INCITE at NERSC

Innovative and Novel Computational Impact on Theory and Experiment

BERKELEY LAB

The U.S. Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program provides computational support for a small number of computationally intensive large-scale research projects that make high-impact scientific advances through the use of a substantial allocation of computing and data storage resources at the NERSC Center.

In 2005, the second year of the INCITE program, three projects were awarded 6.5 million processor hours on Seaborg, NERSC's 6,652-processors IBM supercomputer.

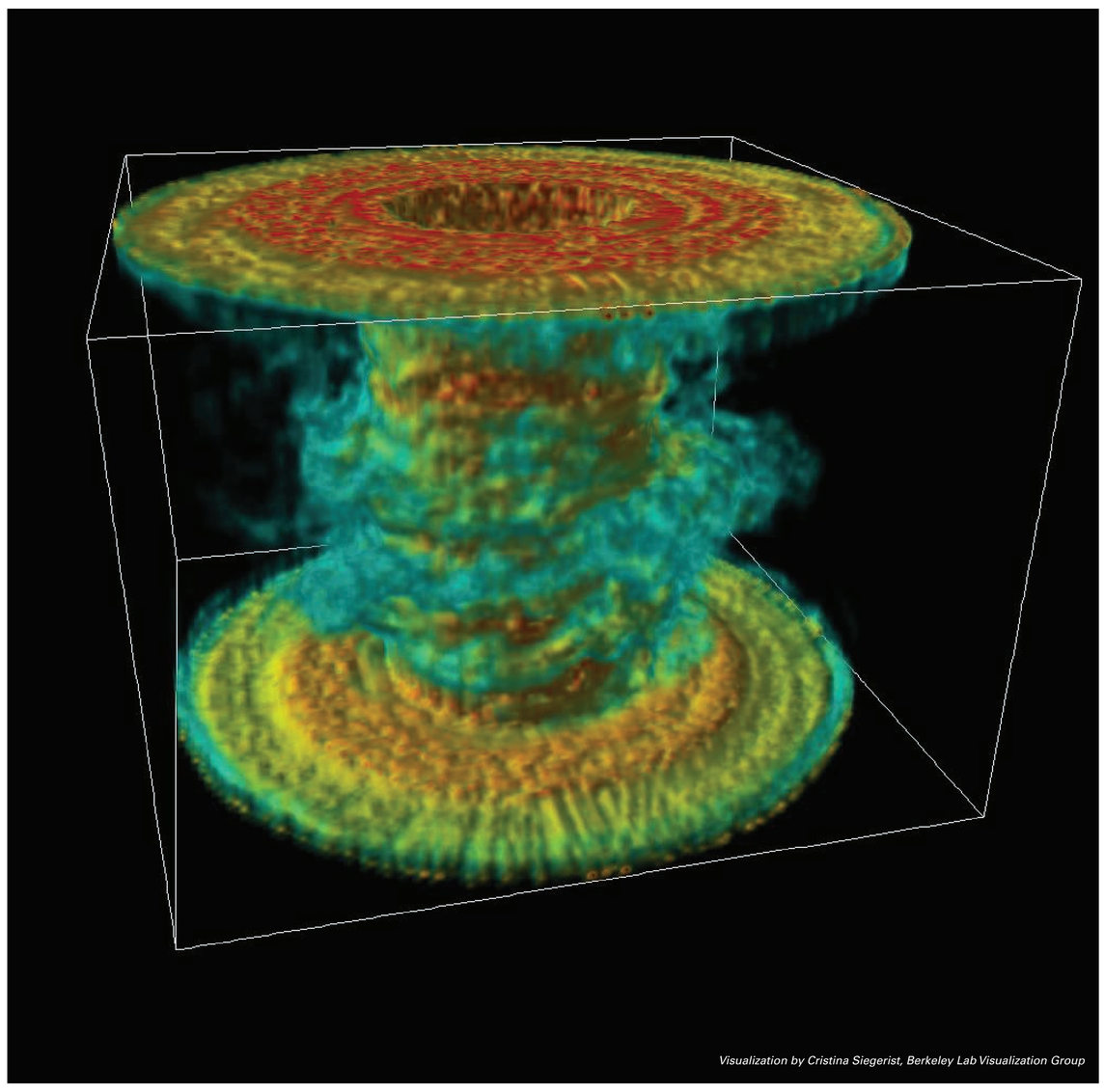
The three projects are aimed at enabling breakthrough research into how stellar bodies form, finding ways to improve energy efficiency while reducing pollution, and preventing disease through understanding protein structure and function.

