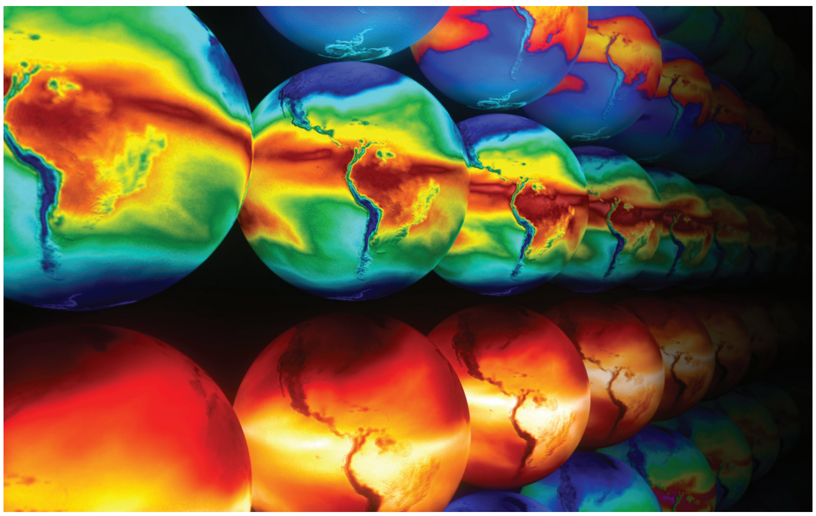
Climate Moves to the Petascale

Unprecedented high-performance computing resources spur partnerships and progress in 2008

Every paramecium, petunia, and person has a stake in global warming. The actions of human stakeholders may make it difficult for the rest to thrive or even survive, indicates the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC), whose authors shared the 2007 Nobel Peace Prize. The report cites about 300 scientific papers that used data from simulations run on supercomputers in 2004 and 2005. It found a greater than 90 percent likelihood that increased greenhouse gases from human activities caused most of the rise in globally averaged temperatures during the 20th century.



These images show the simulated monthly-averaged distribution of the total column water vapor from a high-resolution configuration of the CCSM Community Atmosphere Model. Visualization by Jamison Daniel, ORNL.

In the 21st century the challenge will be to continue to give stakeholders information based on sound science to guide decisions about how to adapt to climate change or lessen its effects. Scientists predict the planet's average temperature will increase 5 to 12 degrees Fahrenheit this century, melting polar ice caps, raising sea levels, fueling extreme weather, displacing populations, shrinking food and water supplies, and driving more than a million species to extinction.

Stakeholders need a crystal ball of sorts to explore future climate scenarios. Among science's best prognosticators are supercomputers, such as those that produced the IPCC data at Oak Ridge and Lawrence Berkeley national laboratories, the National Center for Atmospheric Research (NCAR), and the Earth Simulator in Japan. Supercomputers help stakeholders ask "what if?" What if hurricanes and heat waves become more intense? What if, to displace fossil fuels, we convert forest and food croplands to biofuel crops? What if melting permafrost releases methane, which is 20 times more potent at heating the atmosphere than carbon dioxide? Supercomputers help stakeholders get answers quickly and plan accordingly. DOE, NSF, the National Oceanic and Atmospheric Administration (NOAA), and the National Aeronautics and Space Administration (NASA) are among the U.S. government agencies tasked with assessing climate change. DOE's strength in building and running the world's fastest supercomputers has made its ORNL an interagency crossroads for climate modeling.

"We have started to get the required competencies here at ORNL that build a much stronger program and a capability to respond to national opportunities and national needs in climate," said James J. Hack, director of the NCCS. "Jaguar provides an opportunity for modeling efforts from different organizations to come in contact with each other, leveraging their experience to accelerate progress in climate science," Hack said. In addition, the researchers get help from NCCS experts—scientific computing liaisons, modeling experts, software engineers, and computer scientists—to scale their algorithms to best use Jaguar's 182,000 processors. "Working with domain scientists—to get their applications to scale to more efficiently exploit the computational platforms that we have and that we know are coming—is going to be a critical part of advancing climate science," Hack said. "Models are not going to get faster any more by waiting for CPU clock frequencies to get faster. It's going to happen by learning how to exploit parallelism in a much more efficient way."

Leveraged Investment

Partnerships between government agencies leverage the public investment in research. A case in point is the Climate Science Computational End Station, an alliance of DOE's ORNL, NSF's NCAR, and NASA that organizes efforts to produce simulation data for the fifth IPCC assessment, expected in 2014. ORNL's John Drake is the end station's chief computational scientist, and NCAR's Warren Washington is its chief climate scientist.

