# Transient Molecular Dynamics Simulations of Viscosity and Thermal Diffusivity for Simple Fluids

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A general method is presented for computationally efficient molecular dynamics simulations of viscosity and thermal diffusivity. In this method, the transient decay of an initial velocity or temperature profile during short simulations is fitted to the corresponding macroscopic equations of change, in order to obtain the viscosity or the thermal diffusivity. An initial sinusoidal profile, with nodes at the simulation cell boundaries, is used in this study because: (1) it is compatible with standard simulation algorithms including periodic boundary conditions and Ewald sums; (2) the macroscopic equations have an analytical solution; (3) the analytical solution can be factored into spatial and temporal components that can be fitted to the simulated data separately; and (4) its decay optimizes momentum or heat transfer over the cell domain, thereby improving the statistics of the transport coefficients obtained. Results of multiple transient simulations of very short duration, when averaged, produce quality results comparable to steady-state nonequilibrium and Green-Kubo simulations, which require substantially more simulation time. Results are presented for the application of the transient method for simple Lennard-Jones fluids over the fluid (vapor and liquid) domain. The results are in good agreement with values obtained by other methods. Work is currently underway to extend the method to potential models for more complex fluids.