Stochastic continuum modeling of random interphases from atomistic simulations

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Abstract :

This work is concerned with the construction of an equivalent continuum model for random interphases, based on a set of atomistic simulations. A stochastic representation for the tensor-valued random field modeling the elasticity field in the interphase region is first presented. Sampling issues are then discussed and a new numerical scheme based on stochastic differential equations is provided. Finally, a statistical inverse problem involving the atomistic computations is introduced in order to identify the stochastic continuum model.

Keywords : Stochastic modeling; interphase; molecular dynamics; statistical inverse problem

1 Introduction

Stochastic multiscale approaches have received a growing attention over the past decades, in both computational mechanics and applied mathematics. In addition to the construction of efficient stochastic solvers for uncertainty propagation, the choice and construction of probabilistic representations are now widely recognized as key ingredients for performing robust and predictive simulations. This step turns out to be especially critical for multiscale and/or multiphysics systems, where uncertainties are exchanged back-and-forth as information is passed across scales. In this prospect, and as a complement to the commonly used functional expansions, information-theoretic probabilistic models have been developed and promoted as a valuable way to perform forward simulations, as well as to solve under-determined statistical inverse problems. In this talk, we present a self-contained treatment of information-theoretic models for non-Gaussian tensor-valued random fields and exemplify the proposed framework through the continuum modeling of random interphases from atomistic simulations of nano-reinforced materials.

2 Stochastic modeling and statistical inverse identification

In order to get a physical insight for the local continuum modeling, we first present a set of molecular dynamics simulations performed on a Polyethylene-like polymer containing spherical silica nanoparticles. These simulations provide a complete description of the local morphology of the polymer chains and show particular conformation and density profiles near the filler, hence allowing for the definition of a random interphase region. We then discuss the construction of the random field model along the lines defined in [1]. The representation involves a term with anisotropic fluctuations (which models the finite-size-sampling noise), as well as a term exhibiting transversely isotropic fluctuations (in spherical coordinates) in the bounded domain Ω_{int} corresponding to the interphase. Next, sampling issues for the non-Gaussian random fields are addressed [2]. In particular, a numerical scheme involving stochastic differential equations and allowing for the simulation of the elasticity field in the interphase region (see Figure 2 for instance) is provided. Computational experiments show that the above algorithm performs very well, regardless of the stochastic dimension. In a last step, we dis-

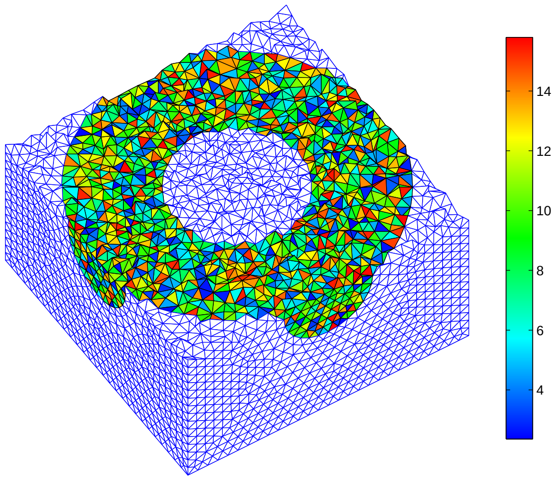

Figure 1: Realization of the random field $\{C_{11}(\boldsymbol{x}), \boldsymbol{x} \in \Omega_{int}\}$ (in GPa) in the interphase region (meshed view of the continuum model).

cuss the calibration of the equivalent continuum representation through a statistical inverse problem involving the atomistic results.

References

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