NERSC NEWS

News from the National Energy Research Scientific Computing Center September 2006

INCITE Allocation Helping Drive Research in Future Accelerator Design

Using an allocation of 2.5 million processor hours on Seaborg at NERSC, a team led by Cameron Geddes of Lawrence Berkeley National Laboratory is creating detailed 3D simulations of laser-driven wakefield particle accelerators (LWFAs), providing crucial understanding of the next generation of particle accelerators and ultrafast applications in chemistry and biology.

The allocation was awarded under DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, which provides large allocations to high-impact projects related to DOE's mission areas. Plasmas are not subject to the electrical breakdown that limits conventional accelerators, and LWFAs have demonstrated accelerating gradients thousands of times those obtained in conventional accelerators using the electric field of a plasma wave (the wakefield) driven by an intense laser.

Plasma-based accelerators hence offer a path to more compact machines, and also to high-current ultrashort electron bunches, which may revolutionize applications of accelerators to radiation sources as well as applications in chemistry and biology.

"Future particle accelerators may use laser-driven plasmas to accelerate particles in as little as a thousandth of the length required by conventional machines, and our INCITE allocation is allowing us

(continued on page 2)

First Cabinet of NERSC's New Cray Supercomputer Arrives for Testing

Lynn Rippe, Jonathan Carter and Nick Cardo of the NERSC procurement team welcome the first cabinet of the new Cray supercomputer and the attached disk storage from Data Direct Networks.

Within weeks of the announcement that NERSC's next large system will be a follow-on to the Cray XT3 supercomputer, the first cabinet of the new machine has been installed for testing at Berkeley Lab's Oakland Scientific Facility.

The new supercomputer, which will be among the world's fastest general purpose system, will have a guaranteed sustained performance of at least 16 trillion calculations per second (with a theoretical peak speed of 100 trillion calculations per second) when running a suite of diverse scientific applications at scale.

Cray will begin shipping the new supercomputer to the NERSC facility at the Lawrence Berkeley National Laboratory later this year, with Complete installation is expected in the first half of 2007 and acceptance in mid-2007.

As part of a competitive procurement process, NERSC evaluated systems from a number of vendors using the Sustained System Performance (SSP) metric. The SSP metric, developed by NERSC, measures sustained performance on a set of codes designed to accurately represent the challenging computing environment at the Center.

"While the theoretical peak speed of supercomputers may be good for bragging rights, it's not an accurate indicator of how the machine will perform when running actual research codes," said Horst Simon, director of the NERSC Division at Berkeley Lab. "To better gauge how well a system will meet the needs of our 2,500 users, we developed SSP. According to

(continued on page 2)

NERSC Calculations Help U.S. Army Corps of Engineers to Improve Gulf Coast Hurricane Defenses

In 2006, the Department of Energy's Office of Science made two separate allocations of 400,000 processor hours of supercomputing time at the NERSC to the U.S. Army Corps of Engineers for studying ways to improve hurricane defenses along the Gulf Coast. The research is being done in cooperation with the Federal Emergency Management Agency (FEMA).

As hurricanes move from the ocean toward land, the force of the storm causes the seawater to rise as it surges inland.

The Corps of Engineers used its DOE supercomputer allocations to create revised models for predicting the effects of 100-year storm surges — the worst case scenario based on 100 years of hurricane data — along the Gulf Coast. In particular, simulations were generated for the critical five-parish area of Louisiana surrounding New Orleans and the Lower Mississippi River. These revised effects, known as "storm-surge elevations," are serving as

(continued on page 3)

A Note About NERSC News

With this issue, NERSC News returns to every-other-month publication after a short hiatus. Highlighting achievements by staff and users of DOE's National Energy Research Scientific Computing Center, NERSC News is published every other month via email and may be freely distributed. NERSC News is edited by Jon Bashor, JBashor@lbl.gov or 510-486-5849.

New Cray System Arrives for Testing (continued from page 1)

this test, the new system will deliver over 16 teraflops on a sustained basis."

The Cray supercomputer at NERSC will consist of over 19,000 AMD Opteron 2.6-gigahertz processor cores, with two cores per socket making up one node. Each node has 4 gigabytes (4 billion bytes) of memory and a dedicated SeaStar connection to the internal network. The full system will consist of over 100 cabinets with 39 terabytes (39 trillion bytes) of aggregate memory capacity.

In keeping with NERSC's tradition of naming supercomputers after world-class scientists, the new system will be called "Franklin" in honor of Benjamin Franklin, America's first scientist. This year is the 300th anniversary of Franklin's birth.

