Computing Sciences at Berkeley Lab
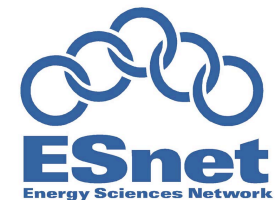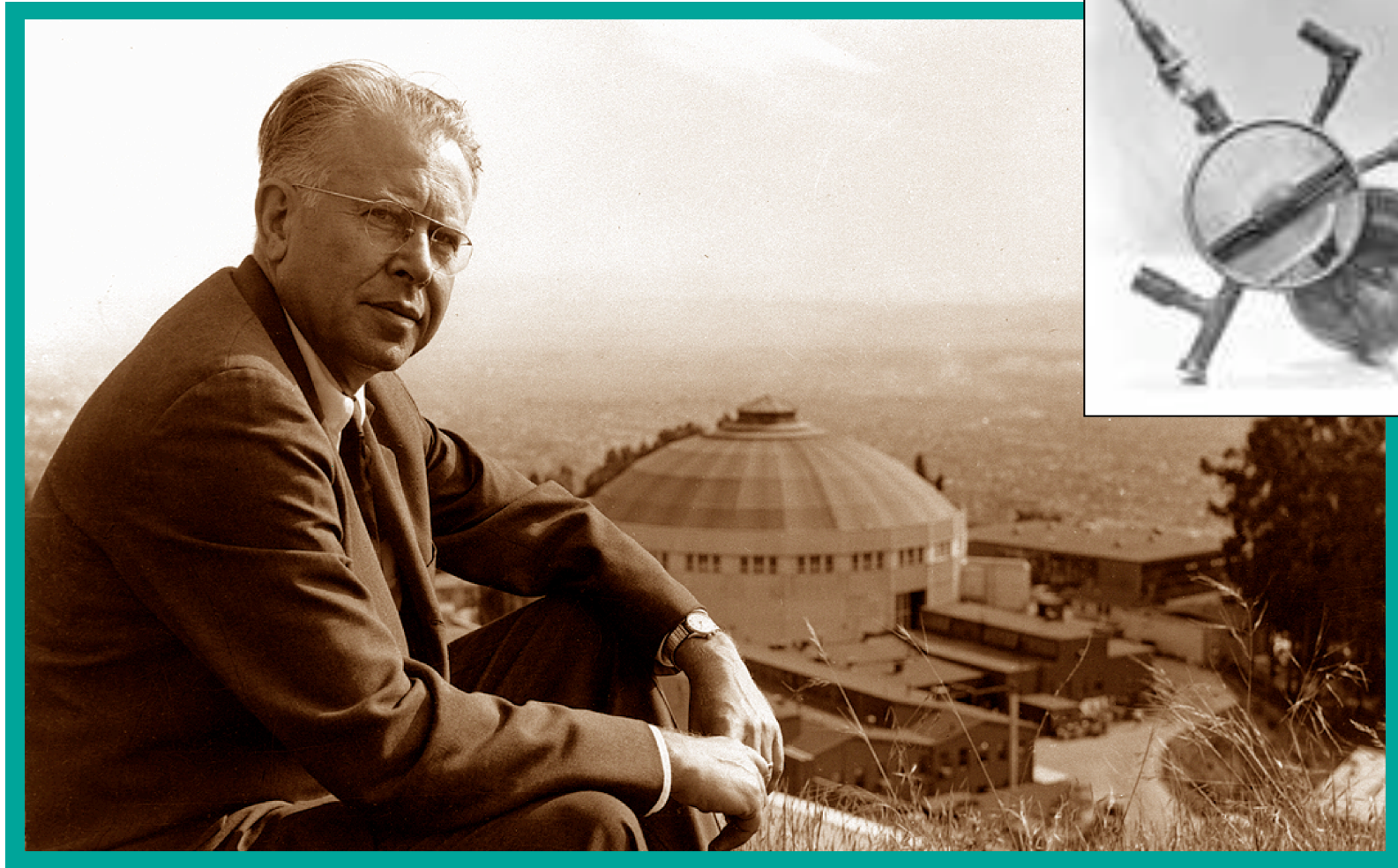
Juan Meza
Department Head
High Performance Computing Research

Lawrence Berkeley National Laboratory
September 9, 2008

Founded in 1931 on the Berkeley Campus
Moved to Current Site in 1940

A National Laboratory Next to a University Campus

Berkeley Lab

UC Berkeley

Berkeley Lab's Major Scientific Facilities Serving Universities, Industry, and Government

88-Inch Cyclotron

National Center for Electron Microscopy

Advanced Light Source

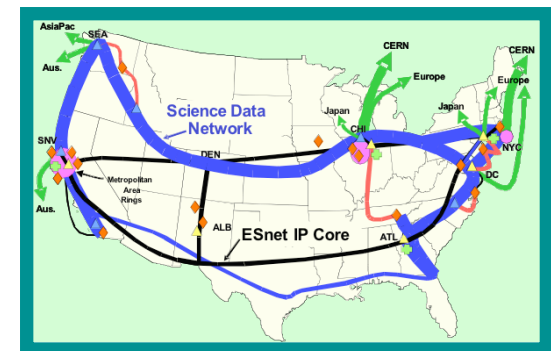**Joint Genome Institute**

National Energy Research Scientific Computing Center

Molecular Foundry

Energy Sciences Network (ESnet)

