A preliminar study on RVE homogenization for phase-field multiscale analysis

Hugo M. Leão[1], Eduarda M. Ferreira[1], Roque L. S. Pitangueira[1], Lapo Gori[1]

[1]*Structural Engineering Department, Federal University of Minas Gerais*
Av. Antônio Carlos, 6627, Pampulha, Belo Horizonte, 31270-901, Minas Gerais, Brazil
hugomleao@yahoo.com.br, eduarda.marques@engenharia.ufjf.br, roque@dees.ufmg.br, lapo@dees.ufmg.br

Abstract. Despite the phenomenological approach presents excellent results in material behavior analysis, real-world materials are inherently heterogeneous. A material is considered heterogeneous when, at a particular observation scale, it becomes feasible to discern multiple mixture phases within it. This level of observation is commonly referred to as the microscale, where interactions between constituents occur, ultimately leading to the emergence of cracks. Modeling a material at the microscale begins with defining a Representative Volume Element (RVE), which is the smallest part of the material that is large enough to statistically represent the entire mixture. This ensures that other samples of the same size exhibit similar properties with minor variations. The analysis of the RVE leads to obtaining the effective properties of a portion of the material. That process is called homogenization. Modeling a RVE can be a challenging task, as it requires the use of highly refined meshes to accurately capture the geometric representation of all mixture components. Therefore, phase-field models present themselves as a suitable choice for this type of modeling, once due to the intrinsic features of its variational formulation, they already need refined meshes and do not present localization effects. Thus, the objective of this work is to model a heterogeneous RVE and obtain its homogenized properties. This homogenization of the material parameters is fundamental for the upscaling operation of multiscale analyses. All implementation were done in INSANE, an opensource software developed by the Engineering Structures Department (DEES) of Federal University of Minas Gerais (UFMG).

Keywords: microscale, phase-field, homogenization

1 Introduction

Majority of the materials used in civil construction are heterogeneous, however, the phenomenological approach is widely used to analyse structural models [1–3]. In this approach, the material is represented by its average behavior, considering a larger observation scale, also called macroscale, where no distinction is made between the different constituents of the mixture. Although this is a cheaper method of analysis from a computational perspective, the explicit representation of the geometry of each phase is important for understanding the complete process of material degradation, since the propagation of cracks in heterogeneous materials can take shapes that would be difficult to predict without considering the interactions between the different phases [4]. Thus, multiscale analysis appears promising given that the behavior of the material's constituents at the microscale provides information about material degradation that affects the macroscopic response. In this work, the principles of FE^2-method, also known as multilevel finite element method [5, 6], were employed. This approach consists on the discretization by finite elements of both macro and microscales, which are solved iteratively by exchanging information between models.

For this type of analysis, it is very important to define a Representative Volume Element (RVE) that consists in a material fraction whose dimensions are large enough to represent the whole and small enough to avoid structural behaviour [7, 8]. The transferring of information between scales are done through an homogenization process that consists in to apply the macroscale internal variables on the RVE boundary and to obtain the effective properties of the mixture.

The objective of this work is to use a macroscopic strain state to construct a boundary value problem in RVEs with a random distribution of particles and to obtain homogenised constitutive relations for the macroscale problem. Although both macroscale and RVE consider a phase-field model for fracture, this work is in its early stages, and therefore the results presented do not yet account for material degradation. The implementation was done in *INSANE* (INteractive Structural ANalysis Environment), an open source software developed in Java by the Structural Engineering Department of the Federal University of Minas Gerais, and has been largely used by the research group since 2002[1].

2 Phase-field models

Based on the variational approach of Griffith's theory, Bourdin et al. [9] have rewritten the energy functional of a solid body Ω in order to transform the sharp crack Γ in a smoothed damaged region $\mathcal{B}$ (See Fig. 1). This way, the phase-field variable is inserted into the problem as a new degree of freedom through an additional equation. That variable varies from zero to unity and quantifies the damage of the material.

