NERSC NEWS

News from the National Energy Research Scientific Computing Center April 2004

NERSC Users Post Impressive Record of Published Results

The Web site for requesting NERSC allocations includes a field requesting information about scientific publications related to research using NERSC resources. In 2003, NERSC users reported a total of 2,404 peer-reviewed papers based, at least in part, on work done at NERSC.

The complete list, organized alphabetically by principal investigator, can be found on the Web at <http://www.nersc.gov/research/ERCAPpubs03.htm>.

NERSC's David Skinner Gets Hands on IBM BlueGene Prototype

David Skinner, who is the lead NERSC consultant for the Seaborg system, was working on a performance monitoring project at IBM's Watson Center in New York earlier this year when an unexpected opportunity presented itself.

"There was a BlueGene/L prototype available while I was there, and IBM Research was interested in getting more experience with real users and codes on the machine," Skinner said. "This was the first real contact NERSC has had with this architecture, which is one of the more novel architectures to come along in a while."

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NERSC News

Welcome to the second 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.

INCITE Supernovae Project Reports Unprecedented Full-Star Simulations

One of three computationally intensive large-scale research projects selected under DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program has achieved unprecedented simulations of stars and supernovae using NERSC's computing resources.

Called "Thermonuclear Supernovae: Stellar Explosions in Three Dimensions," the project is led by Tomasz Plewa of the Center for Astrophysical Thermonuclear Flashes at the University of Chicago and is a collaboration between scientists at the university and at Argonne National Laboratory.

The group, which was awarded 2.7 million processor hours at NERSC, is studying the longstanding problem of thermonuclear flashes on the surfaces and interiors of compact stars. These phenomena are not only fascinating in themselves, but are also important for the light they shed on 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; and Type Ia supernovae for the contribution they make to the abundances of intermediate mass and heavy elements in the galaxy. Type Ia supernovae are also important for their crucial role as standard candles in determining the Hubble constant.

Between January and March of 2004, the group used 168,887.59 CPU hours, just over 6 percent of the total allocation, as

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Combustion Researcher Outlines Advances Resulting from SciDAC Program

The U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program is making important contributions to combustion research, according to Arnaud Trouvé, a professor of engineering at the University of Maryland and a NERSC user.

Trouvé, who has extensive experience in the field of multi-dimensional numerical modeling for turbulent combustion applications, is a leader of SciDAC's Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry project. The project is a multi-institution collaborative effort aimed at adapting S3D, a high-fidelity turbulent reacting flow solver, to terascale computer technology. Ultimately, the project is expected to enable first-principles simulations of pollutant emissions (NOx, soot) from turbulent combustion systems.

"The SciDAC program has been having a multi-faceted impact on our research on numerical combustion," Trouvé wrote. "Perhaps the most obvious aspect is that SciDAC has provided access to a nation-wide high-performance scientific computing infrastructure. Access to resources at NERSC has allowed large-scale computations to be performed, pushing the limits of combustion science."

Additionally, SciDAC has allowed Trouvé's group to adapt their scientific software to large-scale, massively parallel platforms (MPP). The software is currently being re-designed using two standardized frameworks, an adaptive mesh refinement framework called GrACE and the Common Component Architecture (CCA), to enable cross-talk between different projects. Once this is done, Trouvé plans to exchange

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Over the course of three days, Skinner was able to use about 12 hours of run time on the prototype, completing several benchmark runs, as well as a couple of applications. “This data gives NERSC a reasonable starting point for understanding BG/L as an HPC resource,” Skinner said. The results were presented at a recent LBNL seminar and discussions about future work on BG/L are ongoing.

Skinner, who earned his Ph.D. in chemistry at UC Berkeley, primarily consults with NERSC users about improving the performance of their codes on Seaborg. As part of NERSC’s Science-Driven Computing effort, Skinner is also involved in studying performance issues on new architectures such as Blue Planet, BlueGene and parallel vector systems. But he has been branching out into studying various architectures and performance issues.

