Multiscale Coupling Methods for Nanoscale Mechanics and Material Design

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Abstract
In material design, we strive to optimize properties such as strength and toughness through manipulation of the materials microstructure. For efficiency of calculation, the multifield equations can be coupled to a conventional continuum through the Bridging Scale Method. We present a mathematical framework of the Bridging Scale Method for accurately and efficiently simulating dynamics with different spatial scales. We further extend and elaborate the method in two aspects. First, based on normal mode decomposition and a matching differential operator technique, we propose a more accurate multiscale method. Secondly, we develop a releasing zone treatment for effectively damping out reflections across the interface in the presence of a dynamic dislocation.

The characterization and manipulation of complex biological systems has reached a stage to resolve various levels of details. We briefly outline the immersed finite element method coupled with multiphysics features such as protein molecular dynamics for solving a class of bio-nano-fluidics problems. We then apply the multiphysics of the composite electric field for the guided alignment of the carbon nanotube (CNT) and DNA. The aim to use this class of methods to assist the manipulation and characterization of nano scale biological objects, from molecular to cellular levels. In addition, we should use this class of methods to explore the feasibility of various NEMS designs and sensor fabrications by the inclusion of electrophoretic, dielectrophoretic and electroosmosotic forces. The various dynamic processes and assembled patterns are studied by comparing our simulation results with experimental observations. The NEM sensors can be used for the measurement of cell traction forces for the understanding of the focal adhesion complex and cell motility.

Vita
Walter P. Murphy Professor Wing Kam Liu received his B.S. from the University of Illinois at Chicago in 1976; his M.S. in 1977 and Ph.D. in 1981 both from Caltech. His research activities include concurrent and hierarchical bridging scale methods for computational mechanics, in particular, nano mechanics and materials, bio-nano interface, and multi-scale analysis. Selected Liu’s honors include the Gustus L. Larson Memorial Award (1995), the Pi Tau Sigma Gold Medal (1985) and the Melville Medal (1979), all from ASME; the Thomas J. Jaeger Prize (1989) by the International Association for Structural Mechanics in Reactor Technology, and the SAE Ralph R. Teetor Educational Award (1983), the US Association for Computational Mechanics (USACM) Computational Structural Mechanics Award (2001), the International Association for Computational Mechanics (IACM) Computational Mechanics Award (2002) and the Japan Society of Mechanical Engineers Computational Mechanics Award (2004). Liu serves on both the executive committee of the ASME Applied Mechanics Division and the International Association for Computational Mechanics. He was the past president of USACM. Liu is cited by Institute for Scientific Information (ISI) as one of the most highly cited, influential researchers in Engineering, and an original member, highly cited researchers database. He is the director of the NSF Summer Institute on Nano Mechanics and Materials.