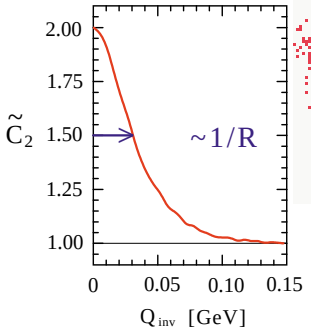
No. 2

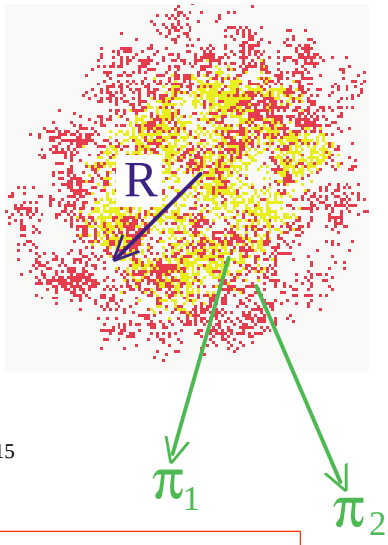
Theoretical Division

quarterly – winter 1997/98

Bose-Einstein Correlations in Relativistic Heavy-Ion Collisions: When pion pairs are emitted totally uncorrelated from a fireball created in relativistic heavy-ion collisions, their field intensities interfere and generate so-called Bose-Einstein correlations, which are functions of the momentum difference of the pion pair. Their inverse widths are approximately proportional to the radius, R, of the hadron emitting source.

1





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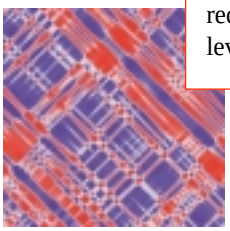
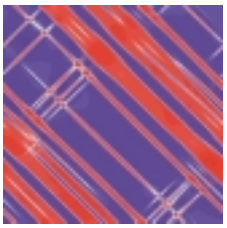
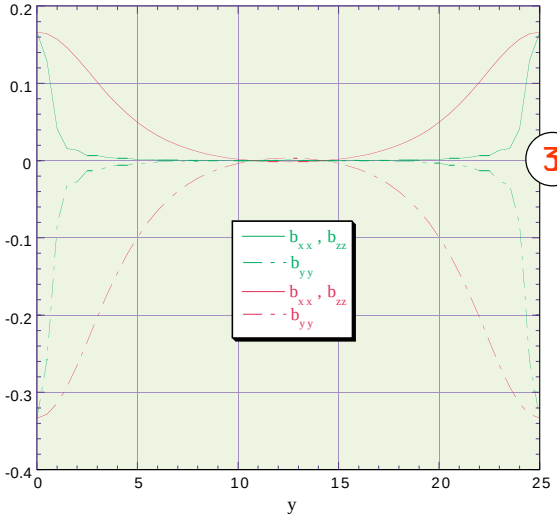


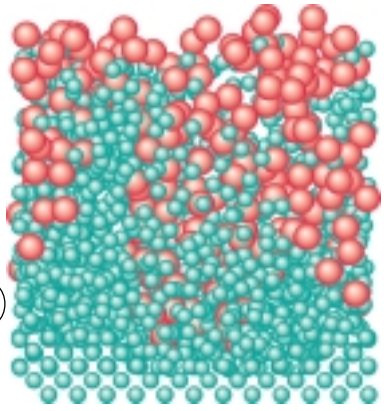


Mesoscopic Dynamics in Highly Nonlinear Solids: The figures show a simulation snapshot in the time evolution of a metallic alloy after it has been rapidly cooled through a symmetry-breaking (cubic to orthorhombic) solid-solid phase transformation. The blue and red represent the two solid phases, which are separated by a white interface. At the micron level one observes needle-like textures evolving from a tweedy precursor phase.



