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Title:	Science Overview, Office of Science, and Energy Work at LANL
Author(s):	Terry C. Wallace and Janet A. Mercer-Smith
Intended for:	Senators Lamar Alexander and Jeff Bingaman Los Alamos, NM, USA 25 August, 2011

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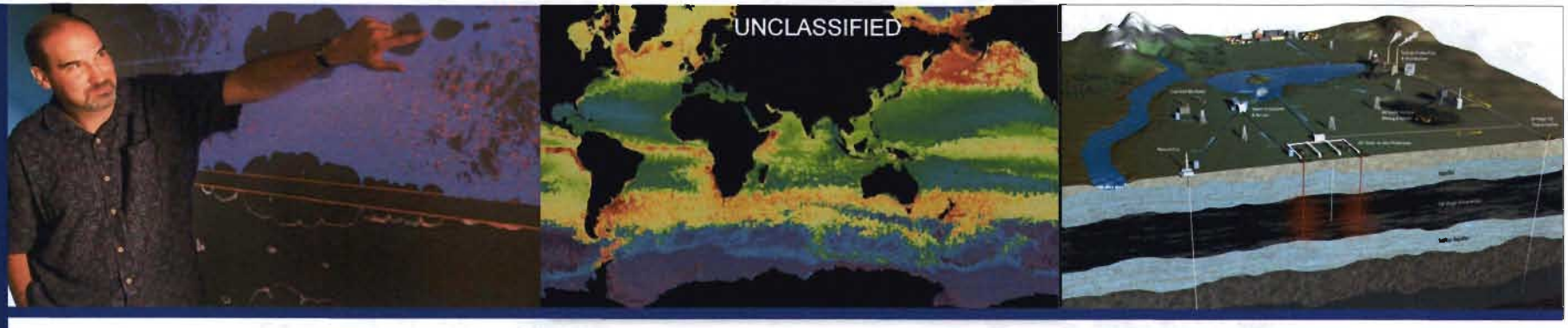
Form 836 (7/06)

Science Overview, Office of Science, and Energy Work at LANL

Terry C. Wallace and Janet A. Mercer-Smith

The Laboratory provides science solution to the mission areas of nuclear deterrence, global security, and energy security. The capabilities support the Laboratory's vision as the premier national security science laboratory. The strength of LANL's science is at the core of the Laboratory. The Laboratory addresses important science questions for stockpile stewardship, global security, and energy security. The underpinning science vitality to support mission areas is supported through the Post Doc program, the fundamental science program in LDRD, collaborations fostered through the Institutes, and the LANL user facilities. LANL fosters the strategy of Science that Matters through investments, people, and facilities. The presentation will focus on research in clean energy and high performance computer modeling and simulation studies of climate change, evolution of the HIV virus, and the mechanism of enzymatic digestion of cellulose.



Science and Technology

Science Overview, Office of Science, and Energy Work at LANL

Terry C. Wallace
Principal Associate Director for
Science, Technology and Engineering

August 25, 2011

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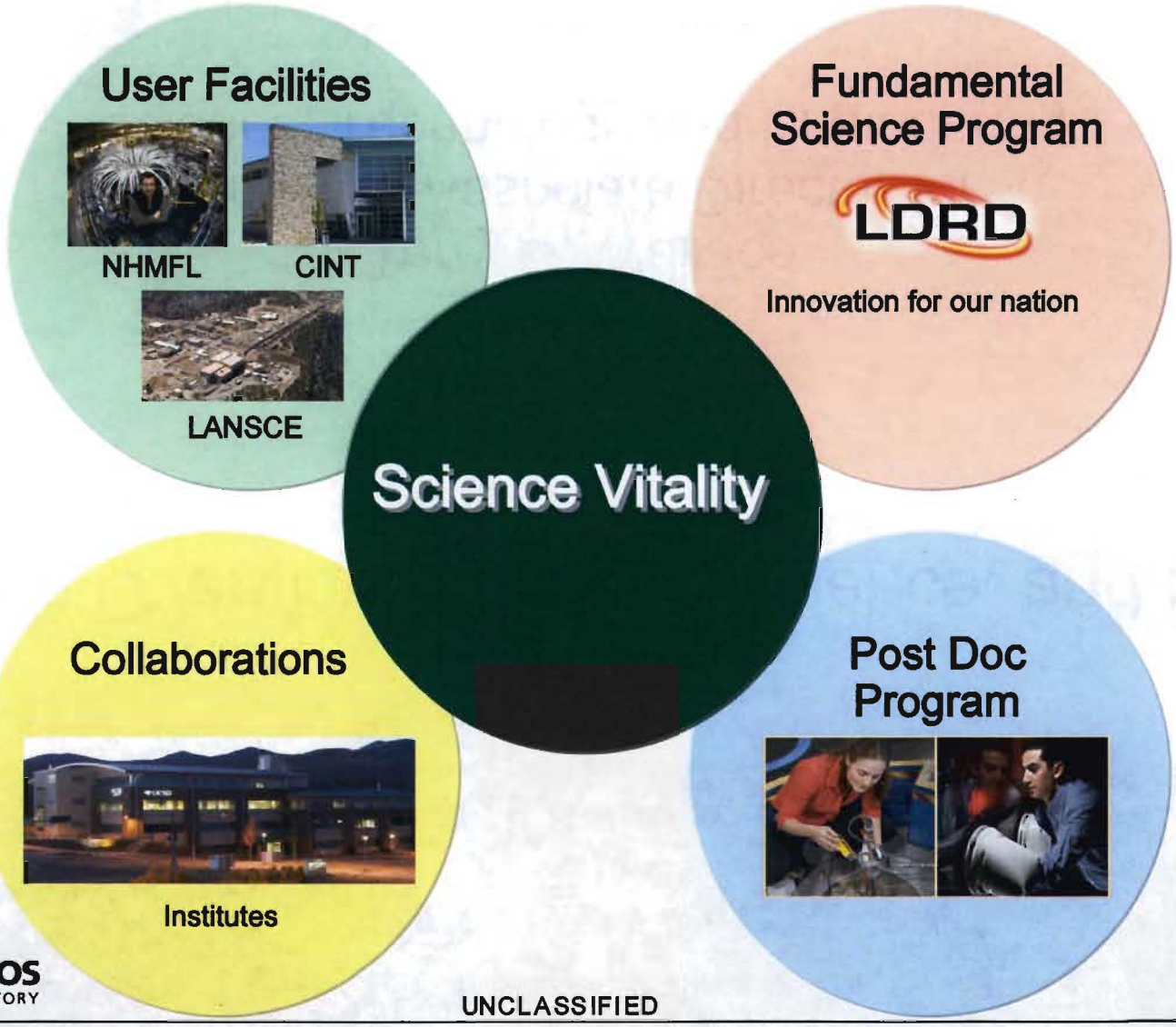
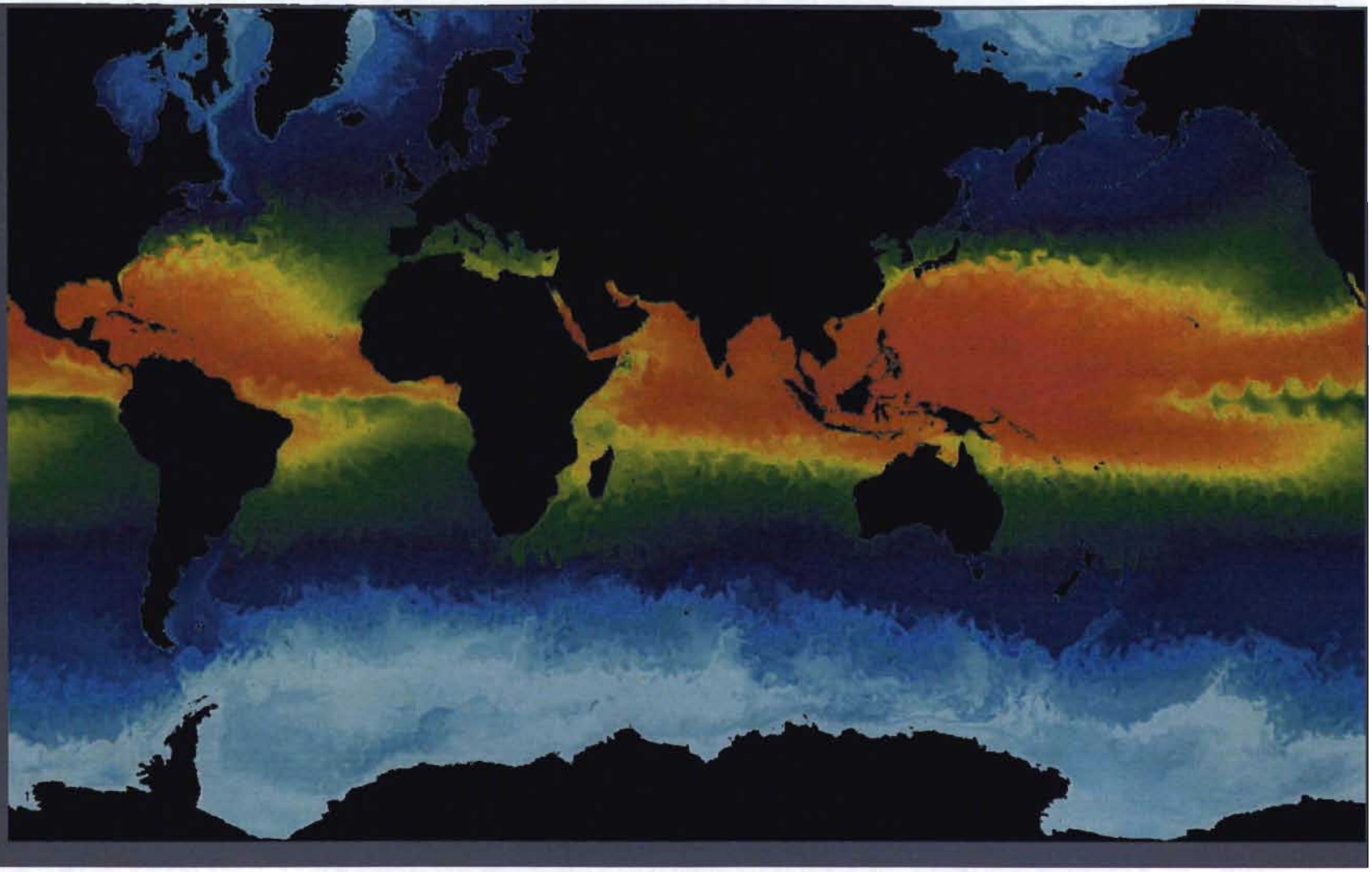
Science vitality underpins the Lab's mission areas.

