A GENERAL MULTISCALE THEORY FOR HETEROGENEOUS MATERIALS

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Characterization of the relationship between material microstructure and overall properties is the key to achieving optimized design of the next generation of lightweight, strong and tough materials. Product performance is ultimately controlled by microscale interactions which occur at several distinct scales of deformation within the material.

Currently, we depend on empirical data to define the microstructure-property link in the material design chain. Direct prediction of material properties through explicit modeling of the microstructure, using techniques such as molecular dynamics, is not yet practical in terms of computational expense. At the other extreme, conventional continuum approximations, originally developed for large structural applications, cannot capture the highly localized deformation fields which occur on the order of the microstructure's characteristic length.

Deformation in many materials can be considered at several separate scales, e.g. alloys often contain distinct populations of embedded *microscale* inclusions, *nanoscale* particles and *atomic* scale dislocations. The behavior of each contributes to the overall properties. A model is proposed here in which a material is physically and mathematically decomposed to each individual scale of deformation in terms of its kinematic response and constitutive behavior.

Extra continuum fields are introduced to describe the deformation resolved at each scale. The internal power is decomposed into the contribution from each scale being considered, resulting in a multiscale set of governing equations. Scale specific constitutive behavior is determined through analytical or computational examination of the micromechanics at each scale through a multiscale representative volume element (RVE) approach. Material deformation can subsequently be concurrently solved at each distinct scale of microstructure.

The theory is illustrated for a polycrystalline material, a granular material, a porous material, a theoretical bio-inspired self-healing composite and an alloy containing particles at two scales [1]. This general theory can be applied to any heterogeneous material via a regular finite element approach. The overall material properties can be elucidated in terms of the constitutive behavior at each scale, which is directly linked to the key microstructural parameters. This is achieved without resorting to empiricism.

An extension of the theory into the atomic regime is proposed in which discrete atomic scale information is utilized through a virtual atomic lattice theory to formulate constitutive relationships 'on the fly' during implementation. A smooth transition from discrete atomic theory to multiscale continuum theory is thus made. During implementation, a pre-formulated constitutive relation or the known atomic scale potentials can be used to represent the material behavior at each scale.

References:

[1] Cahal McVeigh, Franck Vernerey, Wing Kam Liu* and L. Cate Brinson, "Multiresolution Analysis for Material Design" To appear in *Computer Methods in Applied Mechanics and Engineering*

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