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A Novel Approach in Multiscale Analysis of Quasi-brittle Softening Materials

Filip PUTAR, Jurica SORIĆ, Tomislav LESIČAR, Zdenko TONKOVIĆ

Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia

E-mails: {filip.putar, jurica.soric, tomislav.lesicar, zdenko.tonkovic}@fsb.hr

Abstract. A second-order computational homogenization multiscale procedure for the damage analysis of quasi-brittle materials is presented. Higher-order continuum theory embedded into the two dimensional C^1 continuity triangular finite element is employed at both micro- and macroscale. Microscale boundary value problem is based on solving the constitutive relations of gradient elasticity coupled with the isotropic damage law. Softening of an arbitrary heterogeneous material can be captured at the macroscale by the application of the second-order homogenization procedure on the damaged RVE. All the algorithms derived are implemented into the FE software ABAQUS via user subroutines.

1 Introduction

The mechanical response of heterogeneous materials, observed from a macrostructural level, is highly dependent on the microstructural characteristics, such as size, shape, spatial distribution, volume fraction and properties of the individual constituents. Modeling of the microstructure of such materials can be used to assess the overall or effective material properties, and also to predict the occurrence of failure which limits the operational use of many engineering structures. The most efficient way to model the heterogeneous materials with complex microstructure is shown to be via the multiscale methods, where the information is exchanged between different length scales, typically micro- and macroscale, by means of the computational homogenization (CH). There is no need to make any constitutive assumptions at the macroscale, as the response of the homogenized material is determined during the analysis by solving a microscale boundary value problem (BVP) associated with each macroscopic integration point. An important concept here is the representative volume element (RVE), which can be defined as a smallest sample statistically representative for the microstructure, as described in [1].

Classical homogenization techniques are built upon the principle of separation of scales, where the uniform distribution of the macro-strain over the entire RVE domain is assumed. This, however, is violated when the first-order CH schemes, described in [2], are used with the problems where strain softening occurs at the microlevel, associated with the formation of the sharp strain localization zones. When there is no clear separation of scales, capturing of the propagation of the underlying rapidly fluctuating responses can be remedied to some extent by higher-order enrichment of the macroscopic continuum. Besides, standard continuum formulation at the macroscale cannot regularize the formation of the strain localization, which in addition leads to the ill-posedness of the macrostructural BVP. As an improvement to the first-order CH, second-order CH is proposed in [3],[4], which is shown to be successful in treating only the mildly softening materials, specifically the materials not exhibiting the deformation beyond a quadratic nature in the displacements [5]. With the occurrence of the sharp strain localization, homogenized response stops being objective with the respect to the size of the RVE - by increasing the size of the micro-sample, the macroscopic structural response becomes more brittle. In that case RVE stops being statistically representative for the macroscopic material point and should be called a microstructural volume element (MVE) instead, as stated in [6]. Another class of multiscale methods which deal with the strain softening problems is based upon the enrichment of the macroscale continuum with a discontinuity, where the microscale strain localization band is lumped into a macroscale cohesive crack. Taking into account the techniques used for the extraction of the equivalent discontinuity and formation of the corresponding macrostructural effective constitutive relation, several different procedures can be found in the literature [7]-[11]. The existence of an RVE for softening materials undergoing localized damage has been confirmed in [12], where a new averaging technique based on extraction of the deformation of just a localization band is proposed. By using this technique, a CH scheme for discrete macroscopic crack modeling that is objective with respect to the size of the RVE is presented in [10] and [13]. In [14], a new second-order computational homogenization scheme is derived, where the C^1 continuous finite elements are employed at both macro- and microlevel. Employment of the nonlocal theory at the microscale has shown better efficiency compared to available homogenization schemes, additionally offering an advanced frame for damage modeling. Recently, a new damage model employing the strain gradient theory embedded into C^1 continuous finite elements is presented in authors' previous work [15], where the exceptional regularization capabilities of such model are demonstrated.

In the present paper, multiscale scheme based on the combination of work shown in [14] and [15] is realized by implementation of the new damage model at the microlevel. No objectivity issues related to the macroscale discretization are expected since the C^1 continuity should completely regularize the problem. As a starting point of this research conventional homogenization based on averaging over the whole micro-domain is considered, despite the aforementioned problems with the non-existence of the damaged MVE. Derivation of the appropriate homogenization model for the elimination of this unwanted behavior is still under investigation and will be included in authors' following research.

