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A meshfree approach for homogenization of mechanical properties of heterogeneous materials

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A R T I C L E I N F O

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A B S T R A C T

In this paper, asymptotic homogenization and meshfree Solution Structure Method (SSM) are combined to develop a hybrid homogenization technique. This hybrid method makes it possible to capture accurate geometric information of material microstructure, directly from micrographs or Computed Tomography (CT) scans, and offers a completely automated numerical procedure. Homogenization methods often employ FEA to incorporate realistic geometry of the material's microstructure. However, generating a finite element mesh from images or 3D voxel data could be tedious, error-prone, and expensive. Also, in many practical situations, considerable manual modifications are often required. On the other hand, the SSM uses implicit mathematical functions to represent the geometric model. It could be implemented using different types of basis functions, either on a non-conforming structural grid or cloud of points. Adaptive numerical and geometric algorithms assure good geometric flexibility of SSM in handling complex structures. Furthermore, to accommodate material homogenization equations, the SSM is extended so it can provide the exact satisfaction of periodic boundary conditions without using any spatial meshes. To validate the developed method, the architecture of a computer software package is designed that provides an automated computational pipeline for material homogenization. Numerical examples are provided to evaluate the developed platform against other methods and previously published data.

1. Introduction

Advances made in different technological fields have been linked to innovative designs of new materials such as composites which are made from dissimilar constituents formed into an inhomogeneous structure with a methodical or random geometric distribution. Composite materials are widely used in different industrial fields like thermal and acoustic insulations, lightweight structures, biomedical devices, etc. Mechanical properties of such materials are highly dependent on the properties of the constituents, their spatial distribution, geometry and volume fraction of inclusions.

The early analytical methods for finding the homogenized properties of composite materials were relatively simple, such as rule of mixtures [1]. This method was developed into a more advanced variational technique to predict lower and higher bounds of effective properties [2,3]. Later a self-consistent method was proposed which was capable of taking the geometry of composite fibers into consideration [4]. In early 70's Mori-Tanaka method was introduced to calculate the average internal stress in a matrix of composite materials [5]. Also, a modified version of this method was used to evaluate the effective properties of composites [6].

The applications and computational issues of Finite Element Analysis, as one of the most popular numerical methods for solving homogenization problems, have been studied extensively [7–10]. FEA was used to investigate stress and strain distribution of orthotropic composites and determining their effective strain energy [11]. Similar studies were performed to find out homogenized shear and Young's modulus of reinforced composites [12,13]. Also, effective thermal expansion coefficient for two-phase materials was investigated by applying an FEA homogenization scheme [14]. Numerical results of FEA homogenization were applied in topology optimization for structures of anisotropic materials [15,16].

In an FEA package, it is necessary that a computer model of the domain of interest be generated. Then this model has to be discretized into elements via meshes, which should accurately represent the geometry of the model and also be suitable for prescribing boundary conditions. Especially when dealing with homogenization problems, the periodic nature of their boundary conditions could create undesir-

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able complications. The classical method to impose the periodic boundary condition requires identical meshes on opposing sides of the domain, and as the geometric features of the structure gets more complicated, this condition will be *difficult* to satisfy for arbitrary meshes [17–19].

In recent years, several methods have been developed to generate finite element models based on micrograph images of material microstructure [20,21]. These methods use the pixel color data stored in microstructure images to separate different phases of material and extract corresponding geometry of each phase. Even with the implementation of such tool, there is still a considerable amount of manual work required to modify the model and generate a geometry conforming mesh suitable for finite element studies. In many practical cases, generating a good quality mesh requires simplifications of the model which eventually will affect the accuracy of results.

To overcome the drawbacks of the conventional finite element, meshfree or meshless methods have been developed. The idea behind the meshfree paradigm was introduced by Kantorovich in 1950s; he proposed utilizing a solution structure for solving boundary value problems [22]. Later Solution Structure Method (SSM) was improved and generalized by Rvachev and his team [23]. He suggested using functions that vanish on the geometric boundaries in order to satisfy different types of boundary conditions, and he also proposed an algorithmic approach for constructing such functions on complex geometric models using R-functions [23,24]. This algorithm was successfully implemented for functional representation of a variety of geometric structures [25]. Also, other methods such as least square approximation were assessed for generation of functions which has zero values on the boundaries. This resulted in developing a group of distance-like functions which provides and approximate distance field of the points in the domain to its boundaries and can be used to represent solutions to the boundary value problems providing exact treatment of the prescribed boundary conditions [26,27]. The theory behind solution structures and their applications in different fields are extensively studied in [28–32], and it is shown that implementation of SSM can eliminate the necessity of constructing a geometry conforming mesh which provides a considerable geometric flexibility.

In this paper, asymptotic homogenization approach is combined with the Solution Structure Method. Here we will extend the SSM by constructing solution structures that satisfy periodic boundary conditions on the domain boundaries.

