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Computational homogenization of regular cellular material according to classical elasticity

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ABSTRACT

A two-scale computational homogenization method for deriving the effective elastic parameters of regular cell material is presented. In the present application, particle model is used as the micromechanical model and classical linear elasticity as the continuum model. The method is designed to render the same effective elastic parameters irrespective of the Representative Volume Element (RVE) used for a cell structure. This requires simultaneous fulfillment of the kinematic and kinetic conditions of computational homogenization derived in the study. Also, the relationship between the quantities of the micromechanical and continuum model needs to be invertible on a RVE. Effective elastic parameter expressions for eight planar cellular materials obtained with a typical cell as the RVE are compared to their counterparts in literature. As an application example, a new closed-form compliance expression covering e.g. the square, regular hexagon, rhombus, over-expanded hexagon, and re-entrant hexagon cell structures of literature is presented.

1. Introduction

Many engineering materials, for example wood and low density cellular foams (Gibson and Ashby, 1997), have a microstructure consisting of cells that must be taken into account in the analysis of mechanical properties. In addition, 3D printing makes it feasible to create cellular materials with different microstructures from the isotropic base material. The mechanical properties of this type of cellular or granular material can have mechanical properties suitable for various engineering applications. Accurate prediction of the effects of the microstructure and base materials on the effective material properties is a prerequisite for the efficient use and design of cellular materials.

In a rough classification, mechanical modeling of cellular material can be based on a micromechanical or continuum model. The former approach uses a detailed description of the cell geometry and material properties of the cell walls. This separation of the geometrical and material features is advantageous from the modeling viewpoint and enhances the understanding of the effects of geometrical and material parameters on effective mechanical properties. In the continuum approach, the solution domain consists of the regions occupied by cells. Continuum models have some distinct advantages from the computational viewpoint as small scale geometrical details of the cell structure need not to be modeled explicitly. The challenge is placed on the effective constitutive equations that depend not only on the material properties of the cells but also on the geometry of the cell structure.

Computational homogenization is a method for deriving the effective constitutive equation of a continuum model out of the given micromechanical model. The method, based e.g. on matching of the virtual work expressions of the two models, has various applications of which finding the effective elastic parameters of material having a microstructure is the most common. The method applies

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to irregular and regular microstructures although, in the former case, one may have to deal with issues such as modeling of the conditions at the boundaries as discussed e.g. in Nguyen et al. (2011), Larsson et al., 2011, and Coenen et al. (2012). Statistical nature of the material properties and the effect of scale (Kanit et al., 2003) may bring additional complications. Under the regular microstructure assumption, it is sufficient to consider a Representative Volume Element (RVE) with Periodic Boundary Conditions (PBC). With proper kinematic and kinetic conditions on the RVE, the effective constitutive equation obtained describes the behavior of a non-bounded structure consisting of the RVE's. The regular cell structure model gives a particularly clear picture about the effects of the cell geometry and cell wall material properties on the cell structure rigidity as explicit expression for the effective material parameters are often obtained.

Methods for the computational homogenization of regular cell material have been reviewed e.g. by Hohe and Becker (2002), Charalambakis (2010), and Ostoja-Starzewski (2002). According to Hohe and Becker (2002), the methods can be classified into surface average methods, volume average methods, and two-scale expansion methods. In addition, various 'ad hoc' methods ranging from cell-type specific compliance methods to more formal stiffness methods are used in literature. Also, effective elastic parameter expression for the many variants of elastic triangle, rectangle, and hexagon cell structures are well-known (cf. Wang and McDowell (2004) and Gibson and Ashby (1997)). Most results and discussion of literature are related with planar structures and the effective Young's moduli and Poisson's ratios for the plane-stress or plane strain continuum models. The likely reason is that the simple beam-truss cell model is acceptable in the planar case, whereas the corresponding cell description in three dimensions requires the plate-model or a model based on the full set of elastic equations. Aside from the cell application, effective elastic properties of three-dimensional beam-truss structures have been discussed e.g. in Wallach and Gibson (2001) and Vigliotti and Pasini (2012).

Although the same result can be obtained with different combinations of the method and RVE, often the conditions for the correct result have not been explained in detail or the physical meaning of the conditions is not obvious. In addition, sometimes the correct outcome is due to a clever combination of the method and RVE, so that a reader may get an impression that only a certain RVE out of the many possibilities for a given cell structure works. In the writer's opinion, a detailed explanation of the conditions to be imposed on a RVE would improve the understanding in this respect.

