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New Algorithm Speeds Simulations Of Complex Fluids

CHAMPAIGN, Ill. -- Computer simulations play an essential role in the study of complex fluids -- liquids that contain particles of different sizes. Such liquids have numerous applications, which depend on a fundamental understanding of their behavior. But the two main techniques for the atomistic simulation of liquids -- the molecular dynamics technique and the Monte Carlo method -- have limitations that greatly reduce their effectiveness.

As reported in the Jan. 23 issue of the journal Physical Review Letters, researchers at the University of Illinois at Urbana-Champaign have developed a geometric cluster algorithm that makes possible the fast and accurate simulation of complex fluids.

"The main advantage of the molecular dynamics method -- its ability to provide information about dynamical processes -- is also its main limitation," said Erik Luijten, a professor of materials science and engineering at Illinois. "Many complex fluids contain particles of widely different sizes, which move at vastly different time scales. A simulation that faithfully captures the motions of the faster as well as the slower particles would be impractically slow."

By contrast, the Monte Carlo method can circumvent the disparity in time scales, since it is designed to extract equilibrium properties without necessarily reproducing the actual physical motion of the atoms or molecules.

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However, attempts to create appropriate "artificial motion" have been limited to ad hoc solutions for specific situations. Thus, a Monte Carlo method capable of efficiently simulating systems containing particles of different sizes has remained a widely pursued goal.

Luijten and graduate student Jiwen Liu have resolved this issue in a very general way by creating artificial movements of entire clusters of particles. The identification of appropriate clusters is a crucial component of the simulation.

In 1987, researchers at Carnegie Mellon University resolved a similar problem for magnetic materials by simultaneously flipping entire groups (or clusters) of magnetic spins. This finding, which relied on an intricate mathematical mapping dating back to the early 1970s, greatly accelerated calculations for model magnets. Many researchers realized that a similar approach would have an even bigger impact if it could be applied to fluids.

"Thus, a cluster algorithm for the simulation of fluids became a 'Holy Grail' for scientists studying fluids by means of computer simulations," Luijten said. "However, magnetic materials possess a symmetry that is absent in fluids, making it apparently impossible to use the ideas that were so successful in magnets."

Exploiting an idea developed for mixtures of spheres, Luijten and Liu were able to reconcile the asymmetric nature of fluids with the mathematical foundations underlying the identification of clusters. Their simulation method utilizes a geometric cluster algorithm that identifies "natural" groups of particles on the basis of the elementary forces that act between the particles. This approach greatly accelerates the simulation of complex fluids. Indeed, the greater the disparity in size between particles, the more advantageous their method becomes.

"This algorithm provides us with a new tool to study fluids that were not previously accessible by simulations," Luijten said. "It has the potential to advance our understanding of a great variety of liquid systems."

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This story has been adapted from a news release issued by University Of Illinois At Urbana-Champaign.

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