NERSC
National Energy Research
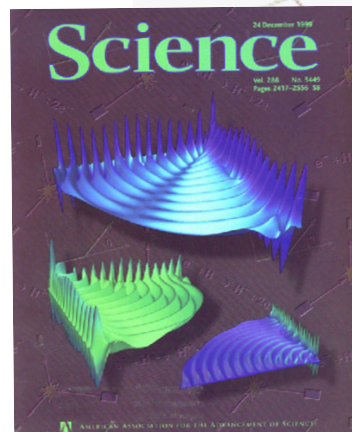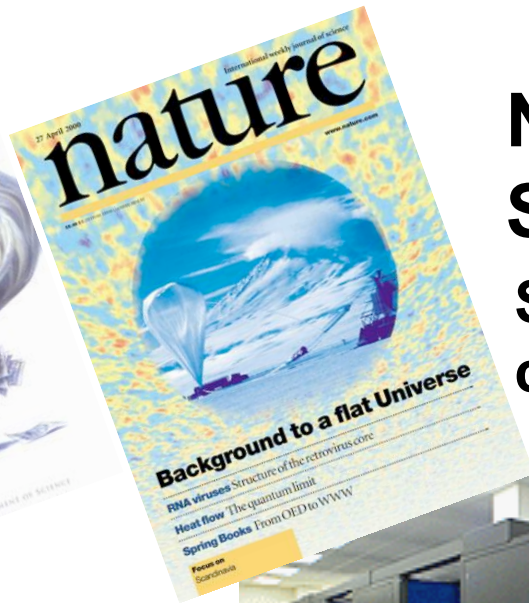# Scientific Computing Center

SCIENCE-DRIVEN SUPERCOMPUTING

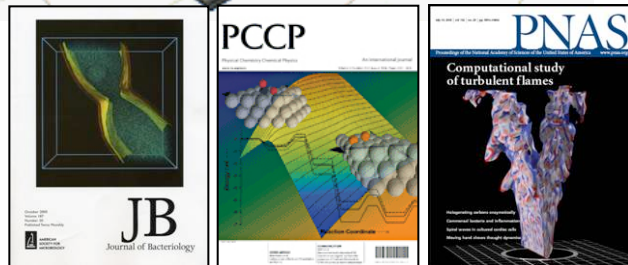# National Energy Research Scientific Computing Center

Serves the entire scientific community

**~3000 Users in
~400 projects
~500 codes**

Focus on large-scale computing
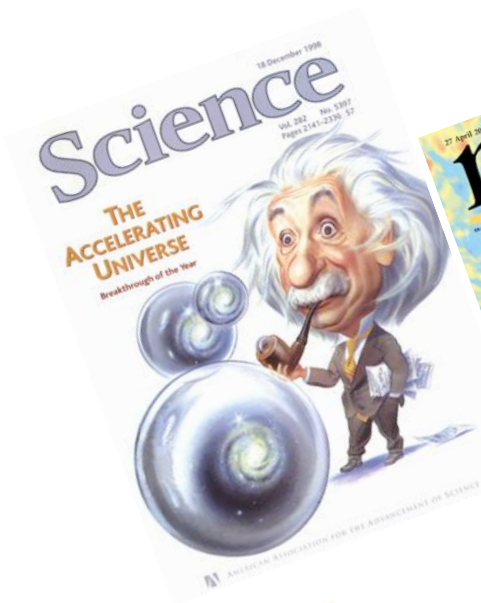
100 Tflops Cray XT-4 at NERSC

Cray XT-4 "Franklin"

19,344 compute cores

102 Tflop/sec peak

39 TB memory

350 TB usable disk space

50 PB storage archive

NERSC is enabling new science

Focus on Science Areas

- Materials Science 13%
- Climate Research 9%
- Lattice Gauge Theory 7%
- Accelerator Physi 7%
- Astrophysics
- Life Sciences 6%
- Nuclear Physics 5%
- Applied Math 2%
- Geosciences 2%
- Computer Science 1%
- Engineering 1%
- Environmental Sciences
- Fusion Energy 28%
- Chemistry 13%
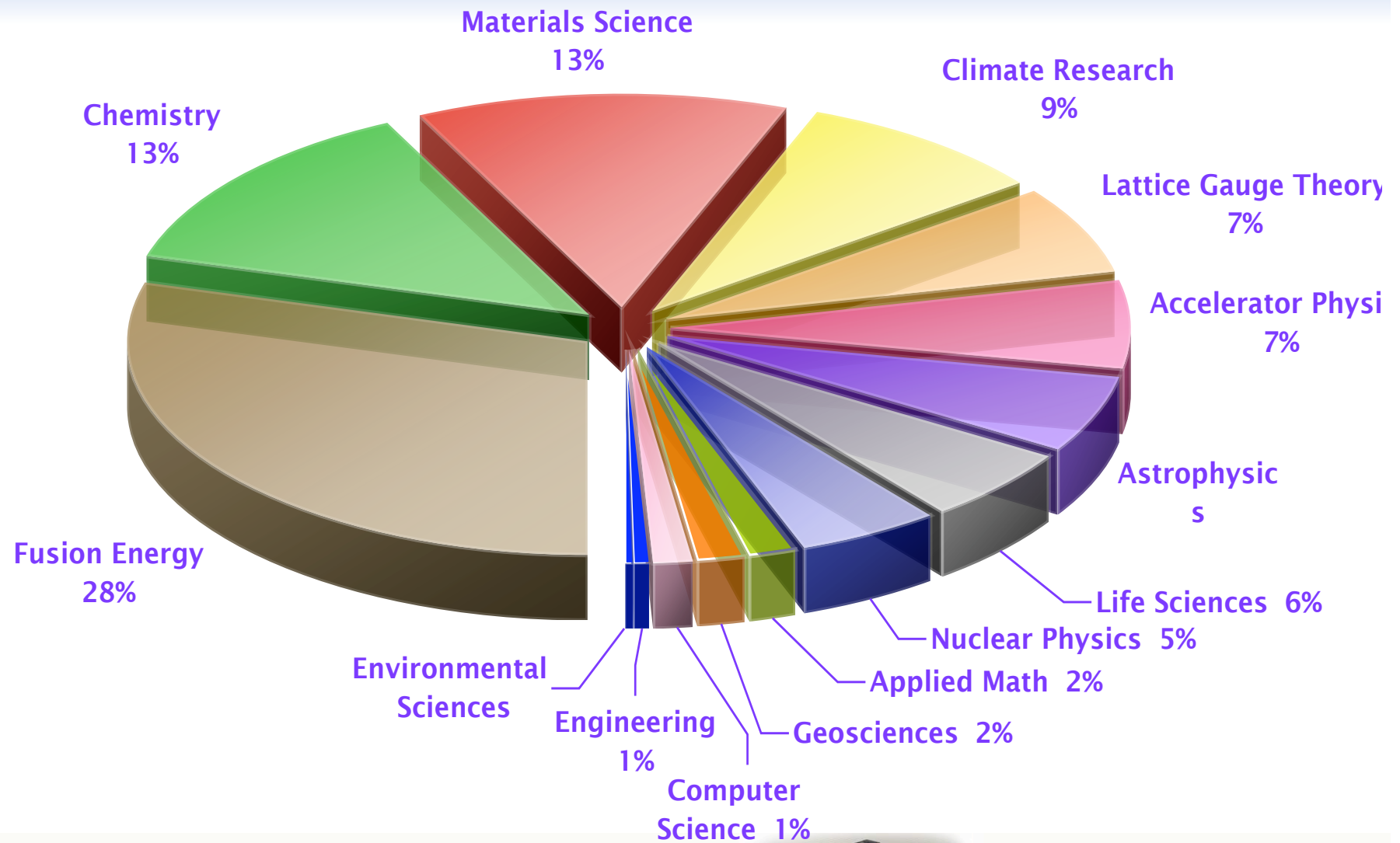
NERSC Systems History

