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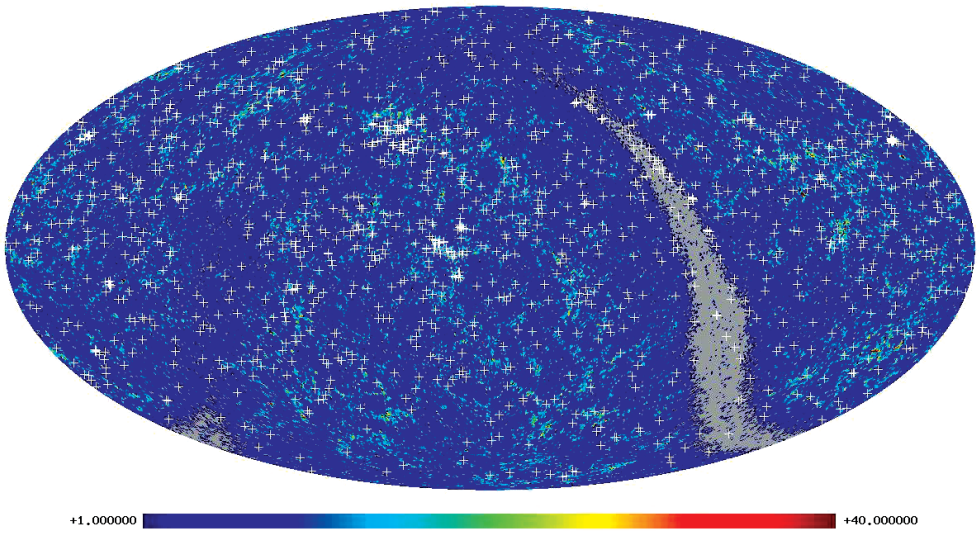
Theoretical Division *Quarterly*

Summer 2004



Hunting for the Intergalactic Magnetic Field

This image shows the distribution of galaxy density in the 2MASS survey in Aitoff projection of equatorial coordinates. White crosses indicate the position of radio sources. Cross-correlating the Faraday rotation fluctuation with local galaxy density is a way of detecting the intergalactic magnetic field.

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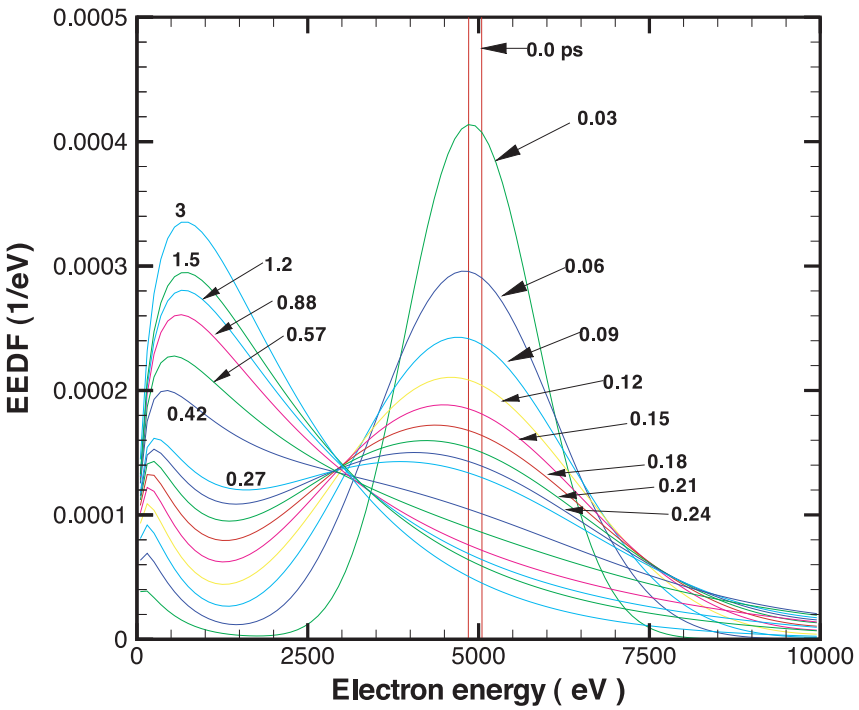

Time Dependent Boltzmann-Kinetic Model of the X-rays Produced by the Ultrashort Pulse Laser Irradiation of Argon Clusters

The Boltzmann equation and a detailed collisional radiative model are solved simultaneously as a function of time to model the time integrated X-ray spectra of the transient plasma produced by a high-intensity ultra-fast laser source. The figure shows the calculated electron energy distribution function (EEDF) for various times between 0 and 3 picoseconds.

