Abstract Submitted
for the DFD19 Meeting of
The American Physical Society

Describing the Mechanics of Fluid-Solid Interfaces using Molecular Modeling NICOLAS HADJICONSTANTINOU, GERALD WANG[1], Massachusetts Institute of Technology — Fluid-solid interfaces are ubiquitous in fluid dynamics, but also particularly important at the nanoscale, where the spatial extent of fluid under bulk conditions is very limited. Predicting fluid behavior at such an interface requires an understanding of the fluid structure, as well as the molecular mechanics of fluid motion under the influence of the solid potential. In this talk, we describe molecular approaches for characterizing these phenomena, with particular emphasis on the resulting slip at the interface. In the case of a simple fluid, we show that molecular-kinetic considerations can be used to develop a universal scaling law for slip that reduces to Navier slip at low shear rates and connects macroscopic transport quantities (e.g. the slip length) to the microscopic system description. In the case of immiscible two-phase flow, we demonstrate that as characteristic length-scales become small, interfacial hydrodynamic bending becomes negligible and, as a result, instead of Tanner's law, the contact angle is described by Blake's molecular-kinetic theory which connects the deviation from the equilibrium contact angle to the amount of slip. Our models are supported by extensive molecular-dynamics simulations, as well as evidence from some directly comparable experiments.

[1]Currently at Carnegie Mellon University

Nicolas Hadjiconstanitnou
Massachusetts Institute of Technology

Date submitted: 27 Jul 2019 Electronic form version 1.4