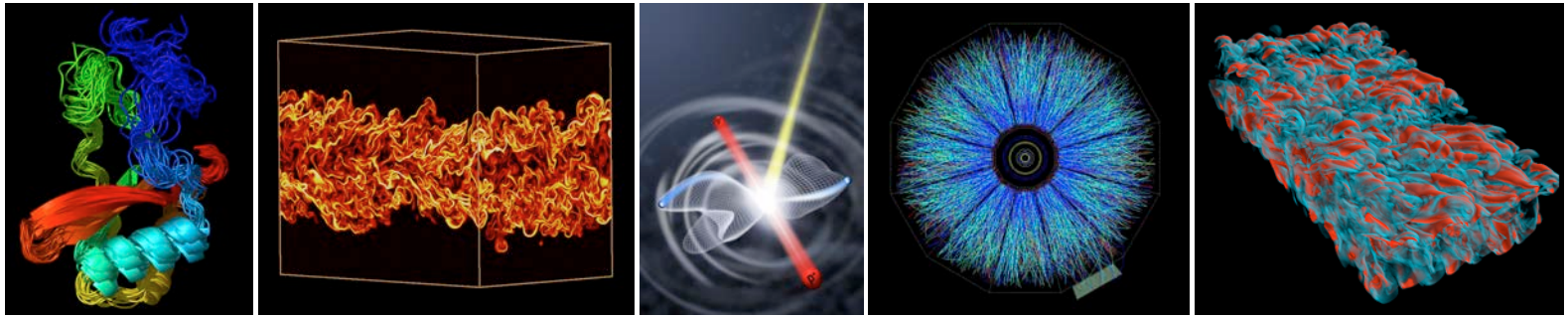
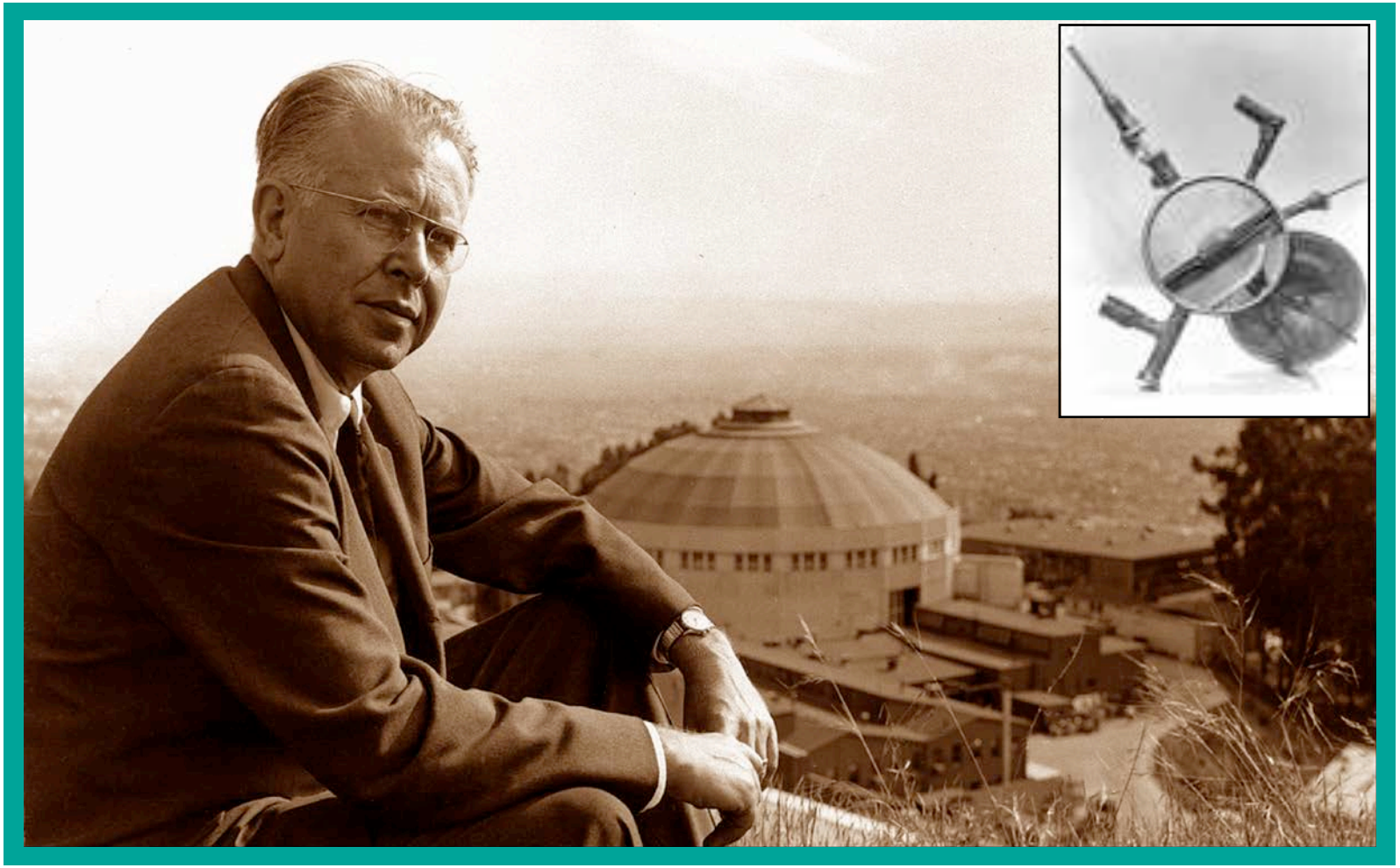