Magneto-rotational instability and turbulent angular momentum transport

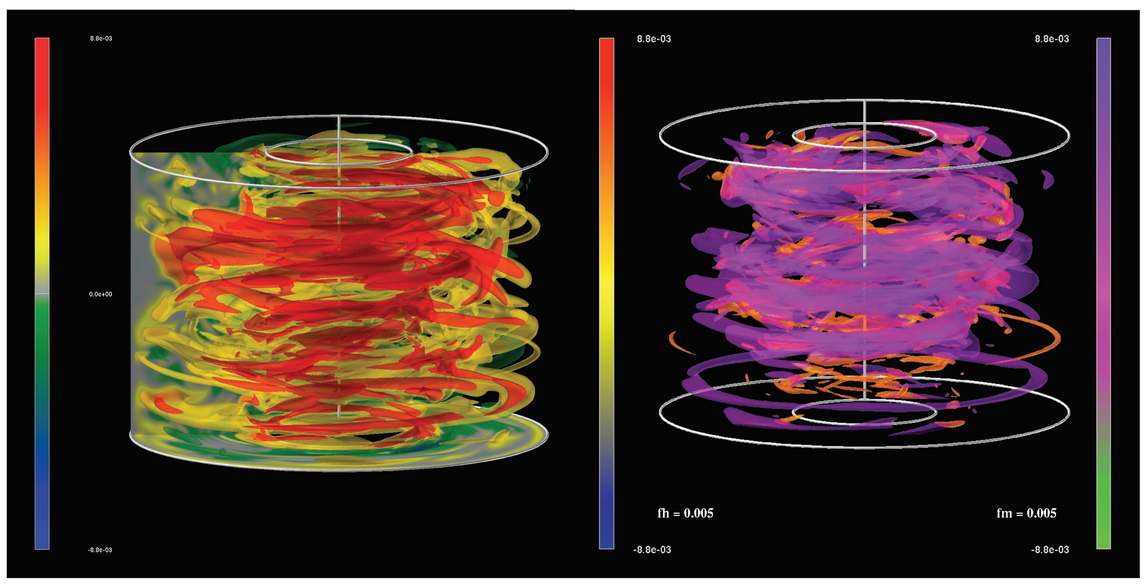
Fausto Catteneo, Aleksandr Obabko, Paul Fischer
University of Chicago, Argonne National Laboratory

This project studies the forces that help newly born stars and black holes increase in size. In space, gases and other matter often form swirling accretion disks around attracting central objects such as newly formed stars. The presence of magnetic fields can cause the disks to become unstable, develop turbulence and loose orbital angular momentum, thereby causing the disk material to fall onto the central object. In recent years, laboratory experiments have been developed to test many aspects of this magnetically caused instability, turbulence and angular momentum transport but on a much smaller scale. The large-scale simulations of magnetized fluid between two concentric cylinders that are carried out on NERSC's Seaborg supercomputer extends the lab experiments by several orders of magnitude and tests theories on how turbulence and angular momentum transport can develop in the astrophysical accretion disks.

"With the help of NERSC staff, we were able to tune our software for Seaborg's hardware and realize performance improvements that made additional simulations possible."

