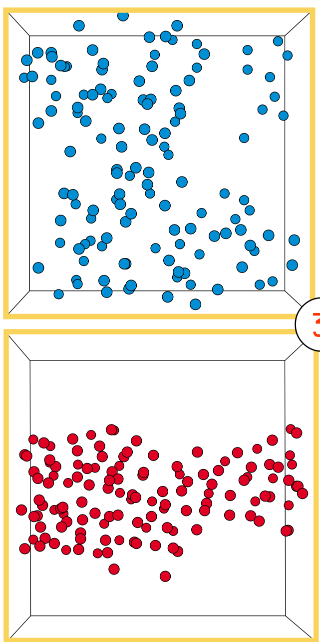

3

Expanded Sodium Near the Liquid-Vapor Coexistence Boundary: Quantum molecular dynamics simulations of a large sample of sodium atoms reveal the mechanics of a vapor (Blue) condensing into a liquid (Red). Transient associations of two and more atoms occur, making the fluid a very complex media in contrast to the usual picture of a continuous molecule to atom transition.

Soliton-Pulse Source for Ultra-High Bit-Rate Optical Transmission Lines: The growth of internet services has created an extraordinary demand for high bit-rate transmission systems. Accurate modeling of light pulse propagation in optical fibers is therefore becoming highly desirable. Figure 4 shows conversion of a single NRZ-phase-modulated bit into a soliton in a transmission line with guiding filters (numerical simulation).

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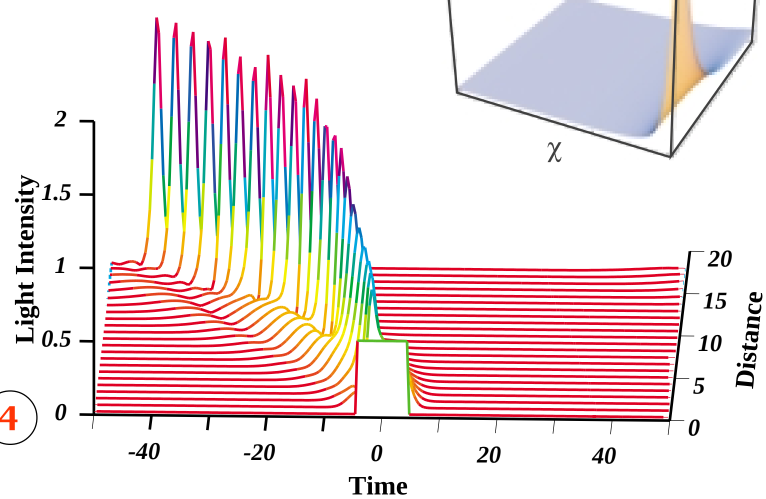