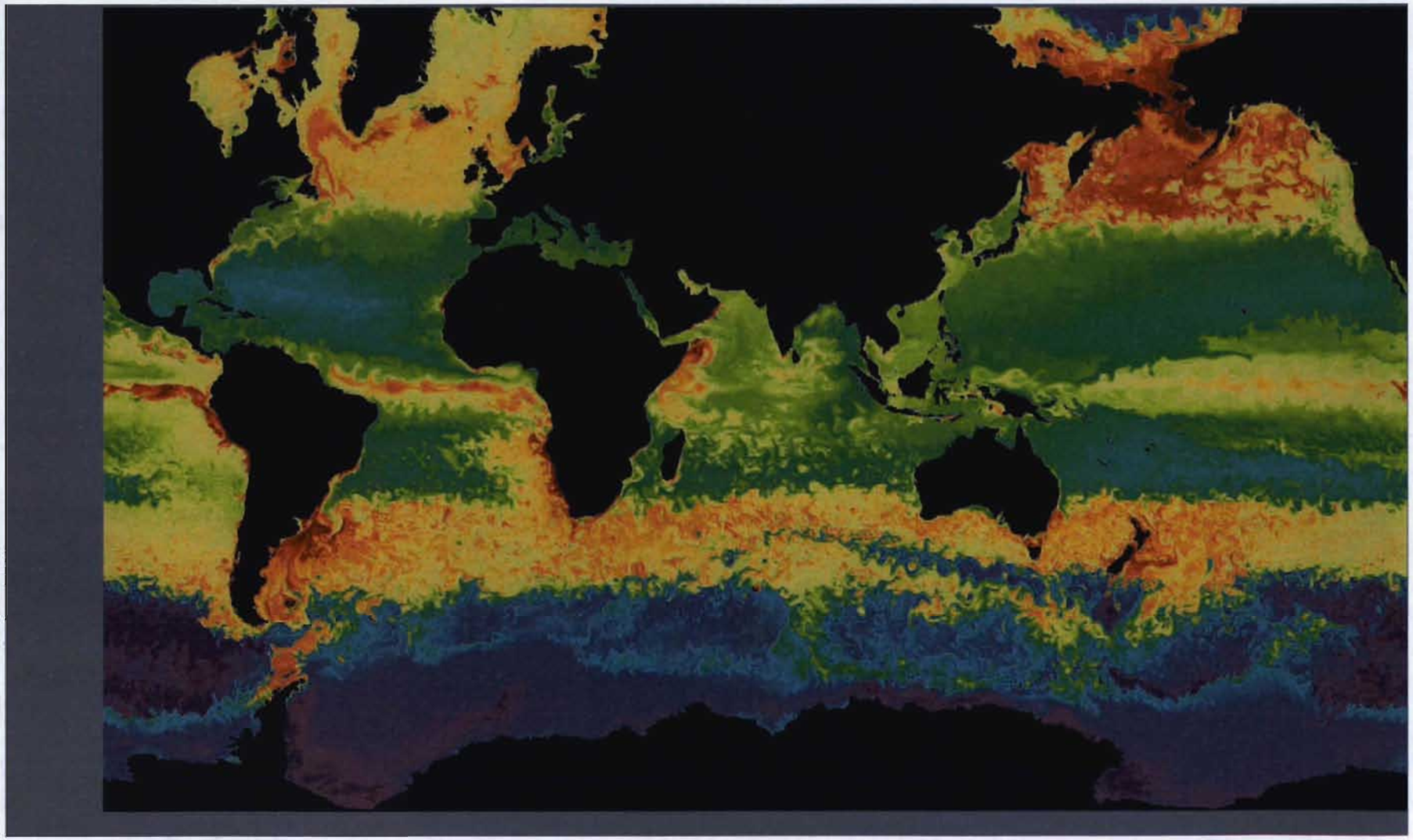


Climate simulation

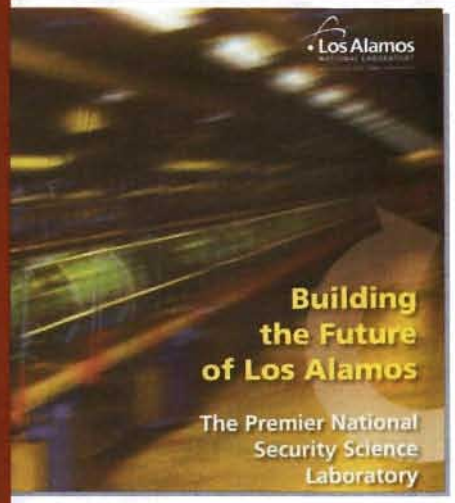
Ocean Circulation



Changes in Chlorophyll Concentration in the Ocean



"Science that Matters" pillars define areas we must sustain.