Computing Sciences at Berkeley Lab

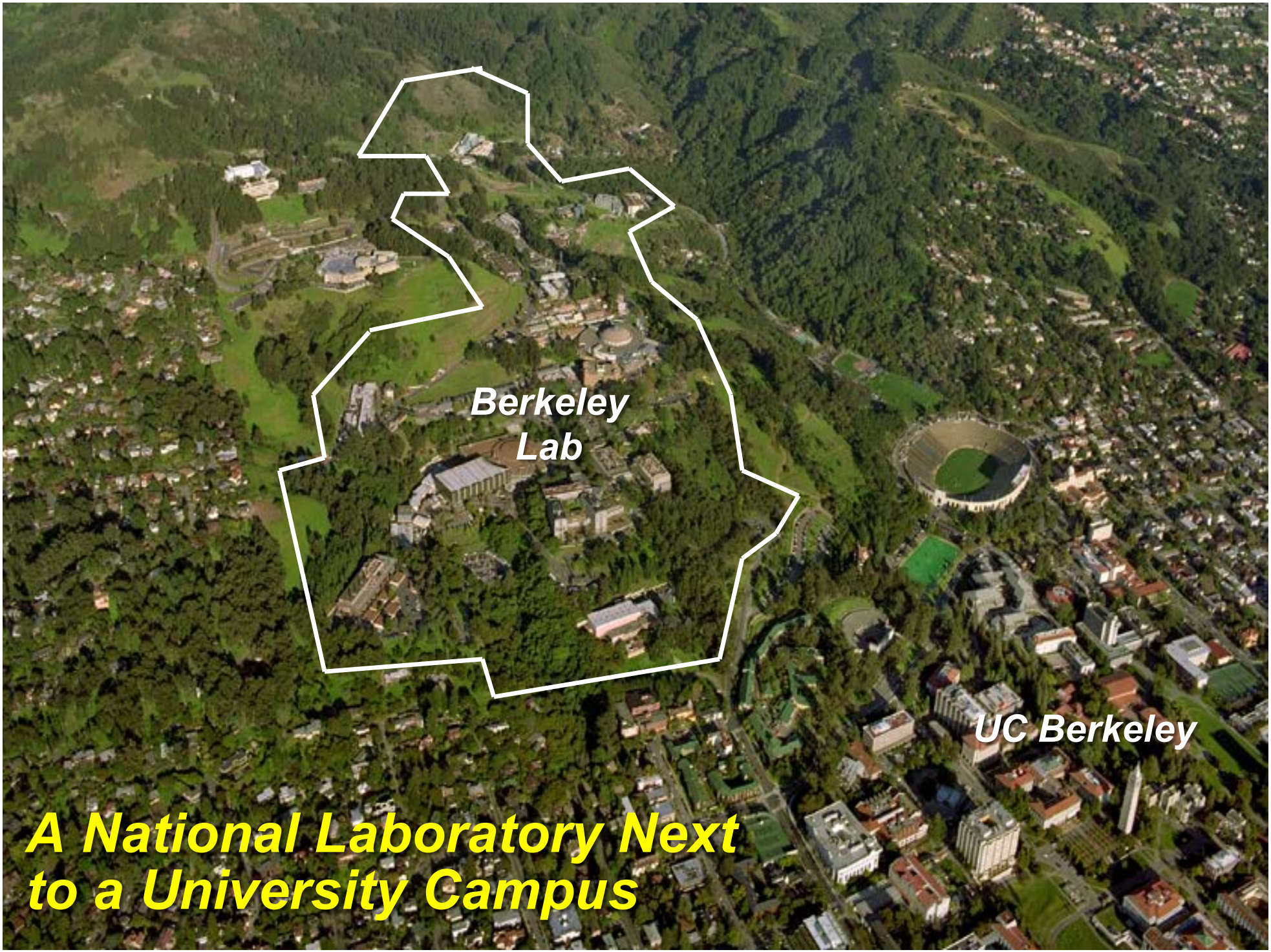
Juan Meza
Department Head, Senior Scientist
High Performance Computing Research
Lawrence Berkeley National Laboratory
June 24, 2009

