Mechanical Engineering Department Seminar

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1130 Mechanical Engineering

Quasi-Continuum Theory for Fluids Under Confinement

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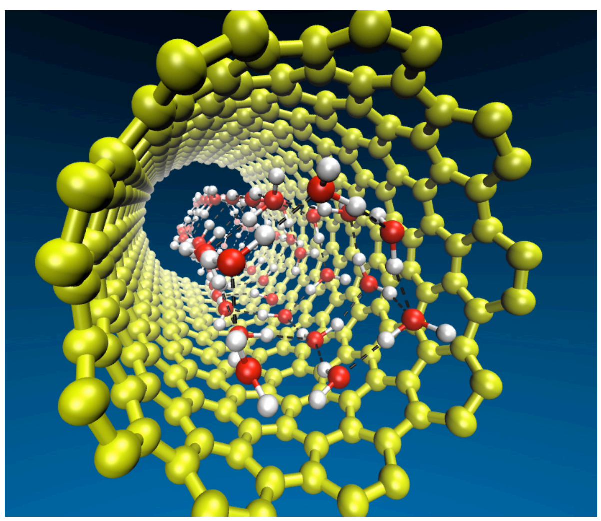
Fluid physics at nanometer scale can be quite different from its macroscopic counterpart. Advances in elucidating fluid phenomena at nanoscale can enable revolutionary advances in numerous applications in engineering and science. Several experimental approaches have been used with increasing success 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? 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. In this talk, we will discuss structure and dynamics of fluids in confined environments, e.g. nanoslits/nanopores. The interfacial structure of fluids is computed by a multiscale quasi-continuum theory. The results from quasi-continuum theory compare well with molecular dynamics (MD) and the quasi-continuum theory is several orders of magnitude faster compared to MD. The structure obtained from the multiscale theory is coupled with the particle transport equation to compute dynamics in nanoslits/nanopores. We will discuss several applications of fluid transport through nanopores.



Bio: N. R. Aluru received the B.E. degree from the Birla Institute of Technology and Science (BITS), Pilani, India, in 1989, the M.S. degree from Rensselaer Polytechnic Institute, Troy, NY, in 1991, and the Ph.D. degree from Stanford University, Stanford, CA, in 1995. He is currently a Richard W. Kritzer Professor in the Department of Mechanical Science and Engineering at the University of Illinois at Urbana-Champaign (UIUC) and Director of the Computational Science and Engineering Program at Illinois. He is also affiliated with the Beckman Institute for Advanced Science and Technology, the Department of Electrical and Computer Engineering and the Bioengineering Department at UIUC. He was a Postdoctoral Associate at the Massachusetts Institute of Technology (MIT), Cambridge, from 1995 to 1997. In 1998, he joined the University of Illinois at Urbana-Champaign (UIUC) as an Assistant Professor.