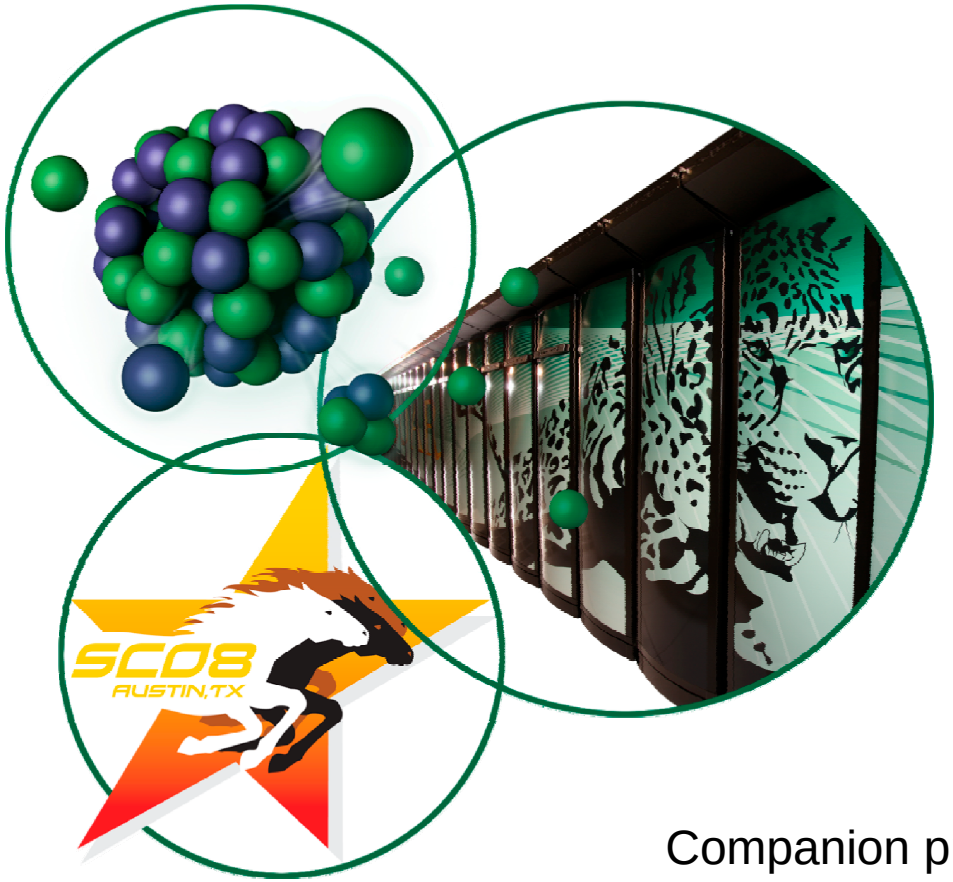
Overview of Science at the ORNL Leadership Computing Facility



Presented by

Douglas B. Kothe

National Center for Computational Sciences

Companion presentations:

"Breakthrough Science in the 2008 INCITE Program at ORNL"

"ORNL Leadership Computing Facility: Preparing for the Exascale"

Enabling breakthrough science

"But one thing is clear from an operational point of view, the Cray XT admin. team did a superb job, and the machine held up very well as we completed the [Q4 Joule] runs on the full system."

- Thomas Schulthess, ORNL

"These are large, demanding jobs. Our resource needs will only increase as we continue our transformation from code development to science."

- Mike Zingale, Stony Brook University

"The queuing policy in Jaguar allows our large simulations to run in a timely manner. The analysis capabilities have also been very valuable. [The NCCS liaison] has been extremely helpful."

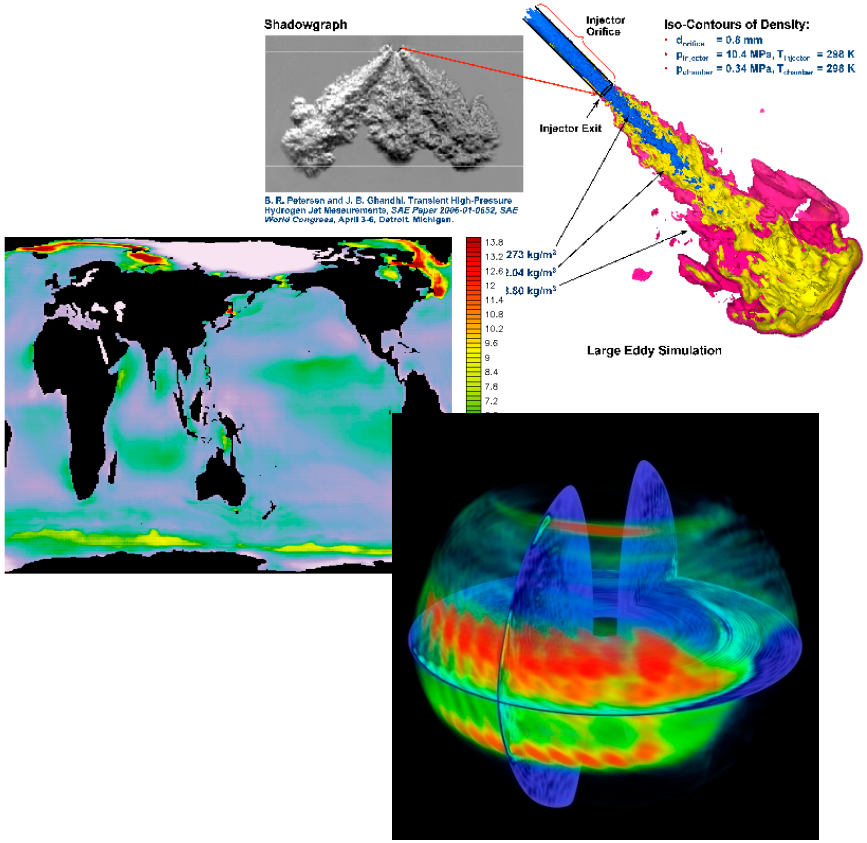
-Jeremy Smith, University of TN/ORNL

These are one-of-a kind simulations. There is nothing like them in the literature to date in terms of breadth and methodology."

-Chris Mundy, PNNL

"The support of the User Assistance Center is highly beneficial to our project. As an example, the support staff has allowed us to use queues that make the completion of our downscaling simulation much faster to produce results needed for a collaborative effort to assess climate change impacts."

- The WRF team, Climate End Station



"In comparison with other systems, we consider the LCF as one of the best. Support was always both beneficial and fast."

- Hermann Fasel, University of Arizona

"Our NCCS staff liaison has been extremely helpful and often proactive in helping us. When asked technical questions, he has always been very responsive. In fact, in all our interactions with NCCS staff, we have found them to be professional and courteous. We greatly appreciate their dedication to us."

- Robert Sugar, University of California−Santa Barbara

ORNL provides leadership computing to 2008 INCITE program

- The NCCS is providing leadership computing to 30 projects in 2008 under DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program
- Leading researchers from government, industry, and the academic world will use more than 75 million processor hours on the center's Cray leadership computers
- The center's Cray XT4 (Jaguar) and Cray X1E (Phoenix) systems provide more than 75% of the computing power allocated for the INCITE program

Project allocations: 145.3 million hours

Industrial allocations: 11.9 million hours

INCITE 2008 projects

Astrophysics

Multi-Dimensional Simulations of Core-Collapse Supernovae
Anthony Mezzacappa (Oak Ridge National Laboratory)

First Principles Models of Type Ia Supernovas
Stan Woosley (University of California−Santa Cruz)

Numerical Relativity Simulations of Binary Black Holes and Gravitational Radiation
Joan Centrella (National Aeronautics and Space Administration)

Biology

Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass
Jeremy Smith (Oak Ridge National Laboratory)

Gating Mechanism of Membrane Proteins
Benoit Roux (Argonne National Laboratory and University of Chicago)

Chemistry

Molecular Simulation of Complex Chemical Systems
Christopher Mundy (Pacific Northwest National Laboratory)

An Integrated Approach to the Rational Design of Chemical Catalysts
Robert Harrison (Oak Ridge National Laboratory)

Computer Science

Performance Evaluation & Analysis Consortium End Station
Patrick Worley (Oak Ridge National Laboratory)

Climate

The Role of Eddies in the Meridional Overturning Circulation
Paola Cessi (University of California−San Diego)

Assessing Global Climate Response of the NCAR-CCSM3: CO_2 Sensitivity and Abrupt Climate Change
Zhengyu Liu (University of Wisconsin−Madison)

Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean
Synte Peacock (ASC/Alliance Flash Center, University of Chicago)

Climate-Science Computational End Station Development and Grand Challenge Team
Warren Washington (National Center for Atmospheric Research)

Modeling Reactive Flows in Porous Media
Peter Lichtner (Los Alamos National Laboratory)

Engineering

High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels
Jacqueline Chen (Sandia National Laboratories)

Clean and Efficient Coal Gasifier Designs Using Large-Scale Simulations
Madhava Syamlal (National Energy Technology Laboratory)

Landmark Direct Numerical Simulations of Separation and Transition for Aerospace-Relevant Wall-Bounded Shear Flows
Hermann Fasel (University of Arizona)

INCITE 2008 projects (continued)

Fusion

Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas Patrick Diamond (University of California−San Diego)
Fluctuation Spectra and Anomalous Heating in Magnetized Plasma Turbulence William Dorland (University of Maryland)
Gyrokinetic Steady-State Transport Simulations Jeff Candy (General Atomics)
High-Power Electromagnetic Wave Heating in the ITER Burning Plasma Fred Jaeger (Oak Ridge National Laboratory)

Materials

Predictive and Accurate Monte Carlo-Based Simulations for Mott Insulators, Cuprate Superconductors, and Nanoscale Systems Thomas Schulthess (Oak Ridge National Laboratory)
Electronic, Lattice, and Mechanical Properties of Novel Nanostructured Bulk Materials Jihui Yang (GM R&D Center)
Development and Correlations of Large-Scale Computational Tools for Flight Vehicles Moeljo Hong (The Boeing Company)

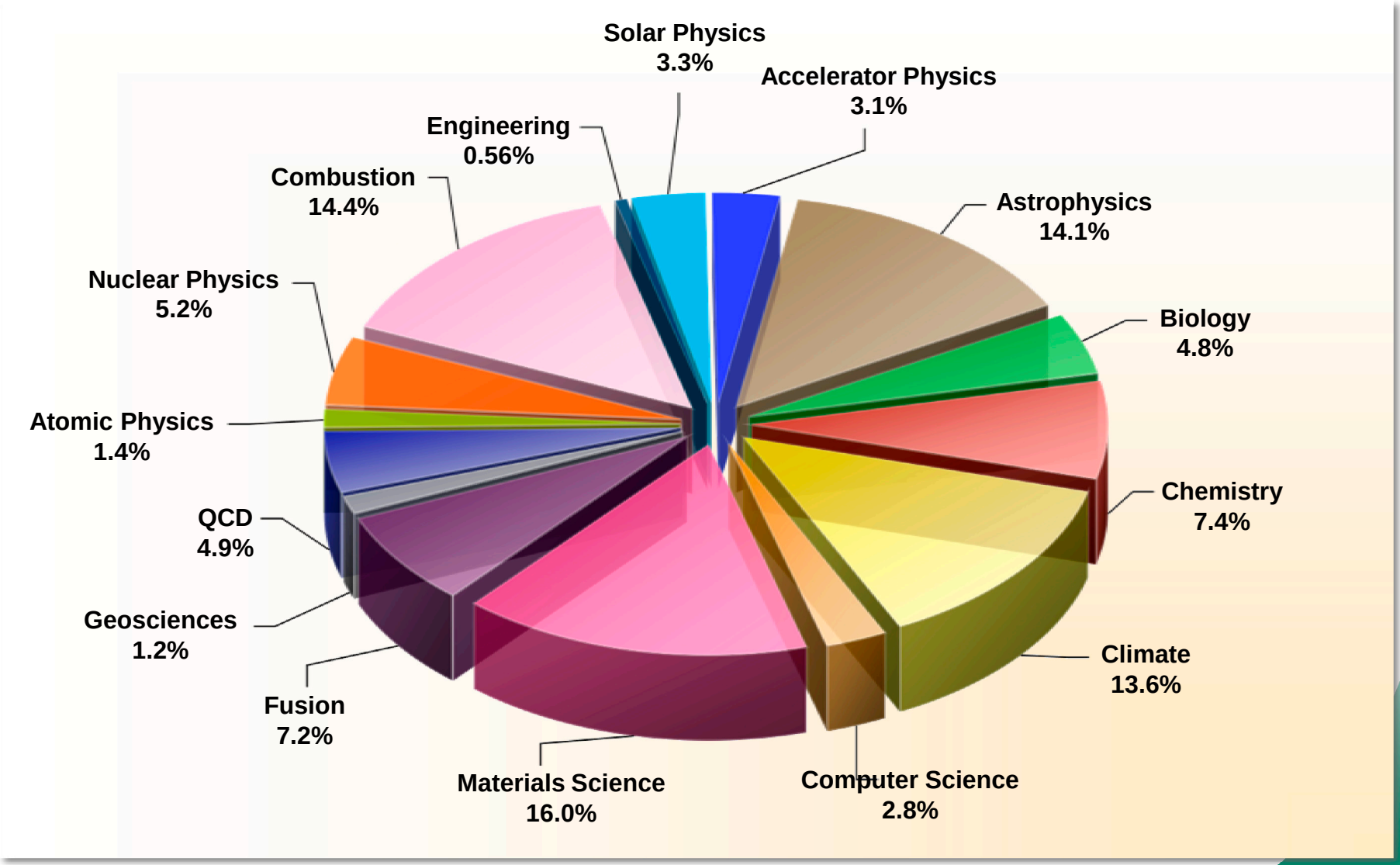
Materials (continued)

Bose-Einstein Condensation vs. Quantum Localization in Quantum Magnets Tommaso Roscilde (Max-Planck -Gesellschaft)
Linear-Scale Electronic Structure Calculations for Nanostructures Lin-Wang Wang (Lawrence Berkeley National Laboratory)

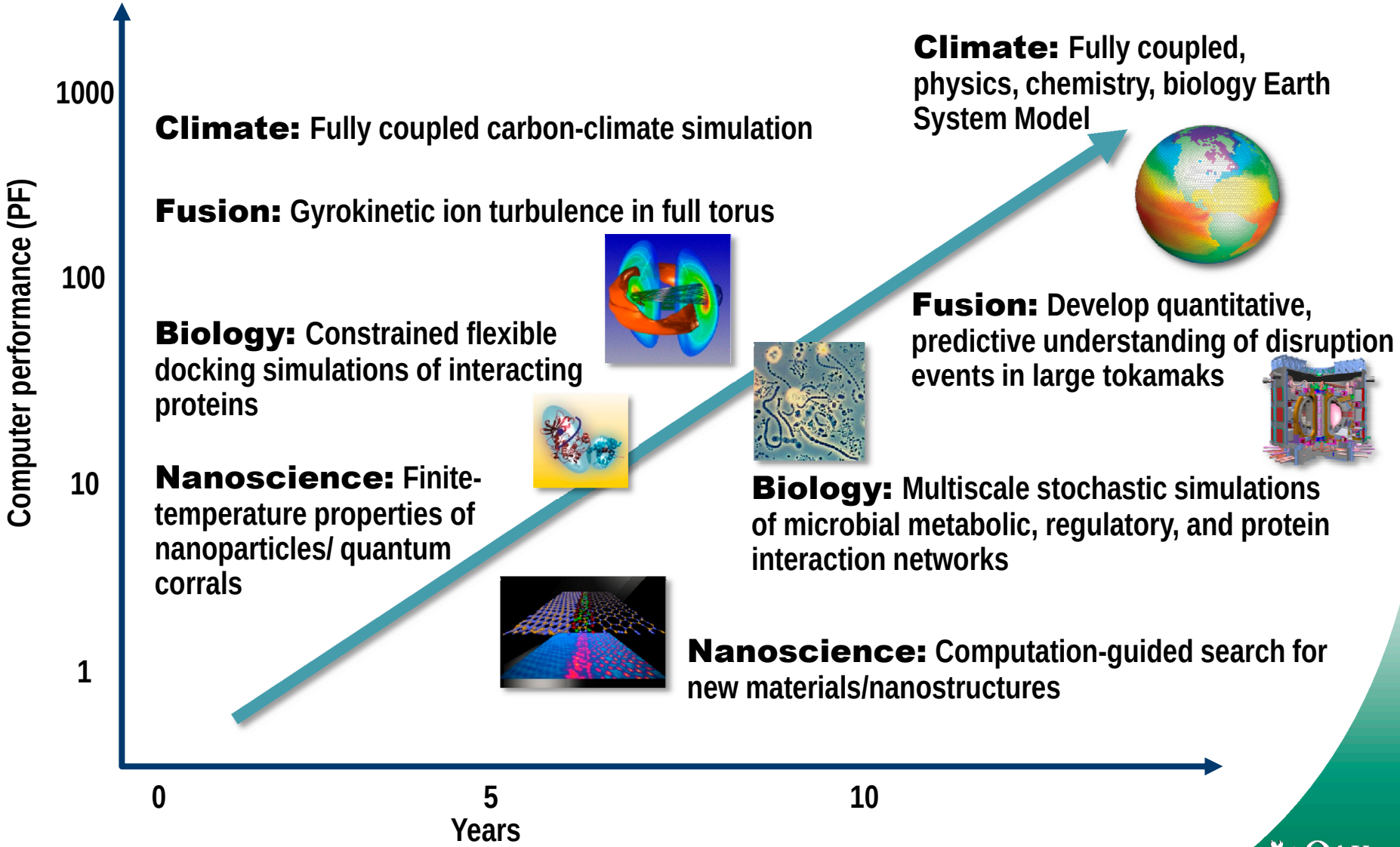
Physics

Computational Nuclear Structure David J. Dean (Oak Ridge National Laboratory)
Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling Lie-Quan Lee (Stanford Linear Accelerator Center)
Lattice QCD Robert Sugar (University of California−Santa Barbara)
Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences, and Fusion Energy Sciences Michael Pindzola (Auburn University)
Modeling Heliospheric Phenomena with an Adaptive, MHD-Boltzmann Code Nikolai Pogorelov (University of California−Riverside)