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



*… as from the beginning the work has been a team effort involving many able and devoted co-workers in many laboratories. As I am sure you will appreciate, a **great many diverse talents** are involved in such developments and whatever measure of success is achieved is dependent on **close and effective collaboration**.*

Ernest O. Lawrence
The evolution of the cyclotron
Nobel Lecture, December 11, 1951



A National Laboratory Next to a University Campus

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

Advanced Light Source

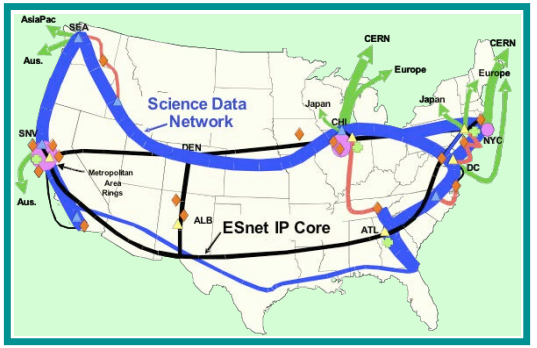
88-Inch Cyclotron

Joint Genome Institute

National Center for Electron Microscopy

National Energy Research Scientific Computing Center

Molecular Foundry

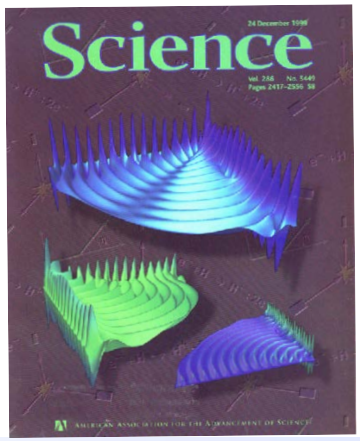


Energy Sciences Network (ESnet)

NERSC
National Energy Research Scientific Computing Center

National Energy Research Scientific Computing Center is enabling new science

- Serves the ***entire*** scientific community
  - Universities use 50% of time
- Focus on large-scale computing
- ~3000 users
- ~400 projects
- ~500 codes



Cray XT-4 “Franklin”

38,288 compute cores
356 Tflop/sec peak
76 TB memory
436 TB usable disk space
50 PB storage archive

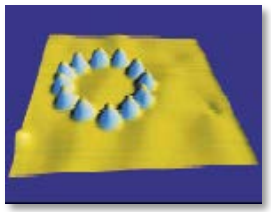
14,000 x

10 x

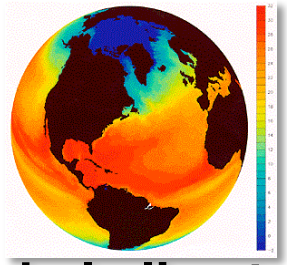
Computational Research Division

Computational Science Mission

The Computational Research Division is engaged in computational science collaborations, creating techniques and tools that will enable ***science-based predictive*** computational modeling and simulation leading to new discoveries and understanding in areas such as:

