Oak Ridge Leadership Computing Facility Snapshot
The Week of January 25, 2010

Turning Exhaust into Power

ORNL supercomputer shines light on thermoelectric material

As it turns out, pushing electrons to the side can turn the tailpipe of your car into an electric generator.

A research team led by General Motors physicist Jihui Yang has used Oak Ridge National Laboratory's (ORNL's) Jaguar supercomputer to nail down the arrangement of atoms within a promising thermoelectric material. In the process Yang and colleagues from the University of Las Vegas–Nevada, ORNL, and Brookhaven National Laboratory (BNL) have advanced the causes of both materials research and vehicle efficiency. They report their findings in the October 2, 2009, issue of the journal *Physical Review Letters*.

The material, known by the acronym LAST, is a mixture of lead and tellurium speckled with small clumps of silver and antimony atoms. These clumps—known as nanoprecipitates—subtly alter the flow of electrons and phonons (units of vibrational energy) through the material, allowing it to convert heat energy directly into electricity. A conventional car engine loses 70 percent of the energy it generates to waste heat. Thermoelectric materials used in the car's exhaust system promise to capture and make use of that energy.

LAST is not new; in fact, it was discovered in the 1950s. But while researchers have long suspected its thermoelectric properties depended on the layout of silver and antimony atoms within the lead-telluride material, they only recently determined that the silver and antimony formed nanoprecipitates rather than blending evenly into the material.

Further, assumptions made for the atomic arrangement within the nanoprecipitates were inaccurate. Yang's team used results from Jaguar to determine that one of the constituents—silver—sits off to the side from its expected position.

Silver to the side

"Imagine you have a cube," Yang explained. "You have atoms populating the center, every corner, and the six surfaces. These atoms are alternating lead and tellurium. That's your basic structure.

"Before our work, people assumed that when you introduce silver-antimony into the material, silver will replace lead, and antimony will replace lead. Our work shows that silver actually will not replace lead. Silver will sit somewhere in the middle of the two adjacent atomic positions. So we pinned down the exact atomic arrangement in the nanoprecipitates and found the results are totally different from what people assumed them to be in the past. We now understand the growth mechanisms of these nanoprecipitates."

The team conducted its investigation with software known as the Vienna Ab-initio Simulation Package, or VASP. With VASP it was able to calculate the structure of the material directly from the principles of quantum mechanics, testing hundreds of possible structures until it found the one with the lowest energy (the structure it would adopt in nature). Yang and colleagues were able to validate their computational results using transmission electron microscopy (TEM) data from BNL on single-crystal samples. According to Yang instruments at BNL were able to resolve the structure of the material to less than an angstrom, or one ten-billionth of a meter.

Recycling energy saves gas

Thermoelectric materials promise an energy boon because vehicle engines are not very efficient at using the energy contained in gasoline or diesel fuel. The heat that goes out the tailpipe represents lost energy. But thermoelectric materials can move electrons from the hot side of the material to the cold side, where they are converted into electricity.

In a hybrid vehicle, this extra power would be routed back to the electric motor to power the vehicle, while in other vehicles it could be used to run components such as the electric water pump, lights, radio, and global positioning system. The result would be a vehicle with substantially improved fuel economy, potentially saving hundreds of millions of gallons of fuel each year.

“The material [LAST] is potentially a good thermoelectric material because it has very low thermal conductivity,” Yang said. “Our ultimate goal is to link this structural property to the phonon density of states, the heat-propagating property of the material. Hopefully this work will provide us with a better understanding of why the thermal conductivity of this material is so low and then, maybe, give us some predicting power.”

The project had to simulate an especially large system—more than 1,700 atoms—because the silver-antimony clumps collect in nanoprecipitates, and these clumps are relatively few and far between.

“This is a grand challenge for material science,” Yang said, “to determine the material structure at the atomic level of nanostructured materials. On a computational level, for the structural calculations you need to have a huge supercell as part of the density functional theory calculation to be able to fully relax your nanoprecipitates, which are comparable in sizes to those observed under TEM in real samples, so that the energetic calculations are done accurately.”