INCITE 2008 allocations by discipline at ORNL

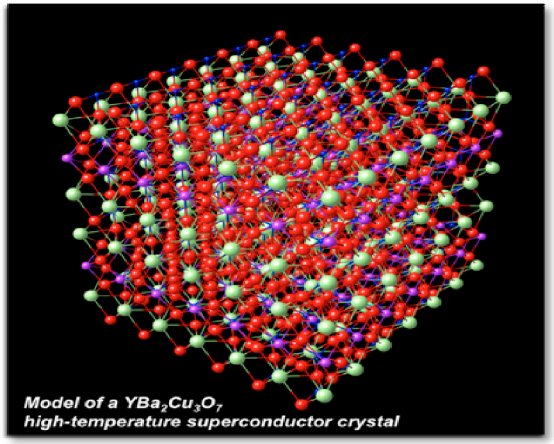


Science advances over the next decade require leadership computing

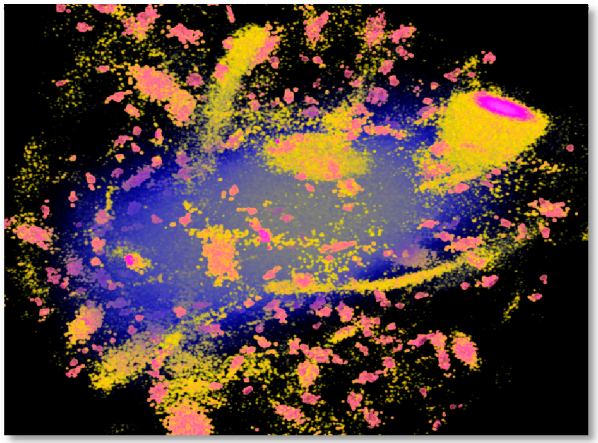


Advancing scientific discovery

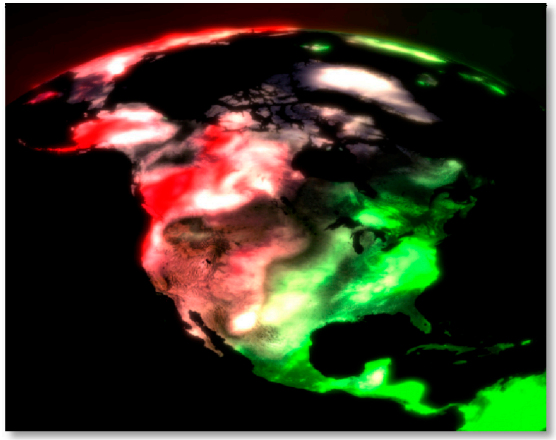
Five of the top 10 ASCR science accomplishments over the past 18 months used ORNL LCF resources and staff



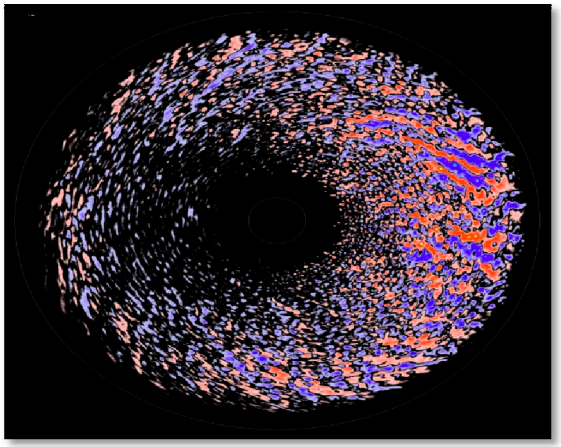
Electron pairing in HTC cuprates*
The 2D Hubbard Model emits a superconducting state for cuprates and exhibits an electron pairing mechanism most likely caused by spin-fluctuation exchange. *PRL* (2007, 2008)



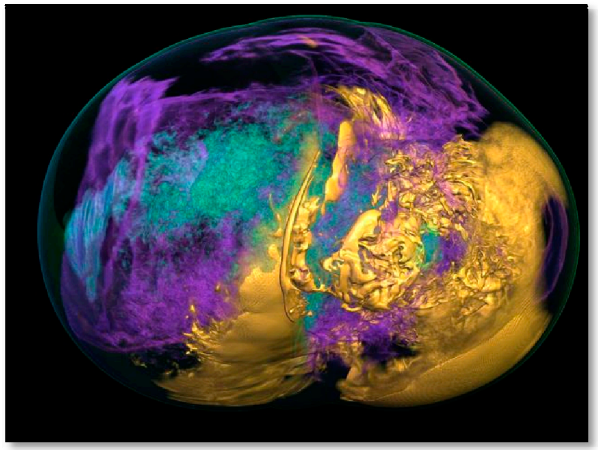
Shining the light on dark matter*
A glimpse into the invisible world of dark matter, finding that dark matter evolving in a galaxy such as our Milky Way remains identifiable and clumpy. Upcoming issue of *Nature*



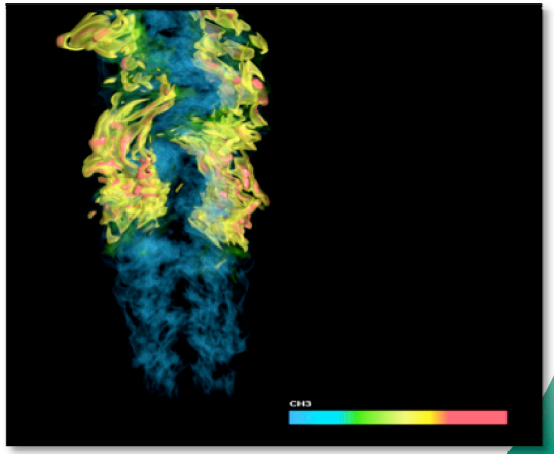
Modeling the full Earth system
Simulated time evolution of the atmospheric CO_2 concentration originating from the land's surface



Taming turbulent heat loss in fusion reactors*
Advanced understanding of energy loss in tokamak fusion reactor plasmas. *PRL* (**99**) and *Physics of Plasmas* (**14**)



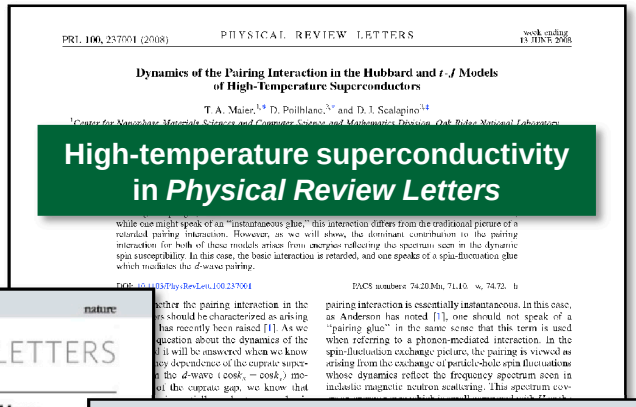
How does a pulsar get its spin?*
Discovery of the first plausible mechanism for a pulsar's spin that fits observations, namely the shock wave created when the star's massive iron core collapses.
Jan 4 2007 issue of *Nature*



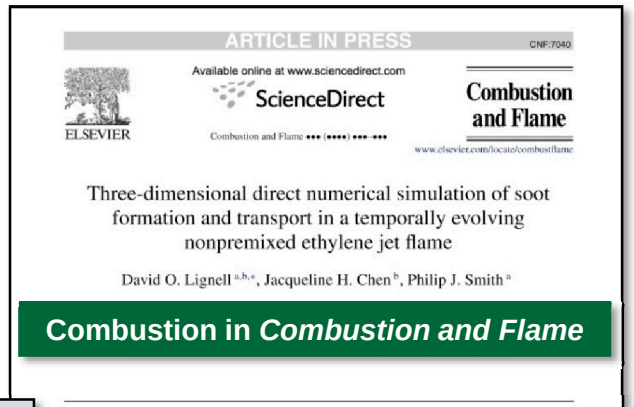
Stabilizing a lifted flame*
Elucidation of the mechanisms that allow a flame to burn stably above burners, namely increasing the fuel or surrounding air co-flow velocity
Combustion and Flame (2008)

*Used ORNL LCF computers

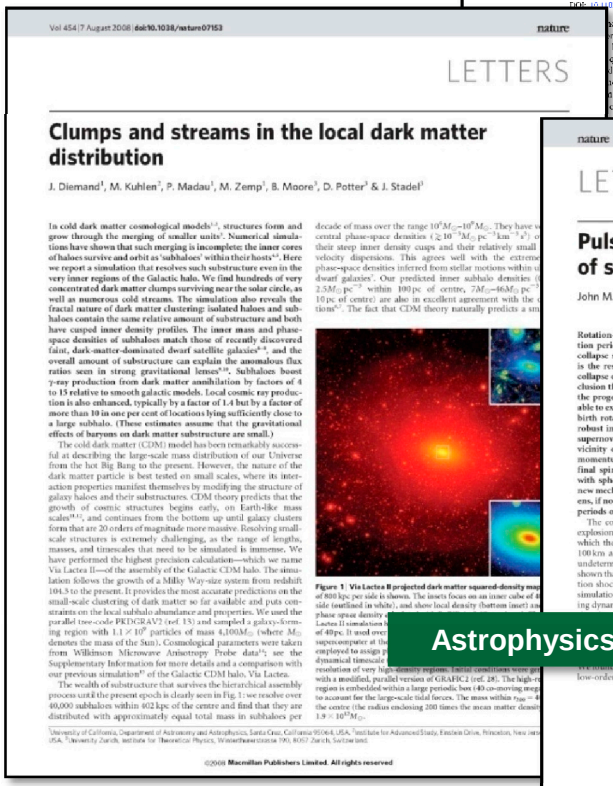
Recent and highly visible science output at the ORNL LCF

