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Nanoscale Hydrodynamics

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ABSTRACT:

Many applications in biology, engineering and sciences rely on efficient hydrodynamic transport through nanometer scale pores and channels. For example, channels and pores in cellular membranes regulate the functionality of the cell by selectively and efficiently exchanging water and ions between extra and intra cellular environments. Selective pores in ultrathin membranes have been shown to be highly efficient for water desalination and power generation. Classical theories often fail to describe fluid physics at nanometer scale. For example, density layering, size dependent fluid properties, restricted translational and rotational motions, charge inversion, flow reversal and several other important phenomena have been observed at nanometer scale. The focus of this talk is to develop efficient theories and computational approaches to accurately describe fluid physics at nanometer scales. First, we will introduce an empirical potential-based quasi-continuum theory (EQT) to accurately predict the structure of confined fluids. We show that the density layering from EQT matches well with molecular dynamics (MD) and EQT is many orders of magnitude faster compared to MD. Next, we show that the EQT framework can be combined with the generalized Langevin theory to compute diffusion of confined fluids and with the classical Navier-Stokes equations to compute the transport of confined fluids. We will show several examples to demonstrate the accuracy and efficiency of the quasi-continuum theory for confined fluids.

BIOGRAPHY:

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, National Center for Supercomputing Applications, 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. He is a recipient of several honors and awards including the NSF CAREER award in 1999, the NCSA faculty fellowship in 1999 and 2006, the 2001 CMES Distinguished Young Author Award, the Xerox Award for Faculty Research in 2002, the ASME Gustus L. Larson Memorial Award in 2006, the USACM Gallagher Young Investigator Award in 2007, was named a Willett Faculty Scholar by the College of Engineering at UIUC for the period 2002-2008, and University Scholar in 2010. He held a William Mong Visiting Research Professorship from the University of Hong Kong and is a Fellow of the United States Association for Computational Mechanics. He currently serves as the Associate Editor of the journal Microfluidics and Nanofluidics and has in the past served as the Associate Editor of IEEE/ASME Journal of Microelectromechanical Systems. He also serves on the editorial board of a number of other journals.