Oak Ridge Leadership Computing Facility Snapshot
The Week of May 17, 2010

Jaguar Explores Carbon–Water Union

Researchers hit jackpot with CASINO code

Some research has potential that's difficult to quantify. The ramifications of a better understanding of a particular phenomenon can sometimes reverberate throughout science, making everlasting waves in multiple arenas.

Take the seemingly trivial properties of a water molecule on graphene, or a single layer of graphite. Water is everywhere, as is carbon. Big deal, right? Actually, it is. Understanding the adsorption, or accumulation, of a water molecule on graphene could influence everything from hydrogen storage to astrophysics to corrosion to geology.

In 2009 a team made up of Dario Alfe, Angelos Michaelides, and Mike Gillan of University College London (UCL) used the Oak Ridge Leadership Computing Facility's (OLCF's) early petascale science period to obtain a full-binding energy curve between water and graphene, research that will impact multiple domains and could only be performed on the world's fastest supercomputer. The project is a collaboration between Oak Ridge National Laboratory (ORNL) and UCL and is supported by the Engineering and Physical Sciences Research Council of the United Kingdom.

Adsorption is the accumulation of atoms or molecules on the surface of a material. The process is possible because unlike the atoms in a material that bond with one another, surface atoms are not wholly surrounded by other atoms and can attract adsorbates, in this case a water molecule.

While the process may sound a bit strange, it turns out that this is the case with most natural surfaces—they are covered by a film of water. It is for precisely this reason that this research is so fundamental. "Water interacts with every surface that we see," said Alfe.

Because of the large numbers of particles and multiple variables involved in the interaction, these systems are difficult to describe. However, science could greatly benefit from a more precise explanation of such systems simply because they occur so often in the natural world.

And as science benefits, so do we. For instance, a better understanding of this particular adsorption process could pave the way for more efficient hydrogen batteries, an integral part of a potential clean energy economy; catalysis, the process of adding an agent to initiate a chemical change, is an important step in countless industrial processes—it could be streamlined to make products safer and cheaper; and adsorption is key to understanding lubrication to reduce friction between moving parts, which plays a role in nearly every nook and cranny of our transportation sector.

And that's just energy. The research will likewise shed light on some of science's most fundamental questions, such as how the Earth forms materials at the extreme conditions deep in its interior, or how molecules form in outer space's interstellar medium. And the methodological advances that result will lead to better predictions of the interaction of water with other materials such as clay particles and proteins, both of which are central to biological and environmental research programs.

Skinning Schrödinger's Cat

Alfe and his team received 2 million hours on Jaguar to calculate a water molecule's adsorption energy and geometry on a sheet of graphene. Using the quantum Monte-Carlo (QMC)–based CASINO code developed at Cambridge University, the team produced an unprecedented depiction of water-graphene adsorption.

By calculating the adsorption energy and geometry in 30 individual steps as the molecule moves closer to the surface, the team made history. "We've been able to obtain a full-binding energy curve between water and graphene," said Alfe. This breakthrough was only possible using CASINO's QMC-based methodology.

Using QMC methodology scientists attempt to solve the quantum mechanical Schrödinger equation, which describes the evolution of a quantum state over time, by simulating a mathematically equivalent random process, such as flipping a coin over and over to predict the chance of achieving heads. The more times one flips the coin, the more precise the prediction.

While there are several ways to solve the equation, QMC delivers the most accurate representation. It is computationally intensive, though, requiring the generation of random numbers across tens of thousands of compute nodes—a technique 1,000 to 10,000 times more expensive, but 10 times more accurate—than standard methods such as density functional theory (DFT).

These standard tools are "okay in giving you answers about the interaction energy between molecules and surfaces where the interactions are strong," said Alfe. If the interaction is weak one must look elsewhere for answers, hence the need for QMC. "QMC is more suited to Jaguar's architecture," said Alfe. Furthermore, he added, it is more befitting to leadership-class machines due to its complexity, and while it is currently more expensive, in the future it will be the more common method in conjunction with the advanced speed of modern supercomputers.

Fortunately, QMC and Jaguar make a good match. CASINO is very parallel in nature, regularly running on 10,000 to 20,000 cores with almost perfect scaling, making it much more parallel than its DFT counterparts. In fact, the researchers recently scaled CASINO to 40,000 cores on Jaguar and envision additional improvements that will enable the code to scale to more than 100,000 cores, making it one of the premier codes in the world.

QMC was also relatively easy to port to Jaguar, said Alfe, primarily because the application was previously running on Hector, a Cray XT4 located at the University of Edinburgh. Given the similar platforms, the researchers didn't even have to recompile their code. And from the looks of things, the team is pleased with Jaguar's performance.

"Jaguar is a fantastic machine," said Alfe, "allowing us to do things we couldn't do without it."

From our origins to our future, Alfe's work on Jaguar cuts a wide swath of discovery. Understanding nature's smallest, most complex systems requires the petascale power of mankind's most powerful computer, making Alfe's project and the OLCF's flagship system a perfect match.

OLCF, NICS Host Spring Hex-Core Workshop, User's Meeting

New and returning users get familiar with upgraded XT5 systems

A workshop was held at ORNL May 10–12 to help new and returning users acclimate to the recently upgraded Cray XT5 machines known as Jaguar and Kraken. Owned respectively by the Department of Energy–supported OLCF and the National Science Foundation–supported National Institute for Computational Sciences (NICS), Jaguar and Kraken underwent the upgrade from four- to six-core processors in late 2009.