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National Nuclear Security Administration

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Investigation of Novel HIV-1 Recombinant Forms Using the Branching Index

In this work we have developed a method for determining if parental DNA sequence representatives are available or are not for recombination analysis.

For many reasons, including future vaccine design and monitoring the epidemic, it is important to accurately describe and classify the forms of HIV-1 that are spreading in different geographic regions and among different risk groups.

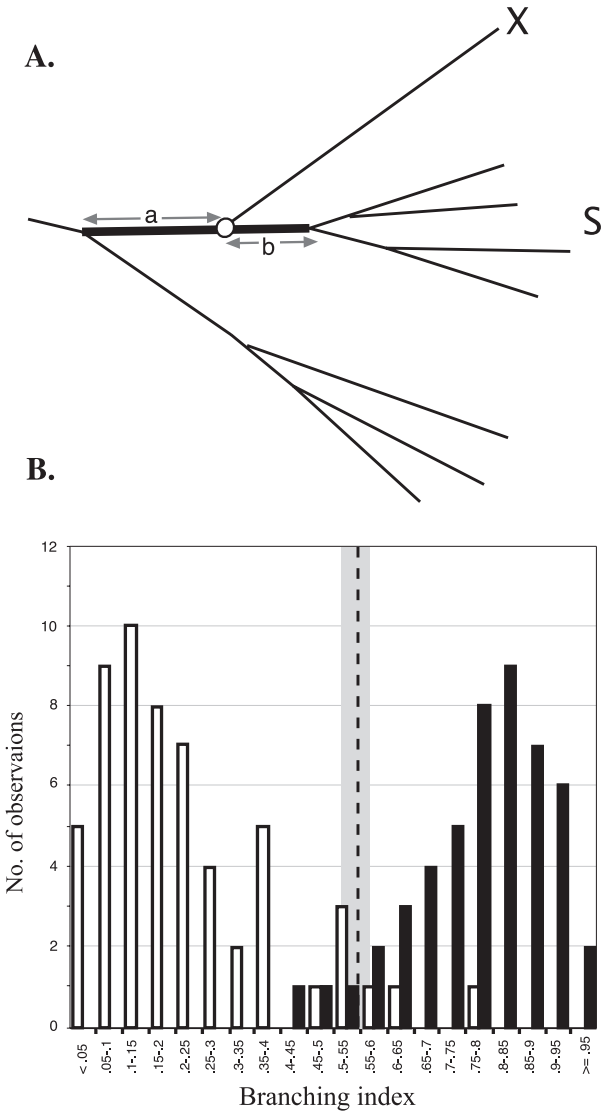

Figure A: Schematic picture of the branching index. Here the association of sequence X to the subtype cluster S is investigated. Letters a and b are genetic distances that depend on the position of the node of sequence X (white circle) at the bold branch. The branching index is defined as a/(a+b) and can take values between 0 and 1. Figure B: Comparison of branching indexes (BIs) from situations when parental representatives are present or not. White bars shows the situation with subtype partners absent, and black bars shows the situation with subtype partners present. The BI categories are shown on the x-axis and the number of observations on the y-axis. The vertical dotted line indicates the suggested cut-off value 0.55 for subtype verification, and the gray zone is a zone of uncertainty (<95% correct classifications).

