Stevens Institute of Technology

Nanotechnology Graduate Program

Multiscale Modeling of Nanostructured and Biological Materials

Wednesday February 7, 2007
Babbio Bldg, Room 122, Time 11am

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One of the central tasks of multiscale material modeling is to develop and apply simulation techniques to uncover the underlying atomistic mechanisms without the significant limitations to the system size and time scales inherent to the fully atomistic models. My current research in this context involves coupling different length- and time-scales to study the deformation and failure mechanisms of nanostructured and biological materials. Depending on the characteristics of the problem under consideration, coupling the length scale can be achieved either concurrently or hierarchically. Concurrent coupling is established through a domain-decomposition scheme in which sub-domains are treated by either coarse (finite elements) or fine (atomistic/quantum mechanics) scale representations, with the key being the coupling strategies at the interfaces of the sub-domains. Differently, hierarchical coupling is established by embedding the fine-scale constitutive relations into coarse-scale material properties. With examples in carbon nanotube fracture and whole-cell deformation, we demonstrate that both methods offer fine-scale resolution, while significantly improve the computational affordability. To extend the time-scale of atomistic simulations, a pathway sampling nudged elastic band (NEB) method is adopted to study the thermally activated process at the crack tip that controls the brittle fracture in solids. Applications of these methods to other material systems are also briefly presented.

Dr. Sulin Zhang received his B.E. from the Department of Engineering Mechanics at Dalian University of Technology in 1994. He was then recommended by the department to the graduate program in Tsinghua University, working with Dr. Wei Yang. Upon receipt of his Master's degree in 1997, he joined the PhD program in the Department of Theoretical and Applied Mechanics at the University of Illinois, Urbana-Champaign (UIUC), and received his PhD in 2002. He then worked as a postdoctoral fellow at Northwestern University with Dr. Ted Belytschko. He was appointed to his current tenure-track assistant professor position at the University of Arkansas in August, 2005. His research interests lie on the multiscale simulations of nanostructured and biological materials.

Light refreshments will be served prior to seminar

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