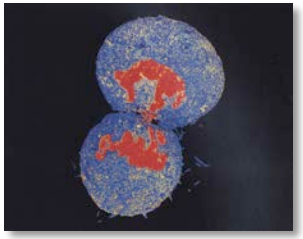


nano systems

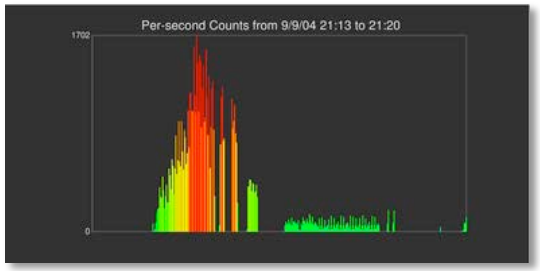


global climate

biological systems



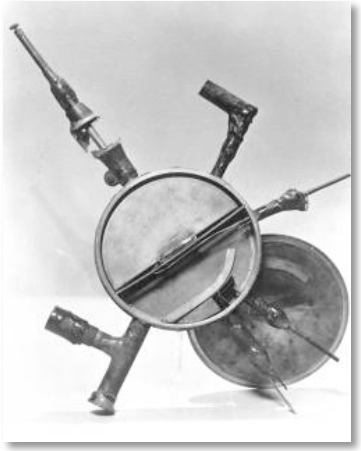
Astrophysics



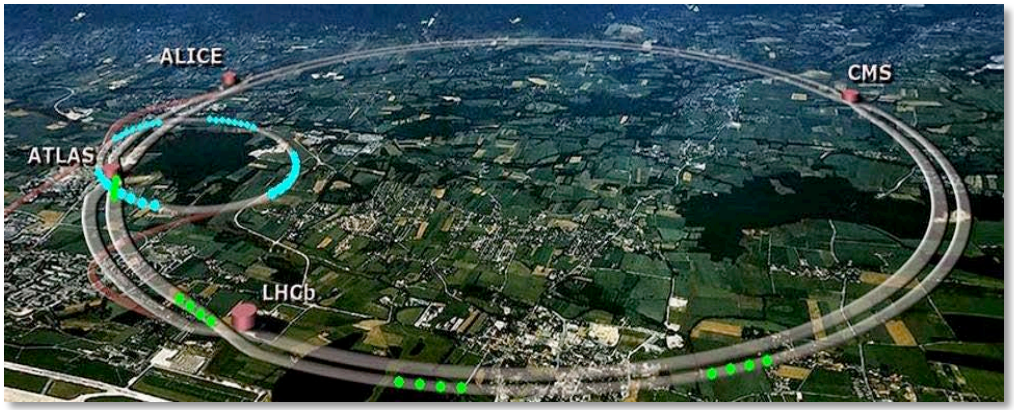
cyber security

combustion processes

Experiments vs. Computational Science



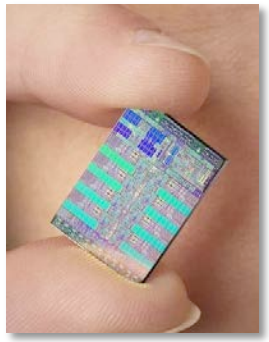
75,000 increase



4.5 inches diameter

27 km circumference, $4B US

500 Million increase



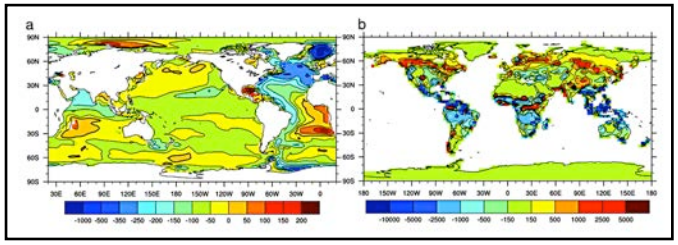
400 operations/s

200 Billion operations/s, $400

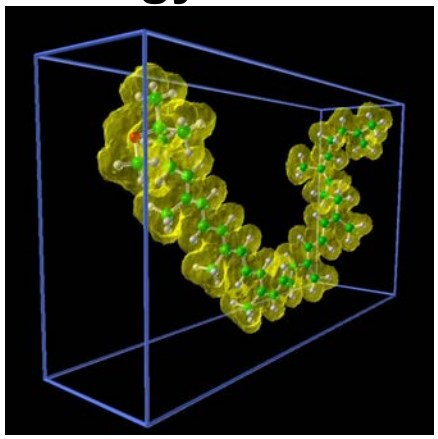
SciDAC - First Federal Program to Implement Computational Science and Engineering