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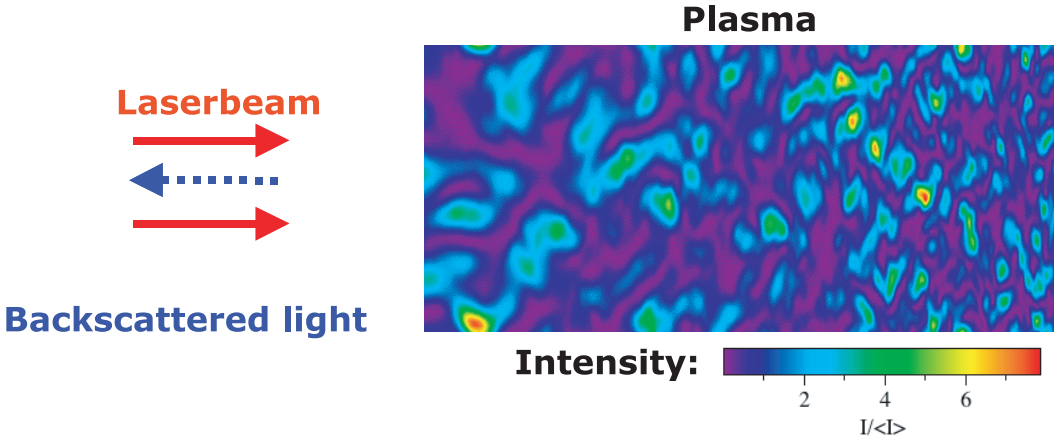

Strong Effect of Doping on Laser Plasma Interaction

Understanding the propagation of high-intensity laser beams in plasma has been an outstanding research objective for more than two decades. As a laser beam traverses plasma, it couples to backscattered light and either an ion acoustic wave (stimulated Brillouin scattering (SBS)) or a high-frequency Langmuir wave (stimulated Raman scattering (SRS)). Typical intensities exceed threshold for a broad spectrum of waves, leading to plasma turbulence.

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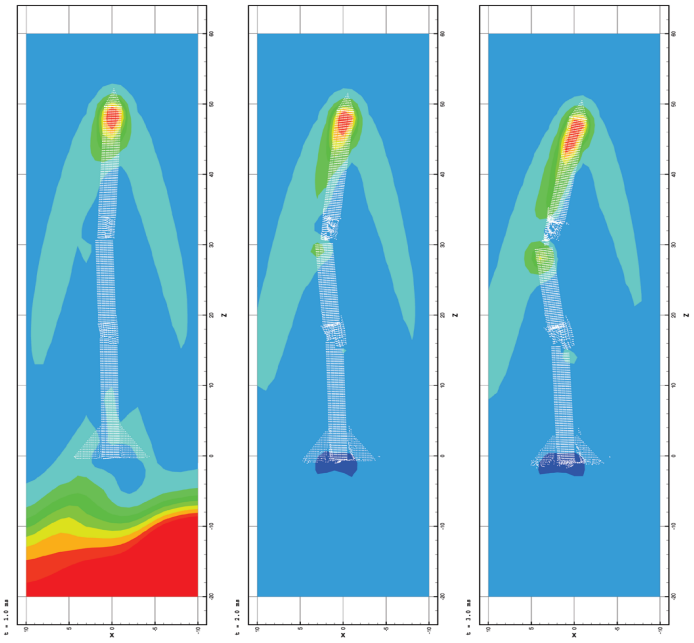

Transition Theory for Fragmentation of Solid Bodies

A physical modeling formalism for solid bodies undergoing fragmentation is being developed. The purpose is to provide a rigorous framework for posing physical models that can be used for the computer simulation of certain problems of current importance in both defense and in industry.

Figure: Brittle steel rod penetrator subjected to a blast impulse during flight. a) 1.0 ms after blast; b) 2.0 ms after blast; c) 3.0 ms after blast.

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The SEL Plasma Simulation Code

One of the major activities of T-15 Group is theoretical and computational studies of magnetically confined plasmas for fusion energy. Numerical simulation of such plasmas presents one of the most difficult challenges in all of computational physics. In response to this challenge, T-15 is developing the SEL code, using some of the most advanced numerical methods in existence.

