INCITE Projects at NERSC Make Major Scientific Advances

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Summary

The Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program provides computing resources and consulting 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 computer time and data storage at DOE high performance computing centers. This paper provides an overview of the INCITE projects that computed at NERSC in allocation years 2005 and 2006.

NERSC has been providing computing, data storage, and consulting services for INCITE and its predecessor programs since 2002 (see https://www.nersc.gov/projects/incite/). The most recent INCITE projects at NERSC are tackling some of the most important and difficult problems in several areas of science.

The *Direct Numerical Simulation of Turbulent Non-Premixed Combustion—Fundamental Insights towards Predictive Modeling* project is led by Jacqueline Chen and Evatt Hawkes of Sandia National Laboratories. They have performed the first 3D Direct Numerical Simulations (DNS) of a turbulent nonpremixed H_2/CO–air flame with detailed chemistry (Figure 1). The simulations, including 11 chemical species and 33 reactions, were performed with up to 500 million grid points and 100,000 time steps, and ran for 2.5 million processor hours on Seaborg and 1.5 million hours on Bassi.

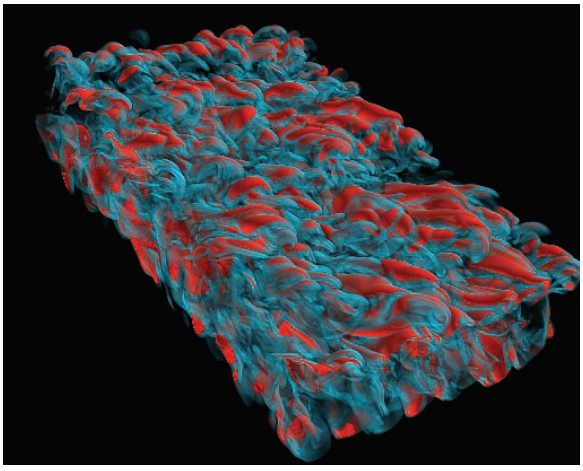

Figure 1. A simulated planar jet flame, colored by the rate of molecular mixing (scalar dissipation rate), which is critical for determining the interaction between reaction and diffusion in a flame.

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The *Magneto-Rotational Instability and Turbulent Angular Momentum Transport* project, led by Fausto Cattaneo of the University of Chicago, is studying the forces that help newly born stars and black holes increase in size. Their simulations are clarifying the mechanisms of angular momentum transport in magnetized, rotationally constrained turbulence.

The *Molecular Dynameomics* project, led by Valerie Daggett of the University of Washington, is combining molecular dynamics and proteomics to create an extensive repository of the molecular dynamics structures for protein folds, including the unfolding pathways. They have used their INCITE grant to simulate proteins from the 151 most common folds, which represent about 75% of all known protein structures (Figure 2).

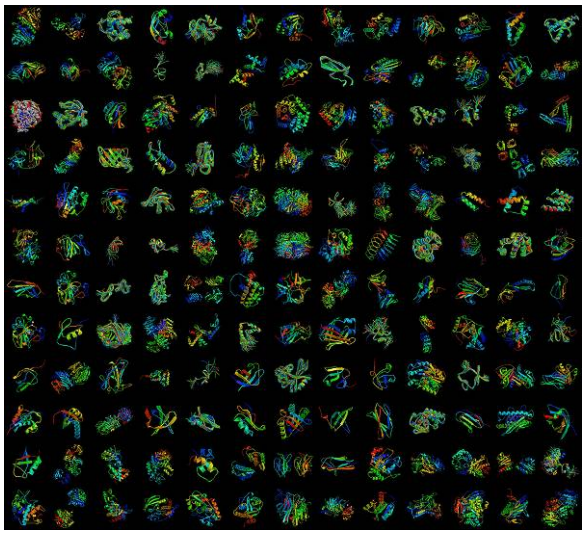

Figure 2. The first 156 dynameomics protein fold simulation targets.

The *Precision Cosmology Using the Lyman Alpha Forest* project, led by Michael Norman of the University of California, San Diego, is aimed at the cosmological goal of precisely measuring the cosmological parameters that describe the shape, matter-energy contents, and expansion history of our universe. The project seeks to increase our understanding of dark energy and dark matter through high-resolution hydrodynamical cosmological simulations of the structure of the high redshift intergalactic medium.

The *Particle-in-Cell Simulation of Laser Wakefield Particle Acceleration* project, led by Cameron Geddes of Lawrence Berkeley National Laboratory, is performing detailed 3D models of laser-driven wakefield particle accelerators, which may accelerate particles in as little as a thousandth of the length required by conventional accelerators. Coupled with experiments, these simulations are developing the detailed understanding of laser acceleration needed to apply this technology to future higher energy particle physics experiments and to compact machines for medicine and laboratory science.

The *Reactions of Lithium Carbenoids, Lithium Enolates, and Mixed Aggregates* project, led by Larry Pratt of Fisk University, is investigating the structure and reactions of some important organolithium compounds. These include lithium enolates, which are among the most important reagents for forming carbon–carbon bonds in organic synthesis. This project is working to uncover the previously unknown detailed reaction mechanisms for these compounds.

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