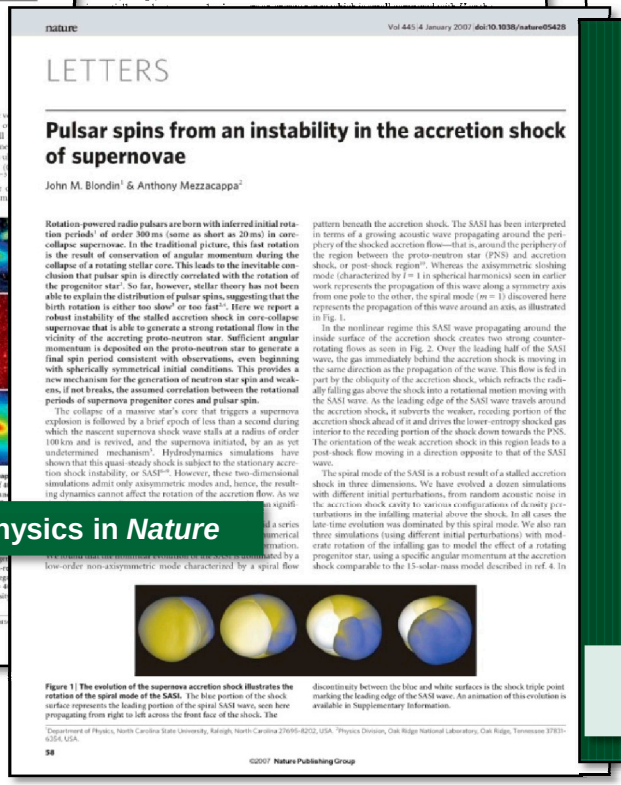


High-temperature superconductivity in *Physical Review Letters*

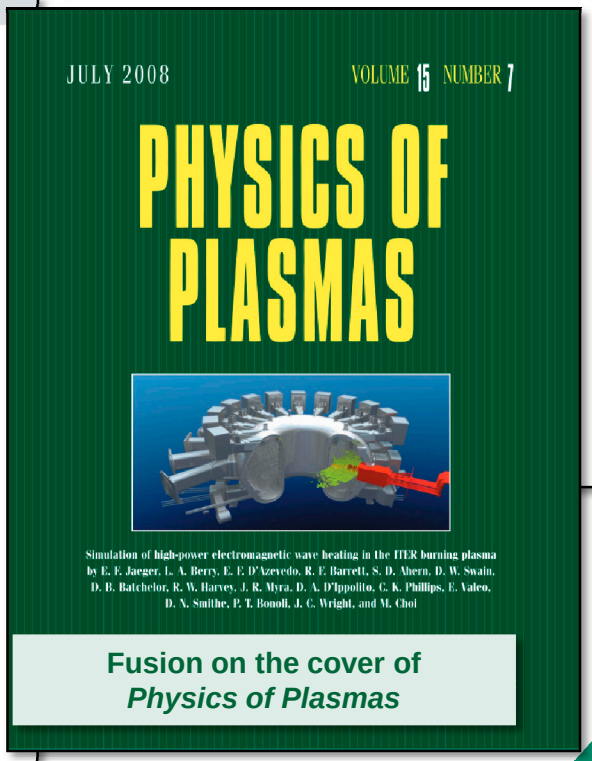


Combustion in *Combustion and Flame*





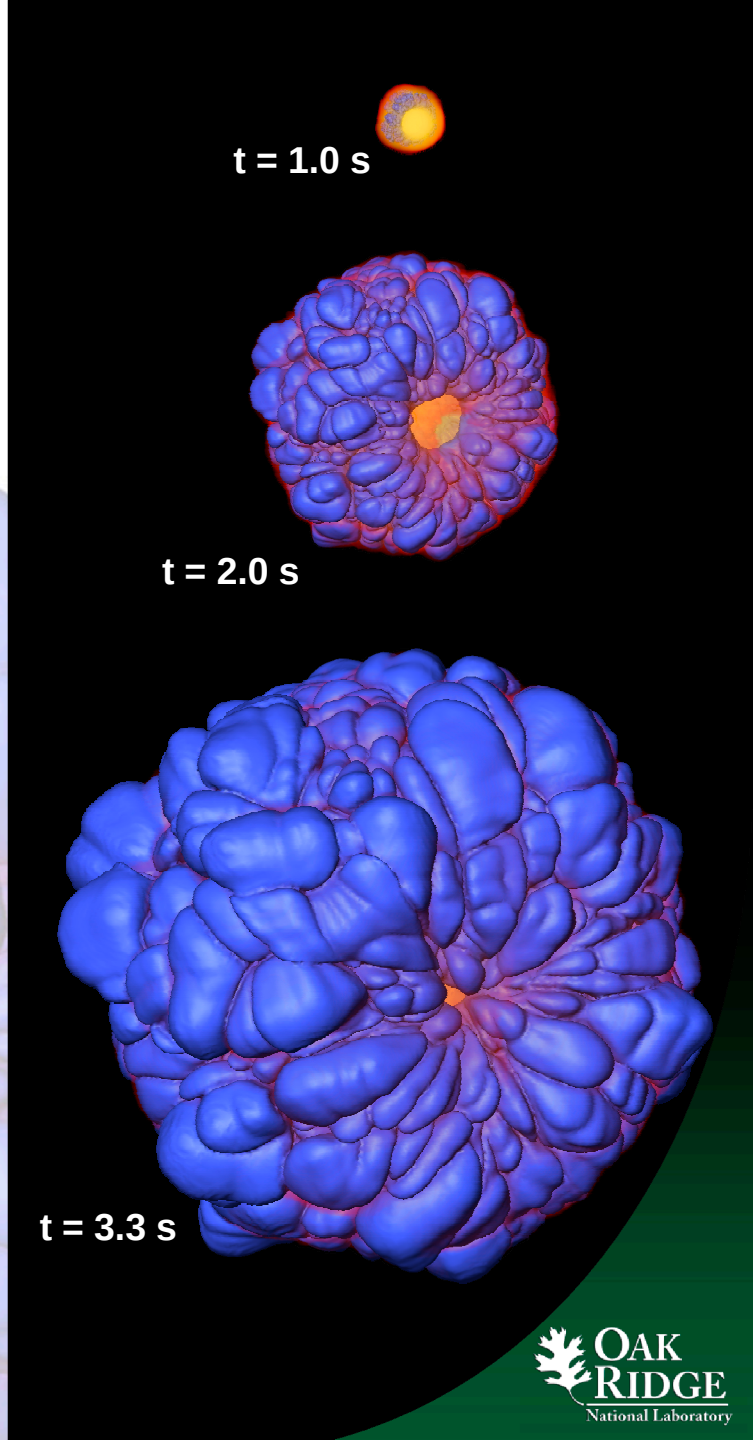
Astrophysics in *Nature*



Fusion on the cover of *Physics of Plasmas*

Creating Type Ia supernova simulations

What begins with a millimeter-sized flame can spark questions that span the universe. Unparalleled computer resources at Oak Ridge National Laboratory enable researchers to span the gap between pencil-sized objects and supernovas

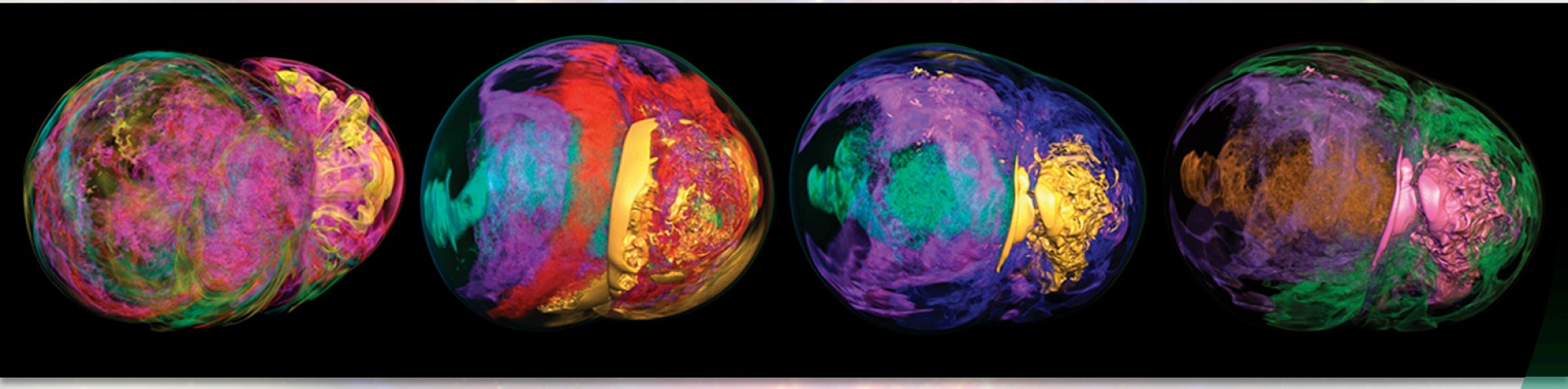


3D thermonuclear supernova model ignited in a bubble 200 km off center

PI: Stan Woosley
University of California –Santa Cruz

Charting the death of massive stars

Understanding the processes behind the explosions of massive stars into supernovas provides insight into how the universe behaves. Supernovas disperse the elements that make up our world and account for baffling phenomena such as black holes and gravitational waves. Three-dimensional simulations at ORNL are providing insights into the mechanisms of supernova creation

