INCITE: INNOVATIVE AND NOVEL COMPUTATIONAL IMPACT ON THEORY AND EXPERIMENT

HIGH-IMPACT COMPUTATIONAL SCIENCE

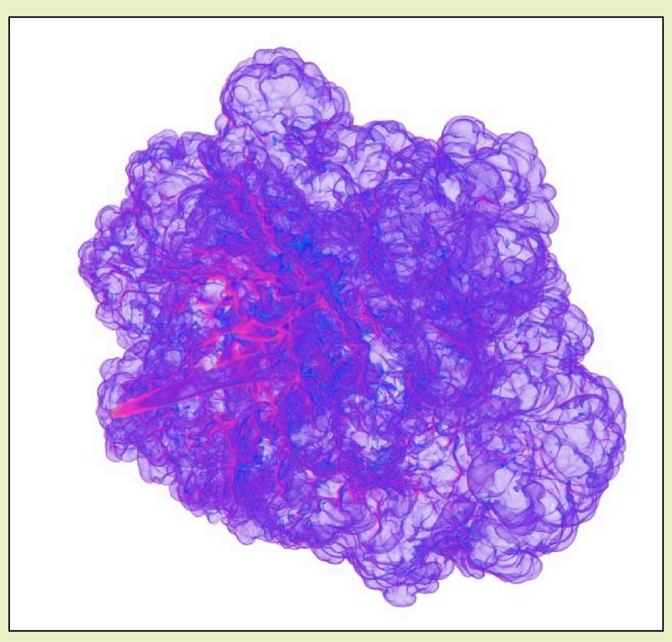
INCITE 2004 Summary

The 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 computer time and data storage at the NERSC Center.

INCITE 2004 consists of three projects using 4.9 million hours on Seaborg, NERSC's 6,652-processor IBM supercomputer.

The projects are expected to significantly advance our understanding of the makeup of the universe, the chemical process by which plants convert sunlight to energy while removing carbon dioxide from the atmosphere, and the turbulent forces that affect everything from weather to industrial processes.

"We have benefited from NERSC HPC staff working on our code performance, innovative ideas for improvement, and diagnostic assistance when problems occur."



Volume rendering of an unstable flame front from a simulation of the deflagration phase of a Type Ia supernova. The flame was ignited as a spherical region slighty off-center in the white dwarf star and results in a rapidly rising reactive bubble.

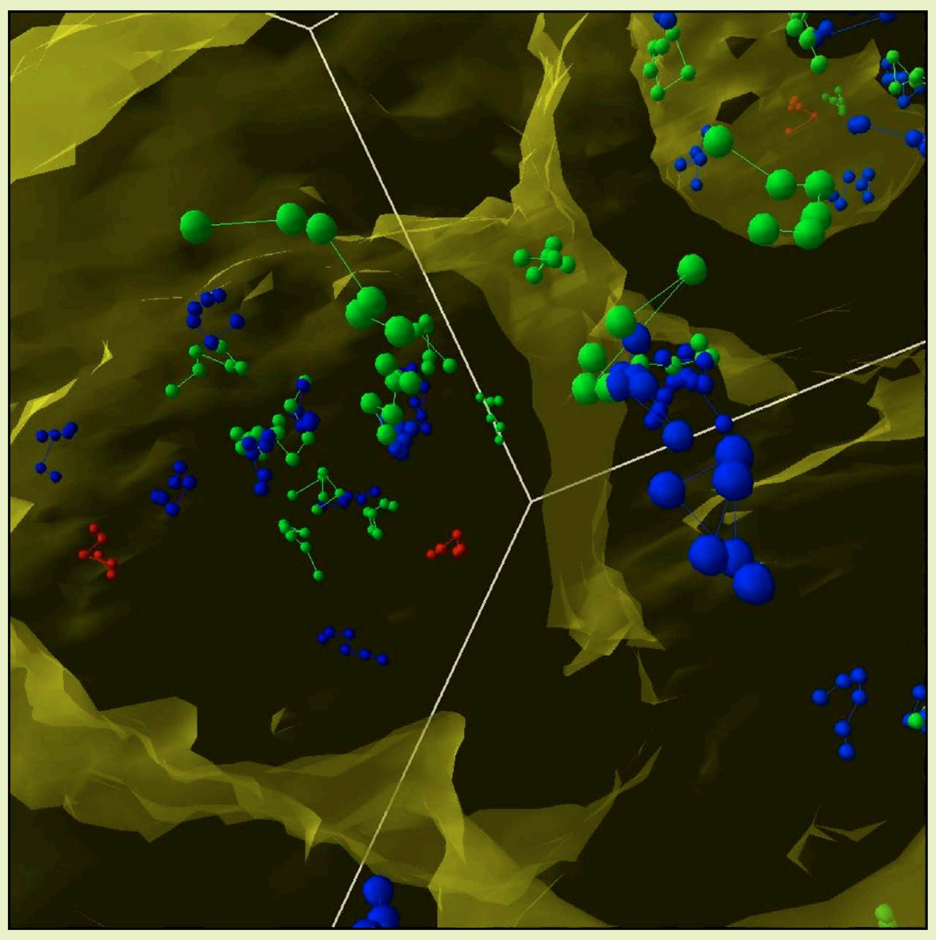
Quantum Monte Carlo Study of Photoprotection via Carotenoids in Photosynthetic Centers

Carotenoids prevent the formation of cell damaging singlet oxygen by quenching the lowest triplet state of chlorophyll.

$$^3Chl^* + {^1Car} \longrightarrow {^1Chl} + {^3Car^*}$$
$$^1O_2^* + {^1Car} \longrightarrow {^3Car} + {^3O_2}$$

The primary objective of this research is to determine the ground to triplet-state energy difference of the carotenoids present in Light Harvesting Complex II and Photo System I using the Zori code for diffusion Quantum Monte Carlo, perhaps the only accurate *ab initio* technique applicable to systems of this size.