- Experimental science focused on materials for the future
- Information science and technology enabling integrative and predictive science
- Science of Signatures for enduring national needs

Materials for the Future

Information Science and Technology for Integrative and Predictive Science

Science of Signatures

Controlled Functionality

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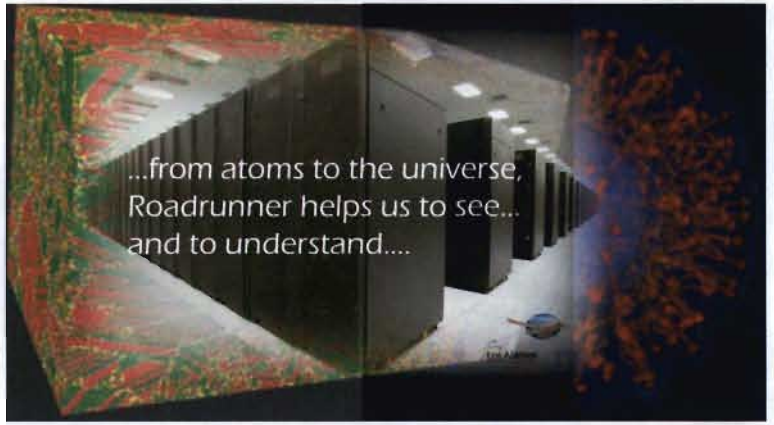
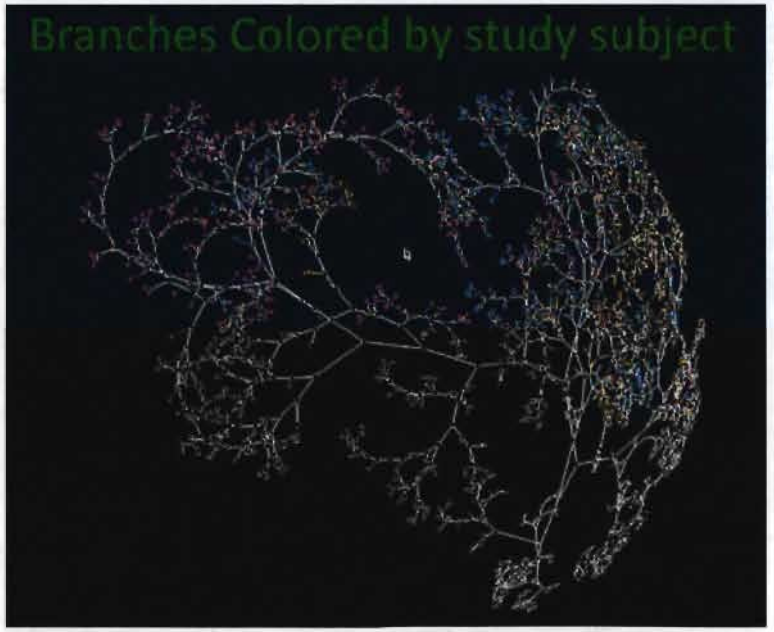
Petaflop computing is a significant step towards exascale.

- Roadrunner was the fastest machine in the world for 18 months.
- Proved that heterogeneous cores could be used to achieve systems breakthroughs.

Applications to HIV Research

- Simulated HIV evolution in patients, using 10,000 sequences from over 400 patients.
- Built an evolutionary tree using a LANL code.
- Bette Korber designed a "mosaic vaccine".
- Medical collaborators will conduct clinical trials with the vaccine as part of the CHAVI consortium.

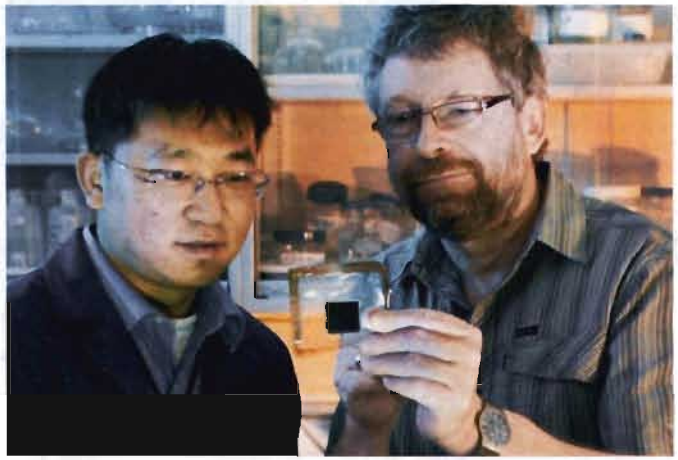




Evolution of HIV

Developed non-precious metal catalysts for fuel cells.

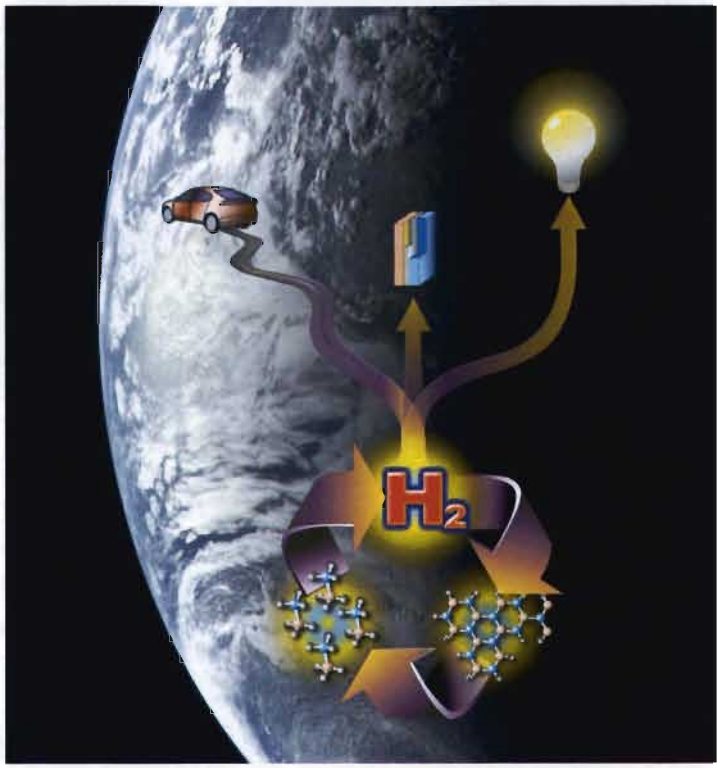
- LANL scientists and an Oak Ridge National Laboratory collaborator developed platinum-free catalysts for the cathode of a hydrogen fuel cell.
- New catalyst uses carbon and inexpensive iron and cobalt instead of platinum.
- Non-precious metal catalyst has good durability, life cycle, and current generation compared with platinum catalysts.
- New catalyst could greatly reduce the cost of fuel cells.
- The journal ***Science*** published the research, and a patent application has been filed.



Los Alamos has conducted research in fuel cells since 1977 and has made enabling breakthroughs in the areas of thin film electrodes and non-precious metal catalysis.

