NERSC NEWS

News from the National Energy Research Scientific Computing Center December 2004

INCITE Awards 6.5 Million Hours at NERSC to Research in Combustion, Astrophysics and Protein Structure

Secretary of Energy Spencer Abraham announced on Dec. 22 that 6.5 million hours of supercomputing time at NERSC have been awarded to three scientific research projects aimed at increasing our understanding of ways to reduce pollution, gaining greater insight into how stars and solar systems form, and advancing our knowledge about how proteins express genetic information.

“As one of the nation’s leading agencies for advancing scientific research, the Energy Department is proud to be able to award these major allocations for studying complex scientific problems that can transform our energy future and boost scientific research,” Secretary Abraham said.

The researchers will use their awards to compute on the IBM supercomputer “Seaborg” at NERSC. The three awards amount to 10 percent of NERSC’s annual computing resources.

The awards are made under the second year of the competitive program, Innovative and Novel Computational Impact on Theory and Experiment (INCITE), announced July 2003 by Secretary Abraham. The program’s goal is to select a small number of computationally intensive, large-scale research projects that can make high-impact scientific advances through the use of a substantial allocation of computer time and data storage at the NERSC Center. The INCITE program specifically encourages proposals from universities and other research institutions.

Two of the projects received 2 million processor-hours, while the third was awarded

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Welcome to the December 2004 issue of NERSC News, highlighting achievements by staff and users of DOE’s National Energy Research Scientific Computing Center. NERSC News is distributed every other month via email and may be freely distributed. NERSC News is edited by Jon Bashor, JBashor@lbl.gov or 510-486-5849.

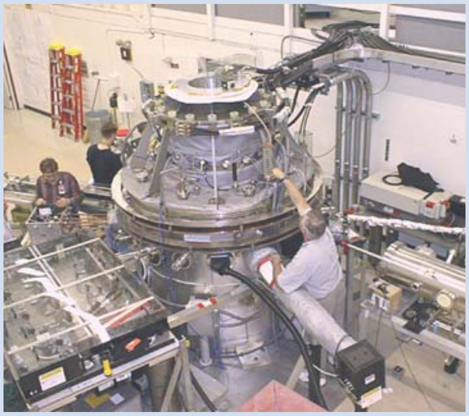
Magnetic Fusion Simulations at NERSC Advance SSPX Research at LLNL

In pursuing the potential of fusion energy, experimentalists try to understand precisely what is going on inside the fusion plasma so they can tune the system to improve the conditions that would lead to a sustained reaction within the heated plasma. If the temperature can be kept high enough and the energy contained, net power can be produced.

A major problem is that determining exactly what is happening inside a fusion plasma is very difficult experimentally. A conventional probe inserted into the hot plasma is likely to sputter and contaminate the plasma, leading to a loss of heat. Experimentalists must use nonperturbative diagnostics, e.g., laser scattering, and measurements with probes and magnetic loops around the edge of the plasma to deduce the plasma conditions and the magnetic field structures inside the plasma.

An important aid to the experiments is work undertaken with computational scientists to create detailed simulations of fusion plasmas. That's what scientists working on the Sustained Spheromak Physics Experiment (SSPX) at Lawrence Livermore National Laboratory have done in collaboration with researchers at the University of Wisconsin-Madison.

The resulting simulations produced using the NIMROD code on NERSC's Seaborg super-



The SSPX at Lawrence Livermore.

computer are very close to the observed results from actual runs on SSPX, giving the researchers confidence in the accuracy of the simulations and increased understanding of the physics in the spheromak.

"These simulations are very important for supporting our experiments," said LLNL's Bruce Cohen, who has been computing at NERSC and its predecessors since the earliest days of the center. "The experimental team has been upgrading the capacitor bank used to drive the reactor, and our simulations confirm

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Two NERSC Users Honored by AGU

At the 2004 American Geophysical Union (AGU) Fall Meeting, NERSC users Inez Yau-Sheung Fung and Garrison “Gary” Sposito were among the 12 recipients of AGU medals for excellence in research. The meeting was held Dec. 13-17 in San Francisco.