2 C^1 continuity triangular finite element formulation

In the presented research, the C^1 continuity plane strain triangular finite element proposed in [16] is used for the discretization of both micro- and macrolevel BVP. The element is based on a small-strain second-gradient continuum theory for which more details can be found in [14]. As shown in Fig. 1, it consists of three nodes, each having 12 degrees of freedom which are two displacements and their first- and second-order derivatives with respect to the Cartesian coordinates. The element displacement field is approximated by the fifth order polynomial.

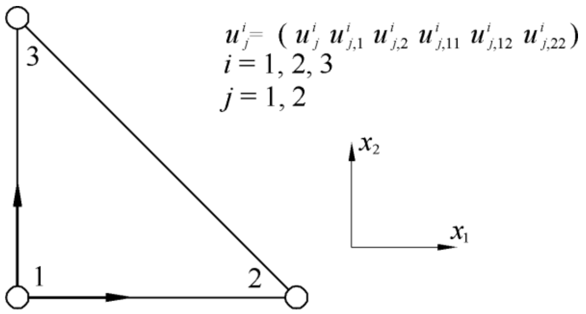

Figure1: C^1 triangular finite element

The finite element equations for both scales are derived from the same form of the principle of virtual work given as

$$\int_A \delta\boldsymbol{\varepsilon}^T \boldsymbol{\sigma}\, \mathrm{d}A + \int_A \delta\left(\boldsymbol{\varepsilon}_{x_1}\right)^T \boldsymbol{\mu}_{x_1}\, \mathrm{d}A + \int_A \delta\left(\boldsymbol{\varepsilon}_{x_2}\right)^T \boldsymbol{\mu}_{x_2}\, \mathrm{d}A = \int_s \delta\mathbf{u}^T \mathbf{t}\, \mathrm{d}s + \int_s \delta\left(\mathrm{grad}\,\mathbf{u}^T\right)\mathbf{T}\, \mathrm{d}s\,, \quad (1)$$

where A and s are area and perimeter of the element, respectively. First term on the left hand side of (1) is well known classical term consisting of the strain $\boldsymbol{\varepsilon}$ and Cauchy stress $\boldsymbol{\sigma}$. The higher-order terms contain the higher-order strain gradients $\boldsymbol{\varepsilon}_{x_1}$ and $\boldsymbol{\varepsilon}_{x_2}$ and their work conjugates $\boldsymbol{\mu}_{x_1}$ and $\boldsymbol{\mu}_{x_2}$, given for both directions of Cartesian coordinates x_1 and x_2. $\mathbf{t}$ and $\mathbf{T}$ are the traction tensor and the double traction tensor, respectively.

2.1 Macrolevel finite element formulation

The stress and the second-order stress increments at the macrolevel, $\Delta\boldsymbol{\sigma}$ and $\Delta\boldsymbol{\mu}$, are computed by the generalized incremental constitutive relations [14] defined as

$$\begin{aligned}
\Delta\boldsymbol{\sigma} &= \mathbf{C}_{\sigma\varepsilon}\Delta\boldsymbol{\varepsilon} + \mathbf{C}_{\sigma\varepsilon_{x_1}}\Delta\boldsymbol{\varepsilon}_{x_1} + \mathbf{C}_{\sigma\varepsilon_{x_2}}\Delta\boldsymbol{\varepsilon}_{x_2}\,, \\
\Delta\boldsymbol{\mu}_{x_1} &= \mathbf{C}_{\mu_{x_1}\varepsilon}\Delta\boldsymbol{\varepsilon} + \mathbf{C}_{\mu_{x_1}\varepsilon_{x_1}}\Delta\boldsymbol{\varepsilon}_{x_1} + \mathbf{C}_{\mu_{x_1}\varepsilon_{x_2}}\Delta\boldsymbol{\varepsilon}_{x_2}\,, \qquad (2) \\
\Delta\boldsymbol{\mu}_{x_2} &= \mathbf{C}_{\mu_{x_2}\varepsilon}\Delta\boldsymbol{\varepsilon} + \mathbf{C}_{\mu_{x_2}\varepsilon_{x_1}}\Delta\boldsymbol{\varepsilon}_{x_1} + \mathbf{C}_{\mu_{x_2}\varepsilon_{x_2}}\Delta\boldsymbol{\varepsilon}_{x_2}\,,
\end{aligned}$$

where the nine different macroscopic constitutive tangents, denoted with $\mathbf{C}$ and appropriate subscripts, are necessary for the description of the arbitrary heterogeneous microstructure. After the homogenization of the damaged microstructure, reduction of the element values of the constitutive tangent matrices leads to the softening of the material at the macrolevel. Finite element equation can easily be obtained by the insertion of (2) into linearized and discretized form of (1), with more details provided in [14].