Oak Ridge National Laboratory

Another important interagency partnership in climate-change research, this one between NOAA and DOE, was established in 2008 to leverage complementary expertise in modeling atmospheric processes. According to a Memorandum of Understanding signed in September, the collaboration aims "to improve the quality of and quantify the uncertainty of climate and weather prediction, including improving the prediction of high-impact weather events, to provide the best science-based climate and weather information for management and policy decisions." NOAA's time on Jaguar rose from 18,171 processor hours used in 2008 to 25.1 million awarded for 2009.

The Climate Change Initiative at ORNL, led by Hack, also awarded its first Laboratory Directed Research and Development grants in 2008 to seed high-impact studies. Hack, who helped lead development of the Community Climate System Model (CCSM) much of America's climate science community uses to simulate Earth's atmosphere, spearheaded the initiative to accelerate discoveries about the planet's climate systems through labwide engagement of researchers from diverse directorates encompassing energy, environment, computing, and national security. Among the new grant recipients were Auroop Ganguly (reducing uncertainty in climate-change models), Kate Evans (decadal prediction of Earth's climate after major volcanic eruptions), and Peter Thornton (biogeochemical modeling of the global carbon cycle when land use changes).

"We are technically and scientifically positioning ourselves to explore the skill of our modeling tools to predict climate change on regional spatial scales and decadal timescales," Hack said. "We never had the resources to do so in the past. Petascale computing provides a first opportunity to see what the modeling tools are capable of in terms of the current state of the science and related computational algorithms."

Accelerating Advancements

In 2008 several climate projects showed they had what it takes to scale up to use greater numbers of processors, providing the higher resolution needed to examine features on finer scales. Simulations on Jaguar's XT4 component were led by Paola Cessi at the University of California–San Diego (atmospheric effects on ocean circulation), Zhengyu Liu at the University of Wisconsin–Madison (abrupt climate change), Synte Peacock at the University of Chicago (first century-scale simulation to track chemicals moving throughout the world's oceans), and Warren Washington at NCAR (development of the Climate Science Computational End Station). In addition, Peacock, who moved to NCAR in 2008, gained early access to the XT4 when it was upgraded from 119 to 263 teraflops in June. Her team's simulation improved understanding of timescales and pathways of oceanic uptake of atmospheric greenhouse gases.

The 2008 accomplishments set the stage for renewed INCITE climate projects in 2009 on Jaguar by Liu (4 million processor hours) and Washington (30 million processor hours) as well as new projects by David Randall of Colorado State University (2 million processor hours to simulate global cloudiness), Venkatramani Balaji of NOAA's Geophysical Fluid Dynamics Laboratory at Princeton University (24 million processor hours to model the Earth system), and Gilbert Compo of the University of Colorado (1.1 million processor hours to study extreme weather).

In November Jaguar was upgraded again with the addition of a 1.4-petaflop Cray XT5 component. The combined XT4/XT5 system features an InfiniBand network to move large data sets from the supercomputer to other computing platforms and a Spider file system that can hold 1,000 times as much data as contained in the printed collection of the Library of Congress, assuming one word is 10 bytes. The massive effort to stand up the DOE Office of Science petascale center began in May 2004 when the federal government awarded ORNL the Leadership Computing Facility project. By November 2008 ORNL had broken the petascale barrier with an upgrade that produced a 1.64-petaflop XT combined system. Scientists immediately ran virtually all of the XT5's processing cores at a sustained speed of 1.352 petaflops to simulate superconducting materials, winning the Gordon Bell Prize for world's fastest scientific computing application.

Thought Leadership

Giving the scientific community the world's fastest HPC system in less than 4 1/2 years required great thought leadership and a sustained effort in delivering on that vision. That said, scientists are already demanding exascale computing systems—1,000 times faster than petascale machines—that promise even greater understanding of complex biogeochemical cycles that underpin global ecosystems and make life on Earth sustainable. One example of the type of thought leadership that will enable continued progress in ultrascale computing is expert testimony Hack delivered in May 2008 to the U.S. Senate Committee on Commerce, Science, and Transportation. "Computational capability remains a significant bottleneck and should remain a high-priority investment," he said, emphasizing the need for balanced expenditures in computational infrastructure, climate science and modeling, climate observations, computer science, and applied mathematics. Congress responded by raising DOE's climate-change-modeling budget from $31 million in 2008 to $45 million in 2009.

UT-Battelle, LLC, which manages ORNL for DOE, has long displayed such visionary thinking, investing in climate-research facilities years before federal research grants became available. UT-Battelle built HPC systems in a town famous for putting the best minds of a generation to work on a global problem of importance to future generations. As a result of this thought leadership, well-positioned Oak Ridge is one of the few places thriving during a worldwide economic downturn. Thanks in part to the watershed achievements of 2008, ORNL announced in 2009 it would hire 1,000 people over 2 years, many of whom will develop new energy solutions and further explore the consequences of our energy use.
–by Dawn Levy

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