Oak Ridge Leadership Computing Facility Snapshot
The Week of October 19, 2009

Scientists Develop New Method to Quantify Climate Modeling Uncertainty
Flux of temperature might play greater role than expected

Climate scientists recognize that climate modeling projections include a significant level of uncertainty. A team of researchers using computing facilities at Oak Ridge National Laboratory (ORNL) has identified a new method for quantifying this uncertainty.

The new approach suggests that the range of uncertainty in climate projections may be greater than previously assumed. One consequence is the possibility of greater warming and more heat waves later in the century under the Intergovernmental Panel on Climate Change's (IPCC) high fossil fuel use scenario.

The team performed an ensemble of computer "runs" using one of the most comprehensive climate models--the Community Climate System Model version 3, developed by the National Center for Atmospheric Research (NCAR)--on each of three IPCC scenarios. The first IPCC scenario, known as A1F1, assumes high global economic growth and continued heavy reliance on fossil fuels for the remainder of the century. The second scenario, known as B1, assumes a major move away from fossil fuels toward alternative and renewable energy as the century progresses. The third scenario, known as A2, is a middling scenario, with less even economic growth and some adoption of alternative and renewable energy sources as the century unfolds.

The team computed uncertainty by comparing model outcomes with historical climate data from the period 2000-2007. Models run on historical periods typically depart from the actual weather data recorded for those time spans. The team used statistical methods to develop a range of temperature variance for each of the three scenarios, based on their departure from actual historical data.

The approach's outcome is roughly similar to the National Weather Service's computer predictions of a hurricane's path, familiar to TV viewers. There is typically a dark line on the weather map showing the hurricane's predicted path over the next few days, and there is a gray or colored area to either side of the line showing how the hurricane may diverge from the predicted path, within a certain level of probability. The ORNL team developed a similar range of variance--technically known as "error bars"--for each of the scenarios.

Using resources at the Oak Ridge Leadership Computing Facility (OLCF), the team then performed ensemble runs on three decade-long periods at the beginning, middle, and end of the twenty-first century (2000-2009, 2045-2055, and 2090-2099) to get a sense of how the scenarios would unfold over the twenty-first century's hundred years.

Interestingly, when the variance or "error bars" are taken into account, there is no statistically significant difference between the projected temperatures resulting from the high fossil fuel

A1F1 scenario and the middling A2 scenario up through 2050. That is, the A1F1 and A2 error bars overlap. After 2050, however, the A1F1 range of temperature projections rise above those of A2, until they begin to overlap again toward the century's end.

Typically climate scientists have understood the range of uncertainty in projections to be the variance between high and low scenarios. But when the error bars are added in the range between high and low possibilities actually widens, indicating greater uncertainty.

"We found that the uncertainties obtained when we compare model simulations with observations are significantly larger than what the ensemble bounds would appear to suggest," said ORNL's Auroop R. Ganguly, the study's lead author.

In addition, the error bars in the A1F1 scenario suggests at least the possibility of even higher temperatures and more heat waves after 2050, if fossil fuel use is not curtailed.

The team also looked at regional effects and found large geographical variability under the various scenarios. The findings reinforce the IPCC's call for greater focus on regional climate studies in an effort to understand specific impacts and develop strategies for mitigation of and adaptation to climate change.

The study was published in the Proceedings of the National Academy of Sciences. Co-authors include Marcia Branstetter, John Drake, David Erickson, Esther Parish, Nagendra Singh, and Karsten Steinhaeuser of ORNL, and Lawrence Buja of NCAR. Funding for the work was provided by ORNL's new cross-cutting initiative called Understanding Climate Change Impacts through the Laboratory Directed Research and Development program.

The paper can be accessed electronically here: http://www.pnas.org/content/106/37/15555

Life and Its Half-Life

Physicists explore what makes carbon-14 tick

For the past half-century, carbon-14 has allowed scientists to date the flotsam of human history: skeletons, ruins, anything that was once part of a plant or body. By existing in all living things and decaying at a steady rate, carbon-14 gives researchers the ability to look at a long-abandoned community, tool, or other artifact and tell us how old it is. And because—for reasons not yet understood—carbon-14 decays far more slowly than most isotopes in its weight class, it allows researchers to confidently date items as far back as 60,000 years.

Now a team led by David Dean and Hai Ah Nam of ORNL is using the unprecedented computing power of ORNL’s petascale Jaguar supercomputer to examine the carbon-14 nucleus. The team, which includes James Vary and Pieter Maris of Iowa State University and Petr Navratil and Erich Ormand of Lawrence Livermore National Laboratory, hopes to both explain carbon-14’s long half-life—about 5,700 years as opposed to a few minutes or even a few seconds—and advance our understanding of what holds all nuclei together.

“Carbon-14 is interesting to us because the physics says it should decay quickly; however, the measured half-life is much longer than expected,” explained Nam, who is a physicist with the OLCF. “The theoretical models people have been using to describe light nuclei such as lithium, with six particles, or boron, which has ten, have been getting some pretty good results. But carbon-14, also a light nucleus, has been elusive.”

