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Homogenization of non-periodic zones in periodic domains using the embedded unit cell approach



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ABSTRACT

In this paper we present the development of the embedded unit cell (EUC) approach, a new concept designed to facilitate homogenization and multi scale analysis of composite materials/domains in cases where the classical theory of homogenization is not valid due to lack of periodic microscopic response, e.g. in the boundary of a periodic macroscopic domain.

The EUC approach is based on a non-periodic formulation of the asymptotic homogenization theory and evaluates the local/micro response of non-periodic zones, based on alternative boundary conditions. Finally, a verification study, which demonstrates the appropriate numerical performance of the suggested homogenization approach, is presented.

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1. Introduction

Composite materials [1–3] are widely used in modern industry, however their underlying inhomogeneity on more than one scale can influence the analysis and research of these materials. This study reports on an analysis of the mutual impact between the properties of the material at the global macroscale and local microscale.

Increasing material complexity at the microscopic scale complicates the analysis of the mechanical response, which is vital for analysis of such structures. A constantly growing number and complexity of structures has prompted the development of preprogrammed simulations of complex structures. One of the alternatives to evaluate the response of such structures is to use the finite element method with mesh refinement, which contains all the data concerning the heterogeneity of the material, such as the amount, type, sizes and shapes of the inhomogeneous inclusions. Consequently, FE model includes a severe number of degrees of freedoms as the macroscopic response solution is based on modeling of the microscopic material properties. The main problem with such a model is the extensive computational resources required to accurately evaluate the material level response.

Multi-scale analysis is a computational method that significantly reduces the computational cost of the models by decreasing the number of degrees of freedom in the macroscopic problem

* Corresponding author. *E-mail addresses:* erezgal@bgu.ac.il, shuhman@gmail.com (E. Gal). [4,5] and often uses homogenization theory, to pass the information between the material scale and structure scale [6–8]. Homogenization theory was developed to overcome these limitations involving the substitution of heterogeneous material by an equivalent homogeneous domain material sample with additional model of the representative unit cell material properties. Among the restrictions of generalized homogenization theory (which is the mathematical formulation of the multi-scale analysis), there is periodicity assumption of the unit cell geometry and microscopic response.

The procedure of evaluating the response of composite materials by applying the homogenization theory on both scales using the finite element (FE) models is well established [9–20]. For an accurate microscopic solution, the finite element model should include a refine mesh that properly represents the material heterogeneity in addition to a coarse FE model of the macroscopic level to obtain the structure response.

The issue of using unit cell in non-periodic domains was reviewed by several researchers. Among them, the minimal kinematic boundary conditions (B.C.) for simulations of unit cell disordered microstructures that were presented by Mesarovic and Padbidri [21]. He compared rigid and periodic boundary conditions to a minimal kinematic boundary condition. It was shown that for this case, rigid or periodic B.C. are: less economical due to additional constraint causing boundary effects; less accurate since additional constraint results in a stiff response; and might not be able to capture some important features of the material's behavior. Mesarovic and Padbidri [21] conclude that the integral constraints



of the minimal kinematic boundary prevail on rigid and periodic boundary conditions for this class of problems. These integral B.C. have the same essence as the suggested EUC approach concept.

Miehe [22] deals with the existence of the quasi-hyper-elastic stress potential that allows to extend the homogenization approaches of elasticity to the incremental setting of inelasticity. Focusing on macro-strain driven micro-structures, Miehe [22] developed a new incremental variational formulation of the global homogenization problem where a quasi-hyperelastic macro-stress potential is obtained from a global minimization problem with respect to the fine-scale displacement fluctuation field. Miehe [22] investigated three different B.C. constraints on the microscopic fluctuation field: (i) linear displacements, (ii) periodic fluctuations and (iii) constant stresses on the boundary of the micro-structure. In [22] it can be observed that the constant stress condition provides the softest response associated with intense deformations of the micro-structures. The linear displacement condition provides the stiffest response. In this paper, we present the development of the special boundary conditions that have the same essence of the constant stress case, yet we add a surrounding domain in order to properly relate the microscopic and macroscopic responses by stiffening the microscopic response according to the location of the unit cell in the macroscopic domain.