The aim of the article is to discuss the kinematic and kinetic conditions to be satisfied in computational homogenization of regular cell structure and the way to satisfy the conditions simultaneously. The principle of virtual work and kinematic assumption are used in the same manner as in the derivation of engineering models (beams, plates etc.) starting from the generic equations of elasticity. It turns out, that computational homogenization of regular cell structure means matching the continuum and particle model virtual work expressions under the kinematic and kinetic conditions of Hill-Mandel type (Larsson and Diebels, 2007). The method of this article is based on the well-known ideas explained e.g. in Charalambakis (2010) and references therein but contains ingredients that are essential when the micromechanical model is essentially a particle one. The particular selection requires an approximation of the gradient operator inside a polyhedron and kinetic conditions of a certain type. Small displacements and rotations are assumed throughout the study to keep focused on the primary goal.

As examples, effective elastic parameters for eight planar cell structures are compared to their counterparts in literature. In the writer's knowledge, the cell-type RVE's have not been used elsewhere although the choice is quite natural for a cell structure. As an application example, a new closed-form compliance expression covering e.g. the square, regular hexagon, rhombus, over-expanded hexagon, and re-entrant hexagon cell structures of literature is presented.

1.1. Dyadic notation

Vector and dyadic tensor notation is used throughout the article. Single and double arrowheads in $\vec{a}$ and $\overleftrightarrow{a}$ etc. denote dyads of order 1 and 2, respectively. Outer products of vectors and dyadic quantities are written in the concise forms $\vec{a}\vec{c} \equiv \vec{a} \otimes \vec{c}$ and $\overleftrightarrow{a}\,\overleftrightarrow{c} \equiv \overleftrightarrow{a} \otimes \overleftrightarrow{c}$, as there should be no danger for misinterpretations. The notations for the inner and cross-products are usual i.e. $\vec{a} \cdot \vec{c}$ and $\vec{a} \times \vec{c}$, and $\overleftrightarrow{a} \cdot \overleftrightarrow{c}$. The double inner product $\overleftrightarrow{a} : \overleftrightarrow{c}$ of second order dyads has the interpretation $\vec{a}\vec{b} : \vec{c}\vec{d} \equiv (\vec{b} \cdot \vec{c})(\vec{a} \cdot \vec{d})$. Finally, the conjugate $\overleftrightarrow{a}_c$ of dyad $\overleftrightarrow{a}$ is defined by $\vec{b} \cdot \overleftrightarrow{a}_c = \overleftrightarrow{a} \cdot \vec{b}\ \forall \vec{b}$ and the second order unit dyad $\overleftrightarrow{I}$ by $\overleftrightarrow{I} \cdot \vec{a} = \vec{a} \cdot \overleftrightarrow{I} = \vec{a}\ \forall \vec{a}$.

Polyhedrons with planar faces and selected points of the polyhedral domain, called as nodes, are used in the cell structure description. Geometry of the polyhedron is taken to be defined by the exterior nodes located on the edges of the planar faces. Position vector of nodes i is denoted by $\vec{r}_i$. Notation $\vec{r}_i i \in I_{\text{ext}}$ is used for the set of exterior nodes located on the polyhedron and $\vec{r}_i i \in I_{\text{int}}$ for the set of interior nodes located inside the polyhedron.

2. Gradient approximation

Approximation of the gradient operator inside a polyhedron is needed later in the discussion. The gradient approximation can be taken as a generalization of the one-dimensional difference approximation to the first derivative and it also shares some of the well-known properties of the one-dimensional version.

For a continuous vector field $\vec{u}(\vec{r})$ of constant $\nabla\vec{u}$ on a polyhedral domain Ω, Gauss's theorem implies that

$$V\nabla\vec{u} = \sum_{\alpha} \vec{A}^{\alpha}\vec{u}^{\alpha}, \tag{1}$$

in which the sum extends over the polyhedron faces, $\vec{A}^{\alpha}$ is the outward directed area of face α, $\vec{u}^{\alpha}$ is the mean value of $\vec{u}(\vec{r})$ on face α, and V is the volume of the polyhedral