UF UNIVERSITY of FLORIDA

Spring 2009 Seminar Series

Department of
Mechanical & Aerospace Engineering

Tuesday, March 17, 2009
4:00 pm
in Room 303 MAE-A

A Material Frame Approach for Calculating Continuum Variables in Molecular Simulations

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Continuum theory can be used to analyze the mechanics of materials and structures. However, in nanotechnology quantities such as stress become ill-defined and the application of continuum mechanics in nanomechanical frameworks becomes suspect. This calls into question whether design tools used for manufacturing can be applied to micro or nano-electro-mechanical systems. While atomistic modeling and simulation methods, e.g. molecular dynamics, can provide a wealth of information for such systems, the use of continuum mechanics to analyze such simulations requires that clear connections between nanoscale mechanics and engineering scale analysis can be made.

The derivation of expressions for calculating continuum variables within an atomic system has a long history, with many articles addressing important issues such as the consistency of stress expressions with the mechanical concept of a force acting on a unit area, and the impact of spatial and time averaging. Among these efforts is the work by Hardy (1982), whose formulation is based on the Eulerian or spatial configuration, where localization (or spatial-averaging) volumes are essentially control volumes fixed in space that matter occupies at a particular time. Hardy's expressions for stress and heat flux contain both “potential” (based on derivatives of potential energy) and “kinetic” (based on the flux of momentum or energy through the localization volume) terms. The validity of kinetic contributions to stress has been an issue of some contention to both the physics and mechanics communities.

An alternative approach is to construct a similar formulation to Hardy's in the Lagrangian or material frame. I will present a material frame formulation whereby expressions for continuum mechanical variables like stress and heat flux are derived from atomic scale quantities intrinsic to molecular simulation. We derive expressions for the 1st Piola-Kirchhoff (P-K) stress (defined as current forces acting over unit areas from the reference frame) tensor and for the material frame-based heat flux vector. Atomistic simulation results are used to compare the stress expression with both the system virial and the Cauchy stress expression developed by Hardy. Our results show that the P-K stress tensor represents a full and consistent measure of stress. We also present an expanded formulation to define continuum variables from micromorphic continuum theory, and show its suitability and necessity for the analysis of materials represented by directional bonding at the atomic scale.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Biography

Jonathan Zimmerman has been with Sandia National Laboratories in Livermore, California since the fall of 1999, and is currently a Principal Member of Technical Staff in the Mechanics of Materials Department. Jon obtained his Ph.D. from Stanford University in mechanical engineering, where he also received a Master of Science degree in the same subject. As an undergraduate, he attended the State University of New York at Binghamton and earned a B.A. in physics and a B.S. in mechanical engineering.

Jonathan's research interests include solid mechanics, material model development, atomistic simulation, fracture mechanics, dislocation and defect mechanisms, and multi-scale modeling methods.

Refreshments served in 303 MAE-A beginning at 3:50 pm