XLVI CILAMCE
VITÓRIA - ES - BRAZIL - 2025
XLVI IBERO-LATIN AMERICAN CONGRESS ON COMPUTATIONAL METHODS IN ENGENEERING

The Influence of the Fluctuation Term on the Accuracy of Multiscale Analysis Results

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Abstract. This work investigates the influence of the fluctuation term in the formulation of the homogenized constitutive tensor within a multiscale approach applied to the analysis of heterogeneous media. A phase-field constitutive model is used, coupled with the multilevel finite element method, which allows for the simultaneous consideration of macro and micro scales. The phase-field model enables the diffuse representation of fractures, capturing the evolution of the displacement field and crack propagation without the need for an explicit description of the fracture geometry. This makes the model particularly useful for materials like concrete, which may exhibit complex cracking patterns. At the macroscopic scale, the material's constitutive behavior is not directly defined; it must be obtained from solving the microscopic scale, where the local material properties, such as variations in stress and strain, are better represented. The connection between the scales requires defining homogenized parameters that adequately represents the material's behavior. Literature suggests that this transition cannot be done through a simple average of the local constitutive tensors, as this approach disregards important fluctuations in the displacement field. To ensure theoretical consistency, the inclusion of a fluctuation term is required, which depends on the inverse of the stiffness matrix of the microscale problem. However, calculating this term results in a significant computational cost. With the multiscale implementation in place, comparative tests were conducted between simulations with and without the fluctuation tensor, evaluating both the accuracy of the results and the impact on processing time. All implementations were carried out using INSANE, an open-source platform developed by the Department of Structural Engineering (DEES) at the Federal University of Minas Gerais (UFMG).

Keywords: Multiscale analysis; Fluctuation; Homogenized constitutive tensor; Phase-field method; Multilevel finite elements.

1 Introduction

Heterogeneous materials, widely used in civil engineering, exhibit macroscopic behavior that is intrinsically linked to phenomena occurring at smaller scales [1]. The damage process in these materials, such as concrete, typically begins with the formation of microcracks at the microscale, which coalesce and propagate until they can be seen in the form of macro-damage ([2]). The complexity of these microcracks patterns, which are difficult to predict without considering the interactions between the different constituent phases, highlights the need for modeling approaches that can capture this heterogeneity.

In this context, multiscale analysis are a valuable tool, allowing the behavior of the material's constituents at the microscale to provide crucial information about the degradation that affects the macroscopic response. Among the various multiscale strategies, the multilevel finite element method (FE^2 method) stands out for discretizing both the macroscale and the microscale using finite elements, solving them iteratively through the exchange of information between the models [3]. This approach is advantageous because it does not require a predefined macroscopic phenomenological constitutive law, which is replaced by a suitable representation of the microstructural scale [3, 4].

A critical challenge in multiscale analysis is defining the Representative Volume Element (RVE), a concept referring to a specimen that is large enough to be statistically representative of the entire material but small enough not to exhibit structural effects. The RVE must contain sufficient information about the microstructure to be representative, and its existence depends on the material's statistical homogeneity and ergodicity [5]. However, for quasi-brittle materials that exhibit a softening response, the RVE may not exist, as the material loses its statistical homogeneity during the localization of damage [5].

A fundamental aspect of multiscale analysis is the influence of the fluctuation tensor on the homogenized constitutive tensor. The literature indicates that a simple average of the local constitutive tensors is not sufficient for the transition between scales, as it disregards important fluctuations in the displacement field. The inclusion of the fluctuation term, which depends on the inverse of the stiffness matrix of the problem at the microscale, is necessary to ensure theoretical consistency [4]. However, calculating this term incurs a significant computational cost. In contrast, taking the simple average of the constitutive tensors of the micro models, here called the Taylor tensor, tends to overestimate the material's stiffness, highlighting the importance of precise homogenization techniques [3, 4, 6].

To deal with the complexity of fracture modeling in heterogeneous media, Phase-Field Models (PFM) prove to be a suitable choice [7, 8]. These models represent fractures in a diffuse way, without the need for an explicit description of the crack geometry, which simplifies the simulation of complex processes such as crack initiation, propagation, coalescence, and branching. Furthermore, phase-field models are robust and work well with heterogeneous media and refined meshes, not presenting localization problems.