- 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

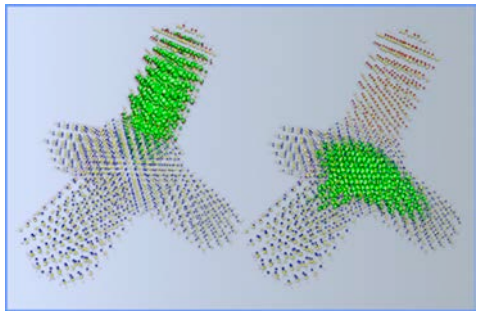
Global Climate



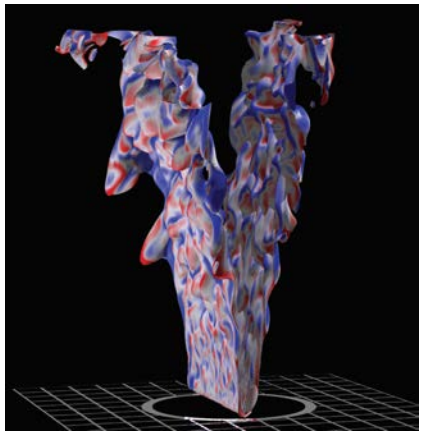
Biology



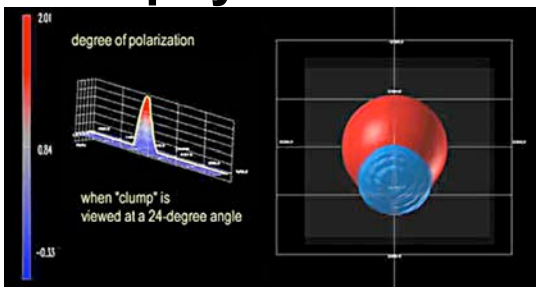
Nanoscience



Combustion

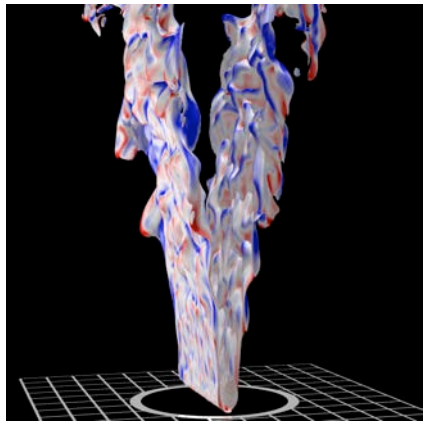


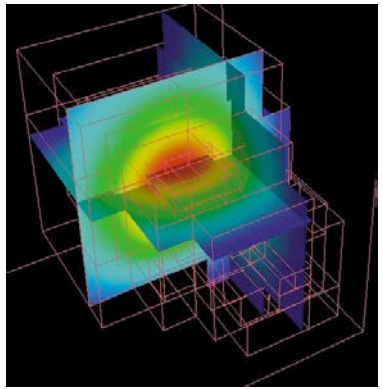
Astrophysics

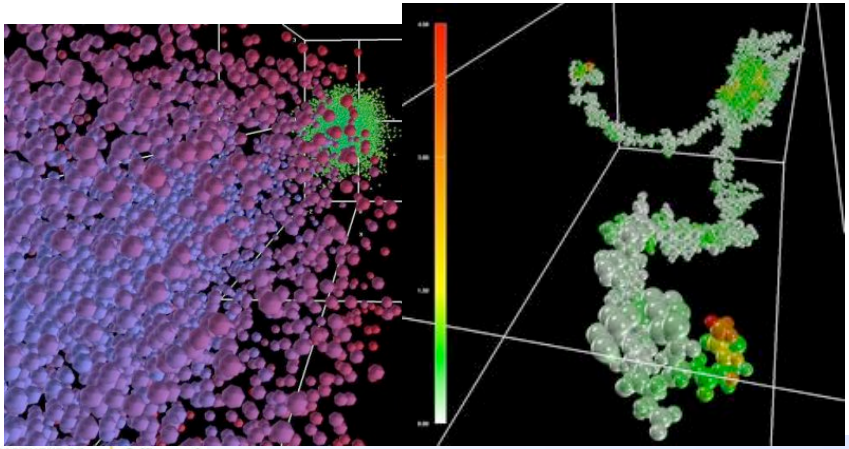


High Performance Computing Research Department

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







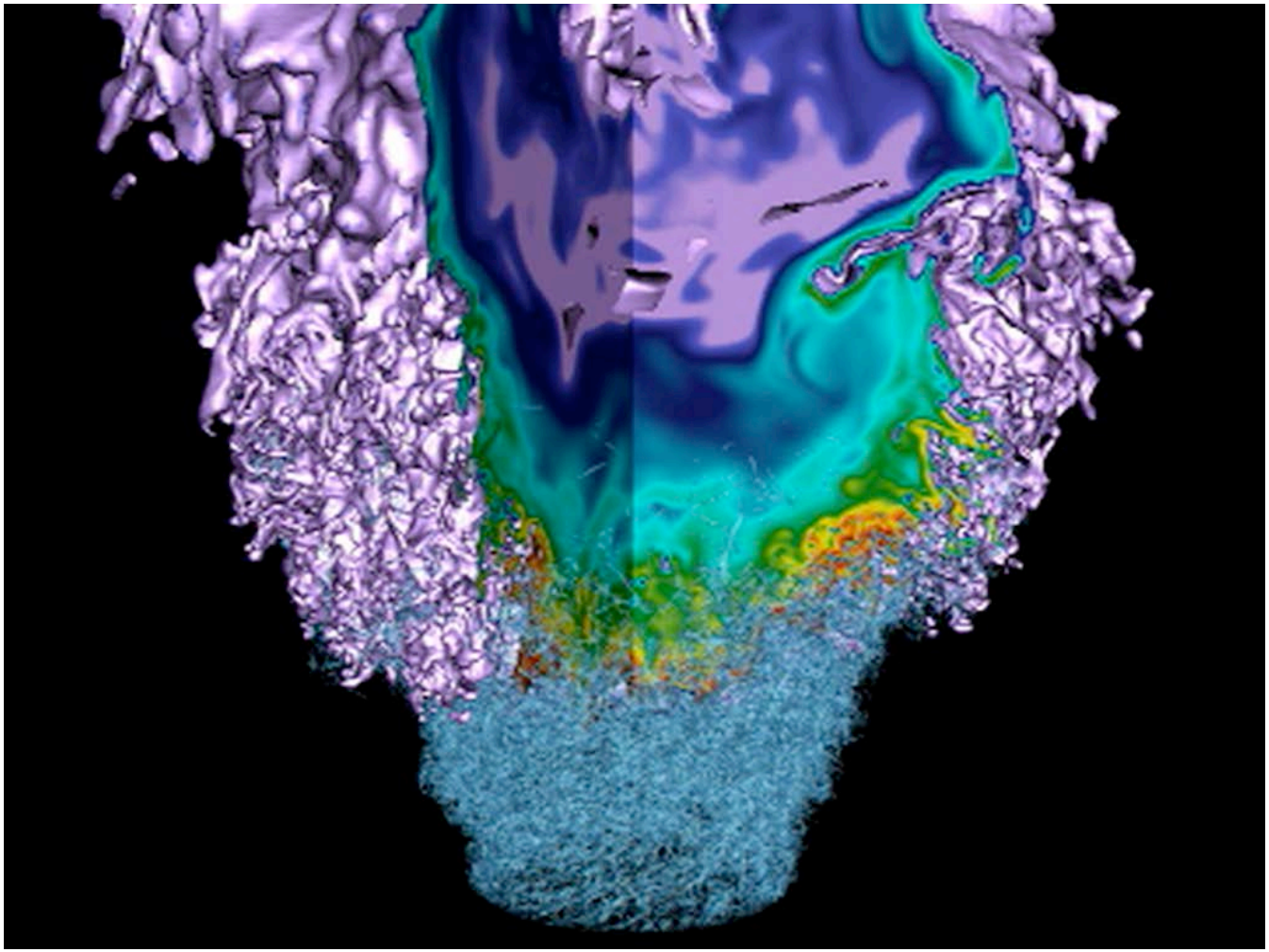
Juan Meza, Department Head

- **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**

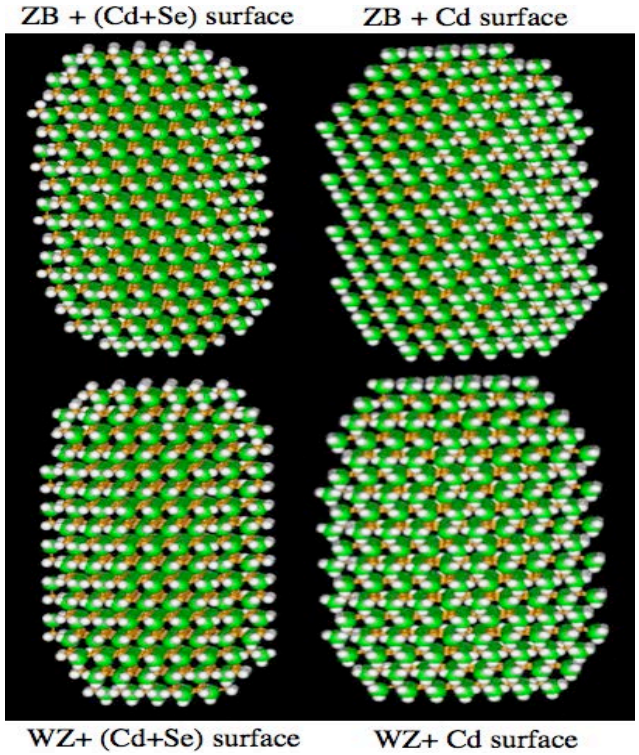