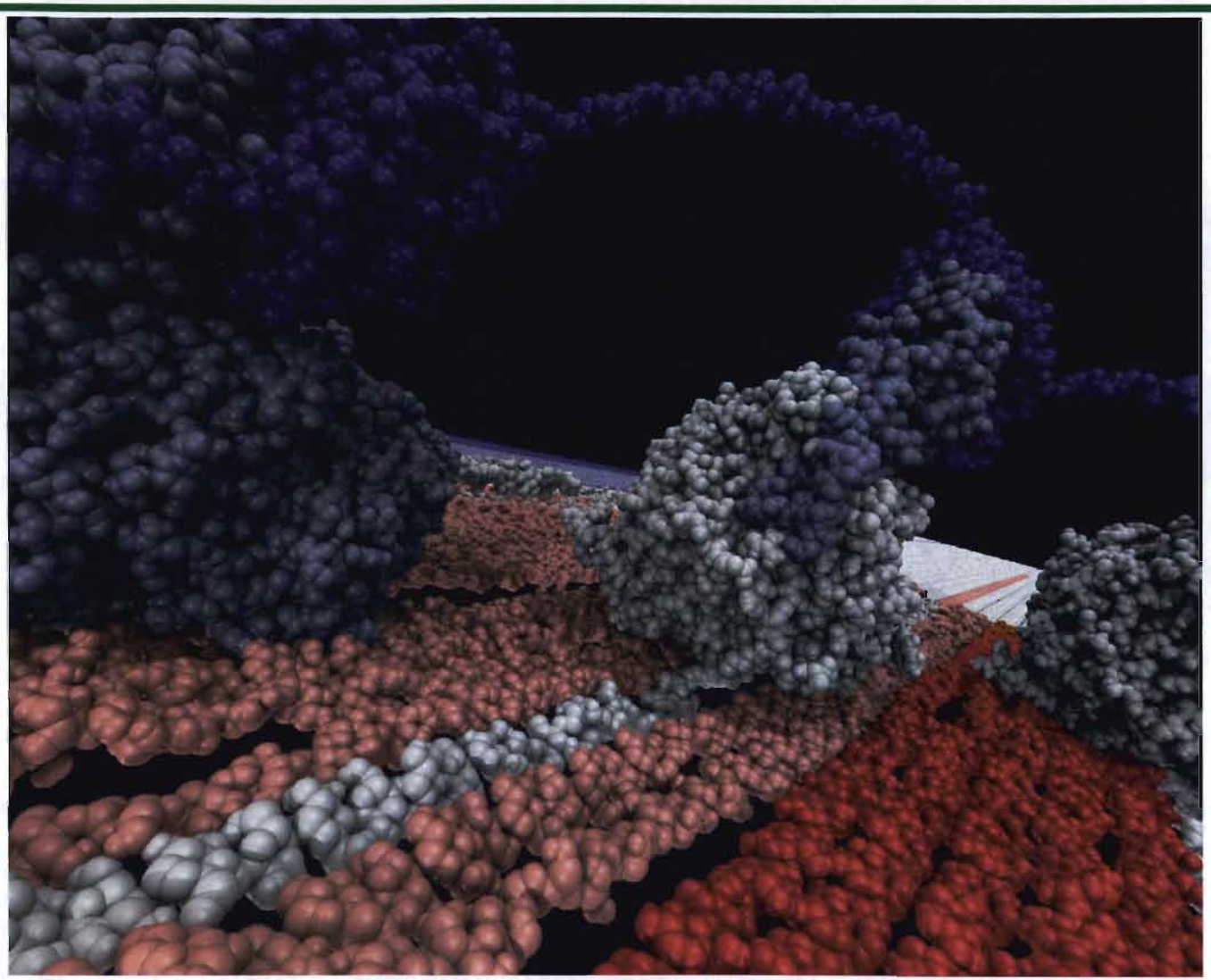
Developed an efficient method to recycle spent fuel for solid hydrogen fuel storage tanks.

- Ammonia borane is an attractive clean fuel because it has a large hydrogen storage capacity.
- A key technical issue is the need for an efficient method to recycle the hydrogen-depleted fuel.
- LANL and University of Alabama scientists have developed a single stage method to regenerate the ammonia borane fuel.
- The journal ***Science*** published the research.



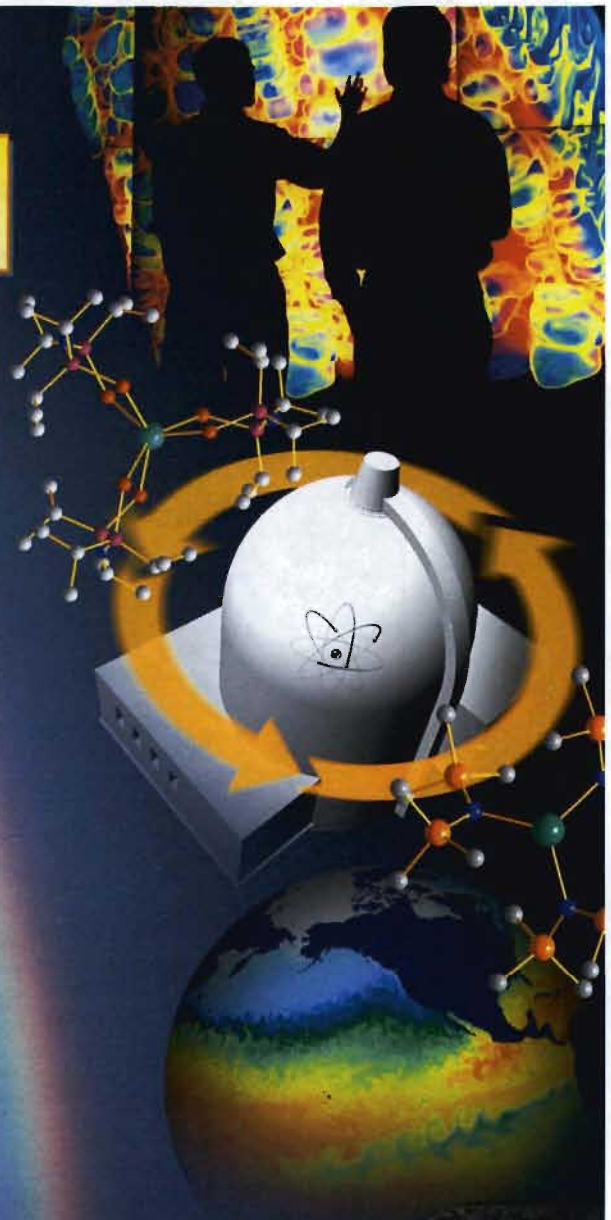
This "one pot" method is a significant step toward the practical use of hydrogen in vehicles by potentially reducing the expense and complexity of the recycle stage.

Understanding the Enzymatic Digestion of Cellulose



Los Alamos Science in the 21st Century

The nation's investment in Los Alamos has fostered scientific capabilities for national security missions.



As the Premier National Security Science Laboratory, Los Alamos tackles:

- **Multidisciplinary science, technology, and engineering challenges**
- **Problems demanding unique experimental and computational facilities**
- **Highly complex national security issues requiring fundamental breakthroughs**

LDRD is *essential* for LANL's science and technology strategy.

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NNSA

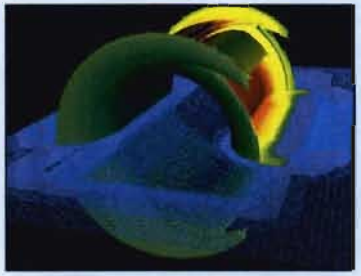
Backup Slides

Backup Slides

Mission

LANL Mission: National Security Science

Stockpile Stewardship

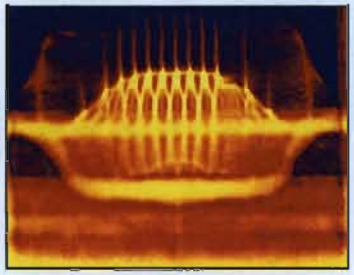


Large-Scale Simulation
Stockpile Stewardship

Pit Manufacturing

B61-7/11 Strategic Bomb

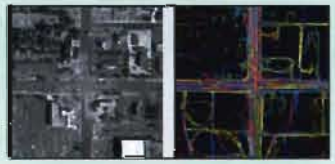
W76, W78, W88
for Trident &
Minuteman III