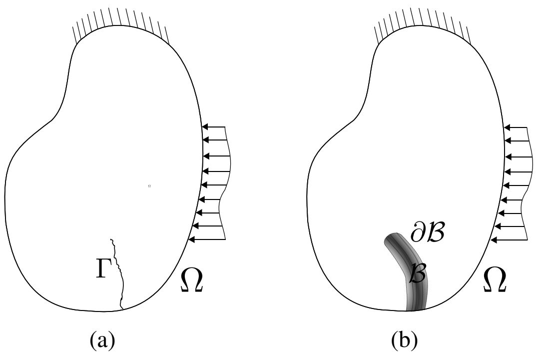

Figure 1. Comparison between (a) Griffith crack and (b) Phase-Field diffuse crack

Therefore, the finite element problem is now solved through a system of equations whose residual form is given by:

$$\vec{r}_I^u = \int_\Omega [\mathbf{B}]_I^{u,T} \, \vec{\sigma} \, \mathrm{d}\mathcal{V} - \vec{f}_I = \vec{0}_I \tag{1a}$$

$$\vec{r}_I^\phi = -\int_\mathcal{B} [\mathbf{N}]_I^{\phi,T} \left(g'\bar{Y} + \frac{1}{C_0 l_0}\alpha' G_c \right) \, \mathrm{d}\mathcal{V} - \int_\mathcal{B} \frac{2l_0}{C_0} G_c \, [\mathbf{B}]_I^{\phi,T} \, \nabla\phi \, \mathrm{d}\mathcal{V} \tag{1b}$$

where eq. (1a) is responsible to calculate the displacements (u) and eq. (1b) the phase-field (ϕ). The parameters of eq. (1b) are related to the material and stand for:

- $\vec{f}_I$ is the external forces vector,
- σ is the stress tensor,
- g is called energetic degradation function and is responsible for degrading the constitutive tensor,
- α gives the shape for the degradation bandwitch,
- C_0 is a constant, dependent on α, and calculated by $4\int_0^1 \alpha^{-1/2}(\phi)d\phi$,
- $\bar{Y}$ is the effective crack driving force, and varies according to the considered constitutive model,
- l_0 is related to the size of the degraded bandwith.

For more informations about the mathematical formulation of phase-field models see Wu et al. [10], Leão [11].

3 FE² strategy

The FE² strategy consists of solving the problem considering two scales of observation, here called macro and microscales. The macroscale is represented by a FEM model whose properties comes from the microscale through an homogenization process. Each integration point of the macroscale FEM model is associated to a microscale FEM model, also called Representative Volume Element (RVE), in which the mixture heterogeneities are geometrically represented. See Fig. 2.

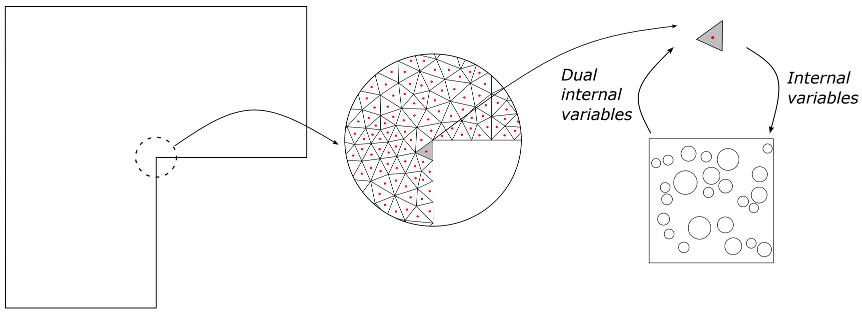

Figure 2. Representation of the homogenized macroscale and the heterogeneous microscale models. Observe that a heterogeneous microscale model is associated for each macroscale integration point. The FE² process ocurrs by transfering internal variables from macro to microscale and dual internal variables from micro to macroscale.

The interaction between scales occurs by applying boundary constraint and conditions to the microscale model according to the multiscale constitutive model in order to represent the macroscale material point. In this work, Neumann boundary conditions were adopted based on a linear displacement model on the RVE contour [5, 12]. For this model, the displacements on the RVE boundary are calculated by:

$$\vec{u} = \langle[\varepsilon]\rangle\,[\vec{x} - \langle\vec{x}\rangle] \tag{2}$$

where $\vec{u}$ is the boundary displacement, $\langle[\varepsilon]\rangle$ the macroscale strain tensor , $\vec{x}$ the boundary point and $\langle\vec{x}\rangle$ a reference point.

3.1 Constitutive tensor homogenization

One of the challenging tasks of multiscale analysis is finding the homogenized constitutive tensor of the RVE to be used at the macroscale level. This process of homogenizing a variable involves obtaining its average value in order to provide an accurate estimate of the RVE's behavior.

