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Topological derivative based optimization of 3D porous elastic microstructures

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As an alternative to the well established microstructural optimization techniques, topological derivative based optimization framework has been proposed and successfully implemented for tailoring/optimizing 2D elastic composites recently, Amstutz et al. [1]. In this paper, an optimization framework for 3D porous elastic microstructures is presented which is based on the notion of topological derivative and the computational homogenization of elastic composites. The sensitivity of the homogenized elasticity tensor to the insertion of infinitesimal hollow spheres within the elastic microstructure is used as the measure for the finite element based evolutionary optimization algorithm. The capabilities of the proposed framework, which is free of any regularization parameter, is assessed by means of example problems including some comparisons with analytical bounds.

1. Introduction

Majority of engineering and natural materials are heterogeneous at a certain scale. Dedicated experimental studies reveal that the superior performance of many natural materials (e.g. sea-shell) is closely linked with such heterogeneities. In fact, attempts to understand and mimic the heterogeneous microstructures observed in nature are considered to be a rational approach to synthesize new engineering materials.

As far as engineering scale component response is concerned, the reliable predictive tools underpinning the microstructure-macroscopic property link are of utmost importance. Therefore, there has been an intensive effort which has resulted in valuable findings in the form of analytical bounds, closed form expressions for effective macroscopic properties and homogenization frameworks combined with efficient computational solution algorithms.

For a considerable group of these studies, the sensitivity of the macroscopic properties to geometrical changes in the microstructure has been the central issue since such an information can be effectively used to optimize or tailor the microstructure to fulfill certain macroscopic performance requirements. In this context, Solid Isotropic Material Penalization (SIMP) method as introduced in Bendsoe and Kikuchi [2], Bendsoe and Sigmund [3], has been the major tool which is used to investigate/synthesize optimum topologies for material microstructures. Essentially, by introducing a smooth fictitious density field, the topology optimization problem is regularized and the optimum microstructure topology is reached through an iterative procedure during which voids are assumed to be forming at the locations where the density falls below a threshold value.

As an alternative, in the realm of topology optimization of continuum structures, the bubble method is proposed and effectively used by Eschenauer and Olhoff [6]. The method is based on the idea of inserting 'bubbles' within a continuum and evaluating approximately the sensitivity of the objective function to the insertion of holes so that optimum locations for material removal can be detected.

In the context of microstructural optimization, a more direct method based on the bidirectional structural optimization (BESO) technique is presented by Huang et al. [10]. Using the homogenization theory and finite element based periodic unit cell solutions, elemental sensitivity numbers are established and used to remove/add elements to construct the optimum porous microstructure.

For microstructural optimization problems, recently an exact analytical formula for the sensitivity of macroscopic elasticity tensor to topological microstructural changes has been proposed, which essentially relies on the notion of topological derivative by Giusti et al. [8,7]. The topological derivative is fundamentally different than the classical derivative notion in the sense that it allows the calculation of derivatives in case of topological singularities such as insertion of holes within an elastic domain. Furthermore this concept has been extended for the calculation of sensitivities in case of elastic inclusion insertion of a different material type than the base material, Giusti et al. [7]. In Amstutz et al. [1], the topological derivative based sensitivities are combined with a level set based optimization algorithm to synthesize

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2D microstructures with desired macroscopic properties including negative Poisson's ratio microstructures.

Departing from the notion of topological derivative and the aforementioned studies, in this paper the exact analytical formula for the sensitivity of the macroscopic elasticity tensor to the insertion of infinitesimal spherical voids into the 3D elastic microstructure is used as the basis for a simple finite element based evolutionary optimization algorithm. The proposed algorithm is implemented by the scripting tools of the commercial FE software Abaqus. The effectiveness of the topological derivative based framework is demonstrated by benchmark problems and the predictions are compared with analytical bounds.

This paper is organized as follows. The homogenization framework used to extract the macroscopic elasticity tensor is briefly reviewed in the next section. Afterwards, the topological derivative concept is introduced and the analytical sensitivity of the macroscopic elasticity tensor to the insertion of infinitesimal spherical void is presented based on the findings of Novotny and Sokolowski [15]. The following two sections are reserved for the details of the finite element based optimization algorithm and the example problems, respectively. Some concluding remarks are made and possible extensions are mentioned in the last section.

2. Homogenization

In this section, homogenization framework used as the basis of this work is summarized. For a detailed treatment, one can consult to Michel et al. [11], Miehe and Koch [12] among others. The presented framework coincides with the asymptotic homogenization, see e.g. Pinho-da-Cruz et al. [16], in case of linear elastic periodic media.

The composition of any heterogeneous solid is generally an assembly of different phases, flaws and interfaces. Almost all variants of homogenization approaches require a properly defined representative volume element (RVE) reflecting the microstructural features in a statistically meaningful way, over which the field variables evolve at the micro-scale. The characteristic length of the RVE is much smaller than the length scale over which the macroscopic field variables vary, which is known as the principle of scale separation. Therefore every material point of the homogenized solid body is equipped with an RVE, reflecting the underlying heterogeneous microstructure, see Fig. 1.