Proton radiography

Global Security

Non Proliferation



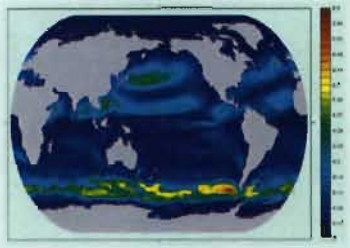
Intelligence Analysis

Space Systems
Six other product lines

Energy Security

Materials and Concepts
for Clean Energy

Nuclear Energy



Climate Energy Nexus

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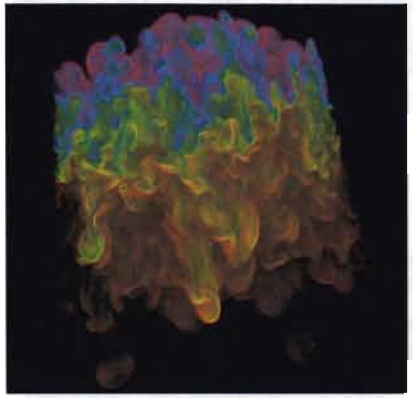
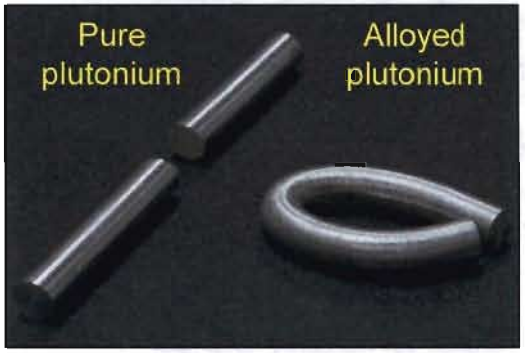
Mission Areas

Science at Los Alamos National Laboratory

Stockpile Stewardship

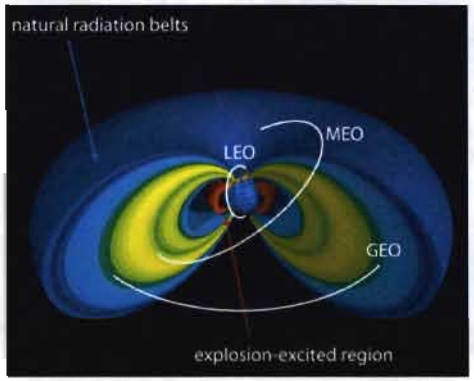


Hydrodynamics: Turbulence

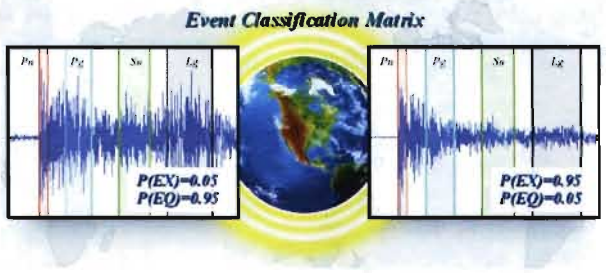


Plutonium Science: Metallurgy

Global Security

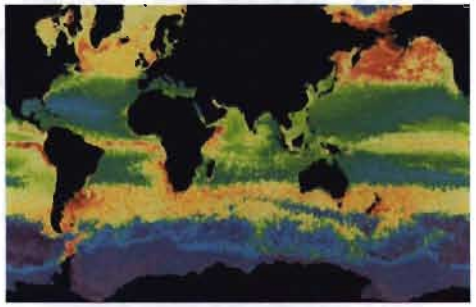


Threats from Space: Dynamic Radiation Environment Assimilation Model



Seismic Detection of Nuclear Explosions

Energy Security



Climate/Energy Impacts: Measurement, simulation, prediction

Materials: Energy generation and transmission

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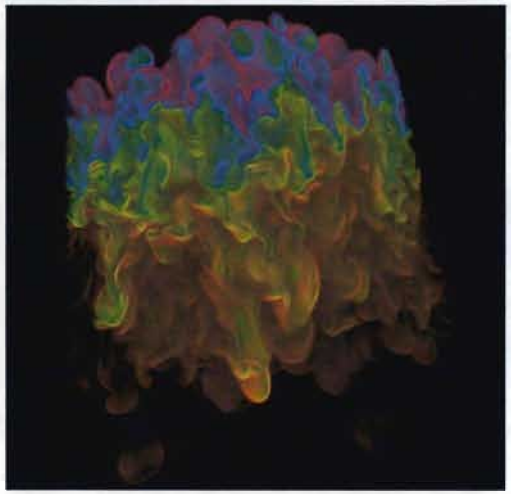
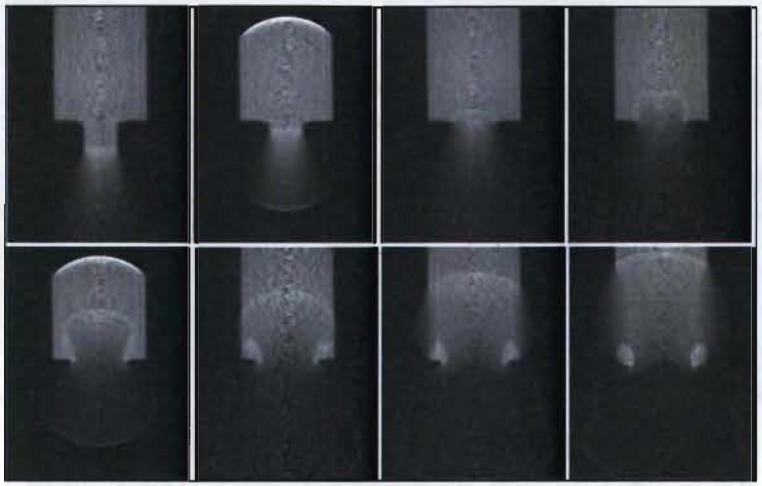
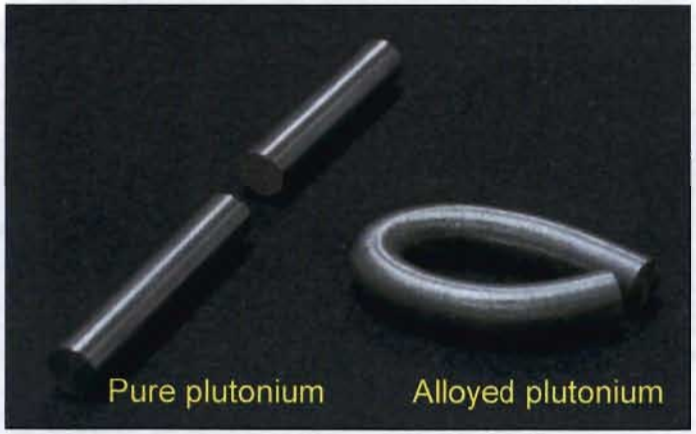
Ensuring a Safe, Secure and Reliable Nuclear Deterrence



Hydrodynamics: Turbulence



Proton Radiography: HE corner turning



Plutonium Science: Metallurgy

SPaSM on Roadrunner:
Materials dynamics in extreme conditions

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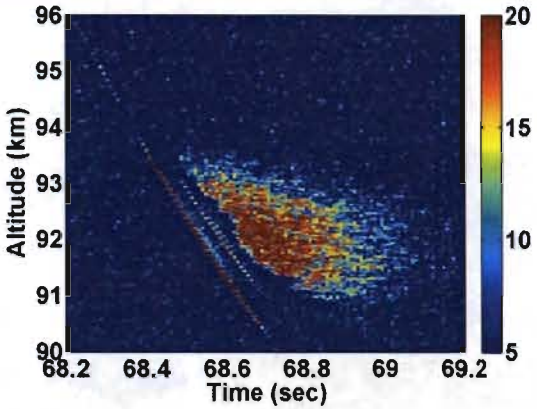
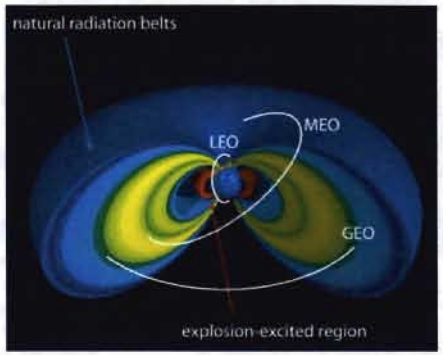
Mission: Science Questions