Fung, director of the Center for Atmospheric Sciences and a professor at the University of California at Berkeley, was awarded the Roger Revelle Medal. Established in 1991, the Revelle Medal recognizes outstanding accomplishments or contributions toward the understanding of the Earth's atmospheric processes. Revelle made substantial contributions to the awareness of global change. The breadth of his research and national/international service made him a statesman of science.

Inez Fung

Fung, who uses “Seaborg” to study carbon-climate interactions, was cited for her work in making “fundamental discoveries on topics before most have even recognized them as important areas of pursuit. Along the way, she has laid the ground work for the now emerging area of biogeoscience, developed many of the key modeling and numerical analysis techniques in use today, and mentored a generation of successful young scientists.”

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NERSC Users Receive AGU Medals (continued from p.1)

The medal citation also notes, "Professor Fung is one of the scientific leaders shaping our current view of the global carbon cycle. She is personally responsible for several of the critical advances in this area since the early work of Roger Revelle's generation. A decade or more ahead of other research groups, she developed a very credible global simulation of the terrestrial biosphere and atmospheric carbon dioxide."

Gary Sposito

Sposito, a professor in Ecosystem Sciences and Environmental Engineering at UC Berkeley, was the recipient of the Robert E. Horton Medal, which recognizes outstanding contributions to the geophysical aspects of hydrology. This medal was established in 1974 in honor of Robert E. Horton's contributions to the study of the hydrologic cycle, work which earned him recognition as "the father of modern hydrology."

Sposito, who was awarded 150,000 processor-hours for 2005 to study clay mineral surface geochemistry, was described in the medal citation as the "undisputed leader in the field of hydrology. Gary's extensive scientific contributions in geochemistry, thermodynamics, mathematics, and subsurface hydrology are legendary. He is largely responsible for bridging the areas of aqueous geochemistry and physical hydrology."

The citation concluded, "As many of us have experienced, Gary is a scholar with an enormous heart and an uncommon graciousness toward younger scientists, offering invaluable help in the form of mathematical derivations and detailed explanations. For his 'spirit of helpfulness and friendliness in unselfish cooperative research,' we can think of no more deserving recipient of the Horton Medal."

INCITE Awards Announced for 2005 (continued from p.1)

2.5 million processor-hours. All three INCITE projects were also awarded significant amounts of data storage at NERSC. Additionally, NERSC's User Services Group will provide specialized technical support to help the researchers make the most efficient use of their computing resources.

Descriptions of the three projects selected follow.

CHEMICAL SCIENCES

"Direct Numerical Simulation of Turbulent Non-premixed Combustion – Fundamental Insights towards Predictive Modeling," by Jacqueline Chen and Evatt Hawkes of Sandia National Laboratories in Livermore, Calif. This project was awarded 2.5 million processor-hours. The researchers will perform detailed three-dimensional combustion simulations of flames in which fuel and oxygen are not premixed. By better understanding the details of such flames, the researchers hope to gain insight into reducing pollutants and increasing efficiency in combustion devices. This research could have applications in such areas as jet aircraft engines, where fuel and oxidizers are not premixed for safety reasons, and in direct-injection internal combustion engines. These simulations would be the first-ever 3D direct numerical simulations with detailed chemistry of a fully developed turbulent, non-premixed flame.

Under certain conditions, this type of combustion can be extinguished, and this project will also try to gain a better understanding of this problem, as well as re-ignition of extinguished flames.

"We are thrilled at the unique opportunity that the INCITE award provides us," Chen said. "This vast award will enable us to make significant contributions to the challenging problem of understanding and modeling the interactions of turbulence and finite-rate chemical effects in non-premixed combustion. Ultimately, our plan is to share the resulting data with the turbulent combustion modeling community at large."