The main contributions of this paper are (1) combination of the asymptotic homogenization approach with meshfree Solution Structure Method; (2) extension of the Solution Structure Method to satisfy periodic boundary conditions; and (3) development of numerical algorithms and software tools to support material homogenization in geometrically complex models. Advantages of the proposed approach include much higher geometric flexibility that makes it possible to easily apply the proposed technique to obtain homogenized material properties from 2D or 3D image data.

This hybrid homogenization technique will inherit careful prediction of homogenized properties from asymptotic homogenization and great geometric flexibility from Solution Structure Method. Solving homogenization equations over a representative volume element (RVE) requires special treatment of periodic boundary conditions, which is usually done via proper mesh generation [17,33]. Meshfree nature of the Solution Structure Method makes it possible to exactly satisfy boundary conditions using so-called solution structures — functions that combine basis functions, approximate distance fields, and prescribed boundary conditions.

Furthermore, a software prototype is developed using the introduced hybrid method. The salient feature of this platform is the ability to calculate homogenized mechanical properties of complex microstructures directly from raw geometric data: micrograph images and CT scans. The prototype uses adaptive numerical algorithms and Solution Structure Method which results in completely automated procedure with virtually no human intervention. The streamlined computational pipeline, absence of the finite element mesh generation makes it possible to provide a fully automated experience from importing micrograph images to the calculation of mechanical properties.

Outline for the rest of the paper is: in Section 2 the idea of MeshFree/Asymptotic homogenization is described and it is followed by three case studies in Section 3. Section 4 summarizes the concept and highlights of our research.

2. Hybrid Meshfree/Asymptotic homogenization

To evaluate effective properties of inhomogeneous materials it is crucial to re-derive governing and constitutive equations in such way that the effect of microstructural inhomogeneities is taken into consideration. Homogenization methods provide the necessary tools to approach this matter. Among different available techniques, Asymptotic method is capable of analyzing inhomogeneous materials with high contrast in the properties of their constituents. And in addition to obtaining effective material properties, it also solves the full structural problem at micro level [9,34]. Although here we have used an Asymptotic method, but the developed platform is not limited to that and can be used to empower any other numerical homogenization technique.

An inhomogeneous material with periodic inclusions can be represented by domain Ω in the global coordinate system $\mathbf{x}$ and the spatially periodic RVE associated with domain Y in local coordinate system $\mathbf{y}$ (Fig. 1). The ratio of macro and micro coordinate systems is defined by ϵ, where $\epsilon \ll 1$ (1). In Asymptotic method, if any physical property of material ($\boldsymbol{\Psi}$) can be related to two distinct macroscale (Ω) and microscale (Y) domains then an expansion in form of (2) can be written with respect to ϵ [15].

$$\mathbf{y} = \frac{\mathbf{x}}{\epsilon} \tag{1}$$

$$\boldsymbol{\Psi}^{\epsilon}(\mathbf{x}) = \boldsymbol{\Psi}^{(0)}(\mathbf{x}) + \epsilon\boldsymbol{\Psi}^{(1)}(\mathbf{x},\mathbf{y}) + \epsilon^2\boldsymbol{\Psi}^{(2)}(\mathbf{x},\mathbf{y}) + \dots \tag{2}$$

where $\epsilon \to 0$, ϵ superscript shows the periodicity of a given variable on the global coordinate system and $\boldsymbol{\Psi}^{(i)}$ function are defined in the domain Ω and they are Y-periodic. On the right-hand side of (2), the behavior of a physical field ($\boldsymbol{\Psi}$) is divided into two parts. The first term ($\boldsymbol{\Psi}^{(0)}$) which is only a function of global coordinates represents the macroscopic (homogenized) part of $\boldsymbol{\Psi}$ and rest of the terms carry the microscopic effects. By using the expanded form of displacement, strain and stress functions and substituting them into macroscale constitutive and balance equations a new form of constitutive equation can be derived which is valid at microscale [35,36,7]:

$$\frac{\partial}{\partial y_j}\left[E_{ijkl}(\mathbf{y})\left(\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial u_k^{(1)}}{\partial y_l}\right)\right] = 0 \tag{3}$$

where E is the material stiffness tensor, $u_k^{(0)}$ and $u_k^{(1)}$ relatively show the components of global and local displacement fields. Mathematical treatment of (3) is extensively discussed in [35] and [36]. It is shown

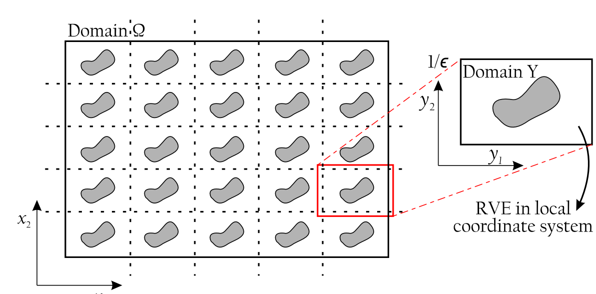

Fig. 1. Schematic representation of global and local coordinate systems.