Study of the Inclusion of Heterogeneity in the Determination of Constitutive Relations for Micromorphic Media through Homogenization

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Abstract. The behavior of quasi-brittle materials, such as concrete, is closely tied to their heterogeneous structure, leading to complex responses to applied loads, including the formation of localized zones of damage. Traditional continuum mechanics models fail to adequately consider the influence of microstructure. To address this limitation, generalized continuum theories have emerged, such as the micromorphic theory, which incorporates additional degrees of freedom to capture the material's microstructure. Additionally, these theories can effectively handle localization issues in quasi-brittle materials represented as elastic-degrading media due to their nonlocal nature. In this study, we investigate the influence of heterogeneity on determining constitutive relations for micromorphic media using a homogenization approach, with a particular focus on quasi-brittle materials. By employing a homogenization technique, the effective constitutive relations for the micromorphic continuum are obtained considering the heterogeneity in a finer-scale. This miscrostructure formed by aggregates and matrix considered in the finer-scale is generated by the take-and-place algorithm and its behavior is described by a classical continuum. Furthermore, an important challenge when modeling with the micromorphic theory is the determination of the 18 elastic parameters required for an elastic isotropic medium. To overcome this obstacle, through this homogenization framework, only classical parameters for the microstructure components are required for the analysis. An analysis is here conducted in order to understand the effect of different characteristics of the finer-scale, as mesh, microcontinuum size, and heterogeneity distribution, on the resulting macroscopic micromorphic constitutive relations. This work could lead to models that are able to capture the microstructure influence, often disregarded when modeling quasi-brittle media, associated to a generalized continuum theory.

Keywords: Micromorphic media, heterogeneity, constitutive relations, homogenization, quasi-brittle materials

1 Introduction

Considering the classical continuum theory, a material is kinematic and statically described based on average macroscopic characteristics. These characteristics are defined adopting the concept of a material particle [1] associated to a representative volume element (RVE) [2–4]. The RVE for a material point of a continuum mass is a material volume that is statistically representative of the infinitesimal material neighborhood of that material point [5–7].

Considering the modeling of damage and fracture for heterogeneous materials (e.g., composite solids, mixtures and multicomponent fluids, soils, and rocks), their internal structure directly influences the structural behavior. This leads to a complex degradation process, which is strongly correlated to the inhomogeneities at the microscales and to defects that may exist at such scales. Therefore, the existence of a representative volume that includes a considerable number of microheterogenities, allowing the representation of local properties by mean values and continuous variables [7], is greatly attractive specially when associated to the idea of Continuum Damage Models. In CDM the medium is modeled as a continuum body macroscopically and the collective effect of damage is described by field variables denominated damage variables [8].

Continuum damage models, however, have a major drawback, as finite element computations based on these models may suffer from a number of issues, being one of the most studied problems in the literature their strong mesh dependency. These issues emerge from the softening behavior of such models characterized by a reduction in the load-carrying capacity of the material when a certain deformation threshold is reached. This leads to the concentration of the degrading phenomena in a certain part of the body, process called numerical strain localization.

One approach described in the relevant literature able to deal with the above shortcoming, is the adoption of generalized continuum theories. Generalized continuum theories are based on the generalization of standard continuum mechanics of Cauchy through the expansion of its basic working hypotheses. These generalizations, first introduced by Voigt [9] and the brothers Cosserat [10], involve additional degrees of freedom (higher order continua) or/and higher order gradients of the displacement fields (higher grade continua) [11–14]. The micromorphic continuum theory [15–17], included in the former category, introduces an internal length in its formulation, which is related to an additional field that enriches the continuum kinematics with effects connected to the microstructure of the material. Hence, this generalized theory is well suited to model heterogeneous materials wherein the RVE concept associated to a classical continuum does not represent satisfactorily all the phenomena related to the influence of the substructure or the structural dimensions are small comparatively to the microstructure.

