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Complex fluid simulation made easier

A geometric cluster algorithm may soon make it possible to get a fast and accurate computer simulation of complex fluids.

Those simulations play an essential role in the study of complex fluids—liquids containing particles of different sizes which have numerous applications that depend on a fundamental understanding of their behavior, said researchers at the University of Illinois at Urbana-Champaign.

Currently, researchers use two main techniques for the simulation of liquids—the molecular dynamics technique and the Monte Carlo method. But both have limitations.

"The main advantage of the molecular dynamics method—its ability to provide information about dynamical processes—is also its main limitation," said Erik Lijten, 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, because it extracts equilibrium properties without necessarily reproducing the actual physical motion of the atoms or molecules. 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.

Lijten 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.

Exploiting an idea developed for mixtures of spheres, Lijten 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," Lijten said. "It has the potential to advance our understanding of a great variety of liquid systems."

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