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Two-scale computational approach using strain gradient theory at microlevel

Tomislav Lesičar, Zdenko Tonković, Jurica Sorić*

Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia

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ABSTRACT

Realistic description of heterogeneous material behavior demands more accurate modeling at macroscopic and microscopic scales. In this frame, the multiscale techniques employing homogenization scheme offer several solutions. Most recently developed two-scale scheme employing second-order homogenization requires the nonlocal theory at the macrolevel, while the classical local continuum theory is kept at the microlevel. In this paper, a new second-order computational homogenization scheme is proposed employing the higher-order theory at both macro- and microlevel. Discretization is performed by means of the C^1 finite element developed using the strain gradient theory. The new gradient boundary conditions employed on representative volume element (RVE) are derived. The relation between the internal length scale parameter and the RVE size has been found. The new procedure is tested on a benchmark example, where the results have been compared to the solutions obtained by the usual second-order homogenization using the local concept on the RVE.

1. Introduction

It is known that all engineering materials can be treated as heterogeneous at some scale of observation. Therein, material heterogeneity and anisotropy play a major role, because almost all materials are heterogeneous and anisotropic due to their natural structure, particularly on the microscopic scale. Profound demands on structural integrity in recent years lead to development and the application of new materials with complex microstructure giving desired material properties. Numerical analysis of mechanical behavior of this new class of materials emerges necessity for an advanced numerical tools employing more realistic material description. Heterogeneous metals such as nodular cast iron are widely used as the material of structural components in mechanical engineering. The ductile nodular cast iron consists of graphite nodules in a ferritic matrix providing large fatigue strength. The geometrical and material properties of the constituents making up the microstructure have a significant impact on the material behavior observed at the macroscale [1]. In addition, the external loading applied at the macroscale might cause changes in the microstructural morphology e.g., void formation, damage as well as cracking, which can put structural integrity at risk. Therefore, in order to assess structural integrity and to predict structural lifetime, an analysis of the evolving microstructure is necessary.

During recent years, a special attention has been directed to the investigation of the relations between the macroscopic material behavior and its microstructure. The determination of an effective material parameters was possible only by experiments or by semi-analytical homogenization methods based on the assumptions of constitutive behavior. Unfortunately, this class of methods cannot adequately capture physical mechanisms managing behavior of the microconstituents. In a multiscale approach, the response of coarse scale problem incorporates physical understanding of material behavior at the lower scales. Firstly, the homogenization concept has been developed in the framework of a classical local continuum theory. In this concept several homogenization approaches are available, such as the mathematical method of homogenization, the Mori-Tanaka method, the double inclusion model, the numerical homogenization, asymptotic homogenization etc., as can be found in [2–4]. However, in more recent formulations several computational homogenization approaches have been used [5–12]. These computational procedures are based on the solution of two boundary value problems, one at the macroscopic and one at the microscopic scale. The results obtained by the simulation of a microscopic representative sample of material named Representative Volume Element (RVE) are used at the macrolevel analysis. Thus, the computational multiscale approach does not require an explicit constitutive relation at the macrolevel, which allows modeling of complex microstructure geometry as well as deformation responses. When in the scale transition procedure only the first displacement gradient is involved, whereby the stress at a material point depends only on the strain (and other state variables) at the same point, this method is referred as the first-order homogenization [13–15]. However, the first-order computational homogenization relies on the intrinsic assumption

* Corresponding author.

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of uniformity of the macroscopic stress and strain fields appointed to a representative volume element (RVE). Due to uniformity assumption, the first-order homogenization is not adequate for the problems dealing with high gradients, where the macroscopic fields can vary rapidly. Therefore, only simple loading cases can be studied, which is considered as a deficiency. Another major shortcoming of the first-order homogenization approach is an inability to encompass microstructural size effects in a material, such as strain localization phenomena and material softening.

