Multiresolution Mechanics for Material Design

Wing Kam Liu, Walter P. Murphy Professor
Director of NSF Summer Institute on Nano Mechanics and Materials
Northwestern University, Department of Mechanical Engineering,
2145 Sheridan Road, Evanston, Illinois, 60208, USA
email: w-liu@northwestern.edu

Abstract

Inadequacies of continuum mechanics and the expense of atomic scale simulations have lead to a recent floury of activity in the area of multiscale theories, which aim to predict material behavior in a manner which takes account of the underlying physics of deformation. We are proposing to develop the next generation of computer-aided design (CAD) simulation theory that integrates nano and microscale physics into CAE capabilities for design and manufacturing. This multiscale approach starts at the most fundamental level of material behavior, the strength of the bonds between atoms, which is predicted by quantum mechanics. These bond strengths determine the sub micro-scale behavior which controls the deformation mechanisms responsible for overall material properties and performance. A mathematical framework, which is capable of bridging the gap between *discrete* atomic scale theory and multiscale *continuum* theory, is proposed. The resulting governing equations are formulated in terms of forces, and a virtual representation of the lattice structure can be used to facilitate a smooth transition between the treatment of discrete atomic displacements and multiscale continuum fields. Hence, constitutive behavior can be determined 'on the fly' during computer implementation by using appropriate atomic potentials. Alternatively, a coarser approximation of the effect of the microscale feature can be gained through an *average gradient continuum* constitutive equation. The proposed multiresolution technique is capable of linking overall material properties to the underlying microstructure via the micro/nano mechanics at each scale of interest. The small scale deformation phenomena which have a profound impact on macroscale properties are captured. The proposed research will be illustrated for a polycrystalline material, a granular material, an alloy containing particles at various scales. A potential use for a bio-inspired self healing composite will also be discussed.

Vita

Dr. Wing Kam Liu, Walter P. Murphy Professor at Northwestern University and Director of NSF Summer Institute on Nano Mechanics and Materials, received his Ph.D. from Caltech. His research activities include bridging scale computational mechanics and materials, multi-scale analysis, and computational biology. Selected Liu's honors include the Gustus L. Larson Memorial Award, the Pi Tau Sigma Gold Medal and the Melville Medal, all from ASME; the Thomas J. Jaeger Prize by the International Association for Structural Mechanics in Reactor Technology; the SAE Ralph R. Teetor Educational Award; the Computational Structural Mechanics Award and Computational Mechanics Award from USACM and IACM, respectively; and the JSME Computational Mechanics Award. Liu serves on both the executive committee of the ASME applied mechanics division (Chair 2005-2006) and the International Association for Computational Mechanics. He was the past president of USACM. Liu is cited by Institute for Scientific Information as one of the most highly cited, influential researchers in Engineering, and an original member, highly cited researchers database. He is the editor and honorary editors of many Journals. Dr. Liu has acted as a consultant to the many organizations.