Computational Research Division
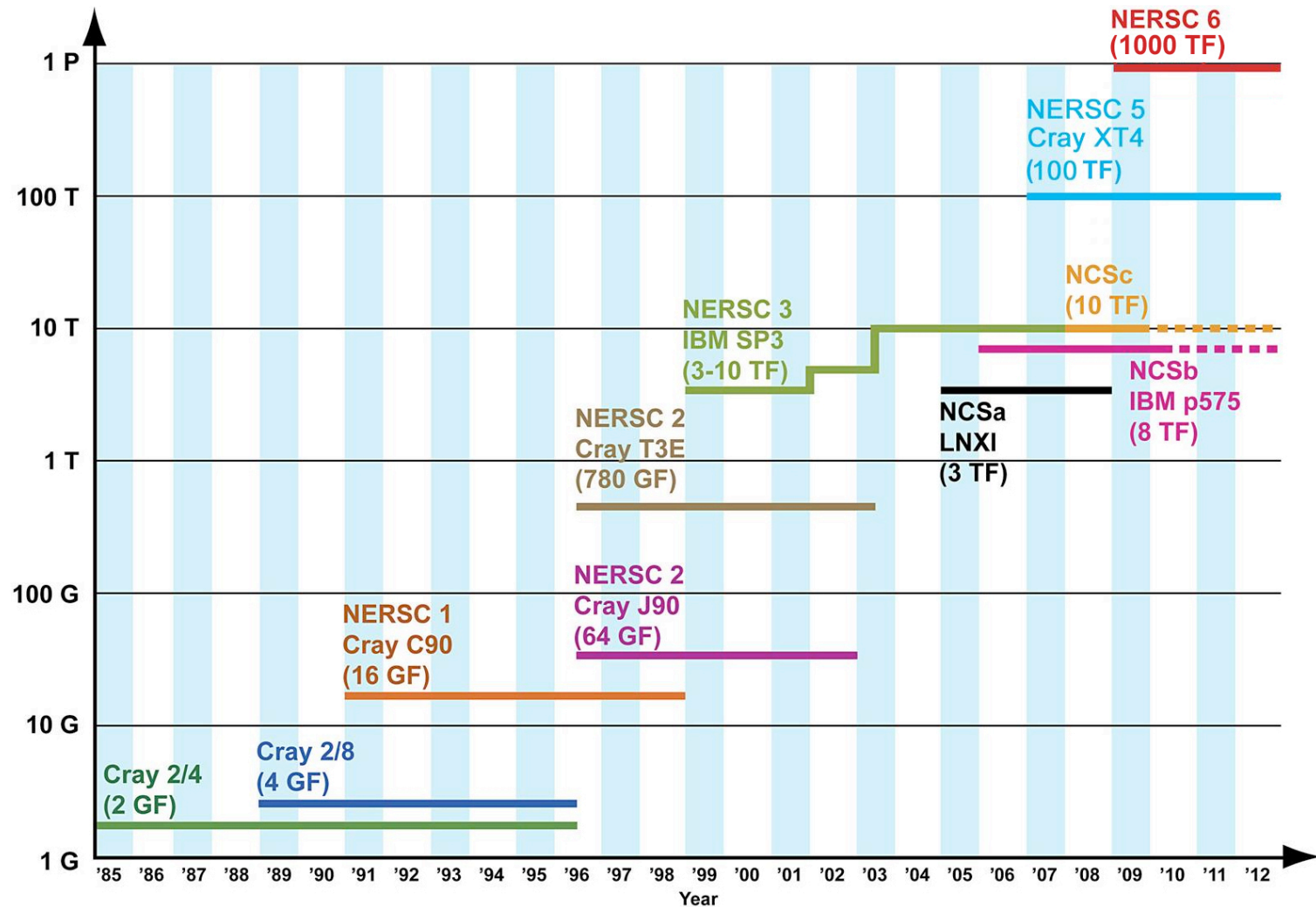
LEADERSHIP IN COMPUTATIONAL SCIENCE
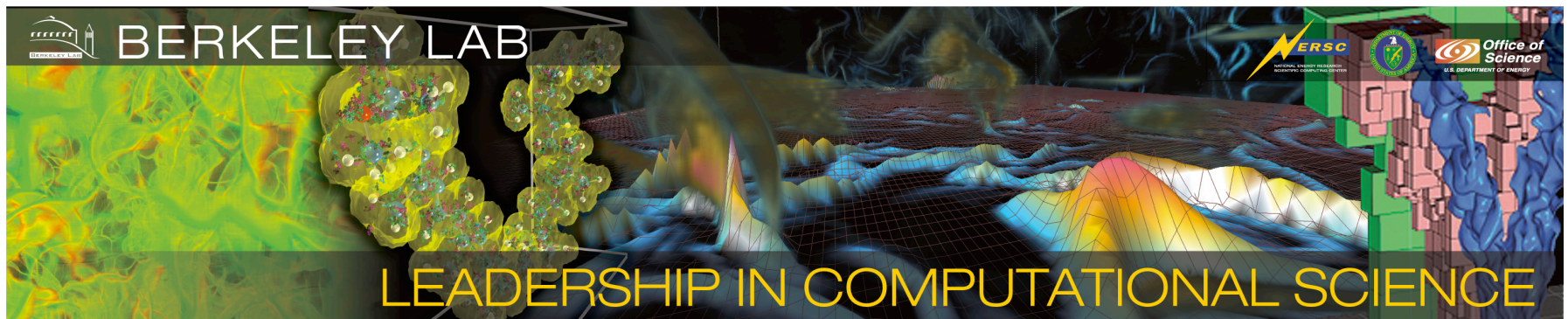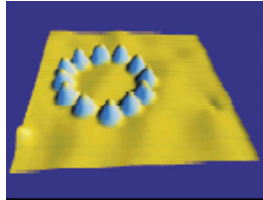
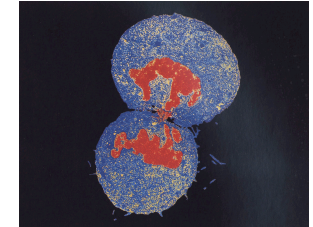# Computational Science Mission

