Semi-Plenary Lecture

Professor N. R. Aluru

Department of Mechanical Science and Engineering
Beckman Institute for Advanced Science and Technology
University of Illinois at Urbana-Champaign

Title: Computational Nanofluidics

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 including water purification, energy conversion and storage, DNA sequencing, etc. 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 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.

Brief Biography:
Dr. N. R. Aluru received the B.E. degree with honors and distinction 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 Professor in the Department of Mechanical Science and Engineering at the University of Illinois at Urbana-Champaign (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. Dr. Aluru received the NSF CAREER award in 1999, the Xerox Award for Faculty Research in 2002, the ASME Gustus L. Larson Memorial Award in 2006, and the USACM Gallagher Young Investigator Award in 2007.