Starting from the definition of the homogenized constitutive tensor

$$\left\langle \hat{\mathbf{C}} \right\rangle = \frac{\partial\,\langle[\sigma]\rangle}{\partial\,\langle[\varepsilon]\rangle}\,\mathrm{d}\mathcal{V}, \tag{3}$$

where $\langle[\sigma]\rangle$ is obtained by the volume average

$$\langle[\sigma]\rangle = \frac{1}{V}\int [\sigma]\ \mathrm{d}\mathcal{V}, \tag{4}$$

using the chain rule, $\left\langle \hat{\mathbf{C}} \right\rangle$ can be obtained by:

$$\left\langle \hat{\mathbf{C}} \right\rangle = \frac{1}{V}\int \frac{\partial\,[\sigma]\,([\varepsilon])}{\partial\,[\varepsilon]} : \frac{\partial\,[\varepsilon]}{\partial\,\langle[\varepsilon]\rangle}\,\mathrm{d}\mathcal{V} \tag{5}$$

But it is considered that, the RVE strain tensor $[\varepsilon]$ can be decomposed into a sum of the homogenized tensor and a fluctuation counterpart $[\tilde{\varepsilon}]$ in such way that:

$$[\varepsilon] = \langle[\varepsilon]\rangle + [\tilde{\varepsilon}] \tag{6}$$

[1] More information on the project can be found at `https://www.insane.dees.ufmg.br/`.

Substituting eq. (6) in eq. (5), and by the definition of $\hat{\mathbf{C}} = \dfrac{\partial\,[\sigma]}{\partial\,[\varepsilon]}$, it arrives to:

$$\left\langle \hat{\mathbf{C}} \right\rangle = \frac{1}{V}\int \hat{\mathbf{C}}\,\mathrm{d}\mathcal{V} + \frac{1}{V}\int \hat{\mathbf{C}} : \frac{\partial\,[\tilde{\varepsilon}]}{\partial\,\langle[\varepsilon]\rangle}\,\mathrm{d}\mathcal{V} \tag{7}$$

The linearized weak form of the balance of linear momentum for the microscale is:

$$\int \delta\,[\tilde{\varepsilon}] : \hat{\mathbf{C}} : \Delta\,\langle[\varepsilon]\rangle\;\mathrm{d}\mathcal{V} = 0 \tag{8}$$

From the definitions of eq. (8), eq. (7) can be rewritten as:

$$\left\langle \hat{\mathbf{C}} \right\rangle = \hat{\mathbf{C}}_{\mathrm{Taylor}} - \hat{\mathbf{F}} \tag{9}$$

with the following counterparts

$$\hat{\mathbf{C}}_{\mathrm{Taylor}} = \frac{1}{V}\sum_{\mathrm{elms}}^{\mathrm{assemb}} \int \hat{\mathbf{C}}\,\mathrm{d}\mathcal{V} \tag{10a}$$

$$\hat{\mathbf{F}} = \frac{1}{V}\sum_{\mathrm{elms}}^{\mathrm{assemb}} \int l^{e,T} k^{e,-1} l^{e}\,\mathrm{d}\mathcal{V} \tag{10b}$$

$$l^{e} = \int B^{T}\hat{\mathbf{C}}\,\mathrm{d}\mathcal{V} \tag{10c}$$

where $\sum_{\mathrm{elms}}^{\mathrm{assemb}}$ represents an assembler operation over all elements (e) of the RVE, $\hat{\mathbf{C}}$ is the RVE constitutive matrix, k^e is the element stiffness matrix and B is the dual internal variables operator.

4 Examples and results

In this section, preliminary results obtained from the homogenization process using the phase-field model during the multiscale analysis will be presented. It is important to highlight that this is an in-progress work and that the multiscale process as a whole is not yet resolved. The results presented in Tables 2 and 3 consist of the homogenized constitutive tensor for one integration point, considering one of the first steps of a non-linear analysis, and Table 4 shows the homogenized stress obtained before analysing the RVE. It is also worth noting that in the analysed step, material degradation has not yet been observed, and thus the phase-field calculation does not affect the results.

For the multiscale analysis, RVEs with a size of 65 mm and material parameters of Table 1 were considered. All the RVEs were meshed using triangular elements with mean nodal distance of 1.5 mm. Five distinct random particle distributions were examined, with particle volume fractions of 25% and 30%. The grading curve was characterized by a Fuller parameter of 0.7909, and the aggregate sizes varied from 4.75 mm to 12.5 mm. See Figs. 3 and 4.