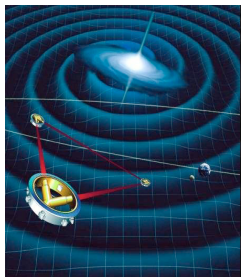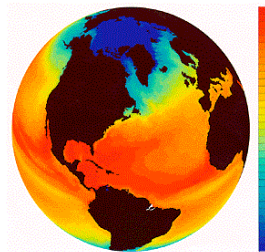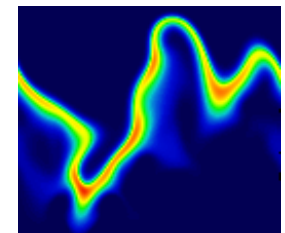**nano systems**

biological systems

The Computational Research Division is engaged in computational science collaborations, creating tools and techniques that will enable computational modeling and simulation, and lead to new understanding in areas such as

astrophysics simulation

global climate

combustion processes

Computer Science and Applied Mathematics Mission

The Computational Research Division is engaged in basic and applied research addressing the following questions of fundamental importance to enabling progress in our ability to use computing and networking technology

develop and analyze computer architectures that are most suitable for scientific applications and measure their effectiveness for science
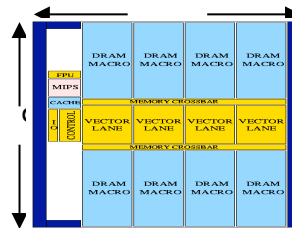
research in algorithms and development of software tools for these new architectures
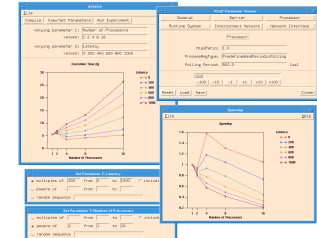
research and development of software tools and technologies in data management, analysis, and visualization
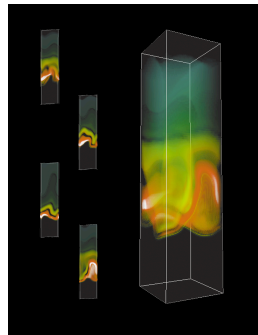
research in networking and distributed computing, and development of grid middleware and collaboration technologies

Simulation Science

Theory

Experiment

Simulation
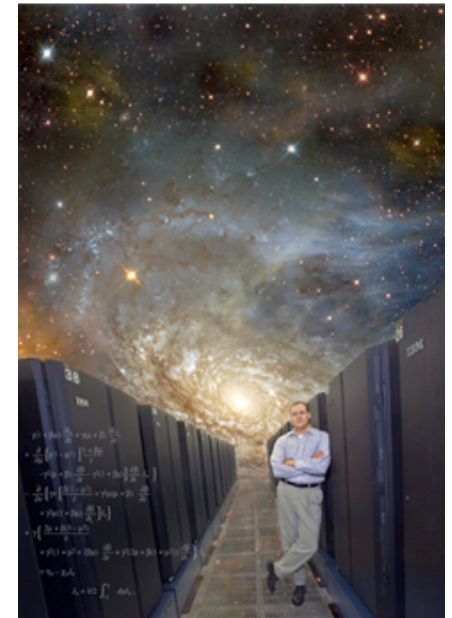
SciDAC - First Federal Program to Implement Computational Science and Engineering

- **SciDAC (Scientific Discovery through Advanced Computing) program created in 2001**
- **SciDAC 2 - new competition in 2006**
  - **About $60M annual funding**
  - **Berkeley (LBNL+UCB) largest recipient of SciDAC funding in both SciDAC1 and SciDAC2**

