

Determine Transport Coefficients and Equation of State of Fluids by Combining Fluctuating Hydrodynamics and Molecular Dynamics Simulations

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The goal of this work is to develop a systematic computational framework to determine the transport properties and equation of states of molecular fluids, especially those with spatial heterogeneity at the nano-scale. The essence of this framework is a direct mapping from the atomic representation of a molecular system to that of continuum mechanics, for which Landau's fluctuating hydrodynamics (FH) is employed. Since transport coefficients and equation of state are the input parameters for a FH representation, this mapping allows the determination of these properties directly from molecular dynamics (MD) simulations that use force fields. The results can also be used to improve molecular force fields in representing transport coefficients and equation of state. A key for this mapping to be meaningful is that the resulting thermal fluctuations of density and momentum fields of the FH and molecular scales need to be matched. By explicitly considering all relevant length-scales, we illustrate that this goal can be achieved. Furthermore, stable solvers for the FH equations are not yet available, especially when large fluctuations and transient flows are involved. We will also present a novel staggered discretization scheme that we developed for solving the FH equations with very small grid sizes (5-10 Å) and transient flows.