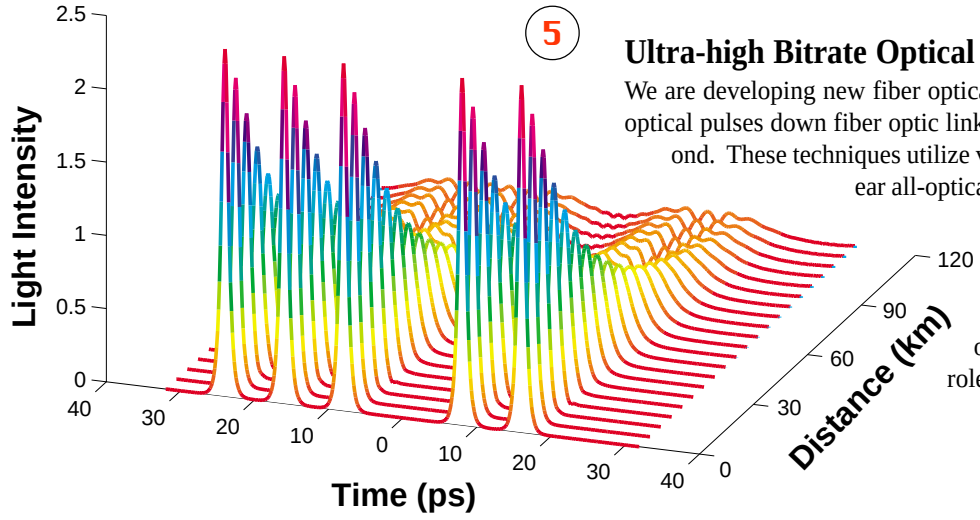
3

Inhomogeneous Turbulence: We have developed a fundamental theory for predicting the evolution of inhomogeneous turbulence based on a random-phase assumption and a new mathematical representation of a bounded fluid. The figure depicts elements of the normalized anisotropy tensor of a fluid between two walls at y = 0 and y = 25 as the anisotropy near the walls (green) diffuses inward (red).



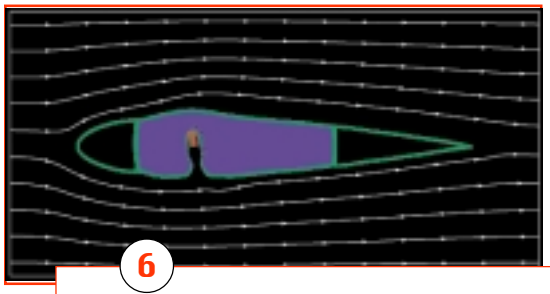
4

Molecular Dynamics Simulations of Si Etching: Molecular dynamics simulations, using classical interatomic potentials, were used to study the reactive ion etching of Si by Cl ions—a common but poorly understood process widely used by the semiconductor industry. The figure depicts a Si surface (green balls) being etched by Cl (red balls) after 6 monolayers of 100 eV Cl^+ ion fluence.



Ultra-high Bitrate Optical Transmission Techniques:

We are developing new fiber optical transmission techniques to send optical pulses down fiber optic links at 100 to 1000 Gigabits per second. These techniques utilize very novel devices, such as nonlinear all-optical interferometers (called loop mirrors) and super-Gaussian filters, as well as specially configured links that minimize dispersion. The mathematical theory of solitons also plays a prominant role in this research.

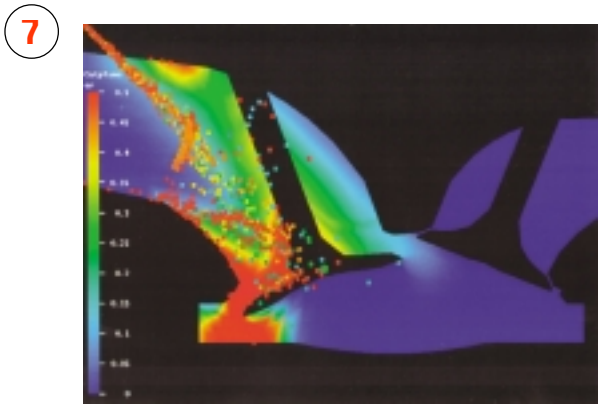


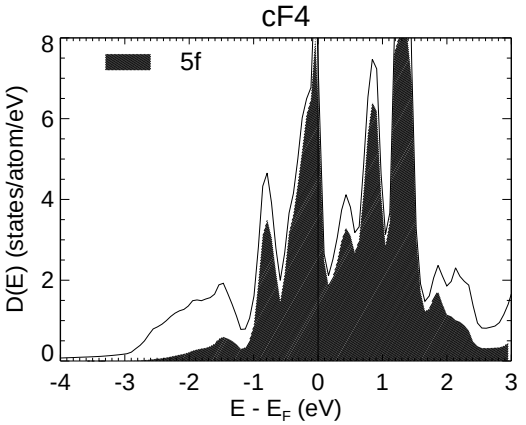
Physics-Based Modeling of Fluid-Solid Interaction Phenomena:

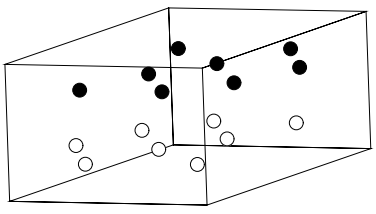
Detailed mathematical descriptions of fluid-solid interaction phenomena are inherently complex due to the nonlinear coupling that develops between the fluid and solid materials and the potentially complex solid material behavior that results. Scientists at LANL are combining a unique computational technique with accurate and efficient solid material models to develop a new, physics-based approach to modeling these phenomena.

Advanced Engine Design:

Tomorrow's automobile, truck, and gas turbine engines demand improved fuel economy, lower emissions, and reduced development time. Three-dimensional computer simulations are increasingly relied upon for understanding engine flows. This is exemplified by this snapshot of port fuel injection in a modern gasoline engine, calculated by the world-renowned KIVA-3V, developed at LANL.







Crystal Structural Stability of Actinide Elements from Electronic Structure Theory:

The structural complexity of actinide elements is being explained using principles of electronic structure theory. The ground-state structures are shown to result from narrow-band metallic bonding. A unique electronic configuration has been developed that predicts many of the anomalous properties of the high-temperature δ phase of Pu.

Loki - Commodity Parallel Processing: Loki is a parallel computer built from off-the-shelf components that provides a general-purpose parallel computing capability for less than one-third the cost of conventional parallel computing platforms. Our novel commodity parallel processor (CPP) design provides a highly reliable and flexible resource ideally suited to a wide variety of large, data-intensive computational problems.

9

Spiral Surface Growth: Film growth is critical to many technologies, including semiconductors, superconductors, and sensors. The growth morphologies are intrinsically multiscale and sensitive to growth conditions. Spiral growth is an important and complex modality. The upper frames are from LANL transmission electron microscopy studies of a high-temperature superconductor film. We have developed a new modeling tool (lower frames) which describes spiral core dynamics and spontaneous spiral pair nucleation.

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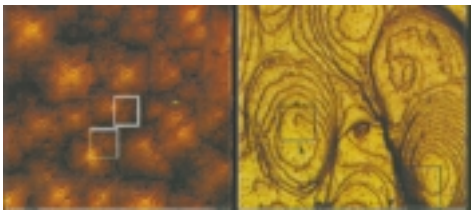
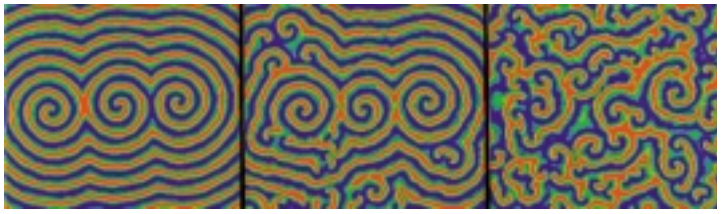
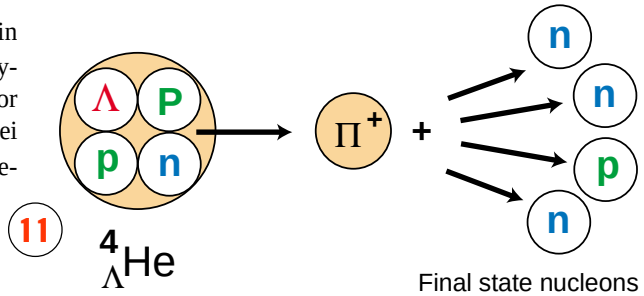




Physical Signature of Virtual Baryons: Hypernuclei contain one or more "strange" baryons called hyperons. The lowest mass hyperon is a Λ, which decays into a nucleon by emission of a negative or neutral pion (π^- or π^0). Emission of positive pions (π^+) from Λ hypernuclei is a 30-year-old enigma. Σ^+s, which are 10% heavier than a Λ and therefore exist only virtually *via* $\Lambda N \leftrightarrow \Sigma N$ conversion, hold the key.