Global Climate
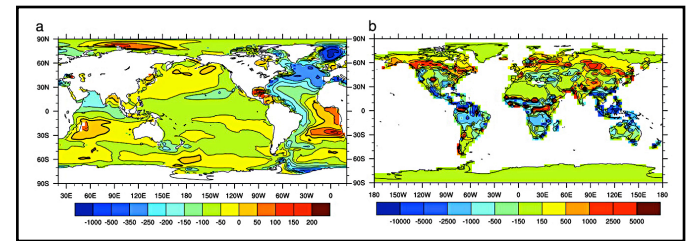
Biology
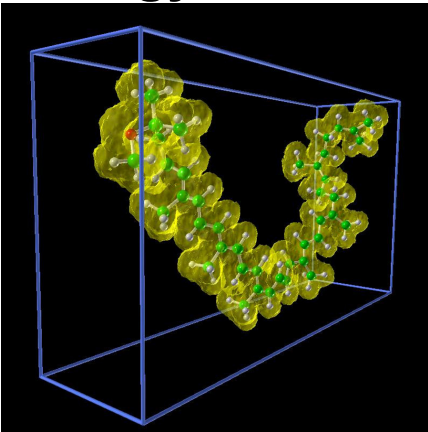
Nanoscience
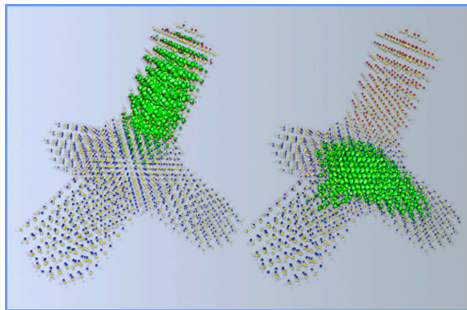
Combustion

Astrophysics

degree of polarization

when "clump" is viewed at a 24-degree angle
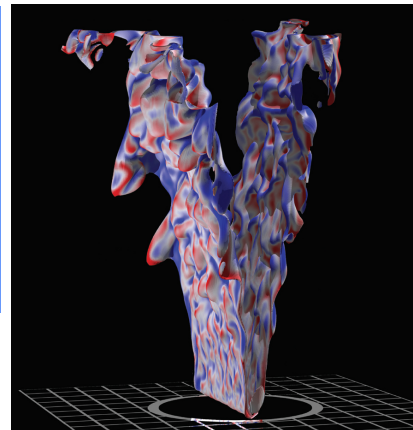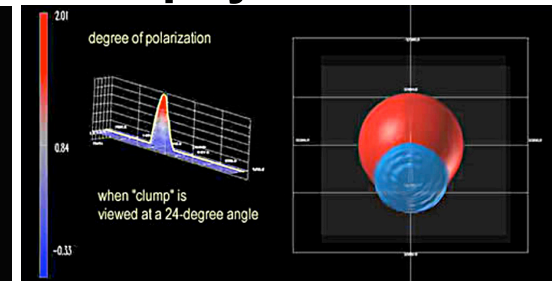
FY07 Highlights

High Performance Computing Research Department

conducts research and development in mathematical modeling, algorithmic design, software implementation, and system architectures, and evaluates new and promising technologies.
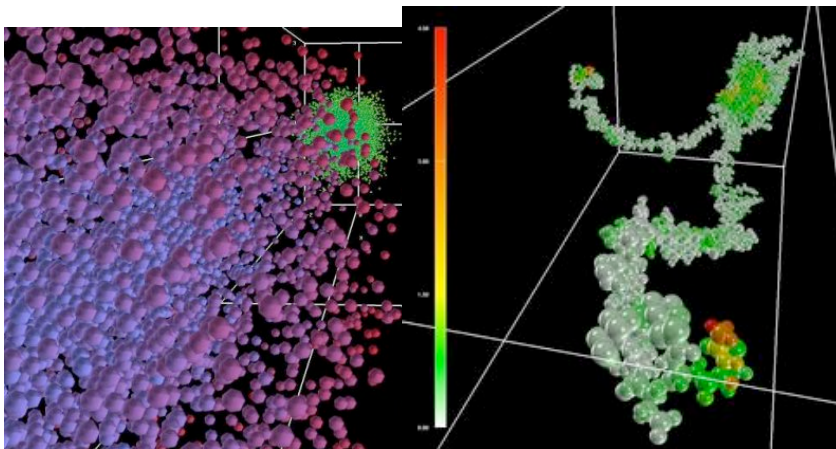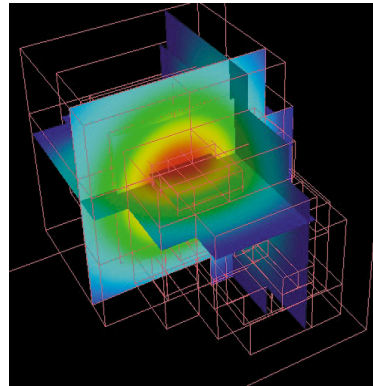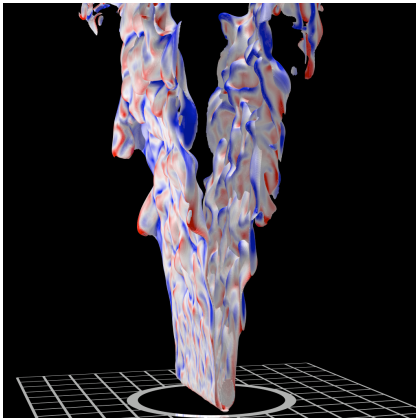
Juan Meza, Department Head

