COMPUTATIONAL RESEARCH in BOSTON and BEYOND SEMINAR

Computational Modeling of Nanoconfined Fluids: Big Surprises Come in (Very) Small Packages

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ABSTRACT:

Nanoscale fluids, unlike their macroscale cousins, exhibit a number of surprising effects that are not present within continuum theories. In particular, the equilibrium and transport properties of nanoconfined fluids can be substantially different from the bulk properties of that fluid. Understanding the physical basis for these anomalous fluid properties including nanoconfined fluid structure, density, and self-diffusivity is central to many pursuits in nanoscale technology. These nanofluidic phenomena afford great opportunities to think big by thinking small specific engineering applications include nanoporous water filters to nanoscale drug delivery mechanisms to nanoscale heat transfer devices (as well as high-efficiency molecular simulation methods, for those of us who identify as computational engineers)!

In this talk, we present a theoretical and computational description of these phenomena in the context of dense simple fluids confined within a variety of nanoscale structures, including carbon nanotubes and graphene nanoslits. We show that the anomalous nanoconfined fluid density can be substantially lower than the bulk density, and that this reduced density is primarily due to repulsive fluid-solid interactions. Using a mean-field approach, we obtain closed-form analytical results for the length-scales associated with fluid layering near the solid-fluid interface. These results allow us to predict the equilibrium fluid density as a function of the confinement length-scale. Our predictions are in excellent agreement with molecular dynamics simulations as well as results from the experimental literature.

We also show that the fluid-solid energy landscape and associated density profile can be used to explain the anomalous diffusive transport observed in such systems. In particular, the presence of a layered structure near the fluid-solid interface implies that fluid molecules near the solid wall exhibit different dynamics as compared to bulk fluid molecules. By constructing different models for diffusion in the near-wall and the bulk regions of the CNT, we show that we can approximately predict the overall diffusive behavior of the nanoconfined fluid. We demonstrate that these results are in agreement with molecular dynamics simulations. We show how several aspects of this theory can be used to model more-complex fluids, including water. Finally, we demonstrate how accurate knowledge of these anomalous fluid properties can inform simple models of nanoscale mass and heat transfer phenomena.

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1:00 PM – 2:00 PM
Building 32, Room 141
(STATA)

Pizza and beverages will be provided.

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