Fish and Fan [23] proposed a formulation based on asymptotic expansion of the displacement field around an arbitrary reference point. The formulation was used to obtain the microscopic large displacement response and also to discuss its ability to predict the response in local-global engineering problems having a non-periodic response. Other investigations of non-periodic problems have been discussed by Cherdantsev [24], who showed that convergence of bi-scale finite element analysis can be achieved without assuming periodicity at the micro scale level. For the homogenization of fracture mechanics of concrete/brittle-materials structure having non-periodic microscale response, Nguyen et al. [25,26] and Verhoosel et al. [27] suggested a homogenization-like procedure based on combining of the enhanced fields with averaging the response at several Gauss points.

Here we present a multi-scale technique based on the theory of homogenization for non-periodic responses based on alternative boundary condition together with surrounding domain, called the embedded unit cell (EUC) approach. In this study, multi-scale analysis is used to evaluate the macroscopic and microscopic responses of heterogeneous materials [28–30], thereby avoiding the assumption of periodic response at the micro-scale, which is required for the classic homogenization theory to be valid. The EUC approach comes to expand the homogenization theory that is based on the assumptions of a periodic unit cell (microscopic) response [31-33] and faces severe restrictions in cases, where separation of scales is difficult to achieve. For example, in concrete structures [34–38], where the heterogeneity of the microscopic structure is more pronounced, the size of the microscopic unit cell is relatively large compared to the size of the macroscopic structure. Another application, where the proposed approach was proved as appropriate homogenization procedure is the analysis of structures having a material matrix that impedes the determination of the repetitive unit cell in a specific zone. A further complication may involve components, where the local/micro responses are expected to develop stress concentrations at specific zones, for example a plate with stress concentration in the vicinity of small holes. The application of the suggested EUC approach for these type of problems is detailed in Grigorovitch and Gal [39]. For the purpose of homogenizing periodic domains with nonperiodic zones, the formulation of Grigorovitch and Gal [39] has been extended in this paper by the development of embedded unit

cell models that contain a set of equivalent springs which represent the surrounding domain. The suggested EUC approach is based on a zone-adapted unit cell, which is restricted by alternative boundary conditions and surrounded by a micro-scale domain that represents the non-periodic features of adjacent cells according to the macroscopic location of the unit cell. This approach can reduce the computational cost of the macroscopic/global models while retaining the precision of the microscale problem solutions. The EUC concept broadens the applicability of multiscale analysis techniques for the evaluation of the mechanical response of a variety of composite materials which are widely used in modern construction industry, in particular highly heterogeneous materials (such as concrete, etc.). In the suggested formulation we use the theory of homogenization as a domain decomposing scheme where multi-scale analysis is used to evaluate the macroscopic and microscopic responses of heterogeneous materials.

The suggested EUC approach is based on a multi-scale formulation of the asymptotic homogenization theory and can be used to evaluate the structure response of non-periodic zones, such as damage zones, where developing of stress concentrations is expected. Finally a numerical implementation and verification study are presented to demonstrate the efficiency and accuracy of the suggested approach.

2. Embedded unit cell formulation

The following sections describe the mathematical formulation of the suggested EUC approach.

The initial assumption is that the macroscopic body Ω is composed of a heterogeneous microscopic structure with a local periodicity set of unit cells Θ (e.g. see [40–43] for more details see [44]), as shown in Fig. 1.

The problem can be described as a coupled pair of more simplified problems, each relating to different scale. The first one comes to describe a macro scale or the structure level, as presented by Ω domain in Fig. 1. The second one describes a micro scale or the material level that composed of microscopic unit cells presented by Θ domain in Fig. 1.

The relation between the macroscopic coordinate system x_i to the microscopic coordinate system y_i is defined by:

$$y_i = x_i / \zeta, \quad i = 1, 2, 3 \dots$$
 (1)

where ζ is the ratio between the scales

$$\frac{\partial \mathbf{x}_i}{\partial y_j} = \zeta \delta_{ij} \tag{2}$$

where δ_{ij} is the Kronecker Delta.

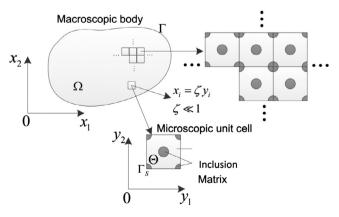


Fig. 1. Heterogeneous microscopic structure with local periodicity unit cells.

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