Micromechanical Modeling of Heterogeneous Materials by Computational Grains

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Abstract
In this study, we review the theory and applications of Computational Grains, for micromechanical modeling of heterogenous materials. Computational Grains are arbitrarily-shaped polygonal elements, modeling real or virtual grains with/without embedded particles, fibers, voids, or cracks. No fine FEM meshing of each grain is needed, thus the preprocessing is greatly simplified. The stiffness matrix of each grain is also directly computed, leading to a great reduction of the computational time. Thus, a direct numerical modeling of the microstructure of heterogeneous materials is realized, which not only gives rapid estimation of macroscopic material properties, but also accurately computes the microscopic stress distribution. One way of computing the stiffness matrix is to use multi-field variational principles together with special trial functions. For example, when studying mechanical behaviors of particulate or fiber composites, Papkovich-Neuber solutions with various kinds of harmonic potentials (spherical, ellipsoidal, cylindrical, etc.) can be used. The other way of computing the stiffness matrix is to re-arrange SGBEM equations, this becomes especially advantageous when modeling microcracks and their growth. Moreover, interface stress effects around nanoparticles/nanofibers, de-cohesions between matrices and inclusions, as well as other interface mechanisms can be easily integrated into the framework Computational Grains, to simulate their influences on the macroscopic material properties. The on-going research & development of Computational Grain is to eventually provide a powerful and easy-to-use suite of tools for the analysis and design of heterogeneous materials.

Keywords: Heterogeneous Materials, Micromechanics, Computational Grains