While it was certainly an accomplishment to work out the atomic structure of this material, the work is not over by any means. Yang’s group is currently investigating the thermal and vibrational properties of LAST, a job that requires even more computing power. Eventually these simulations will help researchers design materials computationally, saving the expense of manufacturing for only those that show the most promise.

<u>Energy Savings Front and Center at ORNL Supercomputing Center</u>
Laboratory reaping benefits of conservation measures

ORNL's Cray XT5 Jaguar supercomputer is allowing researchers to tackle some of today's most daunting energy challenges. Biofuels, nuclear fusion, and next-generation nanotransistors are just a few of the areas being explored on the world's fastest computing system.

Due to their complexity, however, these problems can be addressed only on a machine with Jaguar's raw computing power of more than 2 petaflops, or 2 thousand trillion calculations per second. Achieving that sort of speed is no easy task; maintaining a machine of this magnitude is nearly as daunting as the problems it helps to tackle. Like other leading supercomputers, Jaguar requires robust cooling and support infrastructures that in turn require substantial power consumption. Finding tomorrow's energy solutions requires substantial energy consumption today.

ORNL's computing complex, which also includes the world's third-fastest supercomputer, known as Kraken, has recently begun to reduce its resource footprint by harnessing energy savings wherever possible. As a testament to this philosophy, the laboratory now operates one of the most efficient petaflop-plus high-performance computing (HPC) centers in the country. In other words, the laboratory gets the most computing bang for its power buck among the leading HPC centers, allowing it to tackle big science more quickly and efficiently.

This is a result of innovation across ORNL's entire HPC spectrum, from the building that houses the world's most powerful computing complex (with more than 3 petaflops of computing power) to the machines themselves.

It all starts with the building. ORNL's Computational Sciences Building (CSB) was among the first Leadership in Energy and Environmental Design (known as LEED)–certified computing facilities in the country, meaning that its design satisfies criteria used by the U.S. Green Building Council to measure the efficiency and sustainability of a building.

The CSB, which houses Jaguar, Kraken, and several smaller systems, has a power usage effectiveness (PUE) rating of 1.25— a recent study of 22 large-scale data centers by Lawrence Berkeley National Laboratory reflected an average PUE of 1.83 (the closer to 1 the more efficient). This metric means that for every 1.25 megawatts of energy consumed by the CSB, 1 megawatt is used to power the machines and accelerate science. The other 0.25 megawatts is used for lighting, the dispersion of heat generated by the machines, and various other support equipment. The CSB's PUE rating makes it almost 32 percent more efficient than its average counterpart, a direct result of the laboratory's energy conservation measures.

Take the computer room, for example, where the machines are housed. It's sealed off from the rest of the building by a vapor barrier to reduce the infiltration of humidity. The air pressure inside the computer room is slightly higher than the surrounding area so air will flow out of the computer room without outside air flowing in.

Because ORNL is located in an area of the country with high humidity, keeping moisture out of the air is a priority, one that the building was designed to tackle as efficiently as possible, said Oak Ridge Leadership Computing Facility (OLCF) Project Director Buddy Bland. Too much moisture in the air can lead to water condensation on equipment, while too little can cause static electricity to build up—both of which can be problematic for a room filled with expensive electronics. Removing moisture from or adding it to the air uses a lot of power, so keeping the humidity stable is a great tool for reducing energy consumption.

But the innovation doesn’t stop with the building. There is plenty more under the roof.

When it comes to the machines, it’s all about keeping them cool. Jaguar and Kraken’s combined 288 computing cabinets emit plenty of heat, and the room that houses the world’s fastest supercomputers must stay cool. In its latest attempt to more efficiently cool Jaguar and the University of Tennessee–managed Cray XT5 Kraken, the laboratory recently upgraded all of the fans in the computer room’s air conditioning units (CRUs), which are charged with helping to keep the computer room cool despite the heat generated by the machines.