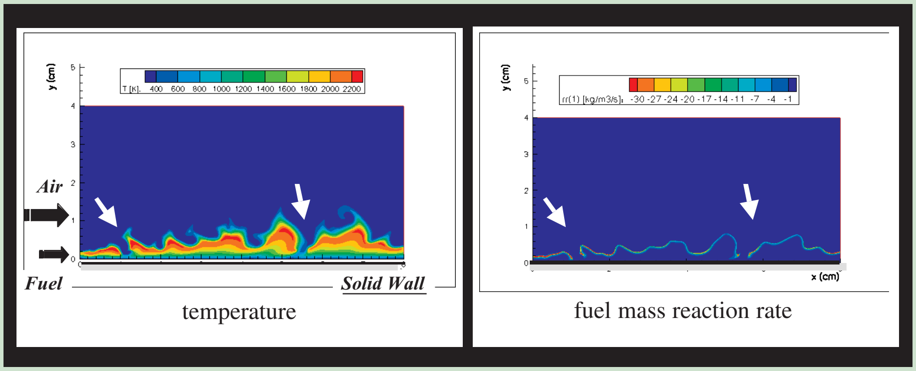
It was this interest that led to informal conversations with IBM staff at scientific computing conferences. From this, Skinner spent a week or so in Yorktown Heights, working on a couple of projects related to hardware performance monitoring. One objective was to improve the scaling and performance of the parallel performance monitoring tools themselves. Performance monitoring that functions efficiently at high concurrency allows researchers to view the performance of an entire parallel calculation in a simple consistent picture. “The work done in January got us a five-fold improvement in profiling a 1,024-way calculation,” Skinner said.

In return, Simone Sbraglia of IBM will be spending two weeks at LBNL’s Oakland Scientific Facility beginning in late April. Sbraglia is the main developer of the Simulator Guided Memory Analyzer (SiGMA), a performance toolkit under development to help programmers understand the precise memory references in scientific programs. The goal for Sbraglia’s visit is to apply SiGMA to examples of the NERSC workload in order to get a better understanding of memory access patterns and performance in scientific codes. It will also help shake out how well a tool like SiGMA can work on real world codes and provide IBM Research some indication about SiGMA’s use as more than a research tool.

“Visiting with developers is a great way to educate one another about what works and what doesn’t,” Skinner said. “Case in point, NERSC has many more applications than most computing centers and we can’t always dig down to the deepest levels for each code. Consequently, tools that can profile with little overhead are especially valuable. There’s a lot of cross-pollination that can go on during these exchange visits.”

For more information, contact David Skinner at dskinner@nersc.gov.

Combustion Research *(continued from p.1)*



Direct numerical study of flame-wall interactions and wall heat transfer. Instantaneous snapshots allow a detailed observation of flame-extinction events.

software components with a closely related project headed by Habib Najm at Sandia National Laboratories.

Trouvé also noted that the team-based, interdisciplinary approach fostered by SciDAC has helped assemble the necessary experts, such as applied mathematicians, computer scientists and application scientists, who are needed to meet the challenges associated with the complexities found in running scientific software on MPP platforms.

In his group’s project, Trouvé said that the applied mathematicians contributed the development of new algorithms; the computer scientists redesigned the software to fit into the standardized GrACE and CCA frameworks, and the combustion scientists contributed in the development of new physical modeling capabilities, including thermal radiation, soot formation and liquid sprays.

“SciDAC has also provided a critical mass of users, which thereby facilitates new software developments, maintenance and upgrades,” Trouvé said, adding that eight other groups are now using the software developed by his group.

For more information, contact Arnaud Trouvé at atrouve@eng.umd.edu or read the project’s most recent update at <http://www.osti.gov/scidac/updates2004/bes_10.html>.

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they tested their applications. The group, according to researcher Timur Linde, expects to typically use 512 to 1,024 processors, then use 4,096 or more processors for their final calculations.

Although only in their testing phase, the group has already achieved significant results.

“We have calculated three Type Ia supernova explosion models, including one octant model with 8 km resolution,” Linde reported. “This was our test run on Seaborg, but it is worth mentioning that this run would already be state of the art in this field.”

The group has also calculated one full-star model with 8 km resolution and 30 km ignition regions and one full-star model with 8 km resolution and 50 km ignition regions.

“These last two runs are the first of this kind ever calculated—no group other than ours has produced full-star simulations before,” Linde said. “We are now moving to 4 km and 1 km resolution models, which will require at least 512 processors and possibly the whole sytem at times.”