Total Staff: 140

Simultaneous rendering of OH and vorticity

John Bell, LBNL



New Linear Scaling Density Functional Method for Electronic Structure Calculations



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

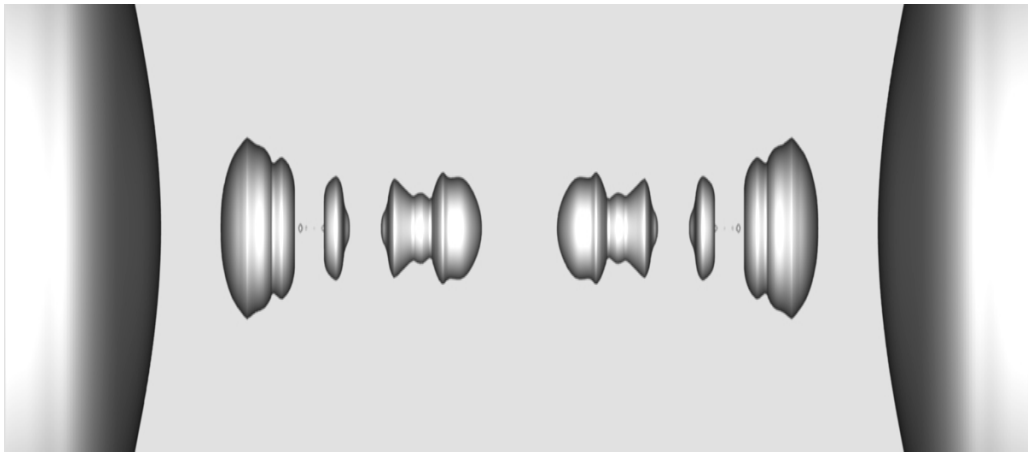
- A new linear scaling three dimensional fragment (LS3DF) method for electronic structure calculations now makes possible the simulation of nanostructures with the same accuracy as a direct *ab initio* method.
- The LS3DF method is based on the observation that the total energy of a given system can 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.

Satellite formation during pinchoff of a drop

- *Fundamental new approach:* Embed interface and potential fluid flow in higher dimensions
- Can pass through the topological/splitting change: study microdynamics
- Mixed boundary integral/level set method/fast multipole boundary solver

$$\mathrm{u} = \nabla\psi \ \text{ in } \ \Omega_d(t)$$
$$\Delta\phi(r,z) = 0 \ \text{ in } \Omega_{\mathrm{d}}(\mathrm{t})$$
$$\Phi_{\mathrm{t}} + \mathrm{u}_{\mathrm{ext}} \cdot \nabla\Phi = 0 \text{ in } \Omega_D$$
$$\mathrm{G}_{\mathrm{t}} + \mathrm{u}_{\mathrm{ext}} \cdot \nabla\mathrm{G} = \mathrm{f}_{\mathrm{ext}} \text{ in } \Omega_{\mathrm{D}}$$