The work aims to investigate the influence of the fluctuation term in the formulation of the homogenized constitutive tensor within a multiscale approach. To this end, comparative tests will be conducted between simulations with and without the inclusion of this term, evaluating both the accuracy of the results (such as stress-strain and load factor-displacement curves) and the impact on processing time.

The central objectives are: to demonstrate the applicability of the FE² method for modeling fractures with the phase-field method in heterogeneous materials; to quantify the difference in the material's mechanical response (stiffness and damage) when including or omitting the fluctuation term; and to assess the computational cost associated with its inclusion.

All computational implementations and analyses in this work were performed using INSANE (Interactive Structural Analysis Environment), an open-source platform developed by the Department of Structural Engineering (DEES) at the Federal University of Minas Gerais (UFMG).

2 Phase-field models for fracture

The phase-field fracture formulation is based on an energy functional that is minimized to find the displacement and phase fields. In the context of small strains, the energy of a fracturing elastic solid is described by the Francfort-Marigo functional [9]. The regularization of a sharp crack is achieved by introducing a diffuse fracture zone whose width depends on the internal length parameter l_0 and an auxiliary scalar variable ϕ [7], that called the phase-field variable, represents the level of material degradation, assuming smooth values between 0 and 1, where 0 represents undamaged material and 1 represents completely damaged material.

The total energy functional E_t for a solid body with a phase-field crack is given by the eq. (1) [8]:

$$E_t = \int_\Omega \psi(\overline{u}, \phi) d\mathcal{V} + \int_\mathcal{B} G_c \gamma(\phi, \nabla\phi) d\mathcal{V} - \int_\Omega \overline{b} \cdot \overline{u} d\mathcal{V} - \int_{\partial\Omega} \overline{t} \cdot \overline{u} d\mathcal{A} \tag{1}$$

where:ψ is the elastic strain energy density; $\overline{u}$ is the displacements vector; ϕ is the phase-field variable;Ω is the body domain; $\mathcal{B}$ is the damaged part of the body; G_c is the critical energy release rate; γ is the crack surface density; $\nabla\phi$ is the nabla operator applied to the phase-field; $\overline{b}$ is the body forces vector; $\overline{t}$ is the surface forces vector; $\partial\Omega$ is the body boundary.

The fields of interest are obtained from the minimization of E_t, which is performed by varying this functional with respect to the displacement u and the phase field ϕ. Therefore, based on mathematical manipulations, the following weak form of the PFM is obtained and shown in the eq. (2) and eq. (3) [8]:

$$\int_\Omega \overline{\sigma} : \delta\overline{\epsilon} d\mathcal{V} = \delta\overline{P}_{ext} \tag{2}$$

$$\int_\mathcal{B} [g'(\phi)\overline{Y}\delta\phi + G_c\delta\gamma] d\mathcal{V} \geq 0 \tag{3}$$

where $\overline{\sigma}$ is the stress tensor; $\overline{\epsilon}$ is the strain tensor; $\delta\overline{P}_{ext}$ is the first variation of the external load potential; $g'(\phi)$ is the derivative of the energetic degradation function; $\overline{Y}$ is the effective crack driving force; $\delta\gamma$ is the first variation of the crack surface density function γ.

3 Multiscale analysis of phase-field fracture

The scale transition, in the context of phase-field homogenization, involves transferring information between the macro- and microscale models (RVEs) [7]. This communication is bidirectional, meaning that some quantities are transmitted from the macroscale to the RVEs, in what is called downscaling, while some quantities are transmitted from the RVEs to the macromodel, in the process of upscaling.

The main term transferred in the downscale process is the strain tensor ϵ_M, which is necessary for constructing the boundary value problem at the microscale. This work employs prescribed displacement boundary conditions in which macroscale deformations are applied in the form of displacements at the boundary of the RVEs as follows: $u_m = \epsilon_M \cdot (X - \bar{X})$, where X is the position vector of a node located on the boundary of the RVE and $\bar{X}$ is the position vector of the RVE centroid.