"The meeting is a good opportunity to introduce new and returning users to the organizations, and relay to them all of the ways in which the center is available to assist them in producing world-class science results," said Ashley Barker, group leader for the user assistance group at the OLCF.

The first day of the workshop was broken into two tracks—Track I for new XT5 users, and Track II for more experienced users. Day two gave participants the opportunity to tour the Computer Room and the EVEREST (Exploratory Visualization Environment for REsearch in Science and Technology) facility.

The workshop included lectures by staff members of OLCF, NICS, Cray, and PGI [provider of compilers and tools for high-performance computers] on such topics as XT5 architecture and programming, AMD six-core processors, and parallel debugging tools. Daily hands-on sessions allowed participants to access Jaguar and/or Kraken using their own codes while working one-on-one with OLCF and NICS staff members to resolve any issues.

The OLCF Users' Meeting was held on the final day of the hex-core workshop specifically for research groups that have been granted allocations on Jaguar through the INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program. OLCF Users' Council also convened on this day to elect Balint Joo, from Jefferson Lab, as chair. Joo will function as the liaison between users and the OLCF management team.

OLCF Hosts Visualization Software Course

Participants explore the capabilities of VisIt

On May 13 the OLCF sponsored a day-long course on VisIt, a software application for analyzing and visualizing very large simulation datasets. OLCF's Cray XT5 called Jaguar is the world's fastest supercomputer, performing at a peak speed of 2.33 petaflops (quadrillion calculations per second). Executing tasks at such light-quick speeds generates some of the world's largest data sets.

"VisIt is unique in that it can handle the largest datasets that users throw at it," said Sean Ahern, OLCF visualization task leader. "Everything researchers do on a small scale can also be done on huge petascale data sets, and that's a very important [software application] for us to be supporting, maintaining, and training users on."

The course included a general overview of how to use VisIt to access data and create visualizations, detailed discussions about how and when to use VisIt's various plots and operators, how to visualize a subset of a database, and how to create derived variables using expressions. The day concluded with lectures about producing presentation-quality graphics and movies through mastery of session files, color tables, annotations, lighting, and scripting. The course alternated between lecture discussions and hands-on exercises and provided an interactive setting in which to explore the software.

"Mathematician Richard Hamming said, 'The purpose of computing is insight, not numbers,'" explained Ahern. "Science happens when someone takes those numbers and creates pictures, statistics, or graphs, and that gives them some understanding about some scientific principle—whether it's the origin of supernovas or modeling a new design of a nuclear reactor."

OLCF Co-Hosts Proposal Writing Webinar

Oak Ridge and Argonne collaborate to help prospective INCITE researchers

On May 17, the OLCF and the Argonne Leadership Computing Facility (ALCF) teamed together for the "INCITE Proposal Writing Lecture/Webinar". The OLCF's Bronson Messer and James Osborn of the ALCF were on hand at the Argonne National Laboratory to answer questions and provide direction to researchers as the event was broadcast online to over 40 attendees. Over one billion processing hours are available through the INCITE program for 2011. The webinar proved timely for researchers as proposals are due by June 30.

"The webinar allowed several people new to the INCITE proposal process, along with a few old hands, to get specific answers to questions about a proposal and review process that might be a bit different from what they are used to. The informal nature of the webinar was designed to help attendees ask about things they might otherwise not try to explore," said Messer.

A presentation from the event is available for download at http://www.nccs.gov/wp-content/uploads/2010/05/2011_INCITE_CFP.pdf and OLCF staff are available to assist with questions by contacting help@nccs.gov For more information about the INCITE program, see www.DOEleadershipcomputing.org or contact the INCITE manager at INCITE@DOEleadershipcomputing.org

ORNL Hosts Students, Teachers for National Lab Day

Six area middle schools take a field trip to see science in the works

On May 6 ORNL hosted students and science teachers from six area middle schools as they explored applications of science as a part of National Lab Day.

"National Lab Day is a nationwide initiative for scientists and engineers to work with educators to help K-12 students experience discovery science," said James Roberto, ORNL director of Strategic Capabilities. "It's about getting students excited about science, engineering, and mathematics—an essential step toward maintaining our competitiveness."

Approximately 120 students from Vine, Jefferson, Harriman, Coalfield, Clinton and Bearden middle schools visited the Spallation Neutron Source—the most intense pulsed neutron beams in the world—as well as the OLCF. At the OLCF, students were treated to a presentation of visualizations on the EVEREST PowerWall, a large-scale venue for data exploration and analysis. Visualizations included images from global population distributions, climate science, and astrophysics projects run on the world's fastest supercomputer, a Cray XT5 known as Jaguar. Students also learned about superhydrophobics, forensic anthropology, and electric cars.

"We wanted to show students that science is not abstract, describe to them that there are people here using computers to answers scientific questions, and that's just one means of exploration," said OLCF visualization expert Ross Toedte. "There are experiments in labs, people taking measurements in the field, and people developing theories about physics and chemistry. These are all ways of exploring science, and they all synergistically support each other."