An important obstacle in adopting the micromorphic theory, despite its advantages, is the need to determine the elastic constitutive parameters required for such theory. In the asymmetric theory more than 1000 constitutive coefficients are involved in the general anisotropic case. Even for isotropic materials, the constitutive equations contain 18 material constants. A homogenization strategy is here used to address this problem [18] and also extended to the case of a heterogeneous material. This work presents a study of this technique applied to heterogeneous quasi-brittle materials, more specifically concrete, building the foundation for subsequent modeling of heterogeneous micromorphic media associated to elastic-degrading models [19].

2 Micromorphic media

In the micromorphic theory, every material point within the macrocontinuum is considered as a continuum of small extent, forming a deformable particle. In a linear approximation, the following strain tensors can be defined [16, 17]

$$\epsilon_{kl} = u_{l,k} - \phi_{lk}, \qquad 2e_{kl} = \phi_{kl} + \phi_{lk}, \qquad \gamma_{klm} = \phi_{kl,m} \tag{1}$$

in which ϵ_{kl}, e_{kl}, and γ_{klm} are the linear strain tensors; u_l is the displacement vector related to the particle centroid; $\phi_{kl} = \chi_{kl} - \delta_{kl}$ is the microdisplacement tensor.

For an isotropic linear elastic micromorphic solid, the following constitutive equations can be obtained [20]:

$$t_{kl} = A_{klmn}\epsilon_{mn} + E_{klmn}e_{mn}, \quad s_{kl} = E_{mnkl}\epsilon_{mn} + B_{klmn}e_{mn}, \quad \text{and} \quad m_{klm} = C_{lmknpq}\gamma_{npq} \tag{2a,b,c}$$

where t_{kl} is the non-symmetric Cauchy stress tensor; s_{kl} is a symmetric stress tensor named micro-stress average [16]; m_{klm} is the stress moments tensor; and $A_{klmn}, B_{klmn}, C_{klmnpq}, E_{klmn}$ are the constitutive moduli.

3 Homogenization of a classical heterogeneous medium towards a micromorphic continuum

In the relevant literature, well-established analytical and discrete formulation of the micromorphic theory can be found. Nevertheless, the identification of the corresponding constitutive laws and the determination of the high number of constitutive parameters limit its practical application. To overcome these obstacles, a homogenization strategy, proposed by da Silva et al. [18] and based on the principles presented by Hütter [21], is employed here. This method involves a multiscale formulation for the construction of macroscopic micromorphic constitutive relations using homogenized microscopic quantities obtained from the solution of boundary value problems at the microscale according to the classical continuum theory. This strategy begins with models of the classical continuum on the microscale, without making any constitutive assumptions on the macroscale. As a result, the required material parameters are those found in the classical theory.

For this formulation, the domain V is conceived as divided into into small finite volumes $\Delta V(\boldsymbol{X})$, here called microcontinuum. For the construction of the constitutive moduli, the material particles are subjected to Cauchy stress states resulting from elementary states of strain. The Cauchy stress states σ_{ij} at the microscale are obtained adopting an analytical formulation presented in da Silva et al. [18]. This method approximates the microscale (microcontinuum scale) stress based on a micromorphic stress state at the macroscale (structural scale). Based on this approximation, the micromorphic stress tensors at the macroscale are then obtained by homogenization. This homogenization strategy can be applied to obtain the initial elastic tensor for the first step of the first iteration of a non-linear analysis. In subsequent works, the authors intend to apply this technique associated with the scalar-isotropic damage models proposed by Reges et al. [19] to model heterogeneous materials.

In order to incorporate the particle heterogeneity, each microcontinuum $\Delta V(\boldsymbol{X})$ is then considered as heterogeneous with a microscale model generated by the take-and-place algorithm. The take-and-place method, based on Bažant et al. [22], Schlangen and van Mier [23], and Wittmann et al. [24], simulates size and spatial distributions of aggregate particles by the random sampling principle of Monte Carlo. In this method, samples of particles are taken from a source that follows a given grading curve and placed one by one into the analysis domain with no overlapping with particles already placed. One commonly used continuous grading curve is given by Fuller (see Wriggers and Moftah [25] for more details).