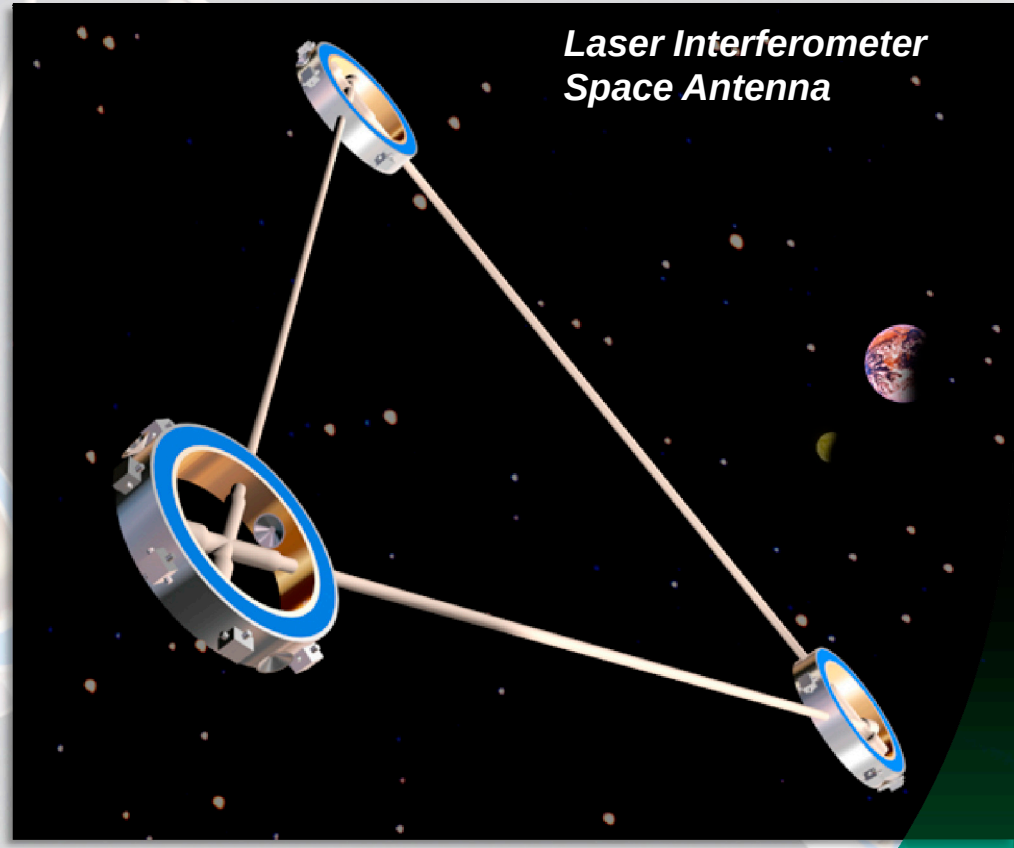


Volume-rendered sequence of the development of the stationary accretion shock instability in a 3D simulation

PI: Anthony Mezzacappa
Oak Ridge National Laboratory

Investigating binary black holes

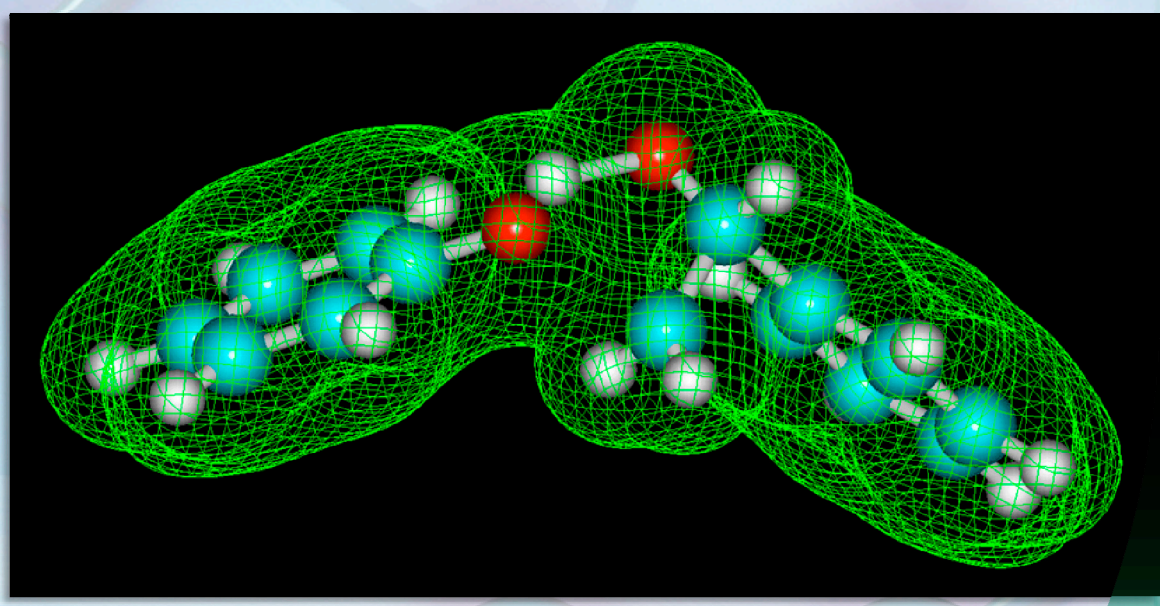
The Laser Interferometer Space Antenna (LISA) is a space-based observatory that will detect and analyze gravitational waves produced when two massive black holes meet and merge. These waves—the most powerful bursts of energy in the universe—can help astrophysicists answer basic questions about gravity, probe the nature of black holes, and explore the evolution of the universe



PI: Joan Centrella
NASA Goddard Space Flight Center

Toward the rational design of chemical catalysts

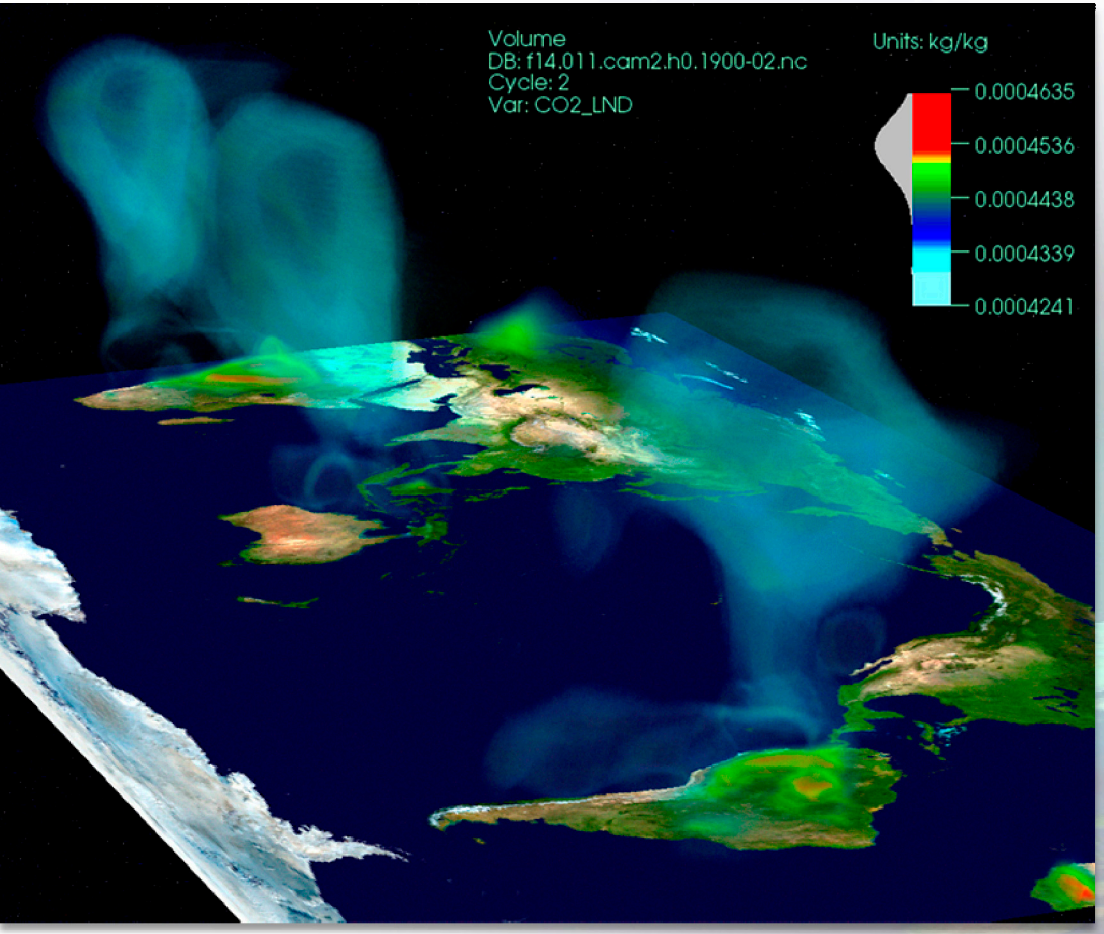
Catalytic processes are directly involved in the synthesis of 20% of all industrial products. Within the DOE mission, catalysts feature prominently in cleaner and more efficient energy production. Understanding and controlling the structures, interactions, and reactions of molecules are of critical importance to a wide range of phenomena, from the fate of contaminants in the environment to the treatment of genetic diseases



Green mesh surrounding constituent atoms in this molecule show results of electron interaction

PI: Robert Harrison
Oak Ridge National Laboratory and University of Tennessee

Forecasting climate change

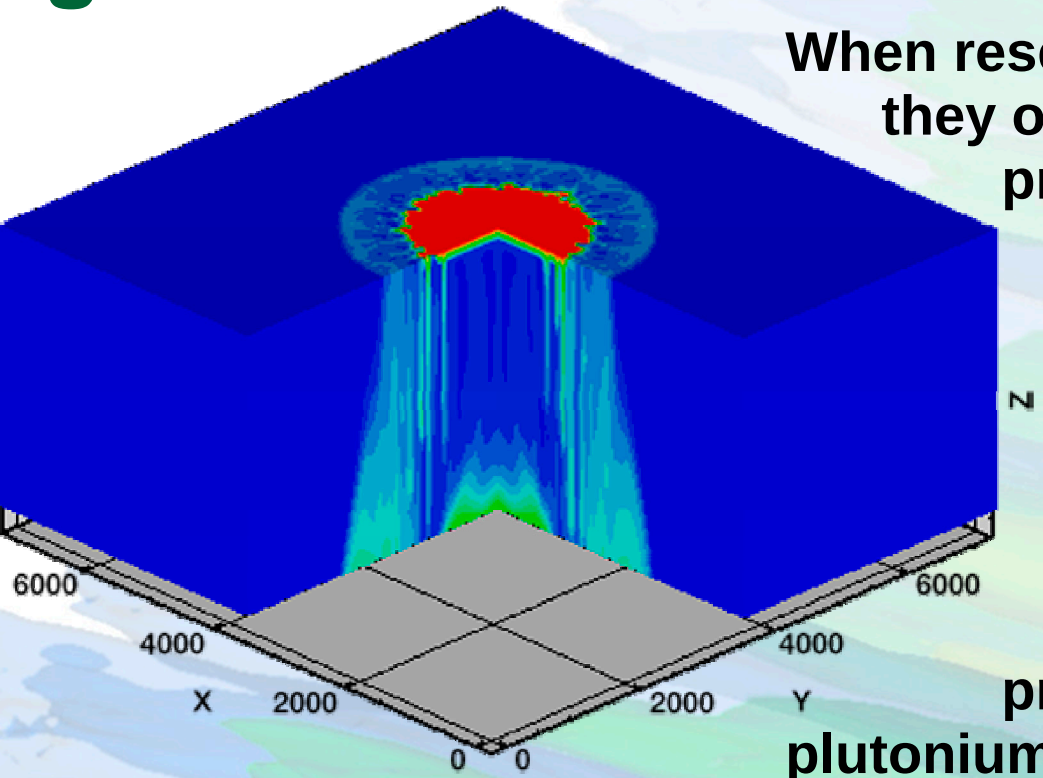


Carbon Land Model Intercomparison (C-LAMP) results showing CO_2 plumes from land due to respiration

PI: Warren Washington
National Center for Atmospheric Research

Upgrading and maintaining the Community Climate Systems Model will aid in its mission of assessing the risk of human-induced climate change. The new model will incorporate the most recent atmospheric, oceanic, and ice data, as well as improved chemistry, biology, and physics and have the resolution capacity necessary to allow for conjectures about regional climate change, a capability that until now has been limited by inadequate computational resources

Modeling uranium transport in groundwater



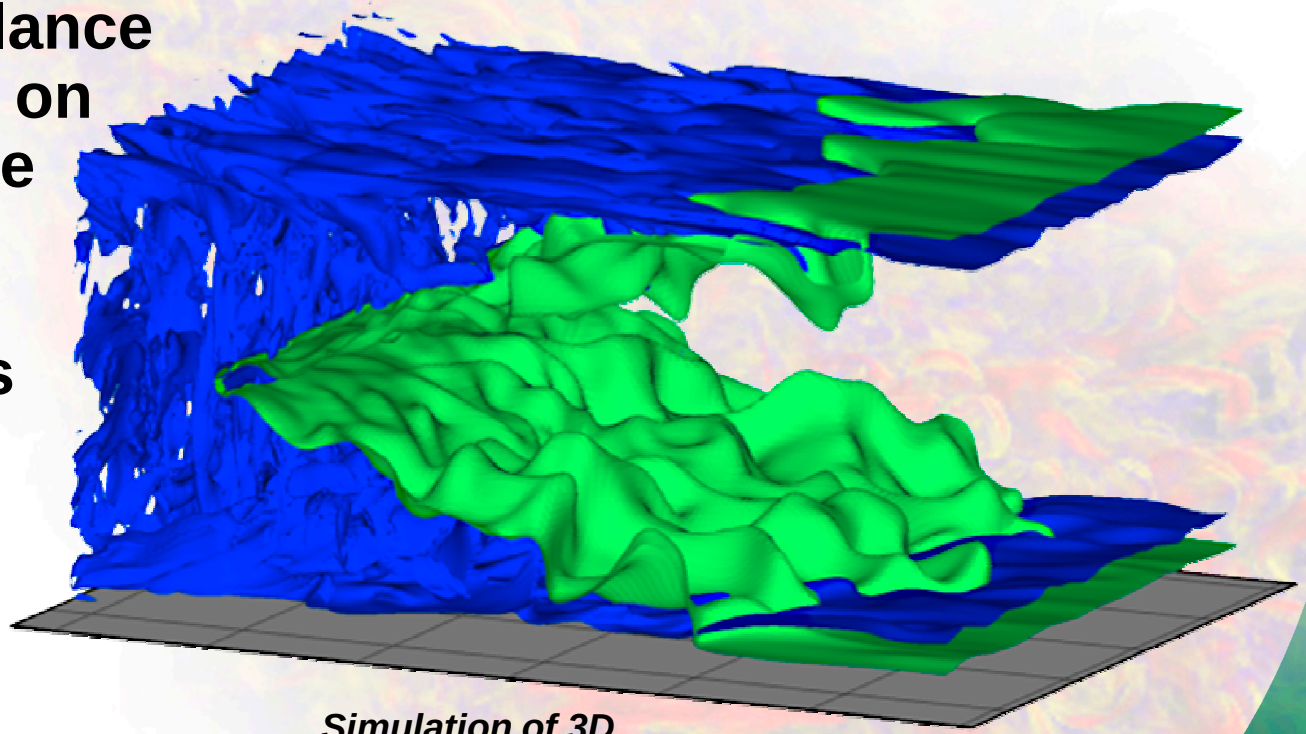
Researchers explore the storage of carbon dioxide in groundwater as a means of removing greenhouse gases from the atmosphere

When researchers model groundwater, they often use supercomputers to predict and simulate aquifer conditions. In this case, researchers are modeling the effects of uranium leakage over time from the Hanford Site in south-central Washington, a U.S. government facility previously used to produce plutonium for nuclear weapons. No longer active, it is now the site of one of the world's largest environmental cleanups

PI: Paul Lichtner
Los Alamos National Laboratory

Understanding turbulent combustion

Optimizing the design of practical combustion devices is of critical importance to the entire world. More efficient and economically feasible combustion devices are needed to balance U.S. dependence on foreign oil and the instability of the Middle East with our energy needs