Results showing fluid pinch-off: Comparison with Experiment



All equations are extended and embedded throughout domain, allowing *seamless* study of breaking and microdroplets

Computed result: Garzon, Gray, Sethian 2009

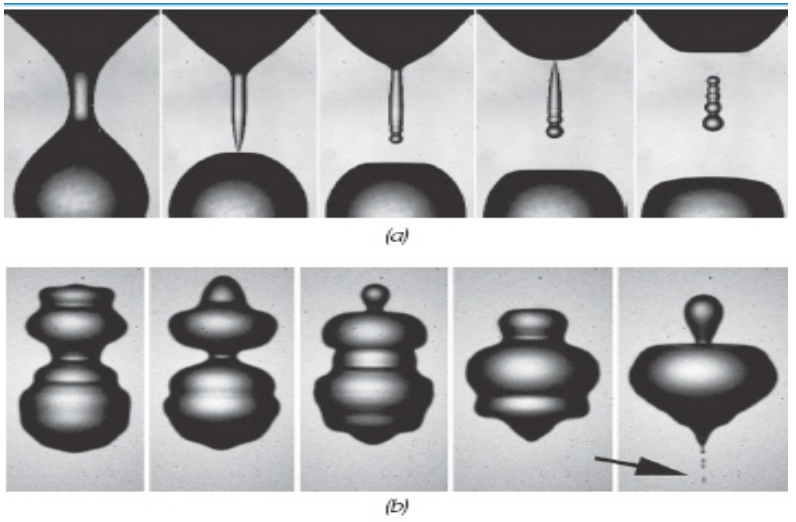
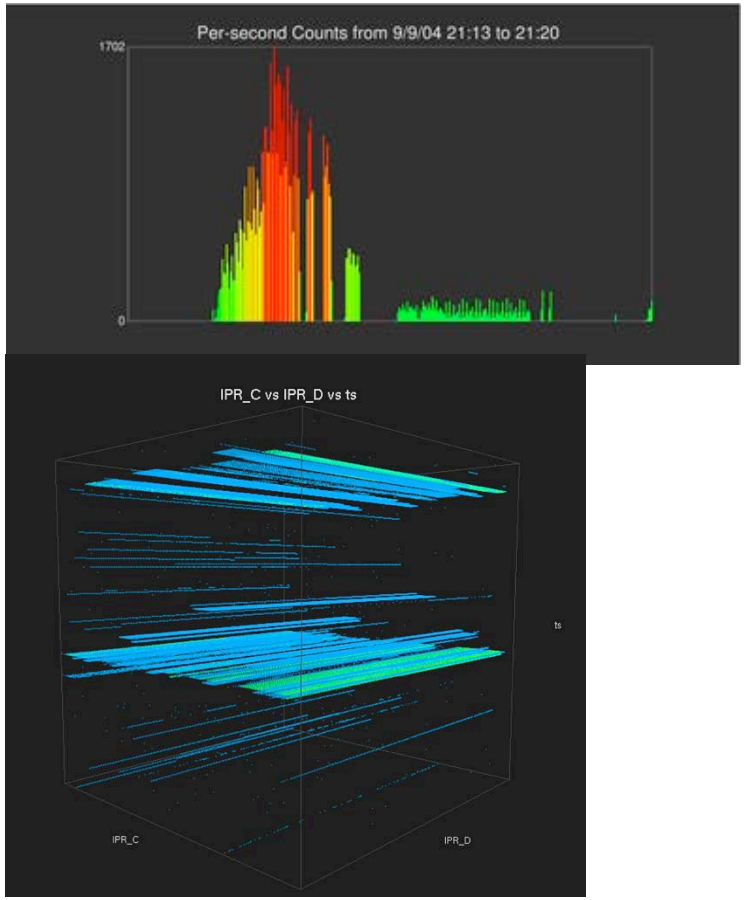


Figure 2: (a) Satellite formation during the pinch-off of a drop from a 5 mm nozzle. (b) Sequence shows the ejection of 30 mm micro-droplets which emerge at 10 m/s.

Experiment: Thoroddsen, 2007, 2008

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.

Summary

- Large-scale mission-focused research in basic sciences
- Access to state-of-the-art facilities
- Proximity to one of the best universities in the world

Great climate!