2.2 Microlevel finite element formulation

After the application of the isotropic damage law, described in [15], to the constitutive relations of the gradient elasticity which can be found in [14], following relations are obtained

$$\Delta\boldsymbol{\sigma} = (1-D)\mathbf{C}\Delta\boldsymbol{\varepsilon} - \mathbf{C}\boldsymbol{\varepsilon}^{i-1}\Delta D,$$
$$\Delta\boldsymbol{\mu}_{x_1} = l^2(1-D)\mathbf{C}\Delta\boldsymbol{\varepsilon}_{x_1} - l^2\mathbf{C}\boldsymbol{\varepsilon}_{x_1}{}^{i-1}\Delta D, \tag{3}$$
$$\Delta\boldsymbol{\mu}_{x_2} = l^2(1-D)\mathbf{C}\Delta\boldsymbol{\varepsilon}_{x_2} - l^2\mathbf{C}\boldsymbol{\varepsilon}_{x_2}{}^{i-1}\Delta D.$$

Here, l represent the parameter of nonlocality, while $\mathbf{C}$ is the classical elasticity matrix which is sufficient for the description of the stiffness behavior of the homogeneous material assumed at the RVE level. D is the damage variable ranging from zero to one, by which the undamaged and fully damaged material are described, respectively. Stress and higher-order stress gradient increments are computed from the values of the last converged equilibrium state (i–1). By using the same procedure as described earlier, finite element equations for the softening analysis of the RVE can be written in the following form

$$\left(\mathbf{K}_\sigma + \mathbf{K}_{\mu_{x_1}} + \mathbf{K}_{\mu_{x_2}}\right)\Delta\mathbf{v} = \mathbf{F}_\mathrm{e} - \mathbf{F}_\mathrm{i}\ , \tag{4}$$

with the particular element stiffness matrices defined as

$$\mathbf{K}_\sigma = \int_A (\mathbf{B}_\varepsilon)^T \left[(1-D)\mathbf{C}\mathbf{B}_\varepsilon - \mathbf{C}\boldsymbol{\varepsilon}^{i-1}\left(\frac{\mathrm{d}D}{\mathrm{d}\boldsymbol{\varepsilon}}\right)^{i-1}\mathbf{B}_\varepsilon\right]\mathrm{d}A,$$
$$\mathbf{K}_{\mu_{x_1}} = l^2\int_A (\mathbf{B}_{x_1})^T \left[(1-D)\mathbf{C}\mathbf{B}_{x_1} - \mathbf{C}\boldsymbol{\varepsilon}_{x_1}{}^{i-1}\left(\frac{\mathrm{d}D}{\mathrm{d}\boldsymbol{\varepsilon}}\right)^{i-1}\mathbf{B}_\varepsilon\right]\mathrm{d}A, \tag{5}$$
$$\mathbf{K}_{\mu_{x_2}} = l^2\int_A (\mathbf{B}_{x_2})^T \left[(1-D)\mathbf{C}\mathbf{B}_{x_2} - \mathbf{C}\boldsymbol{\varepsilon}_{x_2}{}^{i-1}\left(\frac{\mathrm{d}D}{\mathrm{d}\boldsymbol{\varepsilon}}\right)^{i-1}\mathbf{B}_\varepsilon\right]\mathrm{d}A.$$

$\mathbf{B}_\varepsilon$, $\mathbf{B}_{x_1}$ and $\mathbf{B}_{x_2}$ in the upper relations contain the first and second derivatives of the finite element interpolation functions, and $\Delta\mathbf{v}$ is the nodal displacement increment vector. Definition of the external and internal nodal forces $\mathbf{F}_\mathrm{e}$ and $\mathbf{F}_\mathrm{i}$, as well as the detailed information about the higher-order damage model can be found in [15].