Science Questions for Global Security



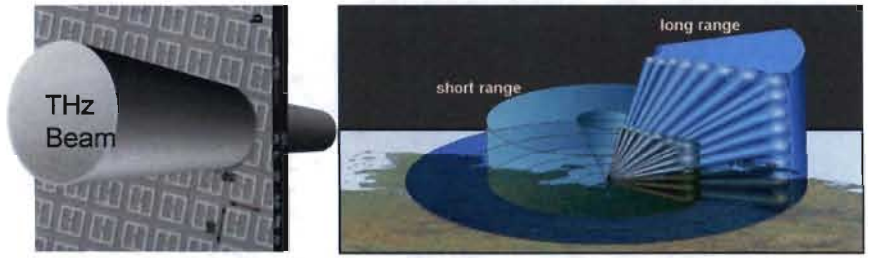
Large interstellar dust



DREAM: Dynamic Radiation Environment Assimilation Model

Actinide particle in soil

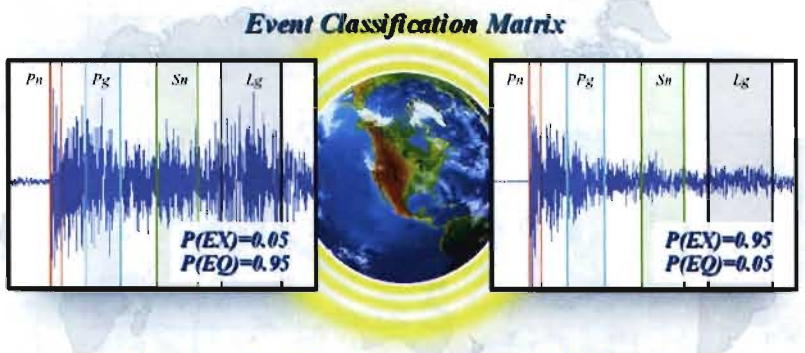
Space Situational Awareness: Threats from space



Terahertz metamaterials that modulate

Electrical and Optical Control of Materials

Nuclear Forensics: Identification & attribution



Seismic Detection of Nuclear Explosions

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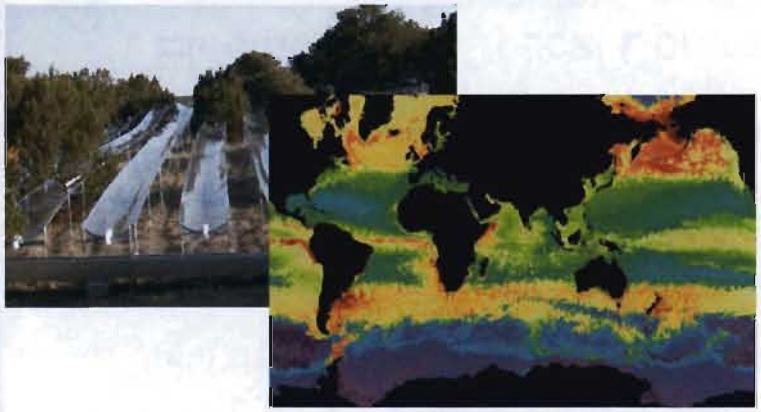
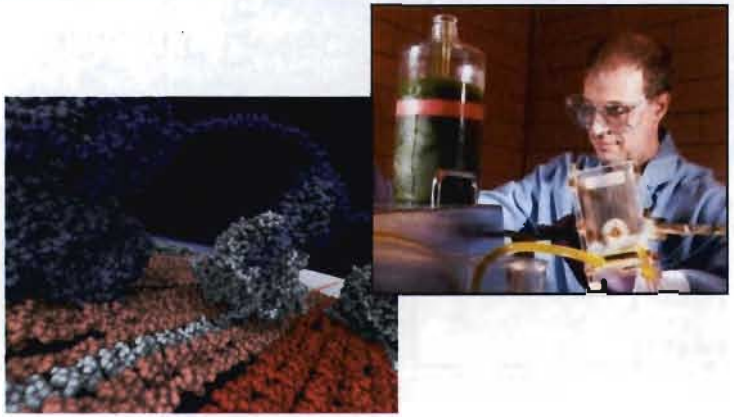
Mission: Science Questions

Questions for Science and Energy

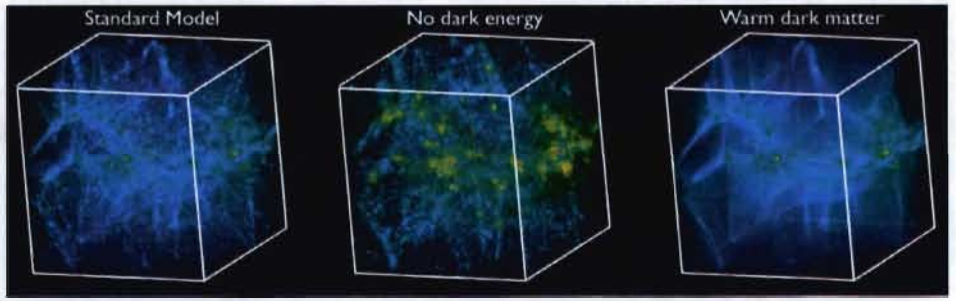


Climate / Energy Impacts:
Measurement, simulation, and prediction



Unconventional Fuels:
Extraction of energy

Theoretical Biology: HIV evolution
and design of "mosaic vaccines"



Simulating the universe on Roadrunner:
Interpreting the world's largest galaxy surveys

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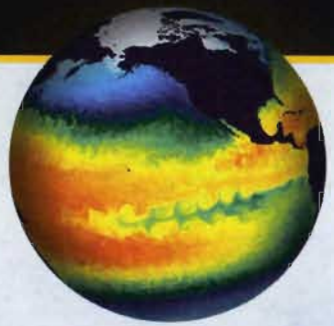
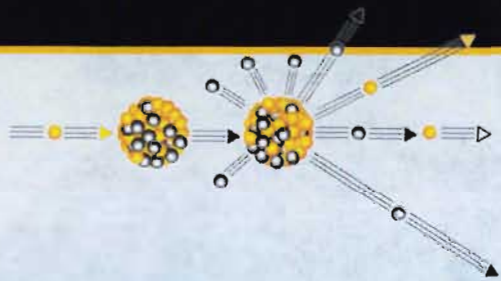
Energy

Los Alamos Energy Security Pillars



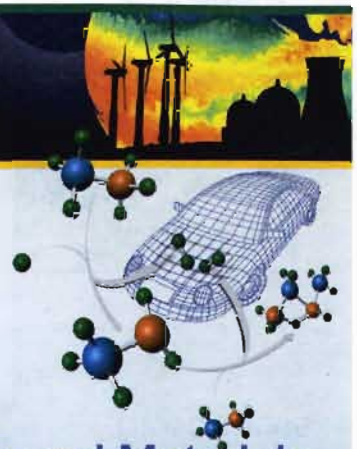
Impacts of Energy Demand Growth

- Coupled predictive models for climate, infrastructure impact analysis
- Prediction of abrupt change at multiple scales (regional to global)
- Global security and policy implications



Sustainable Nuclear Energy

- Efficient extraction of energy content from fuel
- Nonproliferation and safeguards
- Effective waste management



Concepts and Materials for Clean Energy

- Energy storage, generation, and transmission
- Revolutionary alternatives to petroleum
- Clean fossil energy

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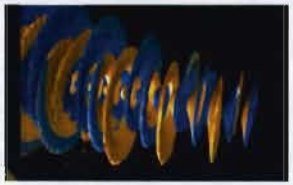
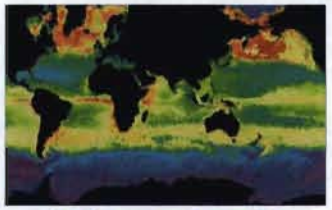
LANL's science capabilities support national security missions and national needs.



