ABSTRACT

Fluid physics at nanometer scale can be quite different from its macroscopic counterpart. Advances in elucidating fluid phenomena at nanoscale can enable revolutionary advances in numerous applications in engineering and science. Several experimental approaches have been used with increasing success in recent years to characterize fluid transport through nanopores of varying diameters. However, many fundamental questions concerning fluid physics still remain. For example, how does confinement affect fluid phenomena? How does surface charge, chemical functionalization and wall structure affect fluid physics? How are rotational and translational motions coupled? How different is diffusion, mobility, osmosis and other fluid transport phenomena at nanometer scale? In this talk, we will discuss how computational approaches can provide fundamental and unique insights into fluid physics at nanoscale. The traditional continuum theory fails to take into account the effects caused by the finite size of the fluid molecules and the fluid accessible volume of the nanopore. This requires atomic scale simulations (e.g. molecular dynamics simulations) where finite size of the fluid molecules is explicitly treated. However, order of the time scales and the length scales possible in atomistic molecular dynamics (MD) simulations is far less than realistic design calculations. Further, it is known that in small diameter nanopores (~3nm and less) quantum-mechanical effects can influence the fluid transport. These can be computed from Density functional theory (DFT) or by semiempirical methods. In this talk, we will show that multiscale methods combining density functional theory, atomistic molecular dynamics, mesoscale particle transport and quasi-continuum theories can be used to understand the fundamental questions posed above. Computational studies on fluid transport through carbon nanotubes, boron nitride nanotubes, and solid-state nanopores will used to demonstrate unique nanoscale fluid transport.

NOTE: If you are interested in meeting individually with Prof. Aluru, please contact Evelyn at 631-5431