Using supercomputer and chemistry to solve global problems

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Depending on how they form and their chemical composition, clouds reflect and absorb varying amounts of the sun's energy. That makes them key players in global climate change. Yet the complex molecular processes underlying cloud formation are little understood.

Now, a team of researchers at the U.S. Department of Energy's Ames Laboratory has been awarded the opportunity to study the problem, using one of the world's most powerful supercomputers, located at another DOE facility, Argonne National Laboratory, in Illinois.

"We know that clouds are formed by aerosol particles," said the team's principal investigator, Theresa Windus, associate scientist at Ames Laboratory and a professor of chemistry at Iowa State University. "The composition of the aerosols determines if a cloud is made up of a lot of small particles or large particles, which in turn impacts the size of clouds, their longevity and the probability they will produce rain."

Other scientists taking part in the research include: Mark Gordon, director of the Applied Mathematics and Computational Sciences program at the Ames Laboratory and Frances M. Craig distinguished professor of chemistry at ISU; Monica Lamm, Ames Lab associate scientist and ISU assistant professor at the Department of Chemical and Biological Engineering; and Michael Schmidt, Ames Laboratory associate chemist.

The team recently received the DOE's coveted Innovative and Novel

Computational Impact on Theory and Experiment (INCITE) award, allowing them access to 8 million processor hours on Argonne's IBM Blue Gene supercomputer.

The amount of processing time is perhaps best understood if you consider a city of 8 million people, in which everyone uses their personal computers to work on the same problem for one hour.

In fact, the award received by the Ames Lab team is part of a total of 1.6 billion hours of supercomputing time granted to 69 research teams by the DOE as part of the INCITE program. Performing research on ultra-high-speed computers allows "scientists and engineers to conduct cutting-edge research in just weeks or months rather than the years or decades needed previously," according to a DOE statement on the INCITE program. "This facilitates scientific breakthroughs in areas such as climate change, alternative energy, life sciences, and materials science."

"Computation and supercomputing are critical to solving some of our greatest scientific challenges," said Secretary of Energy Steven Chu. "This year's INCITE awards reflect the enormous growth in demand for complex modeling and simulation capabilities, which are essential to improving our economic prosperity and global competitiveness."

"The Department of Energy has some of the most powerful computers in the world, and the INCITE program provides time on some of them for researchers to perform complex calculations," said Alex King, Ames Laboratory Director. "Competition for INCITE awards is tough," he added, "and they go to the best and brightest to address the toughest problems that can be solved today. We are very pleased to be part of this important collaboration between national labs."

A key tool that will be used in the Ames Lab team's work is a suite of software programs known as the General Atomic and Molecular

Electronic Structure System (GAMESS), which is designed to run on massively parallel supercomputers, such as the one the researchers will use at Argonne. Gordon is the lead developer of GAMESS code, and he has devoted much of his career to its refinement.

The group's work is expected to generate terabytes worth of novel data. And while other researchers will be able to draw upon that data for future environment-related work, the sheer volume of information available to them may in itself present challenges.

"The more large-scale computing you do, the more you generate large amounts of data. So the issue arises, how do you best manage that data?" commented Gordon.

In addition to modeling aerosol formation, the Ames Lab team will use their allotted supercomputer time to simulate the bulk properties of water. As with the group's work in the area of aerosol formation, the highly detailed modeling of the ways water behaves will provide benchmark data that will greatly facilitate further research into green chemistry, climate change and related areas.

A third portion of the group's allotted computer time will consist of running simulations aimed at better understanding how dendrimers, a kind of polymer, can be used to decontaminate water, an effort that could be of significance to millions of people who live in water-deprived developing nations.

"Clean water is going to be a huge issue as the world's water resources become increasingly stretched in the years ahead," noted Monica Lamm, who is heading up the Ames Laboratory team's decontamination research. "For that reason, the opportunity to have your science run on these machines is very exciting," Lamm said, adding "and the fact that we don't know what the results will tell us is also exciting."

Provided by Ames Laboratory

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