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Atomistic Simulation of the Stochastic Dynamics of Thin Liquid Films ADAM WILLIS, JOHN FREUND, University of Illinois at Urbana - Champaign — For interface flows (e.g. unstable thin films or spreading drops), it has been proposed that at small enough scales classic hydrodynamic continuum equations should be augmented with stochastic terms that model the effect of, for example, thermal noise on the instantaneous geometry of liquid-vapor interface. Since the regions where such effects are thought to be important are challengingly small for experimental diagnostics and sensitive to potential contamination, atomistic simulation provides a clean means of evaluating and testing these theories. We use simulations with a Lennard-Jones potential to investigate the spreading rate of small liquid drops and find deviations potentially consistent with the stochastic model of Davidovitch et al. [Phy. Rev. Let, **95**:244505, 2005] Most Lennard-Jones simulations truncate the interaction potential at a finite radius. This has the effect of also cutting off the disjoining pressure, which is often modeled in continuum expressions as a $1/h^3$ term, h being the film thickness. To properly investigate continuum equations which retain non-local interactions, we have designed a special un-truncated implementation of the Lennard-Jones potential that has an acceptable $O(N \log N)$ computation expense scale with number of atoms N. This will also be discussed in the context of these investigations.

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