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High-performance hierarchically parallel multiscale framework for modeling heterogeneous materials

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ABSTRACT

Heterogeneous multiscale materials are present in our everyday lives, embodied in engineered systems such as filled and layered composites, and in nature as soils and layered rock formations. The overall behavior of these materials is heavily influenced by the widely ranging size, shape, distribution, and material property contrasts of their microscale constituents. Understanding how changes in these microstructure parameters affects the overall behavior of the material is important to optimal design and safety assessment of novel materials. Because of the wide range of spatial scales, Direct Numerical Modeling (DNM) of such composite systems is often too computationally expensive, even for today's super computers. Therefore, we have developed a hierarchically parallel numerical framework based on the Generalized Theory of Computational Homogenization (GTCH). The GTCH assumes a separation of the macro- and microscales and links the overall macroscopic response to the microscale response of a Representative Unit Cell through the variational energy equivalence (Hill's Lemma). No assumption is made on the form the macroscopic response, and the response is governed purely by the interaction of the microscale constituents which are generally well understood. In this way, the GTCH numerical framework provides a pathway towards predictive simulation and design of novel material systems. Wepresent a verification study of the multiscale solver against DNM simulation and show excellent agreement with a reduction in the total number of degrees of freedom required by the multiscale method to achieve an equivalent accuracy. In addition, we present results from highly resolved multiscale simulations of failure of engineering-scale structures consisting of particle reinforced composites or reinforced adhesive layers. Finally, we demonstrate the high-performance aspects of the hierarchically parallel numerical framework by a computational scaling study up to tens of thousands of computing cores.