Supercomputer Study of Water

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Familiar as it is, there's a lot we don't know about water -- such as the structure taken up by liquid water molecules. With a grant of time on one of the fastest computers in the U.S., researchers at UC Davis, Lawrence Livermore National Laboratory and UC Berkeley hope to plunge into the problem and come up with some answers.

"Water is unique. It shouldn't be a liquid at this temperature," said Giulia Galli, professor of chemistry at UC Davis and principal investigator on the project.

Studies on the structure of liquid water date back to 1893. Until recently, water molecules were thought to cluster in tetrahedral groups of four. But in 2004, researchers at the Stanford Linear Accelerator Center claimed to have found structures of rings and chains instead. Another team at the Lawrence Berkeley Laboratory conducted similar experiments and reaffirmed the old tetrahedral model.

The question has yet to be resolved by experiments, which are incredibly difficult to do, Galli said. The problem is also too complicated for a purely theoretical approach, but can be investigated by computational modeling, said co-investigator Francois Gygi, professor of applied science at UC Davis.

Starting from very basic "first principles" about hydrogen and oxygen atoms, Galli, Gygi, David Prendergast and Jeffrey Grossman at UC Berkeley, and Eric Schwegler at the Lawrence Livermore Lab will run computational models of water and see how it ought to behave.

"We start from the beginning and see what comes out," Galli said.

The experiments will run on the IBM Blue Gene supercomputer at Argonne National Laboratory, using a grant of 2.5 million hours of computer processor time awarded through the U.S. Department of Energy's INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program. One of the newest supercomputers in the U.S., the Argonne lab's machine has 1,000 nodes with two processors each. The researchers expect that the experiments will actually take about two months of computer time spread over several months.

The researchers are also interested in how water behaves when it is squeezed into very small spaces, such as a carbon nanotube. That behavior might have implications for using nanotechnology to build very small devices that can handle liquids.