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Green-Kubo relation and hydrodynamic tails of friction at solid/liquid interfaces KAI HUANG, IZABELA SZLUFARSKA, Univ of Wisconsin, Madison — Understanding boundary conditions at the liquid/solid (L/S) interface has been a subject of many scientific investigations. It also has important implications for design of materials for such applications as micro-/nanofluidics. Design of functionalized surfaces and interfaces with optimized friction and slip properties is hindered by existing challenges in measuring these properties either in experiments or in simulations. Here, we have developed a Green-Kubo (GK) relation that enables accurate calculations of friction at L/S interfaces directly from equilibrium molecular dynamics (EMD) simulations and that provides a pathway to bypass the time scale limitations of typical non-equilibrium molecular dynamics (NEMD) simulations. The theory has been validated for a number of different of interfaces and it is demonstrated that the L/S slip is an intrinsic property of an interface. Because of the high numerical efficiency of our method, it opens up new opportunities for computational design of functionalized surfaces for L/S applications. Details of the friction correlation function also permit a full analysis of the time-dependent and frequency-dependent friction in a dynamic system. At the hydrodynamic time scale, the memory kernel of the friction coefficient exhibits an algebraic decay, which leads to a -3/2 power long time tail in the velocity autocorrelation function of fluid particles near a wall. This behavior differs from the predictions of previous theoretical and simulation results, which employed no-slip boundary conditions. Our findings provide new insights into understanding the dynamics of interfacial colloids and nano-particle flow in liquids.

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