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A Slippery Business: Explaining the Wide Range of Water Slip Lengths on Graphene using Molecular-Kinetic Theory GERALD WANG, Carnegie Mellon University — Since the early 2000s, the anomalous transport properties of water confined within carbon nanomaterial environments have attracted an immense amount of attention; the slip length of water has been one topic of particular interest. Accurate modeling of slip phenomena is critical for the design of a wide range of nanofluidic technologies. A scan through the molecular-dynamics (MD) literature reveals that reported slip lengths vary well over a factor of three. This raises the key question: Why do MD simulations yield such an enormous range of water slip lengths? In this work, we present a parsimonious answer to this question, based upon our recently developed molecular-kinetic theory (MKT) for slip. MKT provides an explicit expression that relates the magnitudes of slip phenomena to microscopic parameters describing the fluid-solid interface, along with fluid and solid material properties. We demonstrate that a significant amount of the variation in slip lengths reported in the literature is explainable within the framework of MKT, and can be directly attributed to different models used to simulate water. We briefly comment on a vision for canonical systems and protocol to measure hydrodynamic slip in MD simulations that would enable fair comparison of results.

Gerald Wang
Carnegie Mellon University

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