In a first order homogenization framework, at an arbitrary point $\vec{x}$ within the RVE, the displacement field is decomposed as,

$$\vec{u}_m(\vec{x}) = \vec{u}_M + \mathbf{E}_M\vec{x} + \vec{u}^f_m \tag{1}$$

where $\vec{u}_M$ and $\mathbf{E}_M$ are the displacement vector and strain tensor of the associated macroscopic point, respectively. $\vec{u}^f_m$ is the superimposed fluctuation field due to heterogeneous nature of the RVE. This decomposition leads to the following additive strain field,

$$\mathbf{E}_m(\vec{x}) = \mathbf{E}_M + \mathbf{E}^f_m(\vec{u}^f_m) \tag{2}$$

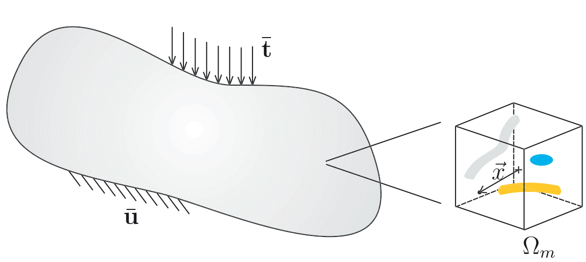

Fig. 1. Macroscopic body and a typical RVE attached to a macroscopic material point.

where the micro-fluctuation strain term is defined as $\mathbf{E}^f_m = \nabla^s \vec{u}^f_m$; ($\nabla^s$ is the symmetric gradient operator). At this stage, it is important to recall the strain averaging assumption which imposes the following integral constraint on the microscopic strain field,

$$\mathbf{E}_M = \frac{1}{|\Omega_m|}\int_{\Omega_m} \mathbf{E}_m \, d\Omega_m \tag{3}$$

where $|\Omega_m|$ is the volume of the RVE. Strain decomposition in turn implies that,

$$\mathbf{S}_m(\vec{x}) = \bar{\mathbf{S}}_m + \mathbf{S}^f_m \tag{4}$$

where the microscopic stress field $\mathbf{S}_m(\vec{x})$ is decomposed into a constant part $(\bar{\mathbf{S}}_m)$ and a fluctuation part $\left(\mathbf{S}^f_m\right)$ given as,

$$\bar{\mathbf{S}}_m = \mathbb{C} : \mathbf{E}_M \text{ and } \mathbf{S}^f_m = \mathbb{C} : \mathbf{E}^f_m \tag{5}$$

respectively. Since linear elastic material behaviour is assumed for every constituent of the RVE, $\mathbb{C}$ is the elasticity tensor of the phase/material point located at $\vec{x}$.

Strain averaging relation, Hill–Mandel principle and additive splits of strains and stresses (Eqs. (2) and (4), respectively) lead to the equilibrium problem of the RVE which can be written as,

$$\int_{\Omega_m} \left[\mathbf{S}^f_m : \nabla^s \delta\vec{u}^f_m + \bar{\mathbf{S}}_M : \nabla^s \delta\vec{u}^f_m\right] d\Omega_m = 0 \tag{6}$$

for which the solution vector is $\vec{u}^f_m \in \widetilde{\mathcal{V}}$ and which has to be fulfilled for every $\delta\vec{u}^f_m \in \widetilde{\mathcal{V}}$. $\widetilde{\mathcal{V}}$ is a subspace of $\mathcal{V}$ which is defined as,

$$\mathcal{V} = \left\{\vec{v}, \int_{\Omega_m} \vec{v}\, d\Omega_m = 0, \int_{\Gamma_m} \frac{1}{2}(\vec{v}\otimes\vec{n} + \vec{n}\otimes\vec{v})\, d\Gamma_m = 0\right\} \tag{7}$$

where $\vec{v}$ has to be square integrable over Ω_m. The problem definition is incomplete without the proper boundary conditions, which are supposed to be fulfilled by the solution $\vec{u}^f_m$. Among various choices, periodically fluctuating displacement boundary conditions are chosen here. For prismatic RVE's, these boundary conditions impose

$$\vec{u}^f_m|_+ = \vec{u}^f_m|_- \tag{8}$$

where $|_+$ and $|_-$ designates the equal sized boundary subset pairs Γ^+ and Γ^- such that $\vec{n}^+ = -\vec{n}^-$, in other words opposite faces of the prismatic RVE. Upon the solution, the macroscopic stresses are obtained by the averaging relation,

$$\mathbf{S}_M = \frac{1}{\Omega_m}\int_{\Omega_m} \mathbf{S}_m \, d\Omega_m \tag{9}$$

2.1. The homogenized elasticity tensor

Since linear elastic behavior is assumed at the micro-scale, the macroscopic response is characterized by the homogenized elasticity tensor $\mathbb{C}_M$ such that,

$$\mathbf{S}_M = \mathbb{C}_M : \mathbf{E}_M \tag{10}$$

The closed form of $\mathbb{C}_M$ can be derived by reconsidering the equilibrium problem (Eq. (6)) as a superposition of multiple linear problems such as,

$$\int_{\Omega_m} \mathbf{S}^f_m : \nabla^s \delta\vec{u}^f_m \, d\Omega_m + \int_{\Omega_m} \mathbb{C} : (\vec{e}_i \otimes \vec{e}_j) : \nabla^s \delta\vec{u}^f_m \, d\Omega_m = 0, \text{ for } i,j = 1,2,3 \tag{11}$$

where $\vec{u}^f_m \in \widetilde{\mathcal{V}}, \delta\vec{u}^f_m \in \widetilde{\mathcal{V}}$ and the particular form of $\widetilde{\mathcal{V}}$ reads as,

$$\widetilde{\mathcal{V}} = \{\vec{v} \in \mathcal{V}; \vec{u}^f_m(\vec{x}^+) = \vec{u}^f_m(\vec{x}^-)\ \forall \text{ pair}(\vec{x}^+, \vec{x}^-) \in \Gamma_m\} \tag{12}$$

$(\vec{e}_i \otimes \vec{e}_j)$ appearing on the right hand side are the independent components of the macroscopic unit strain tensor. The microscopic