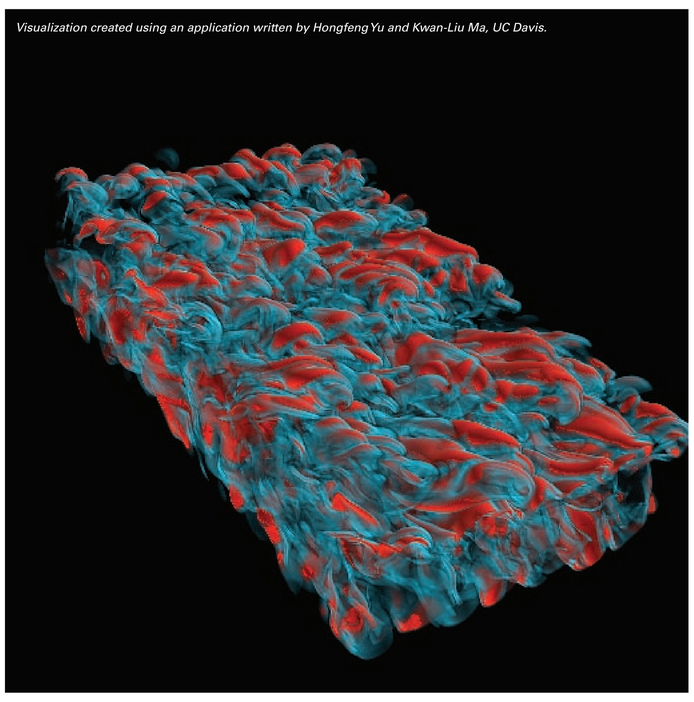


The outward transport of angular momentum controls the rate of accretion, and hence the rate of energy release in astrophysical accretion systems. It is widely believed that magnetic fields play a crucial role in the transport process. These numerical simulations study the mechanism of angular momentum transport in a magneto-fluid bounded by rotating cylinders. Shown in the figures are the energy dissipation rate (top), and angular momentum fluxes carried by velocity and magnetic fluctuations.



Direct Numerical Simulation of Turbulent Nonpremixed Combustion — Fundamental Insights Towards Predictive Modeling

Jacqueline Chen, Evatt Hawkes, Ramanan Sankaran.
Sandia National Laboratories



A complex simulated flame, colored by the rate of molecular mixing (scalar dissipation rate) which is critical for determining the interaction between reaction and diffusion in a flame. The image shows that high scalar dissipation regions exist in thin, highly intermittent structures aligned with principal strain directions.

In recent years, the rapid growth of computational capabilities has presented both opportunities and challenges for high-fidelity simulations of turbulent combustion flows. Realistic simulations that address complex multi-physics interactions, such as the so-called "turbulence-chemistry" interactions in combustion flows, have become accessible through the growth of processor speed, computer memory and storage, and significant improvements in computational algorithms and chemical models. With terascale resources at NERSC we have performed the first three-dimensional (3D) Direct Numerical Simulation (DNS) of a turbulent nonpremixed $H_2/CO/N_2$-air flame with detailed chemistry. This simulation, the first in a series of different Reynolds numbers, is targeted at providing insight into key outstanding issues related to modeling of turbulent nonpremixed combustion: extinction and reignition, flow and flame unsteadiness, the correlation of strain rate and scalar dissipation rate, differential diffusion of species, and turbulent mixing in a finite-rate chemical environment.

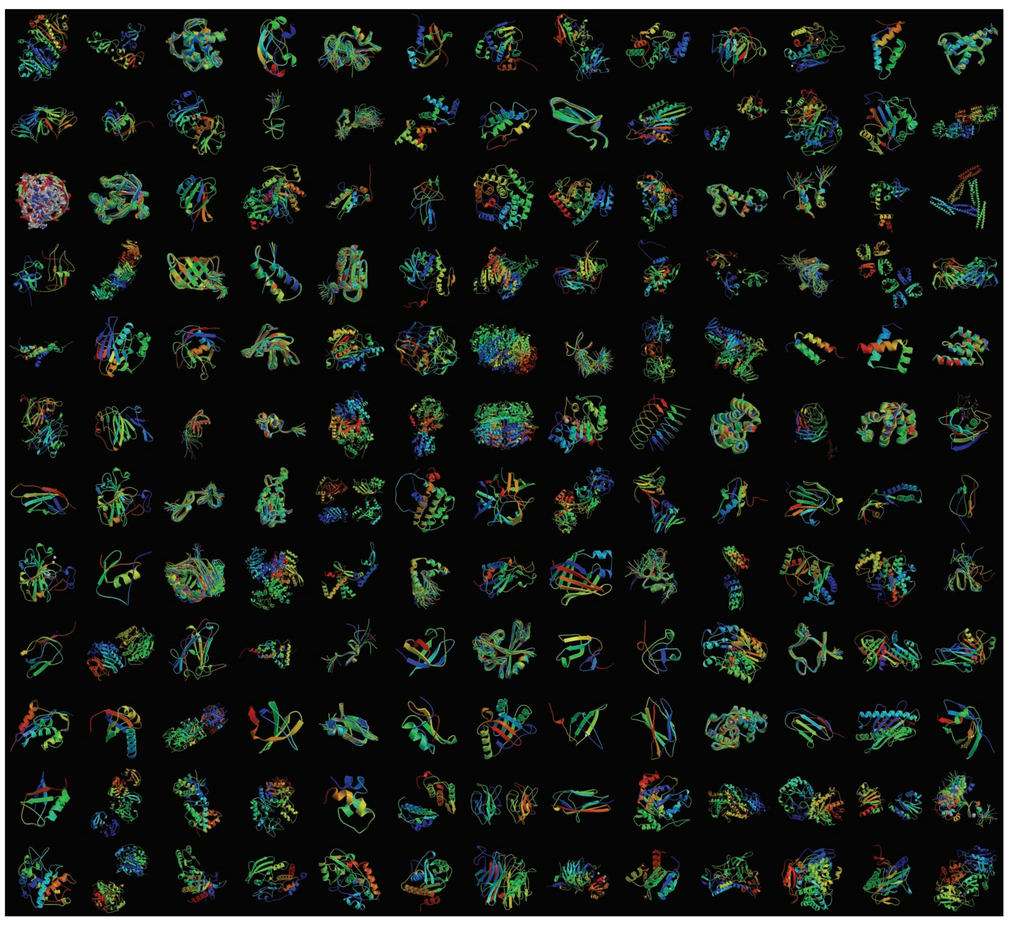
"The assistance we received from the NERSC computing staff in optimizing our code and with terascale data movement has been invaluable. The INCITE award has enabled us to extend our computations to three-dimensions so that we may investigate interactions between turbulence, mixing, and finite-rate detailed chemistry in combustion."