Figure: As a preliminary example of the SEL code, the figure shows the results of modeling 2-D incompressible magnetic reconnection.

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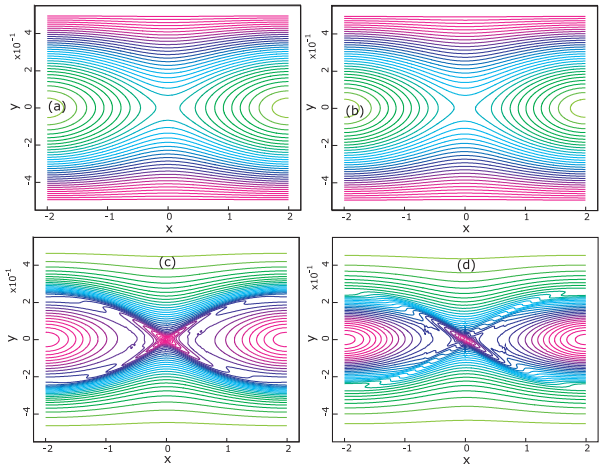

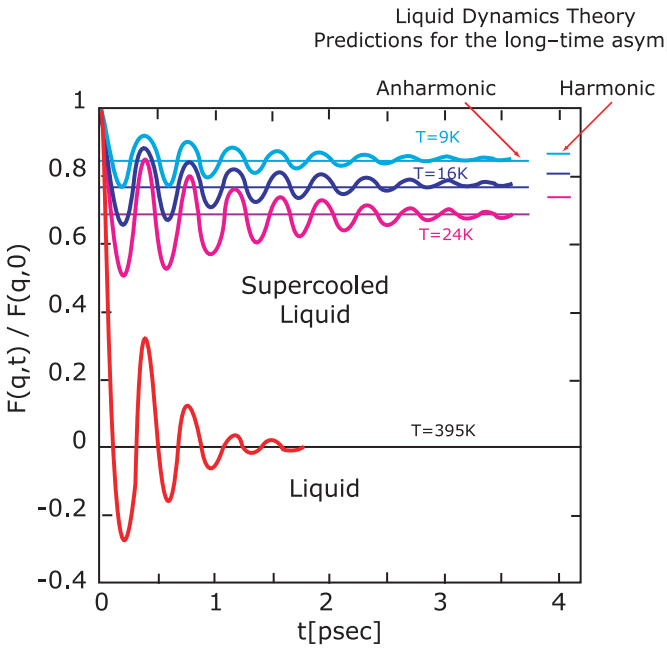

The Promise of Liquid Dynamics Theory

An example of how Liquid Dynamics Theory can explain a result otherwise unexpected, is the case of the intermediate scattering function F(q,t), the Fourier transform of the inelastic neutron scattering cross section S(q,w). Molecular dynamics calculations are shown in the figure for two cases: (a) at three temperatures below the glass transition, where the system is trapped within a single random valley, and (b) in the liquid at T just above melting. The curves are characterized by oscillations at short time, which are the source of the Brillouin peak in S(q,w), and by long-time decay to a constant value.

Figure: Intermediate Scattering Function F(q,t) for q=0.29711 ao-1, on a system of 500 particles of Na. The functions evaluated from molecular dynamics at four differen temperatures are shown, together with the predictions for the long–time asymptotes from Liquid Dynamics Theory.

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New Pseudostructure for α-Pu

We have discovered a new pseudostructure for α-Pu that involves only two atoms per unit cell and is a relatively symmetrical orthorhombic crystal structure and can show that the real α crystal structure only involves small distortions of various atoms around this pseudostructure; the electronic-structure energy of both systems (at least at the band-structure level) is nearly identical. Sophisticated electronic-structure techniques should be just as easy for this pseudostructure as for δ Pu.