The example of the L-shaped panel [13] was used to represent the macroscale of the problem. Due to the high computational cost and the aim of solely analyzing the effect of different particle distributions on the variables transported in the upscale and downscale processes, only one element was extracted from the L-panel mesh, as highlighted in Fig. 2. The integration point of this element provided the strain state at a certain moment in the analysis, given by $\langle[\varepsilon]\rangle = \left\{6.8003\times10^{-5} \quad 8.3682\times10^{-5} \quad 5.4754\times10^{-5}\right\}$. These values were applied as Neumann boundary conditions in the various RVEs studied, and the dual internal variables included in the upscale process were analysed.

Table 1. Material parameters for RVE

Material	Elasticity Modulus (E_0) $[\mathrm{N/mm^2}]$	Poison's rate (ν) $[-]$	Fracture Energy (G_c) $[\mathrm{N/mm}]$	Tensile strength (f_t) $[\mathrm{N/mm^2}]$
Aggregate	100000.0	0.20	0.1300	16.0
Mortar	21876.0	0.18	0.0018	3.48

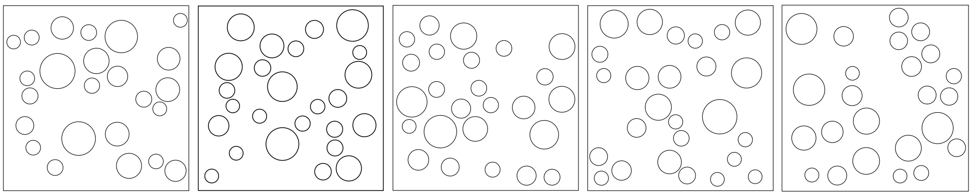

Figure 3. RVEs with random particle distributions for a volume fraction of 25%.

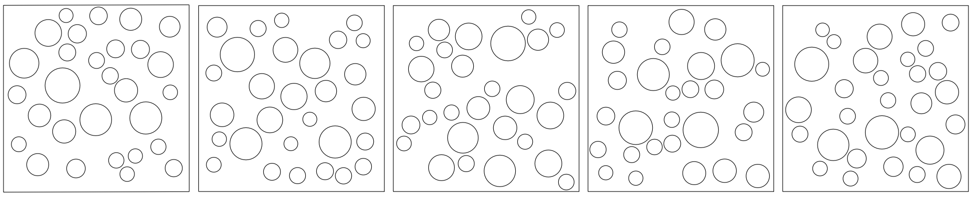

Figure 4. RVEs with random particle distributions for a volume fraction of 30%.

Table 2. Homogenized values considering volume fraction of 25% and different particles distribution. The homogenized strains vector is $\langle[\varepsilon]\rangle = \left\{6.8003 \times 10^{-5} \quad 8.3682 \times 10^{-5} \quad 5.4754 \times 10^{-5}\right\}$. The therms [i,j] in the header corresponds to the position in the constitutive matrix. Terms [2,3] and [1,3] are notably smaller than the others and are therefore omitted from the table.

Distribution	$\hat{\mathbf{C}}_{\text{Taylor}}$ $(\times 10^3\ \mathrm{N/mm^2})$				$\left\langle\hat{\mathbf{C}}\right\rangle$ $(\times 10^3\ \mathrm{N/mm^2})$			
	[1,1]	[1,2]	[2,2]	[3,3]	[1,1]	[1,2]	[2,2]	[3,3]
1	42.016	8.063	42.016	16.976	30.033	5.595	29.748	11.964
2	42.398	8.142	42.398	17.128	29.760	5.682	30.407	12.068
3	42.043	8.070	42.043	16.987	29.838	5.642	29.801	12.014
4	42.083	8.078	42.083	17.002	29.822	5.683	29.845	12.035
5	42.044	8.069	42.044	16.988	29.795	5.637	30.019	12.019
Average	42.117	8.085	42.117	17.016	29.849	5.648	29.964	12.020
Deviation	0.159	0.032	0.159	0.063	0.107	0.037	0.268	0.038

The obtained results indicate that the homogenized constitutive relations exhibit only minor variations, suggesting minimal changes with respect to the random distribution of aggregates within the same particle volume fraction. This consistency is crucial for selecting a sample as a characteristic RVE. It is observed that the values of the homogenized constitutive tensor are significantly lower compared to those of the Taylor constitutive tensor. These results corroborate with Kouznetsova et al. [14], who asserted that the Taylor constitutive model, or constant deformation model in the RVE, tends to overestimate material stiffness. This discrepancy underscores the importance of using accurate homogenization techniques to ensure the reliability of multiscale analyses.