Computational Physics & Applied Mathematics

Accelerators & Electrodynamics



Information & Knowledge Science

Nuclear Physics, Astrophysics & Cosmology

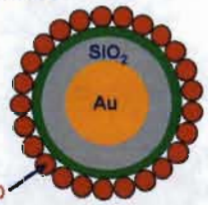
Weapons Science & Engineering

Sensors, Remote Sensing & Sensor Systems

Biosciences

Computer & Computational Sciences

High-Energy Density Plasmas & Fluids



Chemical Science

Materials

Nuclear Engineering and Technology

Earth & Space Sciences

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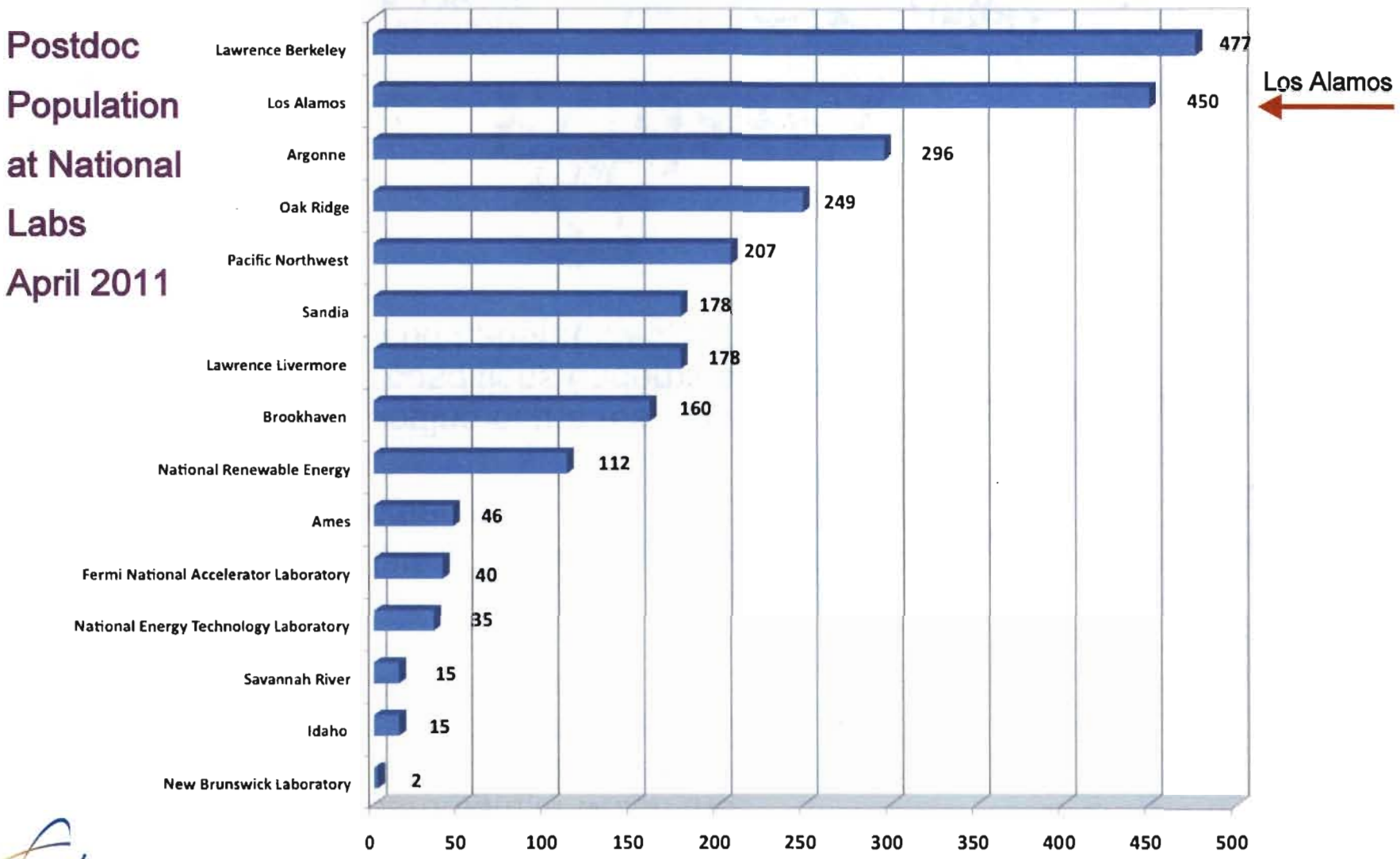
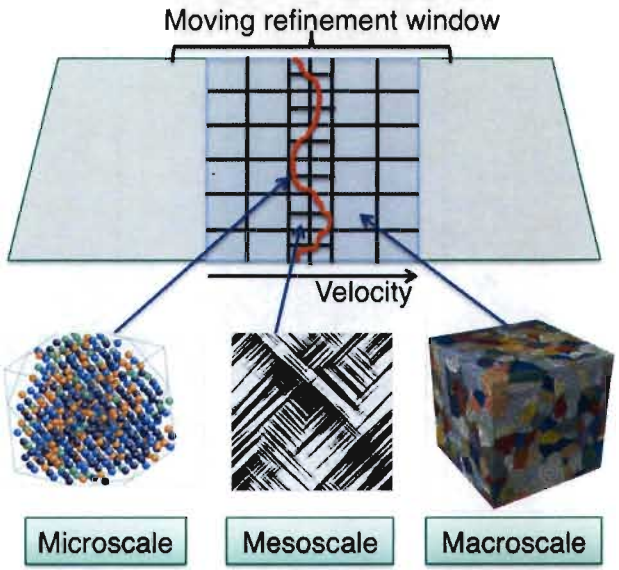
Los Alamos is a national leader for postdoc programs.



Exascale Co-Design Center for Materials

LANL leads the Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx)

- Co-design is a new paradigm in which the exascale hardware, system software, and application codes are concurrently designed to create the exascale simulation environment.
- Goal is to achieve more realistic large scale simulations of materials in extreme mechanical and radiation environments.
- A predictive understanding of the response of materials to extreme conditions underpins DOE and NNSA missions and Laboratory programs.



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Sandia National Laboratories

OAK RIDGE National Laboratory

ExMatEx

Massachusetts Institute of Technology

California Institute of Technology 1891

PRINCETON UNIVERSITY

Lawrence Livermore National Laboratory

CRAY THE SUPERCOMPUTER COMPANY

intel

STANFORD UNIVERSITY

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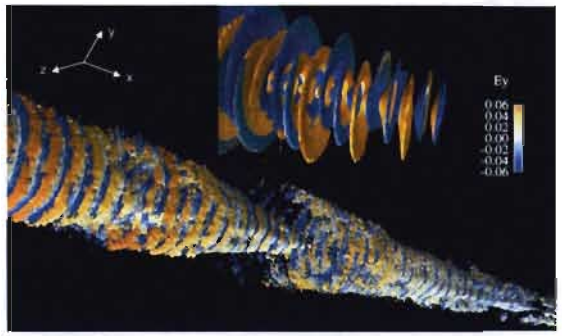
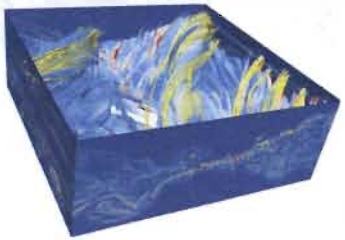
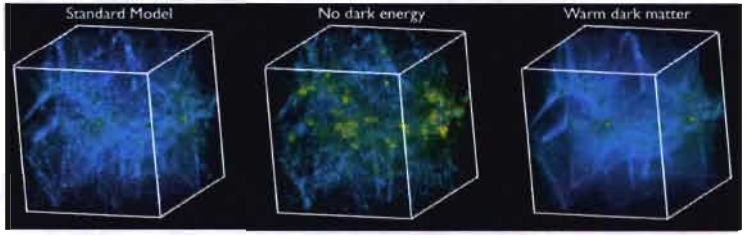
Tremendous science was accomplished with Roadrunner.



