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Multiscale design of nonlinear materials using a Eulerian shape optimization scheme

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Abstract

Motivated by recent advances in manufacturing, the design of materials is the focal point of interest in the material research community. One of the critical challenges in this field is finding optimal material microstructure for a desired macroscopic response. This work presents a computational method for the mesoscale-level design of particulate composites for an optimal macroscale-level response. The method relies on a custom shape optimization scheme to find the extrema of a nonlinear cost function subject to a set of constraints. Three key "modules" constitute the method: multiscale modeling, sensitivity analysis, and optimization. Multiscale modeling relies on a classical homogenization method and a nonlinear NURBS-based generalized finite element scheme to efficiently and accurately compute the structural response of particulate composites using a nonconformal discretization. A three-parameter isotropic damage law is used to model microstructure-level failure. An analytical sensitivity method is developed to compute the derivatives of the cost/constraint functions with respect to the design variables that control the microstructure's geometry. The derivation uncovers subtle but essential new terms contributing to the sensitivity of finite element shape functions and their spatial derivatives. Several structural problems are solved to demonstrate the applicability, performance, and accuracy of the method for the design of particulate composites with a desired macroscopic nonlinear stress-strain response.

KEYWORDS

analytical sensitivity analysis, fixed grid, gradient-based shape optimization, nonlinear GFEM, NURBS

1 | INTRODUCTION

The precise evaluation of the effective properties of heterogeneous materials has a long and rich history, attracting researchers from multiple disciplines. Various theoretical[1-3] and computational[4-6] micromechanics approaches have been widely used to characterize the structure-property relationships of heterogeneous material systems. The primary objective of these studies is to find the effective properties of a heterogeneous material for a given set of phase properties and microstructure. However, over the last two decades, many researchers restated this question as an inverse problem, that is, how can the different phases of a heterogeneous material be distributed to target or optimize a particular macroscopic material property.[7]