Iowa State, Ames Lab researchers preparing for Blue Waters supercomputer

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Iowa State University and Ames Laboratory researchers, left to right, Theresa Windus, Monica Lamm and Mark Gordon are working to scale up their computational chemistry tools for the Blue Waters supercomputer being developed at the University of Illinois and its National Center for Supercomputing Applications. Credit: Photo by Bob Elbert/Iowa State University.

They can't wait to do computational chemistry at a quadrillion calculations per second.

But it's not all that computing power that's driving three Iowa State University and Ames Laboratory researchers as they develop computational chemistry at the petascale. Driving their project is the ability to run complex calculations and do better science.

"Petascale power is required for accuracy," said Monica Lamm, an Iowa State assistant professor of chemical and biological engineering and associate scientist at the U.S. Department of Energy's Ames Laboratory who studies complex molecular binding. "Now we have to use methods that are less accurate and less reliable."

Theresa Windus, an Iowa State professor of chemistry and an associate of the Ames Laboratory, said higher computing power will make a big difference in her studies of atmospheric particles: "This allows us to get results we've never had before."

The source of the new and improved computing power is Blue Waters, a supercomputer that's being developed as a joint effort of the University of Illinois at Urbana-Champaign, its National Center for Supercomputing Applications, IBM, and the Great Lakes Consortium for Petascale Computation, which includes Iowa State.

Blue Waters is expected to be the most powerful supercomputer in the world for open scientific research when it comes online in 2011. It will be the first system of its kind to sustain one petaflop performance - one quadrillion calculations per second - on a range of science and engineering applications.

Blue Waters is supported by the National Science Foundation and the University of Illinois.

Iowa State researchers Lamm, Windus and Mark Gordon, Distinguished Professor and Frances M. Craig Chair in chemistry, Ames Laboratory senior chemist and director of the lab's Applied Mathematics and Computational Sciences Program, are leading Iowa State's work to develop computational chemistry software that can be scaled up to petascale computing systems. The research team also includes Masha Sosonkina, an adjunct associate professor of computer science, of

electrical and computer engineering and an Ames Laboratory scientist; and Brett Bode, the software development manager for the Blue Waters project at the National Center for Supercomputing Applications.

The researchers' work is supported by grants of more than $1.6 million from the National Science Foundation.

The Iowa State researchers are working to scale up two computational chemistry software codes for use on Blue Waters and its thousands of parallel processors and high-speed connections. ("You don't just put a CD into the computer and hit install," Windus said.) One of the codes is called GAMESS and was developed by Gordon's research group at Ames Laboratory and Iowa State; the other is NWChem, for which Windus was the lead developer when she was at the U.S. Department of Energy's Pacific Northwest National Laboratory in Richland, Wash. The computing power of Blue Waters is expected to help the software deliver better, more accurate answers to three specific research problems that have been too computationally demanding to do full-scale calculations with current research tools.

Lamm is studying how dendrimers (large polymers with many branches) bind to ligands (smaller molecules that bind with other molecules to form larger complexes). A better understanding of the binding could have applications in health technologies such as drug delivery and water treatment.

Windus is studying aerosols in the atmosphere and how the tiny particles grow at the molecular level. She said a better understanding of aerosols is important to understanding the chemistry of the atmosphere. She's using NWChem for the research.

Gordon is studying the molecular dynamics of water because many aspects of its behavior aren't very well understood. To do his studies, he's

using a computational method that allows researchers to look at a large molecular system by splitting it into fragments. That allows researchers to make quicker calculations while maintaining accurate results. The method is only available on the GAMESS computational chemistry tool developed by Gordon and his research group.

Lamm said she's hoping the Blue Waters project will help the Iowa State researchers move their projects ahead.

"A problem of computational chemistry has been asking what computing power is available and how can we simplify the science for the computer," she said. "Now we have a chance to do our problems the right way."

Provided by Iowa State University