National Center for Computational Sciences Snapshot
The Week of April 30, 2007

Astrophysicists Close In on Exploding Stars

Researchers come a step closer to explaining the core-collapse supernova

A research group led by Anthony Mezzacappa of Oak Ridge National Laboratory (ORNL) is using the National Center for Computational Sciences' (NCCS's) Cray XT4 Jaguar supercomputer to solve one of the universe's enduring mysteries.

The group is homing in on details of the core-collapse supernova, the explosion of a star at least 10 times as massive as the sun. In doing so, it is helping to explain an indispensable source of elements in the universe and in our own world.

The death of a massive star is determined by the details of its evolution. Over millions of years, the star burns through its nuclear fuel, fusing atoms to create increasingly heavy elements. These elements form into layers—from hydrogen at the surface through helium, carbon, oxygen, silicon, and iron at the core. The process hits a roadblock at iron, which does not create energy when atoms fuse. Eventually, the iron core becomes so heavy that it collapses under its own weight and becomes a mass of neutrons.

The shock wave created when the core reaches the limit of its collapse eventually blows most of the star out into space, but that shock wave stalls as material from the star rains onto the collapsed core. The key mystery of the core-collapse supernova is how the shock wave gets revived to blow the star apart.

While researchers had assumed that the shock wave is revived while it is still within the iron layer, Mezzacappa's research suggests that it is not actually reinvigorated until the infalling oxygen layer reaches it.

"What we have discovered is that at late enough times, the infalling matter will move the shock into the oxygen layer, and that's where the shock wave revives," Mezzacappa explained.

This explanation would add two elements to help explain how the shock wave revives. The first is that the oxygen layer is less dense and falling more slowly than the layers preceding it, meaning the shock wave has less work to do as it pushes toward the surface. The second is that silicon and oxygen falling behind the shock wave undergo nuclear fusion, and the energy they create pushes the shock wave from behind.

The process happens in a fraction of a second, which is auspicious for researchers simulating a process that ranges in scale from the size of the earth's orbit around the sun to the interaction of subatomic particles. Mezzacappa's team, which includes Stephen Bruenn of Florida Atlantic University, John Blondin of North Carolina State University, NCCS scientific liaison Bronson Messer, and Raphael Hix of ORNL, was able to reach its

conclusion by simulating the star for about 0.8 second after the bounce, which is about twice the time previously simulated by his team and others.

"If you look at the dynamics up to that point (0.3–0.4 second), not a lot is going on." Mezzacappa explained. "What we're finding is you just have to run it long enough. Once the shock gets into the oxygen layer, things develop and change."

The team has so far used the 119 teraflops Jaguar system to verify this new explanation in two dimensions using a star 11 times the mass of the sun (i.e., 11 solar masses). The team plans to continue its two-dimensional simulations with 15- and 20-solar-mass stars before repeating the process in three dimensions.

Mezzacappa stressed that the results are preliminary. Nevertheless, he believes they will be important.

"The story that's unfolding is new and exciting," he said. "We don't expect this story to go away in 3-D."

Mezzacappa noted that this research would be impossible without modern supercomputers. Jaguar is the world's most powerful system for open scientific research, and yet the team's simulations took the equivalent of two solid weeks.

"The first issue is, can you run these simulations?" he said. "There are people who don't have these resources, where it would take months or years to run."

Workshop to Show Users How to Get the Most Out of Future Supercomputers

Hands-on event will pair researchers with experts from ORNL and Cray

Experts from the NCCS and Cray, Inc. will work directly with researchers during a 3-day workshop focused on ORNL's upcoming multicore systems.

The NCCS Scaling to Petaflops Workshop, which will help researchers use the center's enormous computing resources to deliver scientific breakthroughs, will be held July 30 through August 1 at ORNL. During this hands-on event, NCCS and Cray experts will meet individually with computational scientists to ensure they can take full advantage of upcoming Cray systems using quad-core processors.

The NCCS will be moving to quad-core supercomputers as it aggressively upgrades its computing power. The center's XT4 Jaguar system will be upgraded from dual-core to quad-core processors in late 2007, taking it to a peak performance of 250 teraflops. In addition, the center will install a petaflops Cray system in 2008 that will also contain quad-core processors. These unique, state-of-the-art systems will enable users to run simulations of unprecedented complexity.

While these systems will be similar to the current dual-core Jaguar, users must nevertheless look closely at the ability of their applications to use more cores per socket because the upgrades will increase CPU speed more than either memory or network bandwidth. The workshop will help them identify areas that might be bottlenecks on the upcoming architectures as well as new algorithms that could aid in scaling the applications to higher node counts.

