



*Friday, December 2, 2011  
3:00 pm, Birck 1001*



**“MD Simulations of Gas Flows in Nano-Channels and Interface Thermal Resistance Between Simple Liquids and Solids”**



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**Abstract:** This talk focuses on our group’s recent research on molecular dynamics simulations of gas flows in nano-scale confined geometries, and interface thermal resistance between simple liquids and solids. Gas flow research demonstrates the importance of wall force field effects that penetrate approximately 1 nm from each surface. Gas density, viscous and normal stress distributions and the velocity profiles within this region show deviations from the Boltzmann equation solutions. Presence of this near wall sub-layer indicates the breakdown of similitude between the rarefied and nano-scale confined gas flows, solely based on the Knudsen number. In addition, MD simulations performed in a wide Knudsen range enable prediction of the Tangential Momentum Accommodation Coefficient for argon gas in contact with FCC surfaces.

The second half of the talk summarizes our research on MD simulations of heat transfer in nano-channels, and our efforts to determine a phenomenological model for the interface thermal resistance (Kapitza resistance) between liquid argon and FCC surfaces. We utilize MD results to extract a model for the Kapitza length as a function of the molecular properties and temperature of the wall, and wall-fluid interaction strength. Specific results for the Kapitza length at argon-silver and argon-graphite interfaces are given; and onset of continuum behavior for liquid argon confined in nano-channels as small as 5 nm is demonstrated.

**Bio:** Prof. Ali Beskok received his B.S. in Mechanical Engineering from Middle East Technical University, Ankara, Turkey in 1988. He received an MS degree in Mechanical Engineering from Indiana University Purdue University in Indianapolis in 1991, and M.S. and Ph.D. degrees from Princeton University, Mechanical and Aerospace Engineering in 1994 and 1996, respectively. Dr. Beskok was a Visiting Scholar at Brown University, Center for Fluid Mechanics from 1994 to 1996, and a Post Doctoral Research Associate at Massachusetts Institute of Technology, Research Laboratory of Electronics from 1996-1998. He joined Texas A&M University Mechanical Engineering Department as an Assistant Professor in 1998, and became an Associate Professor in 2004. In 2007, he moved to Old Dominion University, Mechanical and Aerospace Engineering Department as the Batten Endowed Chair Professor of Computational Engineering. He is the founding director of the ODU Institute of Micro and Nanotechnology.