A Non-Equilibrium Model for the Prediction of Slip for Highly Confined Fluids

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We present a derivation to predict the slip velocity, and hence slip length, for a system of fluid atoms confined by atomistic walls. The derivation is entirely non-equilibrium, and is based upon forming time correlation functions of relevant measurable fluid properties in the steady-state. These correlation functions are formed for increasingly fine-grained slabs of fluid adjacent to the walls. By solving the governing differential equation for the fine-grained slab velocity autocorrelation function, we are able to predict the slab friction coefficient adjacent to the wall in the limit of zero slab width, and hence the slip velocity for a highly confined fluid, to high accuracy. We present numerical results from non-equilibrium molecular dynamics simulations to verify our theoretical predictions and discuss the advantages and limitations of the current model.