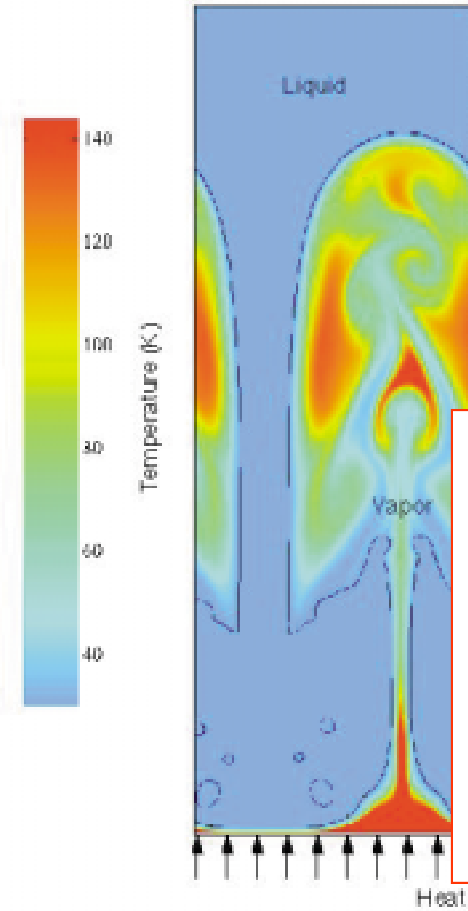

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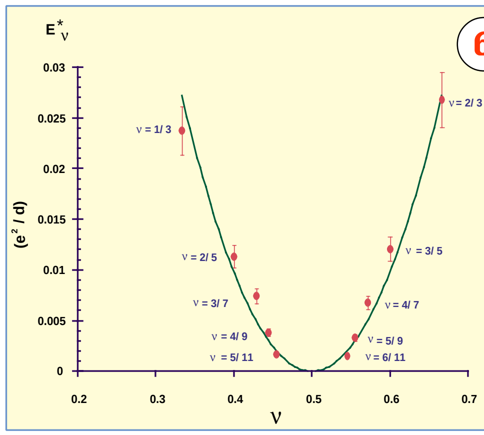
Modeling Boiling Flows: Vapor generation by boiling in two-phase flow is crucial to many processes in the power, chemical, and petroleum industries and is vital for production of electricity from fossil and nuclear fuels. In order to improve the safety and efficiency of these processes, a greater understanding of the fundamental physics of boiling is required. In this computer simulation of boiling, fluid vortices act to mix hot and cold vapor within a rising bubble.



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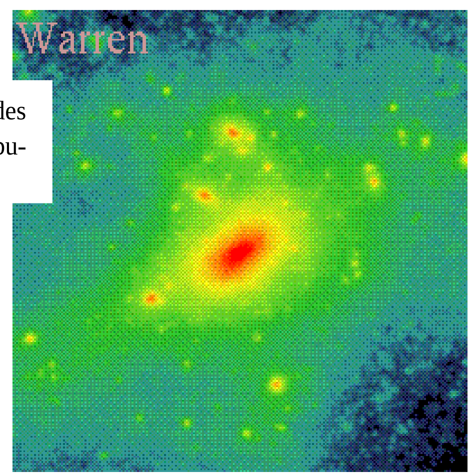
The Fractional Quantum Hall-Effect Energy Gap: Ansatz wave functions have been developed which have the correlations necessary to reduce the Coulomb repulsion between the electrons thereby producing the energy gaps observed in the fractional quantum Hall effect. This energy gap, E^*_ν, as a function of the fractional filling, ν, is compared with the known experimental gaps, and vanishes for $\nu = 1/2$.



In a direct comparison of the top twelve numerical cosmology codes in the world, T-6 performed the highest-resolution calculation of the distribution of dark matter in a galaxy cluster, as shown in the image here.

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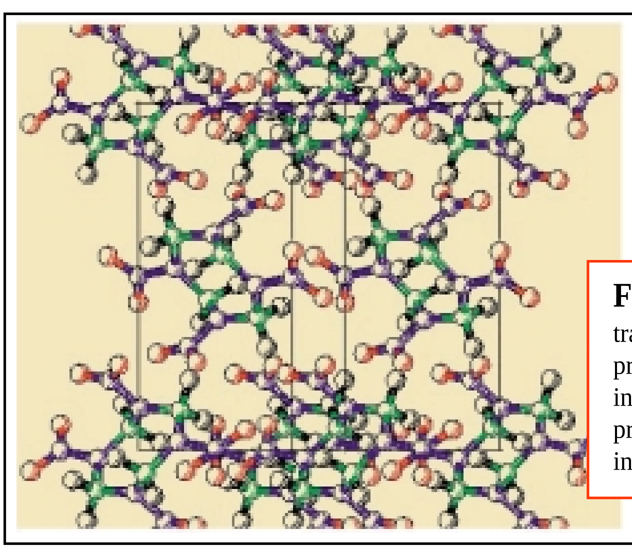
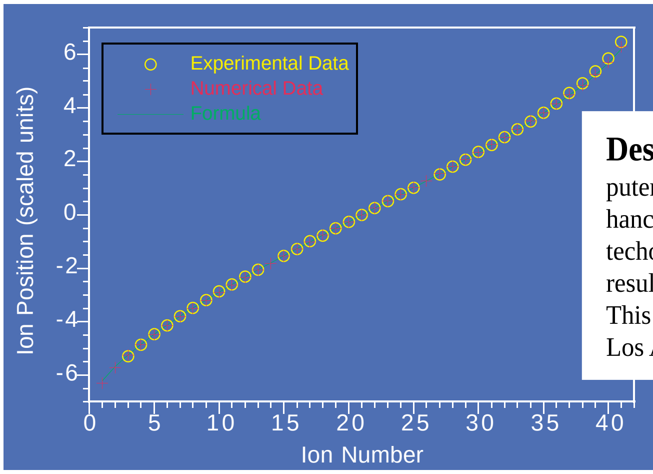


8

First-Principles Studies of Explosive: The vibrational spectra and chemical reactions of explosives are being investigated by first-principles quantum molecular dynamics. This work is used to help interpret experimental data on the fundamental reactions and physical properties of the materials. This will result in improved models for the initiation of high explosives in military applications.