In order to guarantee that all aggregate particles are coated with a minimum thickness of mortar film, a distribution factor (DF) is defined, where an offset on the radius of the particle is set, enlarging the aggregate size prior to checking the existence of overlapping.

Another aspect of the microstructure generator is the definition of the shape of the particles, which is closely related to the aggregate type [26]. For simulating both round and angular shapes, the aggregates can be modeled as circular or polygonal/irregular particles.

After the microstructure is generated, a finite elements mesh is associated to it, wherein triangular and quadrilateral element can be used. The material properties for the aggregates are then set to each element whose position coincides with a particle and the remained elements are set as having mortar matrix properties. The material properties at the microscale are defined as for a linear-elastic classical medium.

After the microstructure generation and the mesh definition, a heterogeneous microcontinuum or RVE is associated to each integration point of the model under analysis. Then, the homogenization technique described in da Silva et al. [18] is processed for each element that composes the RVE. The homogenized stresses are obtained as an average carried over the number of elements n per microcontinuum:

$$\bar{t}_{kl} = \frac{1}{\Delta V\left(\boldsymbol{X}\right)} \sum_{1}^{n} \int_{\partial \Delta V\text{'}(\boldsymbol{X})} \Xi_k \sigma\text{'}_{il} n\text{'}_i ds\text{'}(\boldsymbol{X}\text{'}) \tag{3}$$

$$\bar{m}_{klm} = \frac{1}{\Delta V\left(\boldsymbol{X}\right)} \sum_{1}^{n} \int_{\partial \Delta V\text{'}(\boldsymbol{X})} \Xi_k \sigma\text{'}_{il} \Xi_m n\text{'}_i ds\text{'}(\boldsymbol{X}\text{'}) \tag{4}$$

$$\bar{s}_{kl} = \frac{1}{\Delta V\left(\boldsymbol{X}\right)} \sum_{1}^{n} \int_{\Delta V\text{'}(\boldsymbol{X})} \sigma\text{'}_{kl}\, dv\text{'}(\boldsymbol{X}\text{'}) \tag{5}$$

where $\partial\Delta V$', ΔV' and $\sigma\text{'}_{il}$ represents the contour, the volume and the Cauchy stress for each element in the microcontinuum respectively; $n\text{'}_i$ is the normal to $\partial\Delta V$'; Ξ_k is a position vector; $\bar{t}_{kl}$, $\bar{m}_{klm}$, and $\bar{s}_{kl}$ are the micromorphic stresses obtained by homogenization. The constitutive equations are then defined

$$\bar{t}_{kl} = \bar{A}_{klmn}\bar{\epsilon}_{mn} + \bar{E}_{klmn}\bar{\phi}_{mn}, \quad \bar{s}_{kl} = \bar{E}_{mnkl}\bar{\epsilon}_{mn} + \bar{B}_{klmn}\bar{\phi}_{mn}, \quad \text{and} \quad \bar{m}_{klm} = \bar{C}_{lmknpq}\bar{\gamma}_{npq} \tag{6a,b,c}$$

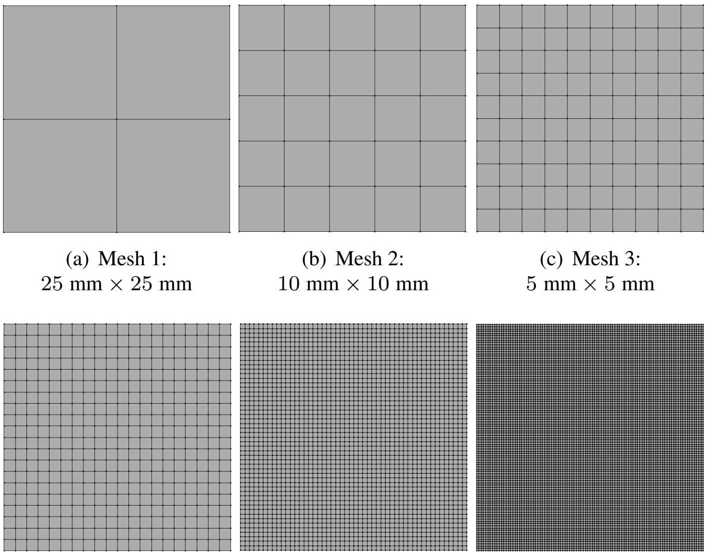
and the components of macroscopic micromorphic stress are determined, which, as a result of elementary states of strain, consist of the terms of macroscopic micromorphic constitutive relations.

