National Center for Computational Sciences Snapshot
The week of December 4, 2006

Combustion Researchers Resolve Turbulence Issue

Combustion researchers using the National Center for Computational Sciences' (NCCS') Jaguar Cray XT3 system have answered a question that defied resolution by experiment.

Specifically, they have shown that the effect that causes a lean, premixed flame to thicken under intense turbulence is more important than a competing effect that causes the flame to become thinner. The finding will eventually increase the efficiency of stationary gas-turbine power generators.

Experiments aimed at identifying the dominant effect produced contradictory results: Some concluded that small eddies that make the flame thicker were more important, while others concluded that the dominant effect was large-scale straining that make the flame thinner. Simulations carried out by the project "High-Fidelity Numerical Simulations of Turbulent Combustion—Fundamental Science Towards Predictive Models" were able to provide an answer and will help answer an even more important question: How fast can these flames burn and remain stable?

The flame being studied contains relatively high concentrations of air and low concentrations of fuel. This "lean" flame burns at a lower temperature and produces less nitrogen oxide (NOx) than a richer flame. Lean combustion has the potential to reduce NOx emissions—which have been linked to acid rain, production of ozone, and aggravation of asthma—from stationary gas turbines.

The simulations fully resolved all turbulence and flame scales. "This work produces highly accurate data that model developers can use to validate and improve models used in engineering computational-fluid-dynamics codes," said Ramanan Sankaran, the NCCS liaison to the project.

The project, led by Jacqueline Chen of Sandia National Laboratories, receives funding from the Scientific Discovery through Advanced Computing program. It also explores stabilization of lifted jet flames and soot formation in turbulent, nonpremixed ethylene flames.

The largest of the simulations used 200 million grid points and ran over the course of 7 to 10 days on 7,200 cores, or about three-quarters of the Jaguar system. Over the last year the simulations have generated 30 terabytes of data.

Acceptance Testing Begins on Cray XT4

All 68 cabinets of the new Cray XT4 have arrived at the NCCS and have been installed on the second floor of the center. The addition of the XT4 will eventually allow the NCCS to produce a machine that performs at a rate of 250 teraflops, or 250 trillion calculations per second.

The High-Performance Computing Operations Group, responsible for the installation, configuration, and administration of NCCS systems, has started the rigorous process of acceptance testing. Working hand in hand with personnel from Cray, the staff is proceeding with hardware evaluation and testing of the machine's operating system.

As part of the acceptance testing, a wide range of diagnostics is being completed to ensure that the hardware is functioning properly. Assessments being carried out on the system include stability, functionality, and performance testing. This includes the use of a locally developed test harness that runs and tests several key applications, as well as testing of several codes on the XT4 by in-house users as well.

Once acceptance testing is completed, current Jaguar users will be transitioned to the new system while the existing Cray XT3 is moved from the first to the second floor of the Computational Sciences Building.

The two systems will be combined in early 2007, resulting in a supercomputer capable of more than 100 teraflops.

Workshop Looks to Future of Biomolecular Simulation

Three dozen research scientists from the United States and Japan will gather at Oak Ridge National Laboratory this month for a 2-day workshop on the future of biomolecular computer simulations.

The NCCS is sponsoring the December 11 and 12 event, entitled "Workshop on the Future of BioMolecular Simulations: From Ab Initio to Nano-molecular Machines." It will give researchers an opportunity to discuss their needs as the field moves into the era of petascale computing. It will also give them a chance to share their ideas with vendors and agencies such as the Department of Energy, National Science Foundation, and National Institutes of Health.

The workshop aims to create three concise plans:

1. a research roadmap defining the scope of the problems and the infrastructure required to tackle large-scale, long-timeframe, and more chemically accurate molecular simulations in the next 5 to 10 years;
2. a software roadmap describing the highest-priority algorithms and codes now available, their limitations, and the highest-priority development needs; and
3. an infrastructure roadmap outlining expected design priorities and specifications for computing platforms suitable for the above problems.

Individual sessions have titles such as "classical simulation codes, strengths, and limitations"; "the future of semi-empirical and ab initio calculations"; and "future machine architecture and software requirements."

More information is available at http://nccs.gov/news/workshops/biomolecular06/.