National Center for Computational Sciences Snapshot The Week of March 10, 2008

Big Machines Model Small Wonders

NCCS supercomputers shed light on nanotechnology

According to Moore's Law, the number of transistors that can be placed on a chip doubles about every 2 years. That means that everything is getting smaller and faster. Nowadays devices are so small, in fact, that it is difficult to study them with theory and experiment alone. Instead, researchers are turning to supercomputers to better understand today's most powerful miniature marvels.

Just ask Gerhard Klimeck, a leading researcher in the field of nanotechnology. The devices in his line of work are really tiny—so tiny that they are on the order of a couple hundred atoms thick. With devices this small, says Klimeck, "electrons behave like quantum mechanical waves. They go around corners and interfere with each other." Klimeck's primary research involves gaining an understanding of how electrons move through semiconducting materials. More specifically, he is interested in making electronic devices smaller and more powerful.

Due to the scale involved, simulating these devices and materials is possible only with extremely powerful computers, such as the Jaguar Cray XT4 at Oak Ridge National Laboratory's (ORNL's) National Center for Computational Sciences (NCCS).

For instance, Klimeck's nanoelectronic modeling code (NEMO) has scaled extremely well on the NCCS's Jaguar. NEMO 3D was benchmarked on a range of high-performance computing (HPC) platforms, five of which ranked in the Top500 list of 2007. An 8-million-atom simulation scaled to more than 8,000 cores ran better on Jaguar than other comparable systems. In fact, it ran so well that Klimeck used the data to bolster his case for a PetaApps award, a National Science Foundation program to identify research that is best suited to petascale computing architectures. His NEMO 1D code, when scaled to 23,000 cores, did in 1 hour what would have taken a serial machine 100 days. A key metric of device engineering, says Klimeck, is reduced wall-clock time. "For real device engineering," he says, "you need turnaround that happens in 1 hour."

Klimeck has been working on the NEMO codes for 18 years. Eventually, he will combine the capabilities of both NEMO 3D and NEMO 1D in a new code dubbed OMEN. This code, says Klimeck, "will scale to 500,000 cores and more and tackle the very relevant problem of semiconductor device scaling. This theoretical and numerical problem makes a grand challenge for petascale computing."

Klimeck describes his research at the NCCS as "very responsive." Besides Jaguar's stability, he cites the "professional people" as another benefit of using the NCCS facilities. "To me it is important to run very high-end simulations so we can calibrate solutions that more engineers can access," says Klimeck. Judging from his work at the NCCS, mission accomplished.

HPCwire Interviews Doug Kothe

NCCS Director of Science waxes petascale

HPCwire contributing editor Steve Conway recently sat down with Doug Kothe, the director of science for the NCCS at ORNL, to discuss how his organization is preparing to enter the era of petascale computing.

The NCCS recently conducted a comprehensive user survey to gauge the needs and capabilities of researchers interested in running applications on the organization's petascale machines, scheduled to come online in 2008. "The survey's main goal was twofold: first, to elicit and analyze scientific application requirements for current and planned leadership systems out to the petascale and second, to identify applications that would qualify for early access to ORNL's 250-teraflop and 1-petaflop systems," said Kothe.

While computing at the petascale does present enormous challenges, the potential payoff is huge. "For the CHIMERA astrophysics code, the expectation is to increase the number of variables from 63 today to more than 1,000," said Kothe, when comparing a 1-petaflop machine to a 25-teraflop one. "With the LAMMPS biology code, today the users are modeling the dynamics of 700,000-atom systems for 5 to 10 nanoseconds of model time per day of simulation time. With a petaflop system, users hope to increase to modeling multimillion-atom systems for 0.1 to 1.0 microsecond per day of simulation time."

Kothe cited the difficulty of conducting such a thorough survey, but remained optimistic about the future. "The HPC community has an opportunity to come together to maximize the science output of tomorrow's hardware systems," he said. "We all have good ideas, and we can share them and come together on this. . . . HPC centers will collaborate to optimally map the applications to the platform and continue to work with the researchers and vendors to ensure that the science demands of today and the future are met with leadership computing resources."

The complete interview can be found at http://www.hpcwire.com/hpc/2150728.html

What a Long, Strange Trip It's Been

NCCS researcher tells history of ORNL

On February 22, Bobby Whitten of the NCCS was the speaker at the University of Tennessee Science Forum, a weekly presentation of a specific scientific issue open to the interested general public.

Whitten outlined the colorful history of ORNL and more specifically the history of the growing NCCS. Taking his audience from the laboratory's early days of secret projects to its current status as a research and development powerhouse, Whitten gave a detailed account of the institution’s chronology, complete with photographs and little-known anecdotes.

The second half of the presentation primarily concentrated on the NCCS and its growing presence in the supercomputing community. First Whitten explained the increasing role of supercomputing in tackling today’s most pressing scientific challenges, such as developing sources of clean energy and gaining a greater understanding of the underpinnings of astrophysics. Then he moved on to describe the impacts that will be possible with tomorrow’s generation of elite computers. He wowed the audience with numbers nearly incomprehensible to the human brain, such as the fact that a petascale computer will be capable of performing a thousand trillion (quadrillion) calculations per second.

“The UT Science Forum was an outstanding venue [in which] to share ORNL’s rich scientific research history,” said Whitten after the event. “It was my pleasure to be a part of the forum as a representative of the NCCS.”