The fan is essentially a 5-horsepower motor within the CRU that pushes air through the CRUs’ coils to remove the heat, said Jim Rogers, director of operations for the OLCF. The new fans allow the center to run the CRUs at a more optimum speed, namely from 60 to 80 percent of their peaks. Instead of being on or off, said Rogers, the CRUs can now “operate more efficiently and in unison.” This upgrade will pay for itself in a year and a half, after which it will save the laboratory $150,000 every year throughout the life of the HPC center.

Combine that with Cray’s latest ECOphlex cooling system, used for both Jaguar and Kraken, and the savings start to add up. The combination of air- and refrigerant-based cooling used by ECOphlex is much more efficient than traditional systems, which rely almost solely on air for temperature control.

ECOphlex also allows ORNL to reduce the amount of chilled water used to cool Jaguar. Considering that thousands of gallons of water per minute are necessary to keep Jaguar cool, a reduction in volume means a proportionate reduction in cooling costs. Simply put, warmer water can mean big energy savings for the laboratory and the taxpayer.

These are just a few of the measures ORNL has taken to ensure its supercomputing program isn’t superfluously greedy when it comes to resources and taxpayer dollars. Because when it comes to solving the nation’s most pressing energy problems and tackling big science, every little bit counts.

OLCF Hosts SciApps-10 Workshop

Interdisciplinary leadership computing researchers share their petascale knowledge on the road to the exascale

August 3–6, 2010, the OLCF will host current and potential leadership computational researchers as they share knowledge and best practices on the implementation of a wide range of computationally intensive applications at the SciApps-10 workshop. The theme of the workshop will be “challenges and opportunities for scientific applications: learning to sustain the petaflop with eyes on the exaflop horizon.”

“What we want to do with this workshop is look at various domains that have been targeted as scientific drivers for the exascale,” explained Ricky Kendall, leader of the scientific computing group at the National Center for Computational Sciences, where the world’s fastest supercomputer—the Cray XT5 known as Jaguar—is housed in the OLCF. Along with the Argonne Leadership Computing Facility in Illinois, the OLCF aims to advance the state of HPC by providing scientists with the most powerful computational tools available, including not only supercomputers, but also state-of-the-art data analysis and visualization technology and highly trained staff who work closely with scientific teams to maximize scientific results.

An endowment from the American Recovery and Reinvestment Act allowed the OLCF to upgrade Jaguar’s four-core processors to six-core ones in late 2009, giving the system a peak performance speed of 2.2 thousand trillion calculations per second, or petaflops. Kendall explained that there is much groundwork to be laid before reaching the exascale, and this workshop seeks to build that foundation. (One exaflop is equal to one quintillion calculations per second, or 1,000 petaflops.)

“We’re looking at what you have to do in these domains—either algorithmically or computationally—to get to 20 petaflops and then to 100 petaflops,” said Kendall. “The title of the workshop is ‘With Eyes Toward the Exascale,’ so really we’re trying to focus on the two steps before we reach exascale.” These “two steps” are called near- and medium-term requirements, which refer to the infrastructure that an application must possess in order to run at roughly 20 and 100 petaflops, respectively.

In addition to the near- and medium-term requirements, leading computational scientists will discuss leadership computing allocation programs, HPC architecture, scientific mission goals, software engineering practices, and case studies for nearly a dozen leading-edge applications in climate science, astrophysics, materials and nanoscience, chemistry, biology, and nuclear energy.

“The applications themselves live many more years than any given piece of hardware,” said Kendall of the overall importance of the SciApps-10 workshop. Three applications that will serve as case studies at the workshop are able to sustain a petaflop or more on Jaguar, serving as examples of codes with the flexible infrastructures necessary to achieve exascale computing.

“The infrastructure of these codes was designed to take advantage of very large-scale machines, but it doesn’t happen overnight,” Kendall explained. “So taking the lessons from those kinds of development projects, listening to what those domains have in place now and where they’re going and the kinds of things they need to do, hopefully we can come up with a least common denominator, a minimum level of requirements that you need to be able to have a really scalable code.”

For more information and to register for the workshop, please see http://www.nccs.gov/user-support/training-education/workshops/sciapps-10/.