Results from these calculations provide the most accurate values of the excitation and total energies of these biologically important systems. A reliable estimate of the relative energies of the triplet states, coupled with information about the separation and relative orientation of the calculated species in the photosystems of interest, leads to an estimate of the quenching rate for triplet excitations in the chlorophyll ring, a quantity presently under discussion in the literature.



Imaginary time paths traversed by electrons in a photosynthetic system. The electrons are colored to make them distinct. The yellow isosurface shows the boundary of the molecular framework.

"We would not have been able to address the systems studied in the INCITE project without the resources made possible in this program."

Zori

College of Chemistry
University of California, Berkeley

Thermonuclear Supernovae: Stellar Explosions in Three Dimensions

X-ray bursts, classical novae, and Type Ia supernovae all have in common a close binary star system in which matter from a companion star accretes onto the surface of a compact star (neutron star or white dwarf). All involve the ignition of a nuclear fuel under degenerate conditions, followed by the thermonuclear runaway burning via a convective or turbulent flame front (or deflagration wave), or via a shock front (or detonation wave).

Type Ia supernovae are thought to be caused by thermonuclear carbon flashes that ignite in the core of a white dwarf whose mass has grown by accretion. Neither laminar deflagration nor detonation alone can account for both the abundances of intermediate-mass nuclei and the large expansion velocity of the ejecta that are produced in a Type Ia supernova. Calculations done on seaborg are aimed at resolving the theory and observed properties of stellar explosions.

Understanding thermonuclear flashes is important to other fundamental questions in astrophysics: X-ray bursts for what they tell us about the masses and radii of neutron stars; classical novae for the contribution they make to the abundances of intermediate-mass elements in the galaxy, and for what they say about how the masses of white dwarfs change with time in close binary systems. Type Ia supernovae are also important for their crucial role as standard candles in determining the Hubble constant.

Advanced Simulation and Computing Alliance Center for Astrophysical Thermonuclear Flashes

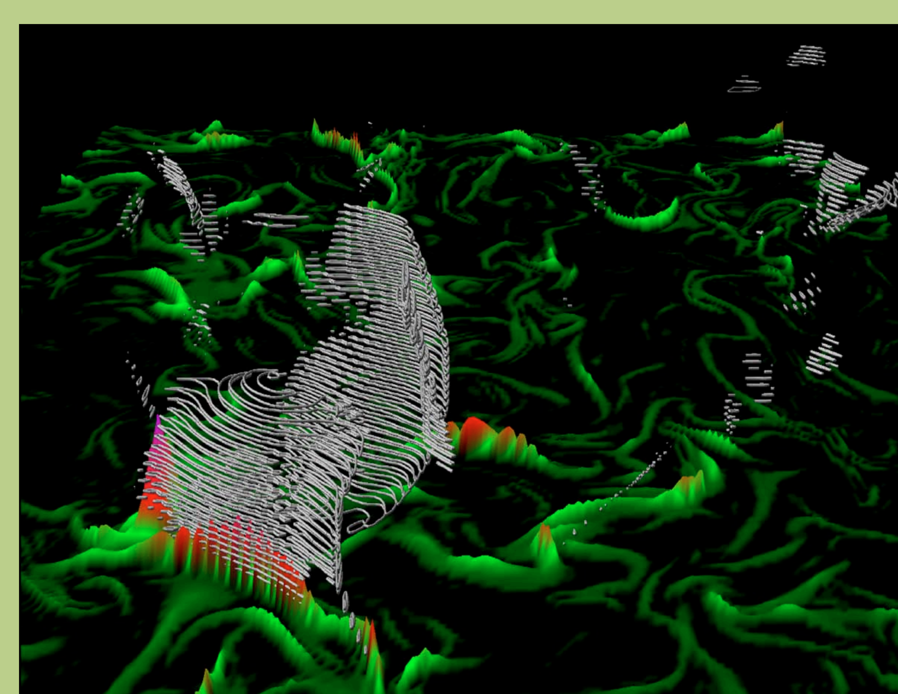
THE UNIVERSITY OF CHICAGO

"We have found NERSC staff extremely helpful in setting up computational environment, conducting calculations, and also improving our software."

Fluid Turbulence and Mixing at High Reynolds Number

This project focuses on the behavior and scaling properties of turbulent velocity fluctuations and the mixing of passive contaminants in such a flow. A pseudo-spectral calculation of the mixing, with Reynolds numbers in the 600-700 range, exceeds the turbulence studied in most controlled laboratory experiments, thus bringing computation closer to real world engineering applications than ever before. The calculations done on Seaborg provide unsurpassed detail and a wider scaling range critical for resolving issues such as small-scale universality, local isotropy, intermittency and inertial-range scaling.

The complexities of fluid turbulence limit our ability to predict natural phenomena and to design improved engineering devices. The calculations carried out on Seaborg at NERSC are novel in terms of their scale and innovative in allowing researchers to address fundamental issues in turbulence theory, including scaling properties of the velocity field, the rate of mixing of passive contaminants, and processes important in atmospheric and aqueous environments. This work is expected to impact both turbulence theory and experiment, as well as other branches of science.



A rendering of the intermittency of a scalar field during turbulent mixing. A 2D surface shows a slice through the mixed volume. Representative 3D structures within the field are shown with gray isolines.

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