Molecular Dynameomics

Valerie Daggett, David Beck, Darwin Alonso
University of Washington, National Institutes of Health

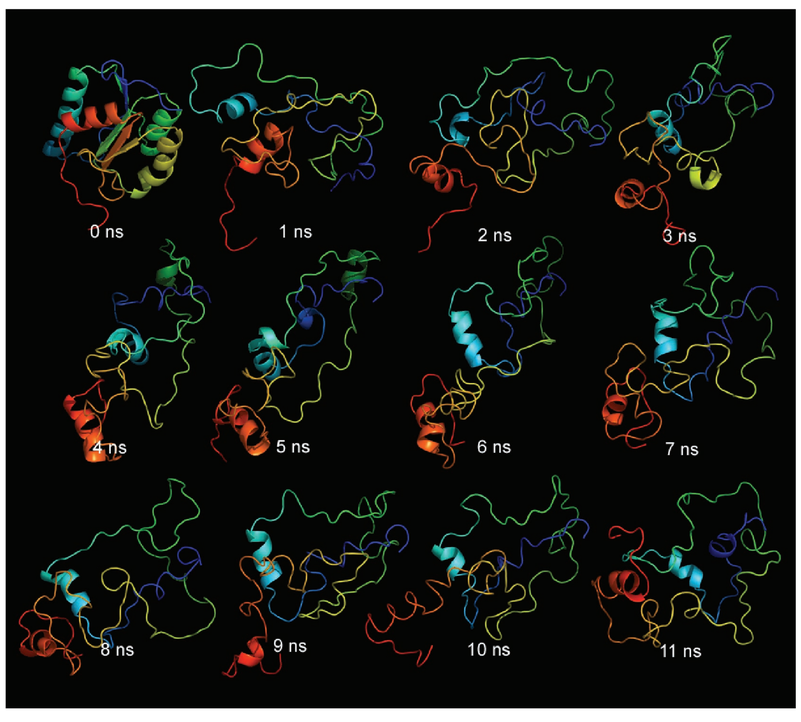
"We are quite satisfied with our experience at NERSC and have made significant progress towards our goal of performing molecular dynamics simulations of the first 150 most populated folds of protein fold space."

The Protein Data Bank (PDB) has been a tremendously useful repository of experimentally derived, static protein structures that have stimulated many important scientific discoveries. While the utility of static physical representations of proteins is not in doubt, as these molecules are fluid in vivo, there is a larger universe of knowledge to be tapped regarding the dynamics of proteins. The goal of this project is to simulate the native (biologically active) state and complete unfolding pathways of important proteins.



The first 156 Dynameomics simulation targets. Each target has been solvated with explicit water and simulated at 298 and 498 Kelvin to observe native and unfolding dynamics, respectively.

Protein target 3rub: Structures taken at 1 nanosecond (ns) intervals from a 21 ns native state simulation of rubisco at 298 Kelvin. Waters, hydrogens and protein atoms included in the simulation are not shown. The protein is depicted with a schematic representation of its secondary structure. The highly dynamic region (image top) is responsible for finding the protein's binding partner (not included in the simulation).



Protein target 1imf: Structures taken at 1 nanosecond (ns) intervals from a thermal unfolding simulation of inositol monophosphatase at 498 Kelvin. Waters, hydrogens and protein atoms included in the simulation are not shown. The protein is depicted with a schematic representation of its secondary structure. Both native and non-native residual helix are observed throughout the unfolding simulation.

Our work is sponsored by:

Office of Science
U.S. DEPARTMENT OF ENERGY

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NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER