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Special Guest Lectures

Adaptive Multiscale Molecular Dynamics Simulations of Soft Matter**Steven O. Nielson, University of Texas at Dallas**Johnston Hall 338
March 15, 2011 - 02:00 pm**Abstract:**

Understanding mesoscopic phenomena in terms of the fundamental motions of atoms and electrons poses a strong challenge for molecular simulation. This challenge is being met by multiscale modeling techniques that aim to bridge between the microscopic and mesoscopic time and length scales. In such techniques different levels of theory are combined to describe a system at a number of scales or resolutions. In adaptive hybrid simulations, the different levels are used in separate spatial domains, and matter can diffuse from one region to another with an accompanying resolution change. Until now, however, adaptive atomistic/coarse-grained (AA/CG) molecular dynamics simulations have had very limited applicability because the on-the-fly CG-to-AA transformation is problematic in all cases with the exception of molecules with a single particle CG representation. Here, we solve this problem by combining a transitional healing region with a rotational dynamics of rigid AA fragments in the CG region. Error control is obtained by analysis of the AA/CG energy flow. We illustrate the method with adaptive multiscale simulations of liquid hexane and of a dilute polymer solution in a theta solvent.

Speaker's Bio:

My research is focused on developing theoretical tools to use in computer simulations of such systems. Specifically, I am combining existing techniques in colloidal modeling with coarse grained methods developed for surfactant modeling. My goal is to study the local self-assembly at the solid-liquid interface and the large-scale self-assembly of the stabilized nanoparticles. I am also working on a closely related project to study the poration of bilayer membranes for use in drug delivery.