"Ben Franklin's scientific achievements included fundamental advances in electricity, thermodynamics, energy efficiency, material science, geophysics, climate, ocean currents, weather, population growth, medicine and health, and many other areas," said NERSC General Manager Bill Kramer. "In the tradition of Franklin, we expect this system to make contributions to science of the same high order."

Artist's rendering of NERSC's new Cray Supercomputer

The new computer and a multi-year services contract are valued at over $52 million. The contract also provides options for future upgrades that would quadruple the size of the system and eventually boost performance to one petaflops (1,000 trillion floating point operations per second) and beyond.

Simulations at NERSC Could Lead to Accelerators of the Future (continued from page 1)

to create simulations with detailed three-dimensional modeling of such accelerators," Geddes said. "These simulations are computationally intensive because the laser wavelength (micron) must be resolved over the acceleration length of centimeters. 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."

In addition to Geddes, the team includes Carl Schroeder, Eric Esarey and Wim Leemans of LBNL, and David Bruhwiler and John Cary of Tech-X Corp.

Recent experiments have demonstrated for the first time the production of high-quality electron beams in a high-gradient laser wakefield accelerator. This was achieved in an LBNL laboratory by extending the interaction distance using a pre-formed plasma density structure, or channel, to guide the drive laser pulse over many diffraction ranges. Such beams allow laser-plasma accelerators to be considered seriously as alternatives to conventional accelerators for a wide variety of applications that demand high-quality electron bunches, making simulations to understand their behavior imperative.

Particle-in-cell simulations are a crucial tool in interpreting these experiments and planning the next generation because they can resolve kinetics and particle trapping. Such simulations have shown that the important physics for production of narrow energy spread in recent experiments is that trapping of an initial bunch of electrons loads the wake, suppressing further injection and forming a bunch of electrons isolated in phase space. At the dephasing point, as the bunch begins to outrun the wake, the particles are then concentrated near a single energy and a high quality bunch is obtained. Only a single wake period contributes to the high energy bunch, and hence the electron bunch length is near 10 fs, indicating that a compact ultra-fast electron source with high beam quality has been developed.

While two-dimensional simulations showed the essential physics and demonstrated the applicability of the VORPAL code used in this project (and its scaling to thousands of processors), substantially higher resolution as well as three-dimensional effects are important in order to allow detailed understanding of the physics of these accelerators and the eventual construction of accelerators for applications, according to Geddes.

Scaling from existing runs, reasonable three dimensional modeling of current experiments (100 MeV class) as well as new GeV-class experiments requires a few hundred thousand to a million hours of Seaborg time per run, and the INCITE program is providing 2.5 million hours to allow several such runs.

"The ability to do such high-resolution runs with full particle models is also vital to the development of reduced models which may reduce computation methods in the future, but which require benchmarking against cases of experimental interest at sufficiently high resolution to give confidence in the results," Geddes said.

Corps of Engineers Simulations to Strengthen Hurricane Defenses (continued from page 1)

the basis of design for levee repairs and improvements currently being designed and constructed by the Corps of Engineers in the wake of Hurricane Katrina's destruction in the New Orleans Metro Area.

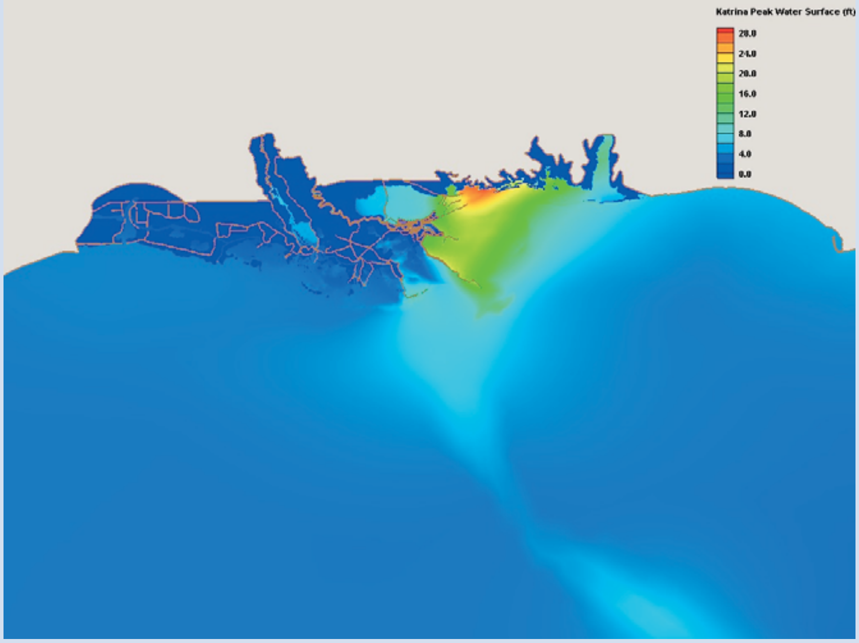
Additionally, Gulf Coast Recovery Maps were generated for Southern Louisiana based on FEMA's revised analysis of the frequency of hurricanes and estimates of the resulting waves. While still preliminary, these maps are being used on an advisory basis by communities currently rebuilding from the 2005 storms. Final maps are expected to be completed later this year.