NCCS and Cray staff will explain the benefits of multithreading application programming interfaces such as OpenMP and POSIX Threads, which can be used to alleviate the limited memory and network injection bandwidth for each node. They will also help users investigate ways the applications can be modified to achieve optimal I/O performance for running larger core counts.

The workshop is open to users and potential users of Cray XT systems. For more information visit http://nccs.gov/news/workshops/fy07scalingworkshop/index.html or contact Don Frederick at frederickdm@ornl.gov.

Fusion Code Breaks Another Record on Jaguar

Simulation moves 74 billion particles

Researchers at the Princeton Plasma Physics Laboratory (PPPL) have once again used the NCCS's Jaguar supercomputer to set a performance record for their application for studying plasma microturbulence in a fusion reactor.

PPPL's Stephane Ethier was able to run the Gyrokinetic Toroidal Code on nearly 23,000 processor cores and push 11.6 billion particles one step per second. The previous record, 5.4 billion particles per second per step, was set on Jaguar in autumn 2006, before the system was upgraded to a peak performance of 119 teraflops.

The team's recent runs also set another record on Jaguar—moving a total of 74 billion particles. Ethier noted that the massive number of particles Jaguar is able to handle will allow the team to eventually simulate additional ion species and kinetic electrons simultaneously. He noted that the high particle-handling capability also allows the team to reduce the amount of statistical noise in the simulations and probe the inner workings of core turbulence at levels of fidelity that were to this point unachievable.

NCCS Staffers Reach Out to Community

Space institute, community group hear about center's work

Representatives from the NCCS have been active in carrying the center's message to interested groups. NCCS Director Buddy Bland was invited to the University of Tennessee Space Institute in Tullahoma to discuss the center's work.

Bland presented an April 18 seminar to students and faculty on high-performance-computing activities, capabilities, and possibilities. He discussed the Cray XT4 Jaguar system's standing as the most powerful system in the world for open science research as well as the history of high-performance computing at ORNL.

Bland also discussed current systems, plans for the future—including a Jaguar upgrade to 250 teraflops in 2007 and the installation of a system capable of 1 petaflops by the end of 2008—and challenges presented by the systems.

Bobby Whitten of the User Assistance and Outreach Group also discussed the NCCS's work when he spoke on the same day to the Friends of Oak Ridge National Laboratory, a group of Oak Ridge retirees and others interested in the work being performed at ORNL. About 40 people attended the meeting at the UT-Battelle Conference Center in which Whitten described the NCCS systems and the research being carried out on them.

ORNL to Host Exascale Town Meeting

Researchers look to build on dramatic gains in computing

ORNL will host a diverse group of prominent computational scientists in a 2-day town-hall meeting in May to help guide research objectives in the coming years.

The meeting, scheduled for May 17 and 18, will help focus a 10-year initiative of the U.S. Department of Energy (DOE) Office of Advanced Scientific Computing Research (ASCR) known as Simulation and Modeling at the Exascale for Energy, Ecological Sustainability, and Global Security (E3SGS). The initiative aims to take the dramatic advances in computing power and computational science that are being achieved at DOE facilities and apply them to some of the world's most important challenges.

The town-hall meeting will include a variety of breakout groups that pinpoint goals for research in a wide variety of critical areas. Topics will include the following:

- exploration of global ecosystems;
- development of renewable energy sources;
- simulation and modeling of the earth's climate;
- development of secure, long-term nuclear energy;
- exploration into the roles played by microbial life and ways to adapt these life forms for human use;
- development of a "cosmic simulator" to capitalize on dramatic gains made in astrophysics; and
- development of hardware and software approaches to accelerate the gains being made in modeling and simulation.

The ORNL event will be the second of three E3SGS town-hall meetings being coordinated by ASCR. The first was held at Lawrence Berkeley National Laboratory in mid-April, and the third will be held at Argonne National Laboratory May 31 and June 1.

Registration for the ORNL meeting is open and can be made at http://computing.ornl.gov/workshops/town_hall/index.shtml.

Network Upgrade Helps Researchers Get Data In and Out of NCCS

Links to ESnet and Internet 2 boosted to 10 gigabits

The speed of data moving into and out of the NCCS increased by up to 20 times on April 11 with a major network upgrade, allowing researchers to handle the increasingly large files generated by the center's state-of-the-art supercomputers.

The center increased its connections to the Energy Sciences Network and Internet2, a high-speed network focused on U.S. universities. The NCCS now has two 10-gigabit connections to the networks, meaning it can send and receive up to 20 billion bits of information each second. The connections replace a single 1-gigabit connection.

According to Josh Lothian of the NCCS, the upgrade has been in the works for more than a year.

"We are very excited about this," he said. "The upgrade will enable our researchers to transfer data to and from their sites with much greater speed."