Table 4 presents the stress results to be applied to the macro-scale integration point in the upscale operation. Again, small variations are observed for different particle distributions. As the deformation applied to the RVEs is the same, particle fractions result in higher values in the constitutive tensor and, consequently, higher stress values.

Table 3. Homogenized values considering volume fraction of 30% and different particles distribution. The homogenized strains vector is $\langle[\varepsilon]\rangle = \left\{6.8003 \times 10^{-5} \quad 8.3682 \times 10^{-5} \quad 5.4754 \times 10^{-5}\right\}$. The therms [i,j] in the header corresponds to the position in the constitutive matrix. Terms [2,3] and [1,3] are notably smaller than the others and are therefore omitted from the table.

Distribution	$\hat{\mathbf{C}}_{\text{Taylor}}$ $(\times 10^3\ \text{N/mm}^2)$				$\left\langle \hat{\mathbf{C}} \right\rangle$ $(\times 10^3\ \text{N/mm}^2)$			
	[1,1]	[1,2]	[2,2]	[3,3]	[1,1]	[1,2]	[2,2]	[3,3]
1	45.865	8.860	45.865	18.503	31.201	6.098	31.307	12.714
2	46.088	8.905	46.088	18.592	31.444	6.109	31.348	12.712
3	46.330	8.954	46.330	18.688	31.865	6.053	31.697	12.752
4	45.885	8.862	45.885	18.512	31.784	5.927	31.572	12.582
5	45.881	8.863	45.881	18.509	31.330	6.085	31.497	12.696
Average	46.010	8.889	46.010	18.561	31.525	6.054	31.484	12.691
Deviation	0.201	0.041	0.201	0.080	0.288	0.074	0.161	0.064

Table 4. Homogenized stress values.

Distribution	Particle fraction					
	25%			30%		
	σ_{xx}	σ_{yy}	σ_{xy}	σ_{xx}	σ_{yy}	σ_{xy}
1	2.347	0.996	2.009	2.433	1.029	2.107
2	2.327	0.996	2.042	2.454	1.033	2.110
3	2.331	0.991	2.004	2.493	1.055	2.142
4	2.328	0.990	2.012	2.470	1.032	2.123
5	2.336	0.992	2.010	2.441	1.029	2.120
Average	2.334	0.993	2.015	2.458	1.036	2.120
Deviation	0.008	0.003	0.015	0.024	0.011	0.014

5 Conclusions

This work presents an initial study on modeling a heterogeneous material using multiscale analysis to determine the initial damage that emerges at the microscale, resulting from interactions between different constituents, and its impact on the macroscale. To model all the mixture constituents, a refined mesh is required. The phase-field model was selected for this purpose because it demonstrated stability and did not exhibit localization effects. From this, a rigorous study was made to obtain the equations for homogenizing the microscale constitutive tensor and for transferring information between the two scales. All the implementation was carried out using INSANE.

In the analysis, the behavior of the Taylor constitutive matrix, the homogenized constitutive matrix, and the stress tensor was examined using a multiscale approach. In this analysis, an L-shaped panel served as the macroscale model and the microscale model of an specific integration point was observed (See Fig. 2). In the microscale model, for modeling the RVE, two different particle fractions were considered, and for each fraction, five different random distributions were analysed.

The results indicate that the different random distributions have minimal impact on the obtained values for both the constitutive matrix and the stress tensor. It is important to note, as previously described by Kouznetsova et al. [14], that the Taylor constitutive tensor tends to exhibit higher values than the homogenized constitutive tensor. Regarding the results for the fluctuation matrix (see $\hat{\mathbf{F}}$ in eqs. (9) and (10)), whose terms can be calculated by the difference between $\left\langle \hat{\mathbf{C}} \right\rangle$ and $\hat{\mathbf{C}}_{\text{Taylor}}$ shown in Tables 2 and 3, its values increases as the particle fraction increases. In an analysis with same mesh and no material variation (not presented in this article) the Taylor constitutive matrix is the same as the homogenized constitutive matrix, i.e. the fluctuation component is zero. This indicates the relationship of the component $\hat{\mathbf{F}}$ with the heterogeneities of the medium. Finally, it could also be observed that, as expected, increasing particle fractions induces higher constitutive matrix values and, consequently, higher stresses.

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