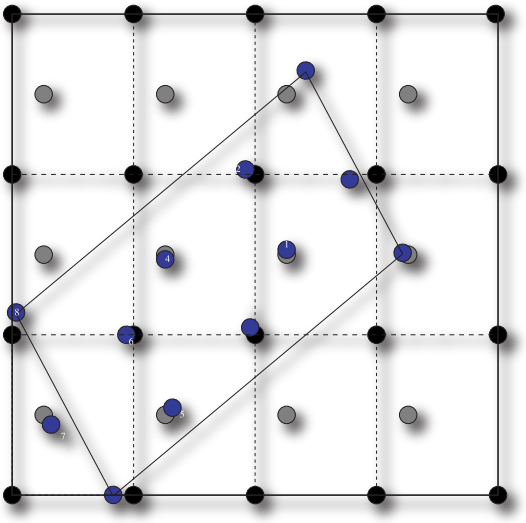

Figure: Pseudostructure in the (011) direction. The blue atoms are the eight positions in the α–Pu structure.

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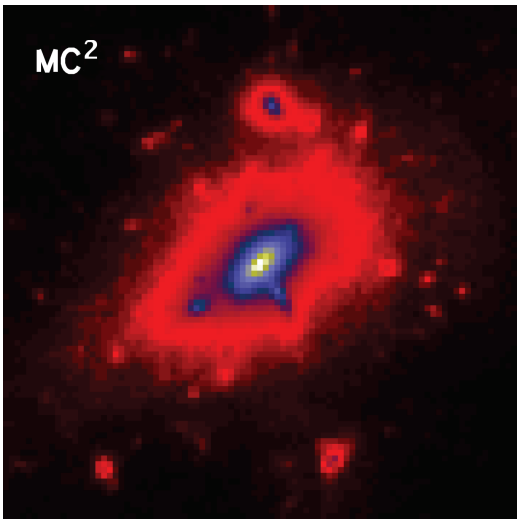

A Flexible Mesh-Based Cosmology Code

There are several different computational approaches to model structure formation in cosmology in the dominant dark matter component. MC^2 is a parallel PM dark matter code based on Vlasov-Poisson solvers developed at Los Alamos (the IMPACT code) and at UCLA (Viktor Decyk's UPIC framework). MC^2 also incorporates a simplified treatment of baryons via the Hydro-Particle-Mesh method; a neutrino module has been recently added, and a more complete hydrodynamic module is under development.

Figure: The density profile of the Santa Barbara cluster from a MC^2 simulation on a 1024^3 grid, projected down to a 1024^2 grid. The box size is 64 Mpc, only the inner 8 Mpc is shown.

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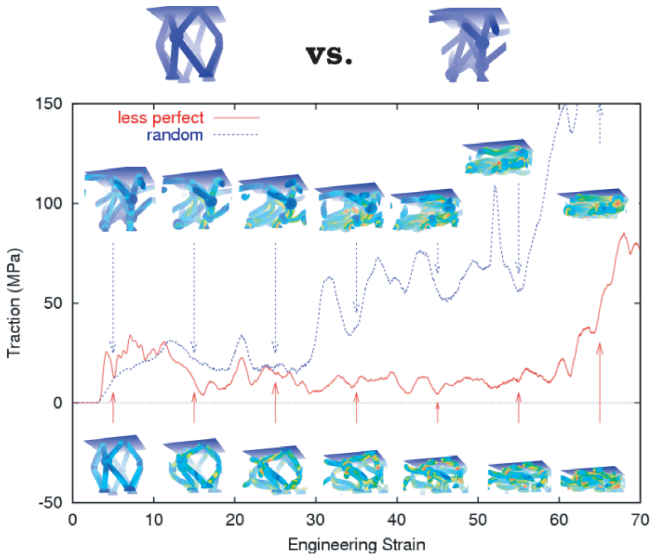

Numerical Simulation of Full Densification of Foams

Foamed materials are increasingly finding application in engineering systems because of their unique properties. They are extremely light weight and can provide gentle packaging or energy absorption during crush-up. The stress plateau and densification deformation regimes may be easily distinguished in the macroscopic stress strain response depicted in the figure. Effects due to regularity of the foam microstructures have also been identified. More regular unit cells appear to exhibit a much flatter stress plateau. Future work includes linux cluster simulations of much larger microstructures, representative of bulk foam material.

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