

Abstract Submitted
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Thermal fluctuations and the hydrophobic effect. HUA-YI HSU, NEELESH PATANKAR, Department of Mechanical Engineering, Northwestern University — Hydrophobic effect typically implies three phenomena widely discussed in literature: depletion of liquid at hydrophobic surfaces, observation of slip at hydrophobic surfaces and the long range attraction between hydrophobic surfaces. The central feature that characterizes all these phenomena is considered to be the formation of thin vapor-like films next to hydrophobic surfaces. Prior work suggests that thermal fluctuations of the liquid/vapor-like film interface near hydrophobic surfaces, and correspondingly, fluctuations in the fluid density play an important role. Fluctuating interfaces are also implied from experiments with a liquid between a hydrophobic and a hydrophilic surface. Thus, it is necessary to develop a way to quantify the interfacial fluctuations to better understand this effect. We present a way to extract this information from molecular dynamic (MD) simulations. Ways to incorporate this information into fluctuating hydrodynamics (FHD) based mesoscale techniques will be proposed. FHD based methods can permit solutions of a variety of dynamic flow problems involving hydrophobic surfaces by using the usual tools available in hydrodynamics studies.

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