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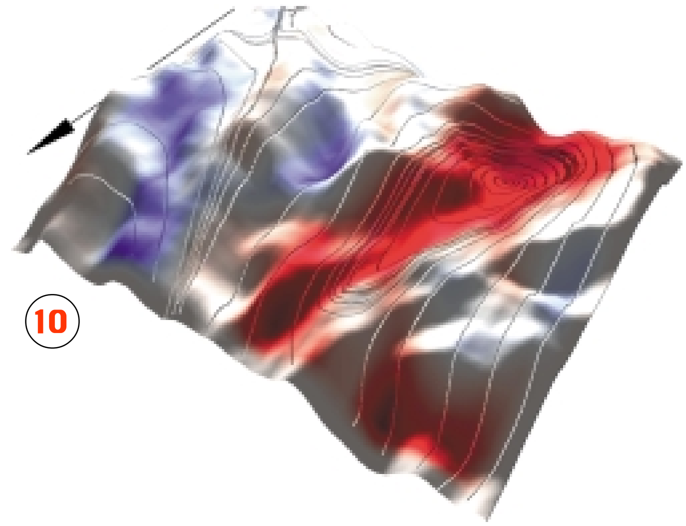
Designing Ion Trap Quantum Computers: Quantum computers are devices that utilize the principles of quantum physics to enhance enormously computing speed. A very promising quantum computer techology is ions confined in an electromagnetic trap. The diagram shows results of simulations of ion positions, compared with experimental data. This is an example of the various theoretical problems involved with the Los Alamos quantum computer project.



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Turbulence in Flowing Soap Films: Soap films, such as ones that form soap bubbles, present a convenient model for many laboratory studies of two-dimensional hydrodynamics. We have developed a diagnostic to simultaneously measure the velocity and thickness fields in the soap film. The image represents a computer-processed snapshot of the flow field in soap film perturbed by a comb.

Phase Front Instabilities in Forced Oscillatory Systems: Periodic forcing can lock oscillatory systems into multiple states with different phases. In spatially extended systems the stability of fronts between these phases controls the transient dynamics and final pattern. The figure shows the collapse of a rotating four-phase spiral-wave into a stationary two-phase pattern.

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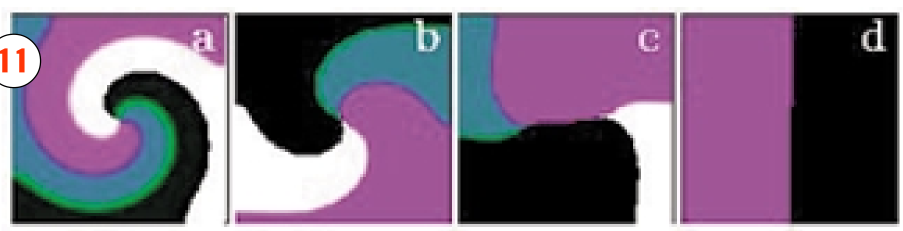

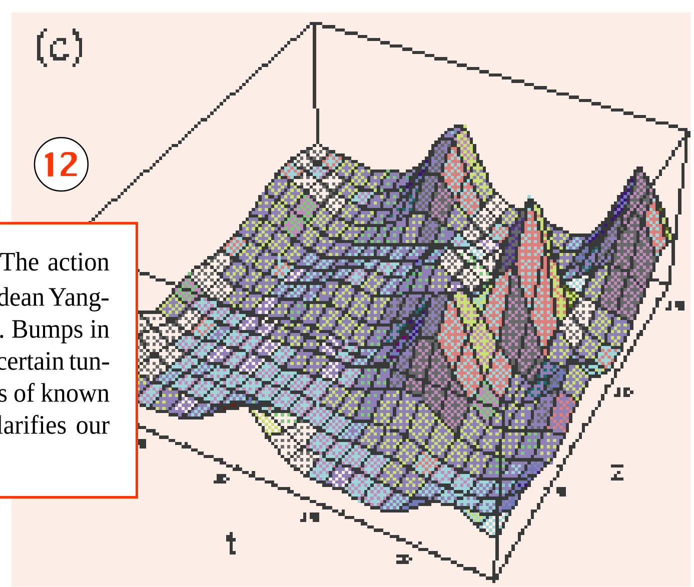

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Modeling the Nonperturbative QCD Vacuum: The action density for nonperturbative gauge field configurations of Euclidean Yang-Mills equations as a function of time and one space variable z. Bumps in this picture correspond to instantons/anti-instantons, which are certain tunneling events connecting degenerate vacua. Physical properties of known and yet unknown particles can be predicted from this and clarifies our knowledge about the strong interactions.

Rhenium Oxidation Chemistry: Concern over the enantiomeric purity of pharmacologically-active compounds has made asymmetric synthesis one of the grand challenges of chemical research. Two outstanding examples are the asymmetric cis dihydroxylation of olefins and the asymmetric epoxidation of olefins. $LReO_3$ complexes catalyze either process depending on the ligand L. Quantum chemistry calculations aid in determining the reaction mechanism.

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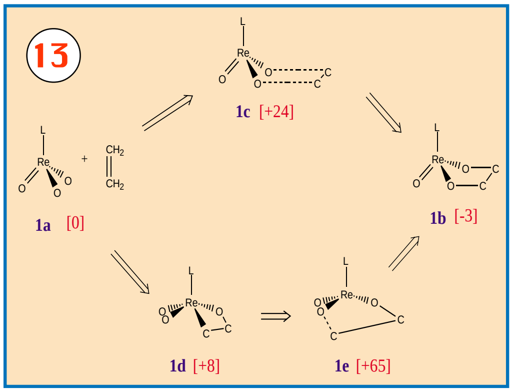

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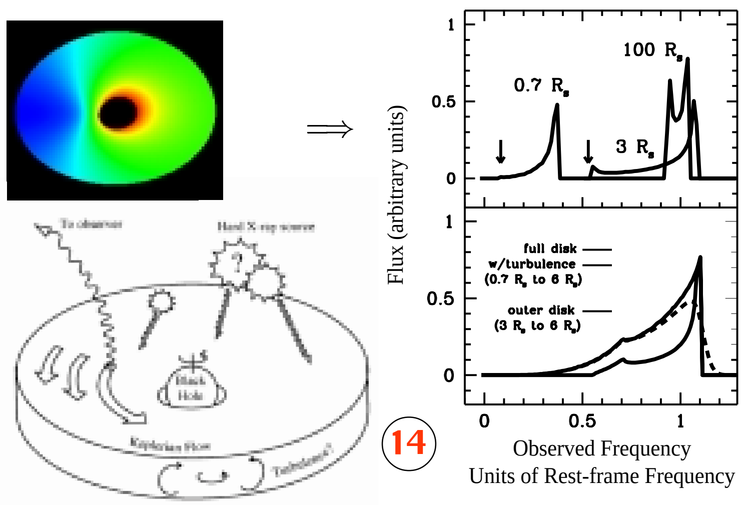

Catching the Spin of a Supermassive Black Hole: Line emission from an accretion disk. Models of the X-ray fluorescence of iron from deep within the gravitational potential of a supermassive black hole. Upper left: computer image of accretion disk showing frequency shift. Right: line profiles from general-relativistic ray-tracing code.

Predictability: Quantifying Uncertainty in Complex Phenomena: Predictions of complex phenomena must include reliable estimates of uncertainty. T-13 is working with X-Division and the NWT Program Office to develop probabilistic methods for prediction that are applicable to SBSS, climate, and other data-limited problems.

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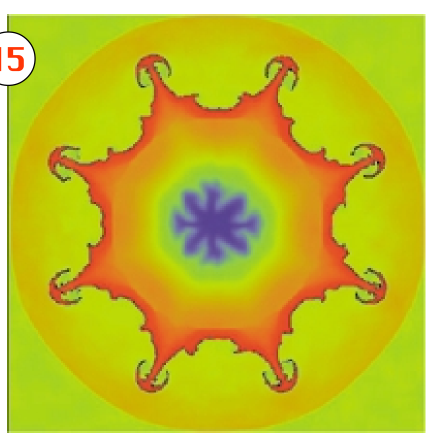

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