3 Scheme of C^1-C^1 second-order CH multiscale algorithm

3.1 Macro-to-micro scale transition

Herein, basic relations of the second-order CH scheme with the non-local theory included at the microscale are provided. Discretization of both levels is made by the above described C^1 triangular finite elements. Considering the subscripts "M" or "m", quantities in the following relations refer to the macrolevel or micolevel, respectively. RVE boundary displacement field is defined according to [14] by

$$\mathbf{u}_\mathrm{m} = \boldsymbol{\varepsilon}_\mathrm{M}\cdot\mathbf{x} + \frac{1}{2}\left[\mathbf{x}\cdot(\nabla\otimes\boldsymbol{\varepsilon}_\mathrm{M})\cdot\mathbf{x}\right] + \mathbf{r}\ , \tag{6}$$

where $\mathbf{x}$ is a spatial coordinate of the RVE boundary, $\mathbf{r}$ the microstructural fluctuation field, and $\boldsymbol{\varepsilon}_{\mathrm{M}}$ and $\nabla \otimes \boldsymbol{\varepsilon}_{\mathrm{M}}$ represent the macrolevel strain and strain gradient, respectively. Microlevel strain and strain gradient can be directly derived from (6) by application of the gradient operators, from where the following relations can be formulated

$$\begin{aligned} &\frac{1}{V}\int_V \left(\nabla_{\mathrm{m}} \otimes \mathbf{r}\right) \mathrm{d}V = \frac{1}{V}\int_\Gamma \left(\mathbf{n} \otimes \mathbf{r}\right) \mathrm{d}\Gamma = \mathbf{0}, \\ &\frac{1}{V}\int_V \left[\nabla_{\mathrm{m}} \otimes \left(\nabla_{\mathrm{m}} \otimes \mathbf{r}\right)\right] \mathrm{d}V = \frac{1}{V}\int_\Gamma \left[\mathbf{n} \otimes \left(\nabla_{\mathrm{m}} \otimes \mathbf{r}\right)\right] \mathrm{d}\Gamma = \mathbf{0}. \end{aligned} \tag{7}$$

Integral constraints (7) are satisfied through appropriate choice of boundary conditions, in this case gradient generalized periodic boundary conditions which are imposed along the boundaries of the RVE, shown in Fig. 2.

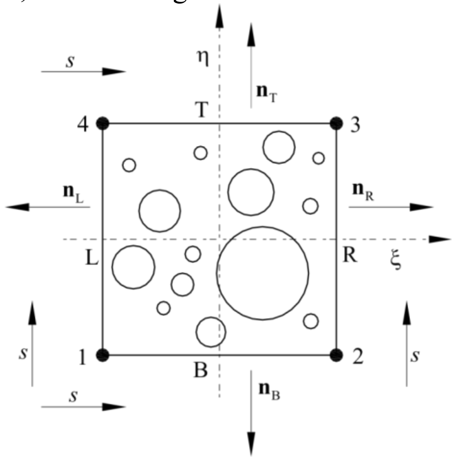

Figure2: Representative volume element [14]

Displacements are imposed on the corner nodes of the RVE boundary as

$$\mathbf{u}_i = \mathbf{D}_i^T \boldsymbol{\varepsilon}_{\mathrm{M}} + \left(\mathbf{H}_1^T\right)_i \left(\boldsymbol{\varepsilon}_{x_1}\right)_{\mathrm{M}} + \left(\mathbf{H}_2^T\right)_i \left(\boldsymbol{\varepsilon}_{x_2}\right)_{\mathrm{M}}, \quad i = 2, 3, 4, \tag{8}$$

where $\mathbf{D}$, $\mathbf{H}_1$ and $\mathbf{H}_2$ are coordinate matrices, described in more detail in [14]. In (8), displacement of the corner node 1 is suppressed in order to eliminate the rigid body movements. Due to periodicity, remaining boundary nodes are kinematically related in the following way

$$\begin{aligned} &\mathbf{r}_{\mathrm{R}}(s) = \mathbf{r}_{\mathrm{L}}(s), \\ &\mathbf{r}_{\mathrm{T}}(s) = \mathbf{r}_{\mathrm{B}}(s). \end{aligned} \tag{9}$$