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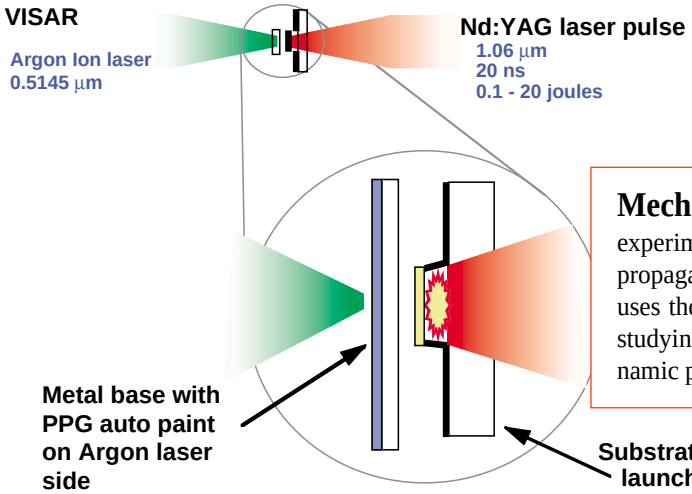
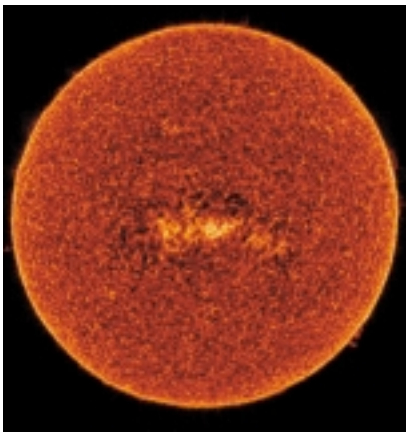


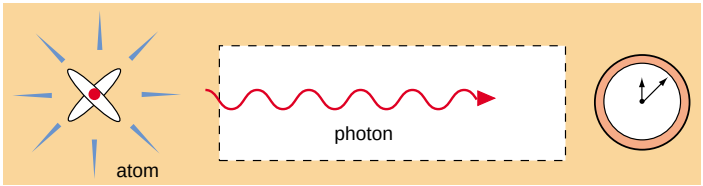
Mechanical Properties of Interfaces: Theoretical and experimental techniques are used jointly to investigate stress wave propagation in multilayered systems. The experimental method uses the Laser-Driven Mini-Flyer, which is an excellent tool for studying high-strain rate damage mechanisms associated with dynamic processes occurring at the multilayer interfaces.

12

Opacities of Mixtures of Atomic Elements: Opacity is a measure of the ability of a substance to absorb radiation and is determined from fundamental atomic properties. The opacities of matter in stars like our Sun and other complex systems are composed of mixtures of opacities of many elements. We have developed a tool that allows users of the world wide web to make opacity mixtures on-line at our web site: http://t4.lanl.gov/opacity/tops.html [13]

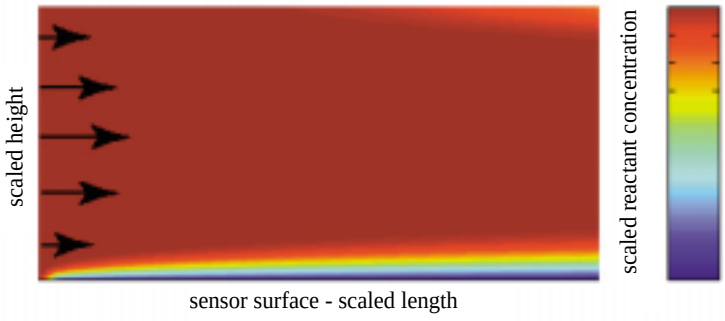


As part of a LANL/UC-Berkeley collaboration [14] we have performed calculations showing that a single photon can in certain circumstances propagate measurably faster in a material medium than in vacuum, and does so without violation of Einstein causality.



Modeling Biosensors: Optical biosensors are becoming the instruments of choice for studying interacting biomolecules. In the most popular design, one of the reactants is coupled to a sensor chip while the other reactant flows past the chip. When the reactants form a bound complex on the chip, the resultant change in the index of refraction is detected. Computer simulations of these instruments are yielding new methods for extracting critical binding parameters.

Simulated reactant concentration in biosensor at t = 2 min [15]



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