ASTROPHYSICS

"Magneto-rotational instability and turbulent angular momentum transport," by Fausto Cattaneo, University of Chicago. This project was awarded 2 million processor-hours and will study the forces that help newly born stars and black holes increase in size. In space, gases and other matter often form swirling disks around attracting central objects such as newly formed stars. The presence of magnetic fields can cause the disks to become unstable and develop turbulence, thereby causing the disk material to fall onto the central object. This project will carry out large-scale simulations to test theories on how turbulence can develop in such disks.

In recent years, laboratory experiments have been developed to test many aspects of this magnetically caused instability, but on a much smaller scale. The INCITE researchers plan to collaborate with the experimentalists in the field and to develop simulations that can extend the lab experiments by several orders of magnitude.

"What we are hoping to achieve is a simulation that matches the experimental work being done at Princeton," Cattaneo said. "If you can do the research both computationally and experimentally, you are much better off than just using one approach. With these INCITE resources, we should be able to do a very good job on the simulations."

LIFE SCIENCES

"Molecular Dynameomics" by Valerie Daggett of the University of Washington was awarded 2 million processor-hours. The project will combine molecular dynamics and proteomics to create an extensive repository of the molecular dynamics structures for protein folds, including the unfolding pathways. According to Daggett, there are approximately 1,130 known, non-redundant protein folds, of which her group has simulated about 30. She plans to use the information from these simulations to improve algorithms for predicting protein structure.

"Structure prediction remains one of the elusive goals of protein chemistry," Daggett wrote in her INCITE proposal. "It is necessary to successfully predict native states of proteins, in order to translate the current deluge of genomic information into a form appropriate for better functional identification of proteins and drug design."

After hearing that her proposal was one of three to receive an INCITE allocation, Daggett said, "We are excited about the massive resources we will have access to now. Our project will run literally hundreds and hundreds of simulations, each a little different, so we will be running a lot of smaller jobs all at once, using up to 1,000 processors at a time."

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Spheromak Simulations Advance LLNL Fusion Experiment (continued from p.1)

how careful tuning of the current pulses can improve plasma performance, such as achieving higher temperatures."

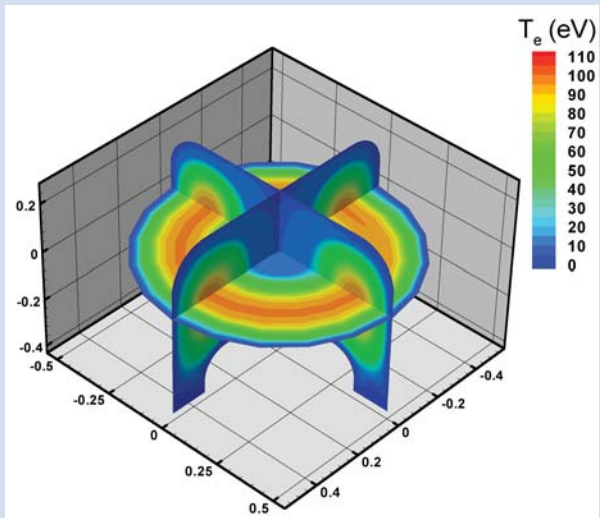
Cohen presented some of the group's latest results in an invited talk at the 2004 annual meeting of the American Physical Society's Division of Plasma Physics, held Nov. 15-19, 2004. In a close collaboration led by Carl Sovinec of the University of Wisconsin-Madison, the Wisconsin-LLNL group recently had a paper accepted for publication by Physical Review Letters.

While the principal magnetic fusion approach focuses on the tokamak, fusion energy scientists are also revisiting the spheromak and other alternative concepts for attaining magnetic fusion. The SSPX spheromak at LLNL is a series of experiments designed to determine the spheromak's potential to efficiently create and confine hot fusion plasmas. The systems differ in that the tokamak's magnetic fields are generated by large, external magnetic coils surrounding the doughnut-shaped plasma (which make the tokamak more complex and expensive), while spheromaks confine hot plasma in a simple and compact magnetic field system that uses only a small set of external magnet coils. The necessary strong magnetic fields are generated inside the spheromak plasma by plasma currents and what's known as a magnetic dynamo.

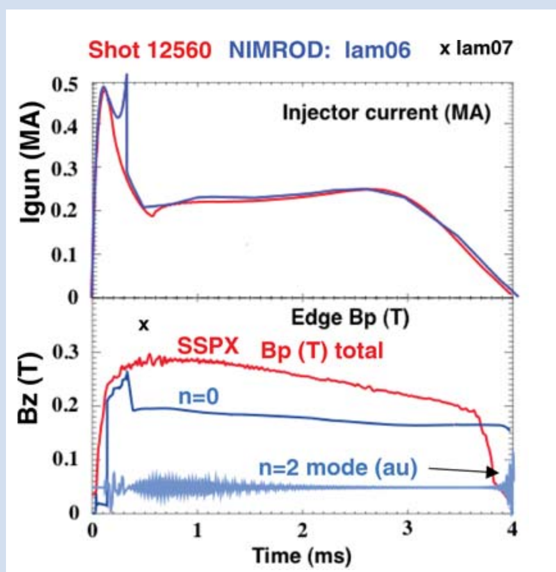
A spheromak can be formed and sustained by injecting magnetic helicity and energy from a magnetized coaxial plasma gun (powered by a capacitor bank) into a conducting shell or flux conserver. Although the physical spheromak design is simple, its dynamo activity produces plasma behavior that is extremely complex and more difficult to predict and control than that found in tokamaks.

"How high a temperature you can achieve and how well you can hold that heat in the plasma are two of the key points on the short list of things you want to understand and optimize in a fusion device," Cohen said. "Minimizing the energy leakage rate relaxes the requirements on how much energy you need to put into the fusion plasma to drive it and makes it easier to achieve sustained thermonuclear reactions."

With recent changes to their code, the Wisconsin-LLNL collaborators have created simulations with temperature histories — measured in milliseconds — that are closer to the temperature histories observed in experiments. This follows the group's prior success in simulating the magnetics of the experiment. "We have the magnetic history captured pretty well," Cohen said. "Energy confinement is closely coupled to the detailed magnetics."



This partial-drive simulation, part of a simulation of the evolution of conditions inside the spheromak, shows the peak temperature of 98.8 eV occurring at 1 millisecond into the simulation.



These graphs illustrate the improved match of NIMROD simulations (in blue) with results from an actual experiment (in red).

Plasma and energy confinement in the spheromak is quite sensitive to the quality and symmetry of the magnetic field lines. As long as the plasma and its confining magnetic field remain relatively axisymmetric with a large volume of closed, nested magnetic flux surfaces, a hot fusion plasma can be confined away from the walls of the device, and a high temperature can be maintained. However, due to magnetohydrodynamic (MHD) instability, small fluctuations and islands develop in the magnetic fields. This disrupts the axisymmetry, undercutting the confinement of the plasma and allowing heat loss. Finding ways to eliminate large-scale magnetic fluctuations and the associated islands would allow the experimenters to improve the energy and plasma confinement, and thereby increase the operating temperature.

"The simulations support experimental findings that controlling magnetic fluctuations is central to improving the quality of the magnetic flux surfaces and the energy confinement," Cohen noted in his talk at the APS meeting.

Future work will also address controlling magnetic fluctuations with a conducting insert along the geometric axis and additional physics improvements to the simulation model.

"We really need supercomputer resources to do these kinds of simulations, which involve massive calculations," Cohen said. Although the simulations cover only four milliseconds in physical time, there are of order 10^5 time steps involved in the simulations. As a result, the group ran each of their simulations in 50 to 80 shifts of 10 to 12 hours each on Seaborg, consuming more than 30,000 processor hours in each complete simulation; and multiple simulations were needed.

This work was performed under the auspices of the U.S. Department of Energy under contracts W7405-ENG-48 at the University of California Lawrence Livermore National Laboratory and grant FG02-01ER54661 at the University of Wisconsin-Madison.