- ❖ **Applied Numerical Algorithms, Phil Colella**
- ❖ **Center for Computational Sciences and Engineering, John Bell**
- ❖ **Future Technologies, Erich Strohmaier**
- ❖ **Mathematics, James Sethian**
- ❖ **Scientific Computing, Esmond Ng**
- ❖ **Scientific Data Management, Arie Shoshani**
- ❖ **Visualization, Wes Bethel**

Total Staff: 140

Studying Supernovae: Low Mach Number Approaches in Astrophysics
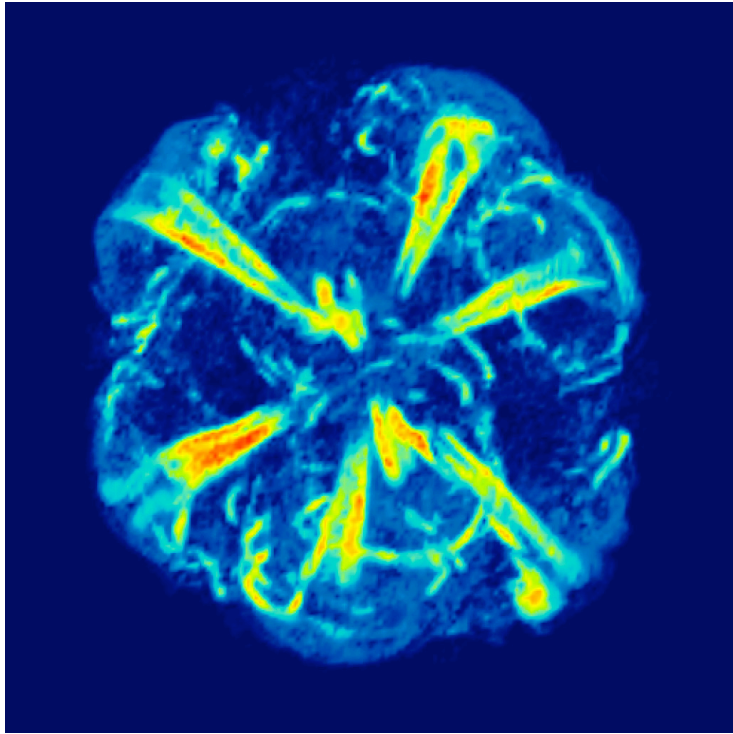
Vortical Structure induced by local heating in a while dwarf. The simulation was performed with the MAESTRO code that is based on the low Mach number analysis developed at LBNL.

A. Almgren, J. Bell, LBNL, Base Math Program

❖ Researchers at LBNL have developed a new mathematical model based on low Mach number analysis.

❖ The new method allows astrophysicists to study the ignition process in Type Ia supernovae.

❖ The low Mach number approach has been validated by comparison with compressible and anelastic approaches and promises significant computational savings.

Scientific Data Indexing Used for Identifying Malicious Network Attacks
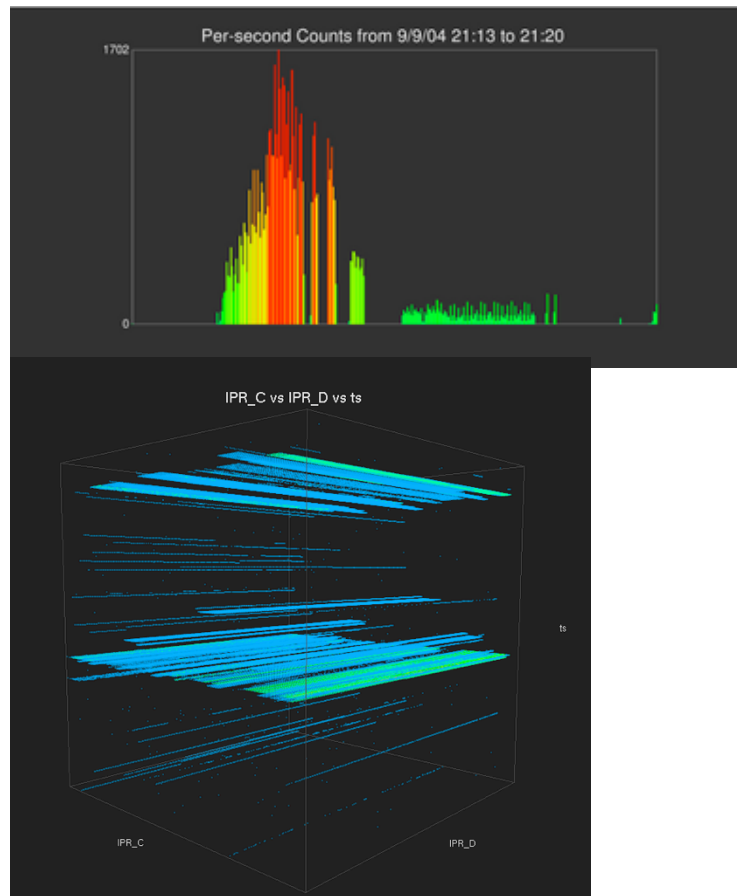
FastBit reveals consecutive regions that represent coordinated attacks.

K. Wu, K. Stockinger, D. Rotem, A Shoshani, E. Bethel, LBNL, Base CS & SciDAC SDM

❖ Network traffic at an average government research laboratory may involve tens of millions of connections per day, comprising multiple gigabytes of connection records between network hosts.

❖ A new tool, based on an LBNL patented fast bit indexing algorithm has been developed that can help reveal a coordinated network attack.

❖ FastBit has been applied to several other application domains, including finding flame fronts in combustion data, searching for rare events from billions of high-energy physics collision events and to facilitate query-based visualization.

New Linear Scaling Density Functional Method for Electronic Structure Calculations

ZB + (Cd+Se) surface   ZB + Cd surface

WZ+ (Cd+Se) surface   WZ+ Cd surface
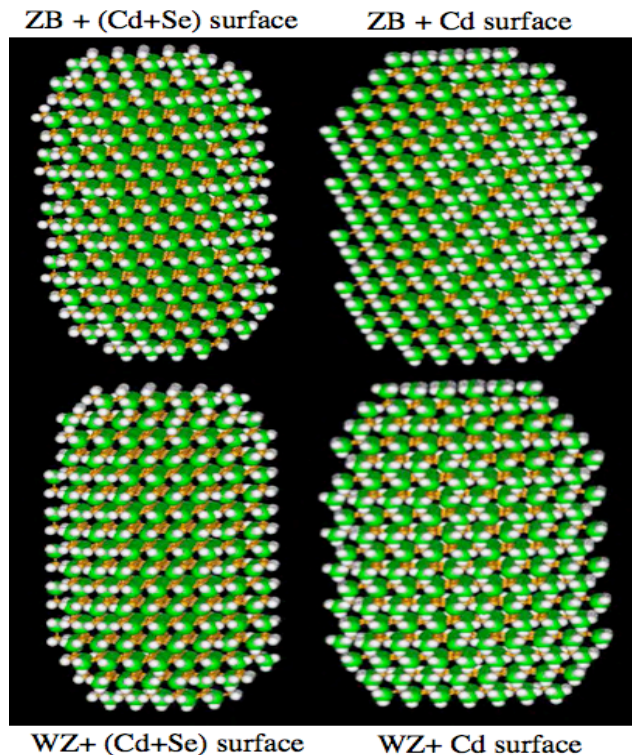
Simulation of CdSe nanorods. The green atoms are Cd, yellow atoms are Se, and white atoms are surface hydrogen. (top) the potential on the central axis; (bottom) the electron state (red) and hole state (green) isosurfaces with an isovalue of 0.0002 e/Bohr^3.

J. Meza, L.-W. Wang, Z. Zhao, LBNL, Nanoscience-Math

- ❖ A new linear scaling three dimensional fragment (LS3DF) method for electronic structure calculations now makes possible the simulation of nanostructures with the same accuracy as a direct *ab initio* method.

- ❖ The LS3DF method is based on the observation that the total energy of a given system can be broken down into two parts:
    - Long-range electrostatic energy
    - Short-range quantum mechanical energy

- ❖ LBNL researchers have used a divide and conquer approach to study the total dipole moments of CdSe quantum dots.

Superconformal Electrodeposition in Semiconductor Manufacturing

50 s   70 s   100 s   130 s   160 s   200 s
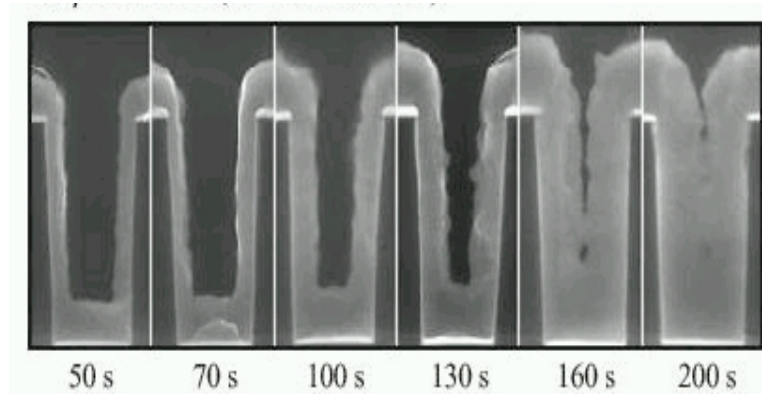
Electrodeposition without Voids

J.A. Sethian, Y. Shan, LBNL, Base Math

❖ Researchers at LBNL have developed a computational methodology to more efficiently simulate and predict some of the most complex processes in semiconductor manufacturing.

❖ This approach is based on a combination of level set methods, Fast Marching techniques, material transport methods, immersed interface schemes and multigrid methods

❖ The methods are applicable to a host of physical phenomena in which one must solve partial differential equations on moving irregular interfaces.

Adaptive Mesh Simulations Reproduce Tokamak Pellet Injection Experiments
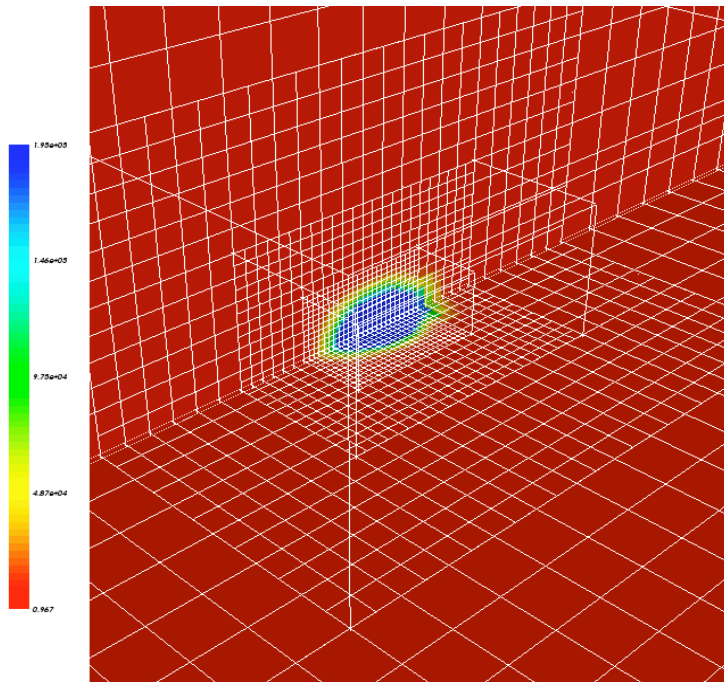
The density (left) and pressure (right) during a High-Field-Scale pellet launch

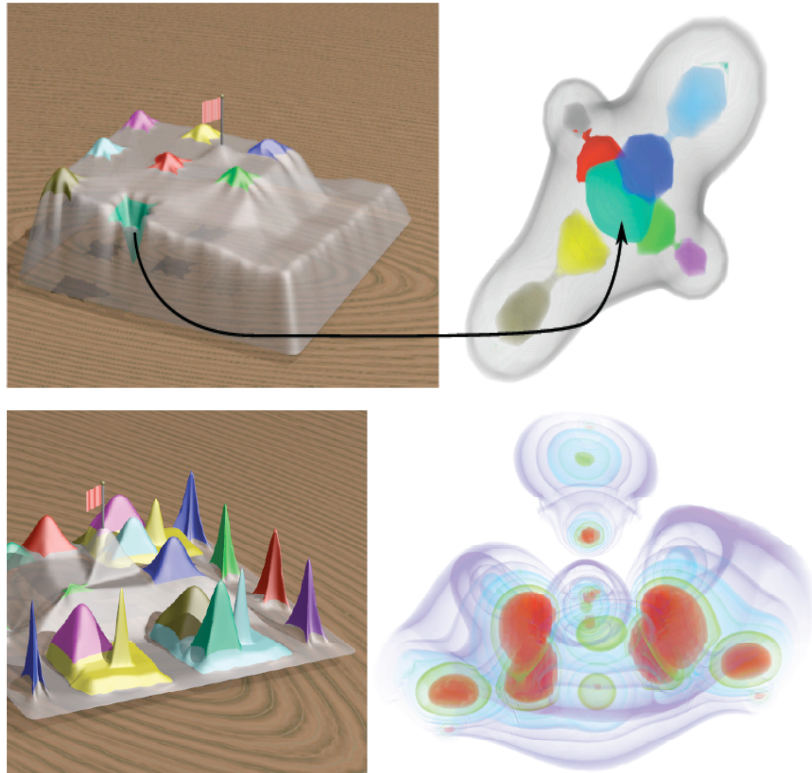**P. Colella (LBNL), R. Samtaney (PPPL), Base Math, SciDAC APDEC**

❖ New simulations using LBNL developed adaptive mesh refinement (AMR) algorithms have for the first time qualitatively reproduced results from a fusion pellet physics experiment.

❖ One can classify pellet injection into two categories:

- HFS (or High-Field-Side) launch in which the pellet is injected from the inside of the tokamak;

- LFS (or Low-Field-Side) launch in which the pellet is injected from the outside of the tokamak.

❖ Simulations using the AMR code were used to investigate the differences and similarities between the two competing techniques of pellet injection.

Novel Visual Presentation of Features Detected via Topological Analysis

Traditional volume rendering of electron density in methane (top) and a protein molecule (bottom) along with the landscape presentation of topological analysis data.

E.W. Bethel, G. Weber, LBNL, Base CS

- ❖ A team of researchers at LBNL has developed a novel technique for effectively presenting the results of features detected in very large and complex datasets through topological analysis.

- ❖ Topological analysis provides a complete study of the variation of a function or field.

- ❖ Describes all features and their location in space either in terms of critical points or in terms of entire regions.

Seismic Velocity Estimation from Time Migration
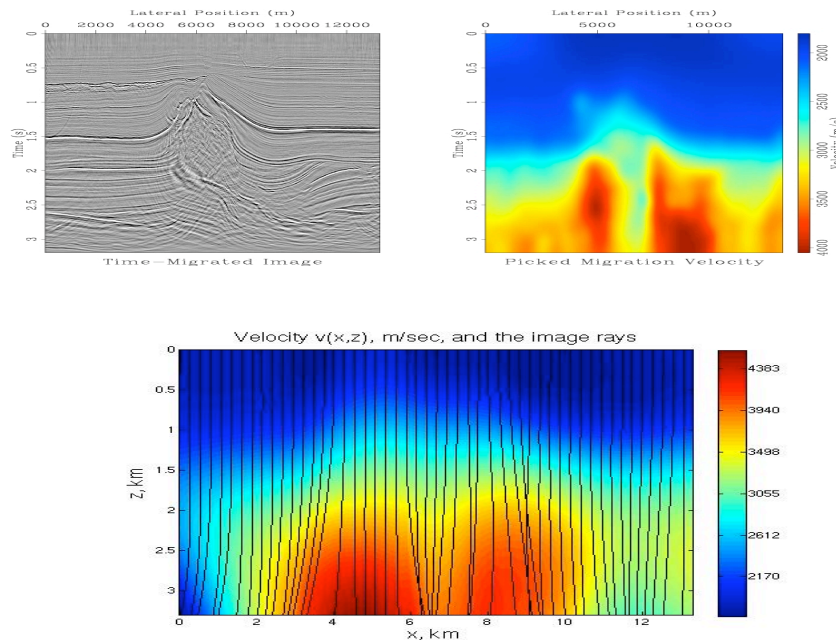
A North Sea salt dome with severe lateral variations. Top left shows the data; top right shows time migration data used to make this image, and the bottom shows reconstructed velocities in depth coordinates, together with the underlying characteristics

M. Cameron, J.A. Sethian, LBNL, Base Math

❖ LBNL researchers have developed an approach that has led to significantly improved seismic images in both two and three dimensions.

❖ The new approach uses a series of algorithms that transform time coordinate data into appropriate depth coordinates and seismic velocity model.

❖ The results rely on a new partial differential equation to describe the evolving wave front of seismic disturbances, as well as new algorithms based on a combination of advanced propagation algorithms as Dijkstra-like schemes.