Transport Coefficients and Molecular Dynamics

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CSTL scientist addresses the need for more efficient simulation methods for industrial modelers.

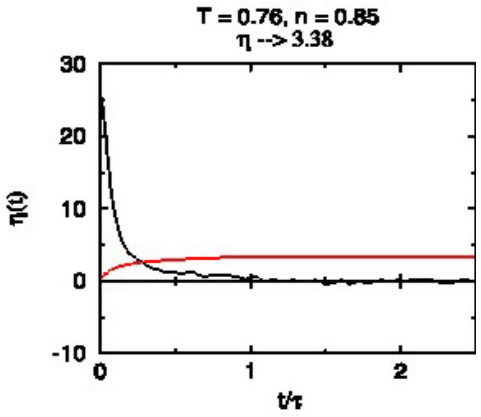
Molecular-level simulation of fluids has been identified as an enabling technology for the efficient determination of physical properties of fluids in conditions where the experiments are expensive and/or hazardous due to toxicity, flammability etc. In order for industrial modelers to realize the potential benefits of molecular simulations, two (at least) issues must be addressed. The first is the need for physically accurate representation of the interactions between the molecules of the fluid and the second is the need to develop more efficient simulation methods than are currently available. This work addresses the second of these issues.

While it has been possible for decades to use molecular simulations to estimate the shear viscosity and the thermal conductivity of a model fluid, the computational resources required have been too large to move it from a research to an industrial setting. Recently, some novel methods for estimating these transport coefficients from simulations have been reported, but no systematic evaluation of the merits of these methods has been produced. The objective of this project is to determine the computational efficiency and accuracy of these methods compared with existing simulation methods.

This project is part of a larger effort in the Physical and Chemical Properties Division to improve molecular simulation methodology to the point where industrial property modelers will be comfortable adding these techniques to their toolkit because it will expand their ability to cope with fluids and state conditions where existing methods fail.

An interagency report, NISTIR 7170 has been issued and an archival publication on system size effects is in the early stages of preparation.

In order to concentrate on the second issue, namely accurate and efficient determination of transport coefficients, this project focused on the Lennard-Jones fluid, a widely studied model system sometimes called the "fruit fly" of simulations. There are sufficient prior results available so that both accuracy and efficiency can be evaluated. Three unconventional methods were examined and one, Reversed Perturbation Nonequilibrium Molecular Dynamics, was found to be competitive with existing methods. This scheme is being further examined to see if the computational efficiency can be improved by reducing the system size without compromising accuracy.



The averaged time correlation functions (solid line) and the time integral for the shear viscosity (dotted line) are shown in the graph