Mechanical Engineering Doctoral Defense

Ultra-efficient and Scalable Uncertainty Quantification and Probabilistic Analysis forHeterogeneous Materials

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Abstract

Ultra-fast 2D/3D material microstructure reconstruction and quantitative structure-property mapping are crucial components of integrated computational material engineering (ICME). It is particularly challenging for modeling random heterogeneous materials such as alloys, composites, polymers, porous media, and granular matters, which exhibit strong randomness and variations of their material properties due to the hierarchical uncertainties associated with their complex microstructure at different length scales. Such uncertainties also exist in disordered hyperuniform systems that are statistically isotropic and possess no Bragg peaks like liquids and glasses, yet they suppress large-scale density fluctuations in a similar manner as in perfect crystals. The unique hyperuniform long-range order in these systems endow them with nearly optimal transport, electronic and mechanical properties. The concept of hyperuniformity was originally introduced for many-particle systems and has subsequently been generalized to heterogeneous materials such as porous media, composites, polymers, and biological tissues for unconventional property discovery. An explicit mixture random field (MRF) model is proposed to characterize and reconstruct multi-phase stochastic material property and microstructure simultaneously, where no additional tuning step nor iteration is needed compared with other stochastic optimization approaches such as the simulated annealing. The proposed method is shown to have ultra-high computational efficiency and only requires minimal imaging and property input data. Considering microscale uncertainties, the material reliability will face the challenge of high dimensionality. To deal with the so-called "curse of dimensionality", efficient material reliability analysis methods are developed. Then, the explicit hierarchical uncertainty quantification model and efficient material reliability solvers are applied to reliability-based topology optimization to pursue the lightweight under reliability constraint defined based on structural mechanical responses. Efficient and accurate methods for high-resolution microstructure and hyperuniform microstructure reconstruction, highdimensional material reliability analysis, and reliability-based topology optimization are developed. The proposed framework can be readily incorporated into ICME for probabilistic analysis, discovery of novel disordered hyperuniform materials, material design and optimization.