4 Study of the homogenization technique

In order to model non-linear problems with the micromorphic theory associated to a heterogenous microcontinuum, an initial study of the proposed homogenization strategy is here presented aiming to evaluate the influence on the constitutive relations of the type and size of the elements that compose the mesh for the microcontinuum as well as the impact of the microcontinuum size. The results are presented in the following sections.

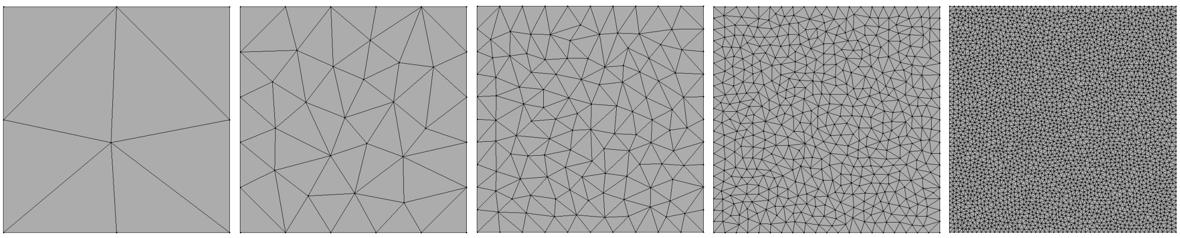
4.1 Mesh study

To evaluate the impact on the homogenized constitutive operator of the type and size of the element that composes the microcontinuum discretization, the meshes illustrated in Fig. 1 for quadrilateral elements and in Fig. 2 for triangular elements were studied. A square heterogeneous microcontinuum of size 50 mm was considered for all the meshes and, for the microstructure, the following parameters: maximum sieve size $d_{max} = 19$ mm; minimum sieve size $d_{min} = 9.5$ mm; continuous particle distribution; spherical particles; particle fraction PF $= 30\%$; distribution factor DF $= 0.2$; $n = 0.5$ for the Fuller's distribution [25]; Young's modulus for the aggregates $E_{particle} = 300$ GPa; Poisson's ratio for the aggregates $\nu_{particle} = 0.2$; Young's modulus for the matrix $E_{matrix} = 30$ GPa; Poisson's ratio for the matrix $\nu_{matrix} = 0.2$.



(a) Mesh 1: 25 mm × 25 mm
(b) Mesh 2: 10 mm × 10 mm
(c) Mesh 3: 5 mm × 5 mm
(d) Mesh 4: 2.5 mm × 2.5 mm
(e) Mesh 5: 1 mm × 1 mm
(f) Mesh 6: 0.5 mm × 0.5 mm

Figure 1. Mesh study: quadrilateral microcontinuum meshes



(a) Mesh 1: average size 25 mm
(b) Mesh 2: average size 10 mm
(c) Mesh 3: average size 5 mm
(d) Mesh 4: average size 2.5 mm
(e) Mesh 5: average size 1 mm

Figure 2. Mesh study: triangular microcontinuum meshes

To each discretization, the same heterogeneous microstructure was associated, obtaining a heterogeneous microcontinuum. Subsequently, the homogenization process was carried out and the elastic constitutive operator for the micromorphic continuum obtained containing $\bar{A}_{klmn}$, $\bar{E}_{klmn}$, $\bar{E}_{mnkl}$, $\bar{B}_{klmn}$, and $\bar{C}_{lmknpq}$ (Eq. 6). Some values obtained for the components of the constitutive tensors versus the element size are presented in Fig. 3.