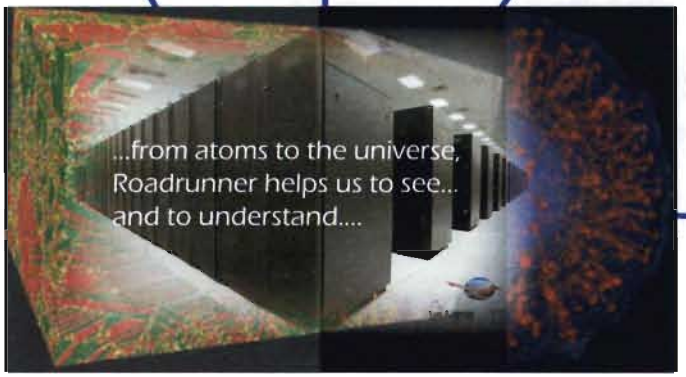
3D simulations show the nonlinearity of laser-plasma instability under NIF hohlraum plasma conditions.

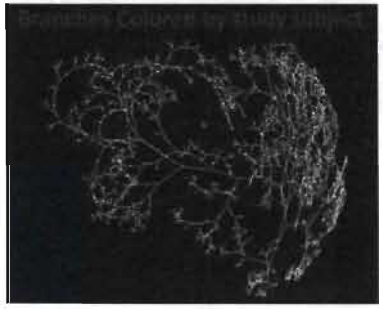


Development of turbulent reconnection in flux ropes



Roadrunner simulation of the universe guides the interpretation of the world's largest galaxy surveys.





Simulating the evolution of HIV virus assists vaccine design.

Molecular dynamics simulation enables understanding of how materials deform and fail, allowing better materials design and prediction of their lifetime.

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Now Roadrunner is a workhorse for classified simulations.

Climate modeling: global through regional scales

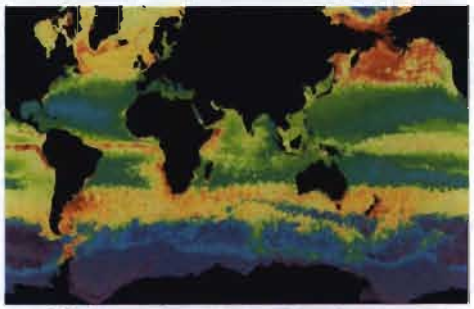
Global to regional scales

- Parallel Ocean Program (POP)
- New multi-scale ocean (MPAS-O)
- New multi-scale atmosphere (MPAS-A) with NCAR
- Los Alamos Sea Ice Model (CICE)
- Ice sheet model (Glimmer-CISM)
- Ocean, ice components of Community Climate System Model (NSF/DOE)
  - IPCC Assessments

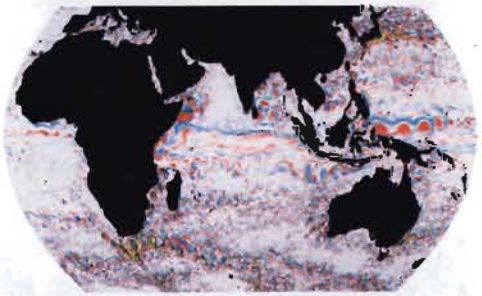
Regional to high resolution scales

- Weather Research and Forecasting (WRF)
- High resolution atmospheric fluid dynamics (HIGRAD)
- Cloud-aerosol and hurricane processes
- Hydrology and water resources
- Ecology and landscape processes

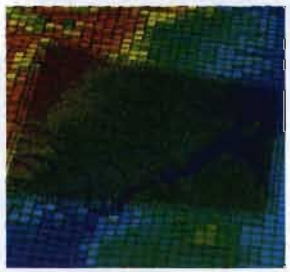
Knowledge of climate system is needed for future climate projection.



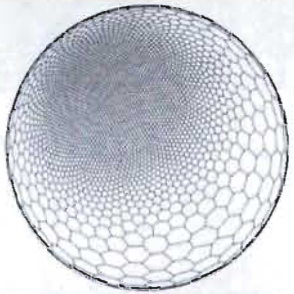
Chlorophyll concentration in the ocean



Ocean vorticity simulation



Hydrology



Model for Prediction Across Scales (MPAS)

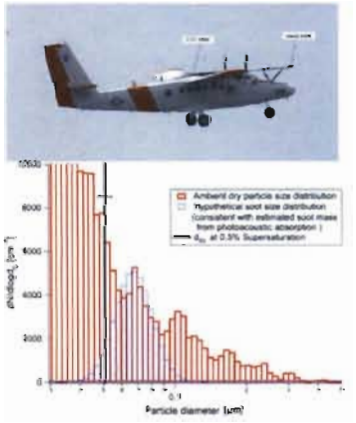
Energy Security

LANL's climate science addresses major issues.

From ecosystems … to regional atmosphere… to global ocean

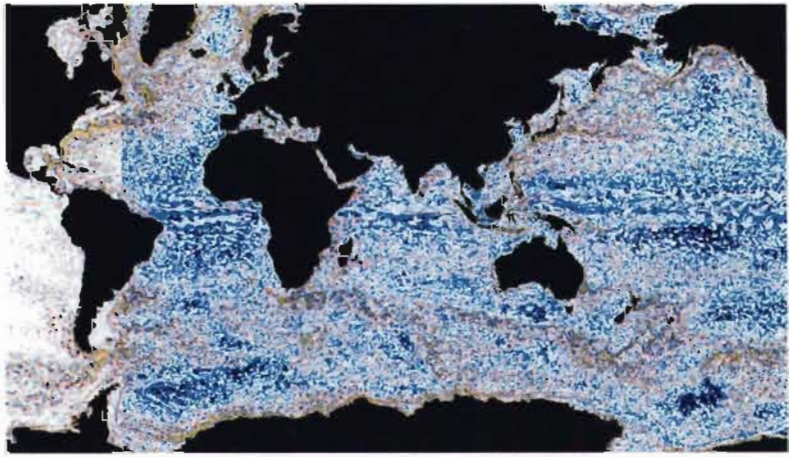
Climate-induced tree mortality

Measurement of climate change processes

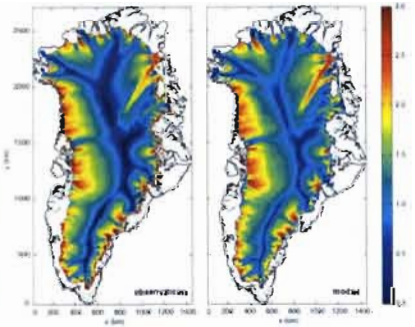


Aerosol (top) and cloud (bottom) property measurements

Coupled Ocean and Sea Ice Model (COSIM)



Vorticity from an eddy-resolving ocean simulation after 120 simulated years



Ice sheet dynamics

Linked, alternating pattern of warming trends in the Arctic and Antarctic (*Geophys Res Lett 2010*)