The Corps used its first NERSC allocation, announced in February, to conduct storm-surge simulations using the ADvanced CIRCulation (ADCIRC) coastal model and Empirical Simulation Technique (EST) to study both how high the storm-surge waters would rise and how often such surges would occur.

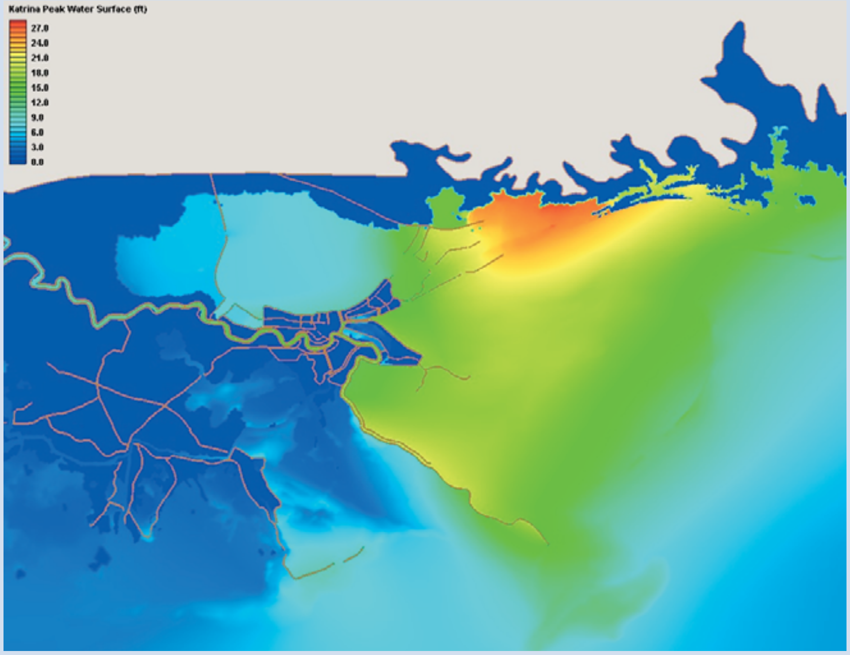
The Corps of Engineers plans to use the second NERSC allocation, announced in July, to finalize the revised stage frequency relationships by the end of 2006. Having access to the NERSC supercomputer will allow the Corps of Engineers to create more detailed models of the effects of Hurricane Rita and other storms along the Texas-Louisiana coasts. Increased detail will give the Corps of Engineers and FEMA more information about the local effects of such storms. For example, storm-surge elevations are greatly influenced by local features such as roads and elevated railroads. Representing these details in the model greatly improves the degree to which computed elevations match observed storm-surge high-water marks and allows the Corps to make better recommendations to protect against such surges.

At NERSC, the Corps of Engineers team is running their simulations on an 888-processor IBM cluster called "Bassi." The cluster is powered by IBM's newest Power5 processors and is specially tuned for scientific computation. The Corps' simulations typically use 128 to 256 processors and run for two-and-a-half to four-and-a-half hours per simulation batch.

As a result of the runs, the Corps determined that the applications produced incorrect results at topographic boundaries in some instances and codes were modified to improve the accuracy of the results. For example, the runs at NERSC have improved the Corps' ability to model the effects of vegetation and land use on storm surges which propagate far inland, as Hurricane Rita did on Sept. 24, 2005.



Overview simulation showing elevated storm surges along the Gulf Coast.



Simulation detail showing highest surge elevation (in red) striking Biloxi, Miss. New Orleans is the dark blue crescent to the lower left of Biloxi.