Observing all the results obtained for each constitutive tensor, its is possible to identify a convergence in the values for element sizes smaller than 5 mm for quadrilateral and triangular elements. For more refined meshes the quadrilateral element presented a lower time for obtaining the constitutive tensor by the homogenization technique due to the presence of fewer elements in the mesh.

It is important to note that the results for this study apply for a heterogeneous microstructure with the parameters previously specified for particle fraction, distribution factor, and sieve sizes. For other distributions, another study should be conducted to determine the element type and size that yield better results with the lowest processing time.

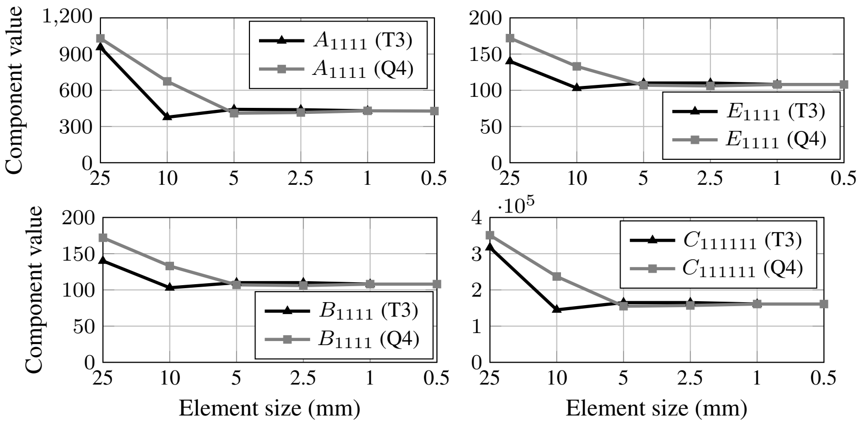


Figure 3. Mesh study: samples of components of the constitutive operators A_{ijkl}, E_{ijkl}, B_{ijkl}, and C_{ijklmn}

4.2 Microcontinuum size and distribution study

After the definition of the appropriate size and type of the element for the microstructure discretization, a study of the microcontinuum size associated with an analysis of the influence on the constitutive operator of the distribution randomness was conducted.

Adopting quadrilateral elements with dimension 5 mm, square RVE's with sizes varying from 20 mm up to 120 mm were studied. For each microcontinuum size, 200 particle distributions were generated to evaluate the variation of the components of the constitutive operator due to the randomness of the take-and-place algorithm. Figure 4 shows some examples for the microstructure generated for the same input parameters considering a microcontinuum of size 100 mm. Figure 5 illustrates the values for some components obtained for a microcontinuum of size 100 mm for the 200 distributions generated.

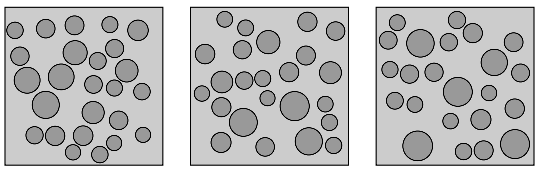


Figure 4. Distribution study: random generation of particles with same input parameters for microcontinuum of size 100 mm

The observed behavior for the tensors A_{ijkl}, E_{ijkl}, E_{klij}, and B_{ijkl} is similar, where components with indexes 1111, 1122, 2211, 2222, 1212, 1221, 2112, and 2121 tend to an average value and the remaining components oscillate around zero. This corresponds to the expected behavior of these tensors for a plane analysis due to the uncoupling of the corresponding stress-strain measures. The components of the tensor C_{ijklmn} present a tendency to fluctuate around a average value, what also fits with the anticipated behavior for this type of analysis.