The periodicity relations for the available nodal degrees of freedom are then derived by using (6), (8) and (9), in form of

$$
\begin{aligned}
\mathbf{u}_{\mathrm{R}} - \mathbf{u}_{\mathrm{L}} &= \left(\mathbf{D}_{\mathrm{R}}^{T} - \mathbf{D}_{\mathrm{L}}^{T}\right)\boldsymbol{\varepsilon}_{\mathrm{M}} + \left[\left(\mathbf{H}_{1}^{T}\right)_{\mathrm{R}} - \left(\mathbf{H}_{1}^{T}\right)_{\mathrm{L}}\right]\left(\boldsymbol{\varepsilon}_{x_1}\right)_{\mathrm{M}} + \left[\left(\mathbf{H}_{2}^{T}\right)_{\mathrm{R}} - \left(\mathbf{H}_{2}^{T}\right)_{\mathrm{L}}\right]\left(\boldsymbol{\varepsilon}_{x_2}\right)_{\mathrm{M}}, \\
\mathbf{u}_{\mathrm{T}} - \mathbf{u}_{\mathrm{B}} &= \left(\mathbf{D}_{\mathrm{T}}^{T} - \mathbf{D}_{\mathrm{B}}^{T}\right)\boldsymbol{\varepsilon}_{\mathrm{M}} + \left[\left(\mathbf{H}_{1}^{T}\right)_{\mathrm{T}} - \left(\mathbf{H}_{1}^{T}\right)_{\mathrm{B}}\right]\left(\boldsymbol{\varepsilon}_{x_1}\right)_{\mathrm{M}} + \left[\left(\mathbf{H}_{2}^{T}\right)_{\mathrm{T}} - \left(\mathbf{H}_{2}^{T}\right)_{\mathrm{B}}\right]\left(\boldsymbol{\varepsilon}_{x_2}\right)_{\mathrm{M}}.
\end{aligned} \tag{10}
$$

3.2 Micro-to-macro scale transition

Once the microstructural BVP is solved, the homogenization of the macrostructural stress tensors and constitutive matrix has to be performed. The starting point for the derivation of the required relations for the homogenized stresses is Hill-Mandel energy equivalence condition, defined for the non-local continuum theory on both structural levels as

$$
\frac{1}{V}\int_{V}\left(\boldsymbol{\sigma}_{\mathrm{m}} : \delta\boldsymbol{\varepsilon}_{\mathrm{m}} + {}^{3}\boldsymbol{\mu}_{\mathrm{m}} \vdots \left(\nabla_{\mathrm{m}} \otimes \delta\boldsymbol{\varepsilon}_{\mathrm{m}}\right)\right)\mathrm{d}V = \boldsymbol{\sigma}_{\mathrm{M}} : \delta\boldsymbol{\varepsilon}_{\mathrm{M}} + {}^{3}\boldsymbol{\mu}_{\mathrm{M}} \vdots \left(\nabla \otimes \delta\boldsymbol{\varepsilon}_{\mathrm{M}}\right). \tag{11}
$$

Following the procedure given in more detail in [14], the stresses are obtained as

$$
\begin{aligned}
\boldsymbol{\sigma}_{\mathrm{M}} &= \frac{1}{V}\int_{V}\boldsymbol{\sigma}_{\mathrm{m}}\,\mathrm{d}V, \\
{}^{3}\boldsymbol{\mu}_{\mathrm{M}} &= \frac{1}{V}\int_{V}\left({}^{3}\boldsymbol{\mu}_{\mathrm{m}} + \boldsymbol{\sigma}_{\mathrm{m}} \otimes \mathbf{x}\right)\mathrm{d}V.
\end{aligned} \tag{12}
$$

Based on the generalized Aifantis macroscopic constitutive relations assumption, nine different constitutive tangents are introduced to describe the microstructural effects that occur on the RVE. Derivation of the tangents is performed by using the static condensation procedure, resulting in their dependency on the condensed stiffness matrix $\tilde{\mathbf{K}}_{\mathrm{bb}}$ and appropriate combination of coordinate matrices, as shown in [14].

4 Conclusions and following steps

Multiscale scheme with the non-local continuum theory implemented at both macro- and microscale is extended to the consideration of the softening behavior of quasi-brittle materials. The non-local continuum theory in form of the gradient elasticity is embedded into the C^1 three node triangular plane strain finite element. Additionally, isotropic damage law is introduced in the RVE finite element formulation, providing in this way a complete regularization of the microstructural boundary value problem. Homogenization over the whole domain of the RVE is considered in this paper and will be used in a numerical example as the first step of the following research, together with a completely homogeneous microstructure. In this way, comparison with the results of the one-scale damage model could be made due to the fact that a moderate localization is expected at the microscale, for which the existence of the RVE can be proven. By using the standard heterogeneous RVE, formation of the sharp localization zones is anticipated and the existence of the RVE comes into question when a described homogenization is used. Therefore, an enhancement of the proposed homogenization model has to be derived for the elimination of this non-physical problem, which will be the topic of authors' further research.

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