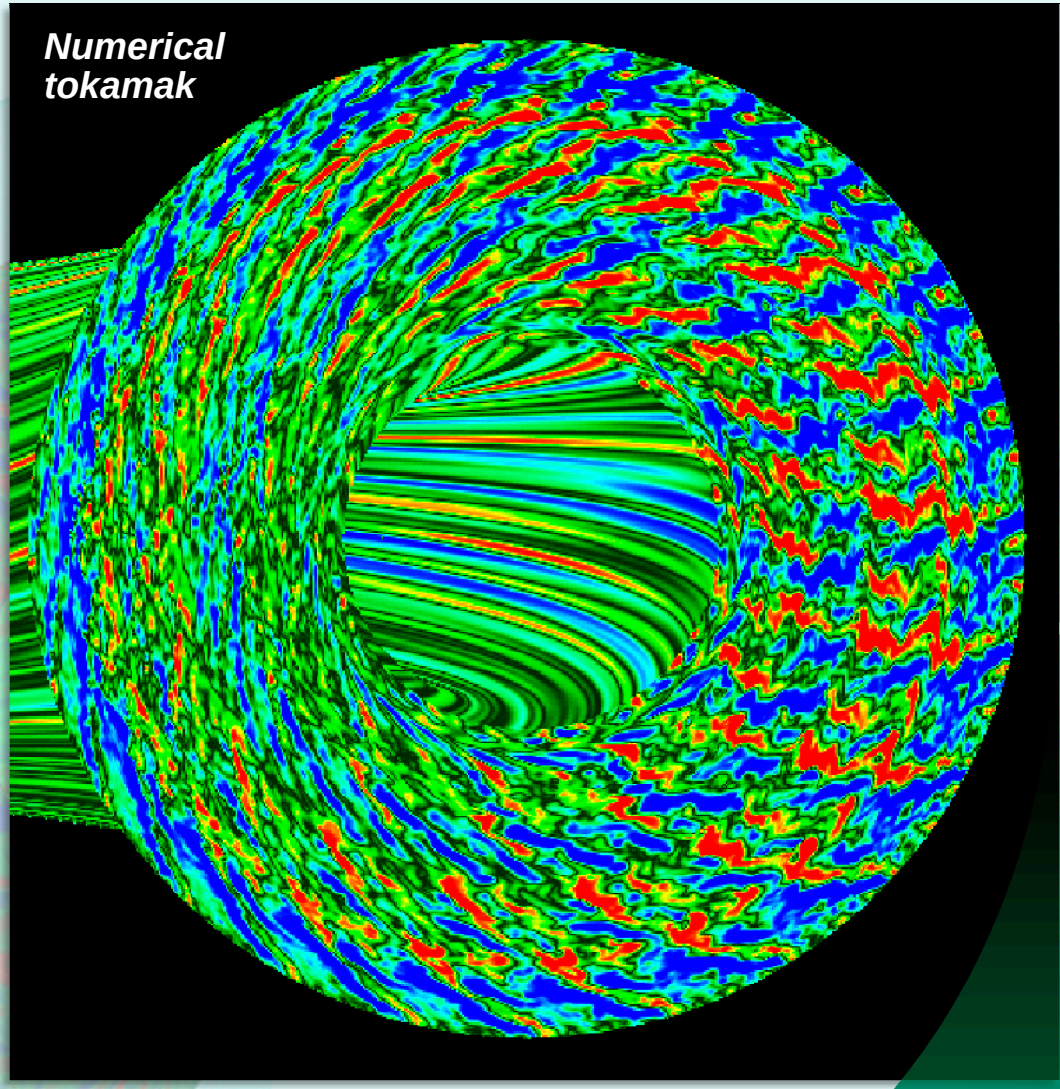


Simulation of 3D turbulence and complex chemistry

PI: Jacqueline Chen
Sandia National Laboratories

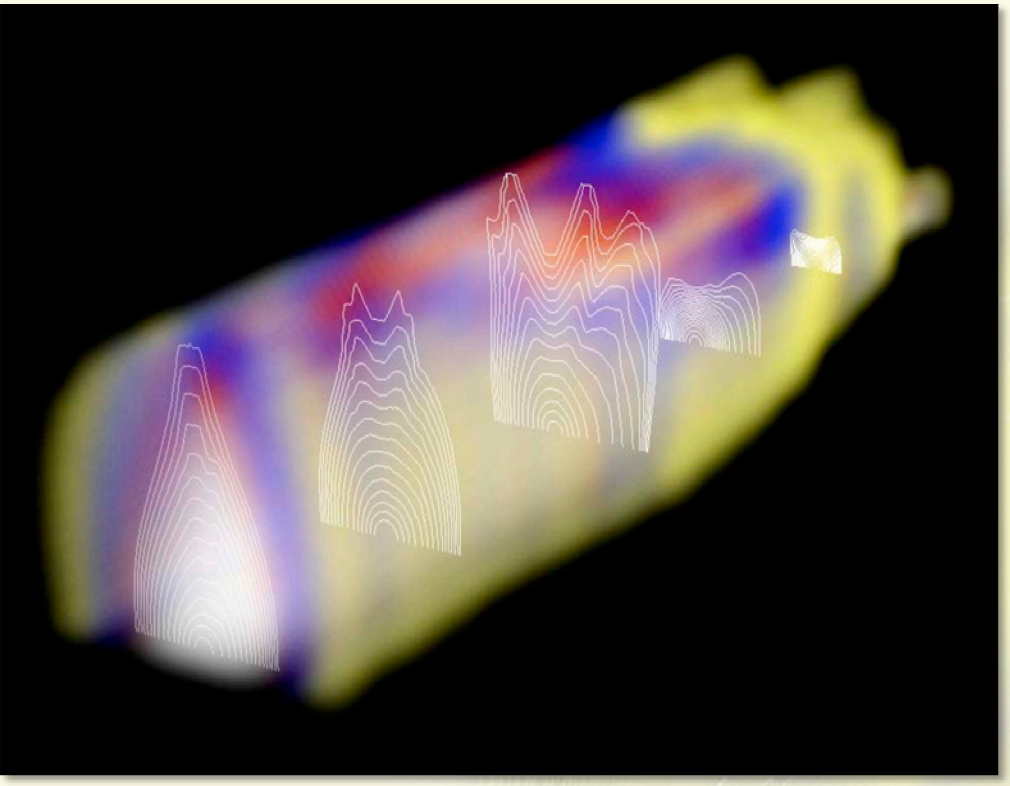
Solving the riddles of fusion power production

Researchers are trying to find a better way to manage heat and particle loss in a tokamak reactor. If successful, the world could one day have a more abundant, cleaner energy source with virtually no waste and almost zero risk of a nuclear accidnent



PI: Jeff Candy
General Atomics

Electromagnetic wave heating in fusion plasmas



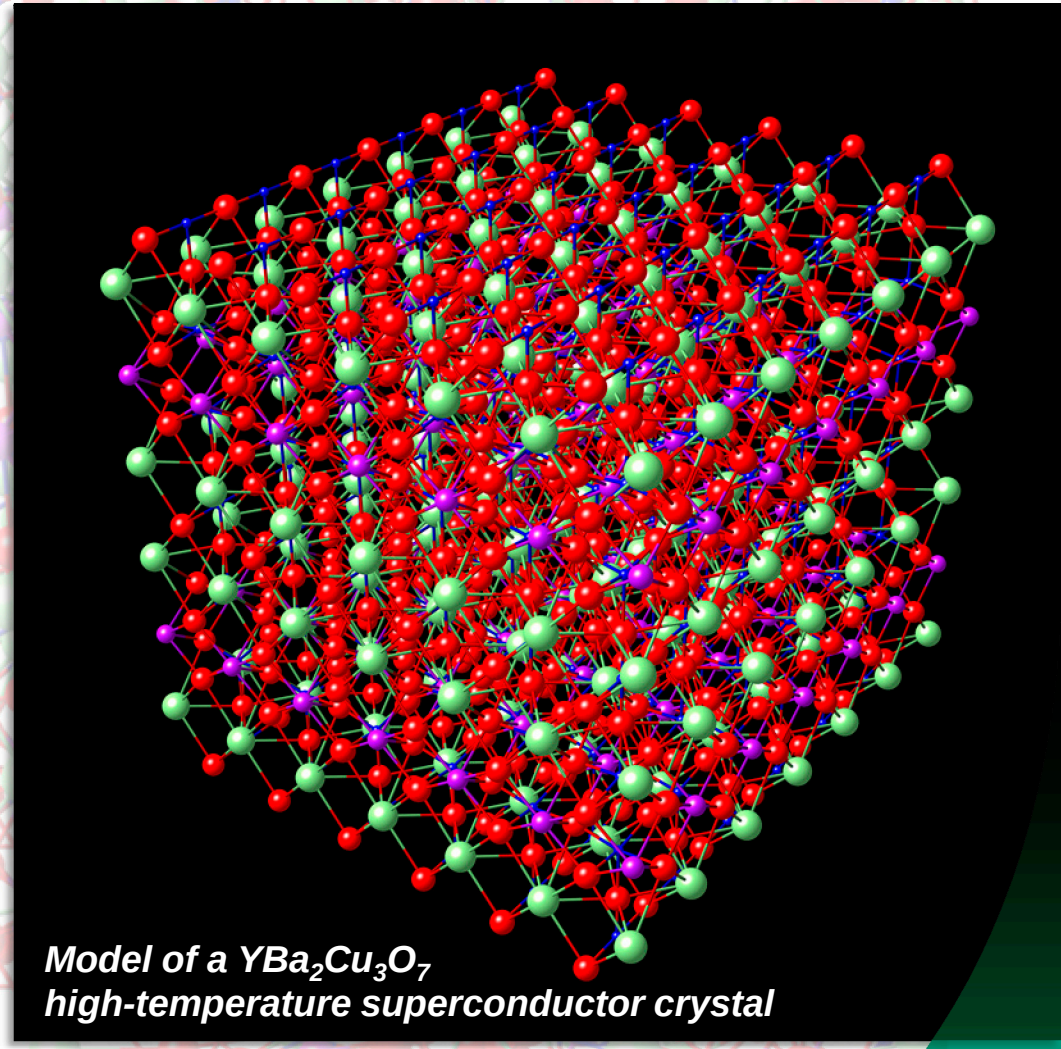
Bounce-averaged velocity distribution function for ions in a tokamak plasma

The production of energy by means of a fusion reaction could one day supply the world with a much cleaner, more abundant energy source. High-power electromagnetic waves in the radio-frequency range have shown great potential in managing plasma heat and behavior, possibly bringing this revolutionary technology one step closer to reality

PI: Fred Jaeger
Oak Ridge National Laboratory

Designing advanced materials

Every technological field benefits from progress in materials research. This team is performing high-power computational simulations to aid in the development of classes of advanced materials that will affect daily life in significant ways, such as revolutionizing electrical power systems with high temperature supercnductors

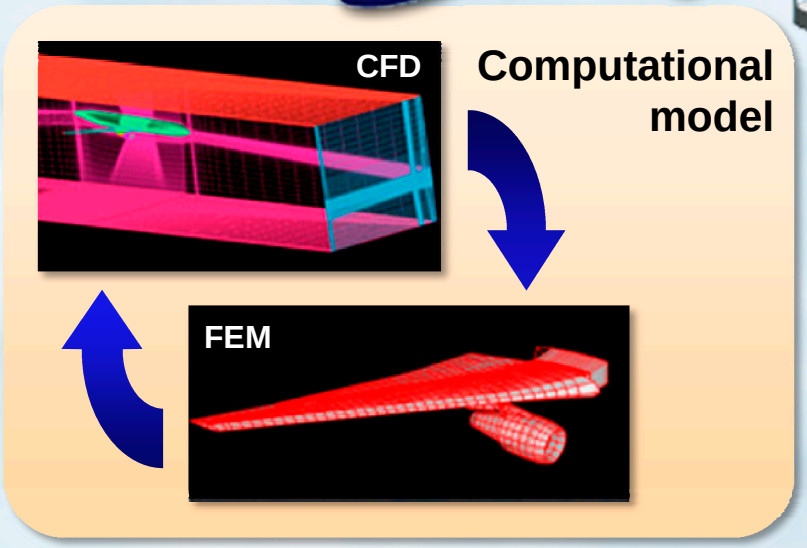


Model of a $YBa_2Cu_3O_7$ high-temperature superconductor crystal

PI: Thomas Schulthess
Oak Ridge National Laboratory

Developing and correlating large-scale computational tools for flight vehicles

Computational development and correlations/validations of large-scale computational tools for flight vehicles will give industry a better understanding of aerodynamics, help prevent unnecessary maintenance, and allow for more aggressive designs



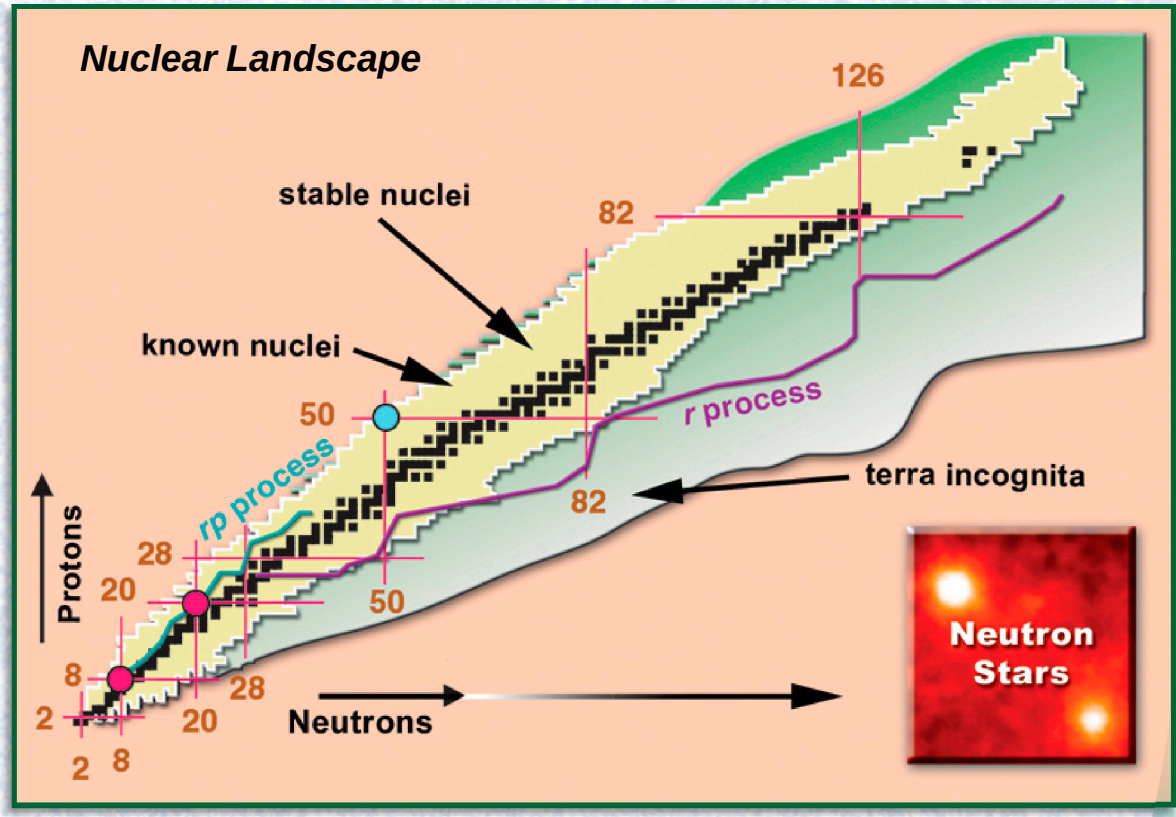
Static aeroelastic modeling

PI: Moeljo Hong
The Boeing Company

OAK RIDGE National Laboratory

Building nuclei from the ground up

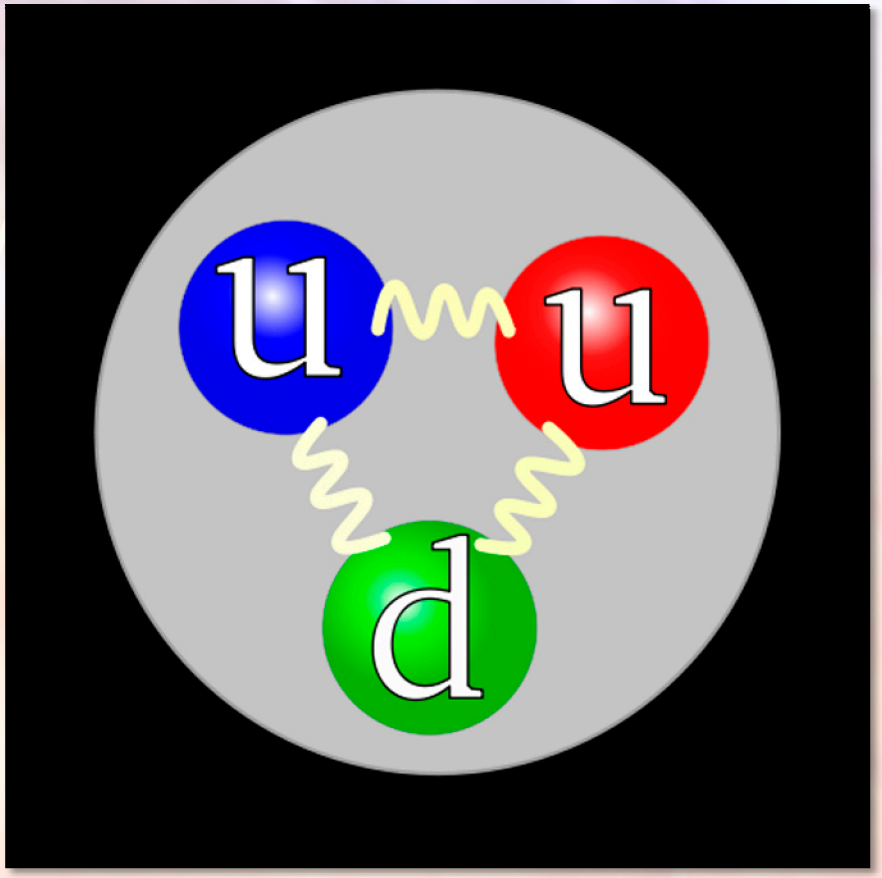
Researchers are undertaking the ambitious task of arranging the microscopic nuclear physics of the atom into a theoretical model that accurately predicts the mass, shape, size, and basic energy spectrum of intermediate-mass elements such as oxygen and calcium.



This model will help us to better understand the processes by which stars burn and how the elements in our universe were formed

PI: David J. Dean
Oak Ridge National Laboratory

Lattice QCD for hadronic and nuclear physics



Only the most powerful computers can tease apart the "color" interactions between quarks and gluons, the building blocks of atomic nuclei

Quark structure of a proton

PI: Robert Sugar
University of California –Santa Barbara

Contact

Douglas B. Kothe

Director of Science
National Center for Computational Sciences
(865) 241-9392
Kothe@ornl.gov

For a detailed list of science achievements, see the companion presentation "Breakthrough Science in the 2008 INCITE Program at ORNL"