Binding a nucleus

A radioactive isotope’s half-life is the time it takes half the atoms in a sample to decay. A simulation that can make us understand why carbon-14’s half-life is so long has the potential to illuminate all half-lives. The task is especially challenging because we don’t quite know how an atom’s nucleus is held together. We know that the nucleus is made up of protons and neutrons, known generically as nucleons. We know further that these nucleons are made up of even smaller particles known as quarks and gluons, which hold together through the “strong force.” The tail of the strong force yields interactions among nucleons that hold the nucleus together. A holy grail of nuclear physics, then, is to theoretically describe the properties of all nuclei, stable and unstable, mundane and exotic, large and small.

Dean and his colleagues have an allocation of 30 million processor hours on Jaguar to dissect the secrets of carbon-14 with an application known as Many Fermion Dynamics, nuclear (MFDn), created by Vary at Iowa State. According to Nam, MFDn is an especially good code for this application because it scales very well. Dean’s team will be using nearly 150,000 of Jaguar’s more than 180,000 computing cores on the project (the entire XT5 partition of the machine), and the application is ready to scale to even more cores as they become available.

The team is using an approach known as the nuclear shell model to describe the nucleus. Analogous to the atomic shell model that explains how many electrons can be found at any given orbit, the nuclear shell model describes the number of nucleons that can be found at a given energy level.

Using the power of the petascale

Jaguar’s unprecedented power allows the team to depart from other nuclear structure studies in several respects. The team is able to take an ab initio (or first principles) approach, working directly from the strong-force interactions of the quarks and gluons within each nucleon. In addition, Dean’s team takes a “no-core” approach that incorporates all 14 nucleons—without assuming an inert set of particles—and includes more energy levels in the model space. And lastly, the simulations go beyond two-body forces, which include the interaction of every nucleon with every other nucleon two at a time, to incorporate three-body forces.

“Previously we could only consider two-nucleon interactions because the number of combinations needed to describe all the different interactions is really big, even for only two particles at a time,” Nam explained.

Jaguar makes these calculations possible not only because it is capable of up to 1.6 thousand trillion calculations a second, making it the world's fastest scientific supercomputer, but also because, at 362 terabytes, it has three times more memory than other system on the planet.

"These types of calculations for carbon-14 were previously not possible because it's a memory-intensive calculation," explained Nam. "Accounting for the three-nucleon force amounts to storing tens of trillions of elements … that's hundreds of terabytes of information."

By making use of Jaguar's power, the team hopes to push us a little closer to an understanding of the atom's nucleus. In doing so it will make carbon-14 an even bigger star than it already is.

ORNL Project Director Speaks at 2009 Computing in Atmospheric Sciences Workshop
Bland discusses challenges facing HPC centers

The OLCF's project director, Arthur S. "Buddy" Bland was a keynote speaker at the 2009 Computing in Atmospheric Sciences Workshop. The workshop, held Sept. 13-16 in Annecy, France, was the ninth meeting in a series of biennial workshops hosted by the National Center for Atmospheric Research, sponsored by the National Science Foundation (NSF). The workshop serves as a forum for international specialists to discuss advances in information technology and the evolving infrastructures that allow scientists to explore atmospheric issues as part of the Earth system model.

Topics discussed at the forum included international progress reports and plans from national weather, climate and research laboratories, challenges facing high performance computing facilities, and performance of weather forecasting and Earth system model applications on high-end supercomputers.

Bland's presentation at the workshop focused on challenges facing high performance computing facilities such as the National Center for Computational Sciences located at ORNL, home of the world's fastest supercomputer for open research, the Cray XT4/XT5 known as Jaguar. As supercomputers continue to grow in speed, their power usage grows as well. Jaguar, currently at 1.64 petaflops, uses over seven megawatts of power, and it is expected that high performance machines will use in excess of 10 megawatts of power in the next few years. Bland discussed the forces that drive the power requirements of high performance systems, the demands placed on the facilities that house these systems, and how ORNL is dealing with both of these issues.

2009 Hex-Core Workshop Announced
Event to focus on recent upgrades to ORNL's Jaguar and Kraken

The OLCF and the NSF-sponsored National Institute for Computational Sciences (NICS) are upgrading their Cray XT5 systems from quad-core to hex-core processors. To assist developers and users as they scale their applications to accommodate the increased number of processors, a workshop has been scheduled at ORNL on December 7-9, 2009. The goal of the workshop is to help users take advantage of the new architecture with a focus on sustained performance.

Topics to be covered include: an overview of the Cray XT5 architecture, discussion of the AMD hex-core CPU unit, Cray XT5 NUMA issues, and tutorials on effective programming for the systems. The workshop will have lectures from the OLCF, NICS, and Cray staff as well as hands-on sessions, offering users the opportunity to work on applications with staff. For more information, including a draft agenda and link to register, please see: http://www.nccs.gov/user-support/training-education/workshops/fall-2009-cray-xt5-hex-core-workshop/