Considering all the microcontinuum sizes analyzed, the average value for each component for each RVE size was calculated. The results are presented in Fig. 6 for the average values obtained versus the microcontinuum size. The results for the tensors A_{ijkl}, E_{ijkl}, E_{klij}, and B_{ijkl} are similar, where non-zero components tend to a certain value with the increase in the microcontinuum size, probably due to the better representation of the microstructure and its particles. For tensors A_{ijkl} and E_{ijkl} components that were expected as null presented a negligible fluctuation around zero values. The average values obtained for the tensor C_{ijklmn} present an exponential growth as the microcontinuum increases, with no convergence to a value. These results may be correlated to the formulation of the micromorphic theory where the tensor C_{ijklmn} is more significant with the increase of the size of the material particle, but further studies are necessary to attest this hypotheses.

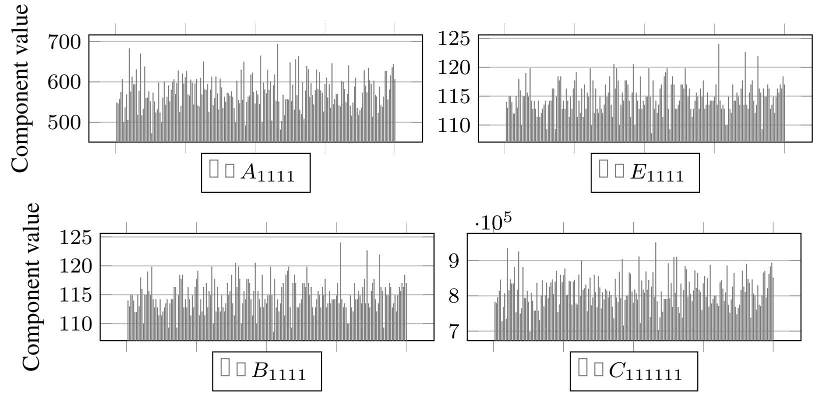


Figure 5. Distribution study: components of the constitutive operator A_{ijkl}, E_{ijkl}, B_{ijkl}, and C_{ijklmn} (microcontinuum 100 mm)

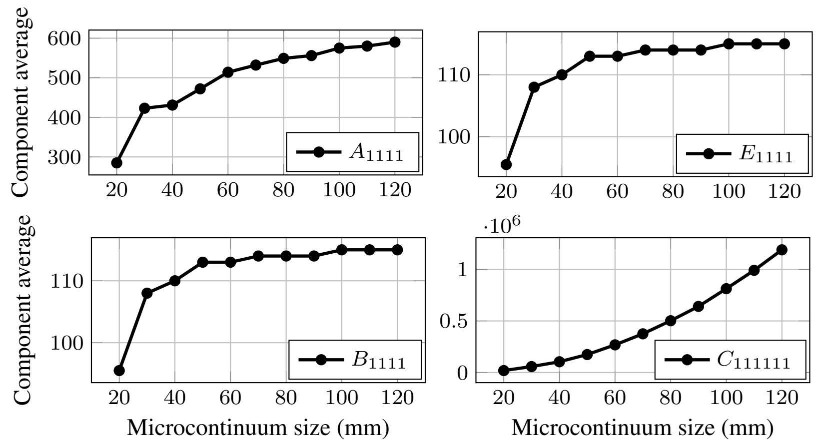


Figure 6. Distribution study: average of the components of the constitutive operator A_{ijkl}, E_{ijkl}, B_{ijkl}, and C_{ijklmn} versus microcontinuum size

5 Conclusions

Considering the great potential of the micromorphic theory for properly representing materials with heterogeneous microstructure, this work presents an initial study of the adoption of a homogenization technique over a concrete RVE described by classical continuum mechanics. The microstructure is generated through the take-and-place algorithm in which, for the aggregate size distribution, a Fuller curve was used associated to the sieve sizes specified by ABNT NBR 7211 [27] (25.0 mm to 4.75 mm). The behavior observed in the micromorphic constitutive operators when considering heterogeneity agrees with the expected results, verifying the proper functioning of the technique.

This work presents multiple possibilities for the study of the influence of the heterogeneous microstructure in the structural behavior with the use of the micromorphic theory. The inclusion of voids in the microstructure and the adoption of this strategy to model non-linear problems associated to the elastic degradation models proposed by Reges et al. [19] are topics to be further explored by the authors.

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