The mentioned shortcomings of the first-order approach have been overwhelmed in an extended formulation proposed in a second-order computational homogenization procedure [8,16,17]. This computational strategy comprises a nonlocal continuum theory at the macroscale, which takes into account the influence of a surrounding material on the behavior of a considered material point [18,19]. Herein, the size effects can be accounted for through the RVE size. The microstructural level represented by the RVE is treated as an ordinary local continuum, see [20,21], which is in this case able to capture more complex deformation modes. For the numerical implementation of the multiscale framework, finite element method is the most popular approach. To solve boundary value problems employing the nonlocal theory which is in second-order homogenization adopted at the macrolevel, C^1 continuous interpolations should by applied in appropriate finite element formulations, where displacements, as well as displacement gradients (strains) should be continuous functions. On the other hand, at the microstructural level classical theory is preserved, where the standard finite elements employing C° continuity are usually used for discretization. Thus, based on the aforementioned numerical implementation aspects, the multiscale scheme employing the second-order computational homogenization, which comprises the nonlocal theory at the macrolevel and the local theory on the microlevel in the following text will be referred as the NL-SL (nonlocal-standard local) second-order homogenization. Unfortunately, the NL-SL second-order computational homogenization approach suffers from difficulties in the scale transition methodology due to the coupling between the nonlocal theory at the macroscale and the local concept on the RVE. Namely, the second-order macrolevel gradient cannot be related to the microlevel higher-order gradient as a true volume average. Therefore, in the micro-to-macro scale transition, after resolving Hill-Mandel energy condition, the homogenized double stress requires a modified definition at the microstructural level. Furthermore, in case of generalized periodic boundary conditions, an artificial stress concentration appears at the RVE corner nodes, as result of suppressed microfluctuations at the RVE corners [17]. In order to cope with this problem, some regularization methods have been proposed. A substantially different approach has been derived in [21,22] for the multiscale kinematics, where zero projection of the microfluctuations at the macrolevel is enforced through the principle of orthogonality. The orthogonality is enforced by a vanishing surface integral of the micro-macro variable scalar product. Even though such formulation has notable advantages, again, some relaxed constraints on the fluctuation field are required to avoid stress concentrations at the corners. Similar solution has been recently proposed in [23], using the method of multiscale virtual power. In this approach, the external body forces and macroscale displacements are used in the macro-to-micro scale transition. A novel concept of conservation of kinematical quantities is introduced and used for derivation of the boundary conditions and homogenized quantities. This approach can be considered as an extension of the framework derived in [17,22], since the resulting relations in the absence of the volume forces and inertia effects coincide with the relations derived in the above mentioned references. Even though significant research has been published on the macro-to-micro scale transition in the second-order homogenization framework, this challenging problem still remains open for further studies.

In addition, the discretization of the macrostructural level in the NL-SL scheme is usually performed using mixed finite element formulations, where the C^1 continuity requirements are fulfilled in a weak sense, via Lagrange multiplier or penalty method [24–29]. But, the mixed finite element formulations show a poor behavior compared to the C^1 finite elements [29–31]. Besides the mixed finite element formulation, other approaches can be used for solving gradient problems, such as the discontinuous Galerkin method [32,33], the meshless methods [34–36], or the boundary element methods [37–39]. A comprehensive overview can be found in [40]. Despite large efforts, an efficient numerical formulation for solving strain gradient problems is still unresolved.

In this paper the authors propose a new second-order computational homogenization scheme employing the nonlocal theory at both scales. Therein, the mathematical consistency of the transition methodology is ensured, considering conforming continuum theories used at different scales. The computational scheme is derived adopting the gradient elasticity theory and small strain setting. The discretization at both the macro and microlevel is performed by the C^1 continuity plane strain triangular finite element derived and verified earlier in [41,42]. In that sense, the newly proposed framework derived in this contribution will be referenced as the NL-NL (nonlocal-nonlocal) second-order computational homogenization. The macro-to-micro scale transition methodology is derived using the gradient displacement and gradient generalized periodic boundary conditions. A consistent NL-NL homogenization scheme has been proposed. The derived scale transition methodology, as well as homogenization procedure were embedded into the finite element program ABAQUS by means of FORTRAN subroutines. The performance and accuracy of the proposed approach has been verified on an elastic shear layer example.

The paper is organized as follows. In Section 2 the gradient theory is discussed and the constitutive relations of the Aifantis gradient elasticity theory are displayed. Section 3 deals with the numerical implementation of the Aifantis theory into finite element method. The basic relations of the C^1 triangular finite element are derived. Also, the physical role of the element nodal degrees of freedom is discussed. Some issues of implementation of a non-standard finite element into the commercial FE software ABAQUS are described. In Section 4, a new gradient-enhanced second-order computational homogenization is developed, where the complete micro-macro transition procedure is explained. The dependence of the RVE size on the length scale parameter of the Aifantis gradient theory is investigated. The performance of the newly developed homogenization procedure is verified in Section 5. The standard benchmark problem of shear layer is discussed, where the accuracy of the results obtained by the NL-NL algorithm is confirmed by the comparison to the NL-SL homogenization scheme available in the literature.

2. Higher-order continuum theory

2.1. Small strain second-gradient continuum formulation

In a classical small strain continuum theory, kinematical behavior at time t is described by the vector of the displacement field $\mathbf{u} = u_i\mathbf{e}_i$. The displacement gradient describes the second-order strain tensor expressed by the components as

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}). \tag{1}$$

In the second-gradient continuum theory, a third-order strain gradient tensor ${}^3\boldsymbol{\eta}$ is introduced, which is defined as gradient of the strain tensor

$${}^3\boldsymbol{\eta} = \eta_{ijk}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k = \nabla \otimes \boldsymbol{\varepsilon}, \tag{2}$$

with a minor symmetry in the last two indices $\eta_{ijk} = \eta_{ikj}$, [43]. Accordingly, the variation of the strain energy density function may be expressed in terms of both the strain and the strain gradient as