After the RVE analysis, some quantities of interest are homogenized to provide the effective material properties at the macroscale. Among them is the homogenized constitutive tensor, which relates macroscopic stresses to macroscopic strains, whose response is crucial for the correct representation of material and structural behavior. In computational homogenization approaches, this tensor is obtained from the microscale.

The consistent macroscopic constitutive tensor ($\overline{\mathbb{A}}$) is a measure of the material's stiffness at the macroscale. It is calculated from the condensation of the microstructural stiffness, and its final expression, as presented in eq. (4), exhibits two main terms [6]:

$$\overline{\mathbb{A}} = \mathbb{A}^{Taylor} - \frac{1}{V} L^T K^{-1} L \tag{4}$$

Where $\mathbb{A}^{\text{Taylor}}$ represents the volumetric average of the microscopic constitutive tensors, analogous to the Taylor assumption [3], the term $L^T K^{-1} L$ is the fluctuation term, which depends on the structural fluctuation stiffness matrices (K and L) of the discretized microstructure. The $\mathbb{A}^{\text{Taylor}}$ term tends to overestimate the material's stiffness, while the fluctuation term corrects this overestimation. The computational cost of calculating the homogenized constitutive tensor is significantly impacted by the presence of the inverse of the stiffness matrix of the micromodel, which is contained in the fluctuation term.

An important aspect of the multiscale analysis adopted in this work that should be highlighted is that the inelastic process, including the calculation of the phase field that represents material degradation, occurs only at the microscale. This means that the phase field calculations are performed exclusively within the RVE, reflecting the interactions and behavior of the material at a microstructural level, and are then homogenized so that it can be visualized, in the post-processing phase, on the macroscale.

4 Examples and results

In this section, some numerical results are presented to investigate the influence of the fluctuation tensor on the accuracy of the multiscale analysis, as well as the impact of failure zone homogenization. The simulations were executed using the INSANE software under three distinct scenarios, each designed to isolate and evaluate specific aspects of the homogenization scheme:

- **Case 1: Failure Zone Homogenization and Taylor Term Only.** In this scenario, failure zone homogenization was applied, that is, the variables that are transferred in the upscale process have their average calculated taking into account only the failure region of the RVE. This approach was proposed by Nguyen et al. ([10], who highlight the importance of defining an adequate homogenization region during the softening regime of the material. Additionally, only the Taylor term, which represents the volumetric average of the microscopic moduli, was used for the homogenization of the macroscopic constitutive tensor, disregarding the fluctuation term.
- **Case 2: Without Failure Zone Homogenization and With the Fluctuation Tensor.** In this case, failure zone homogenization was not employed, that is, the average of the variables upscaled is calculated considering the entire domain of the RVE. The homogenized constitutive tensor included the fluctuation term, which is crucial for correcting the overestimation of material stiffness and capturing the internal deformation modes of the RVE.
- **Case 3: Without Failure Zone Homogenization and Taylor Term Only.** Similar to Scenario 2 in terms of the absence of failure zone homogenization, however, for the homogenization of the constitutive tensor, only the Taylor term was considered, excluding the contribution of the fluctuation tensor. This scenario serves as a baseline for comparison to isolate the effect of the fluctuation term when failure zone homogenization is not active.

It is worth noting that a fourth case considering failure zone homogenization and the fluctuation tensor cannot be evaluated using the formulation employed. The fluctuation tensor, given by the second term of eq. (4), depends on the inversion of the domain stiffness matrix, which can only be performed by applying boundary conditions that make the matrix non-singular, and the boundary definition is lost when defining a region for homogenization that no longer encompasses the entire RVE.

The problem analyzed consists of a multiscale approach that couples the macro and micro scales using the multilevel finite element method (FE^2). As illustrated in Fig. 1, the macrostructural model is discretized, by four quadrilateral elements with 4 nodes (Q4) and each of its Gauss points is associated with an RVE that captures the material's heterogeneities. The communication between the scales, known as downscaling and upscaling, allows the behavior of the microstructure to influence the global response of the problem, which is essential for modeling the fracture process, which begins at the microscale. The microscale is discretized by triangular elements (T3) and consists of two materials: random aggregates embedded in the mortar. It is worth noting that all macro-scale elements have a uniform thickness, except for the first element, which has a thickness of 0.9 in order to induce the strain location and damage evolution in this region.

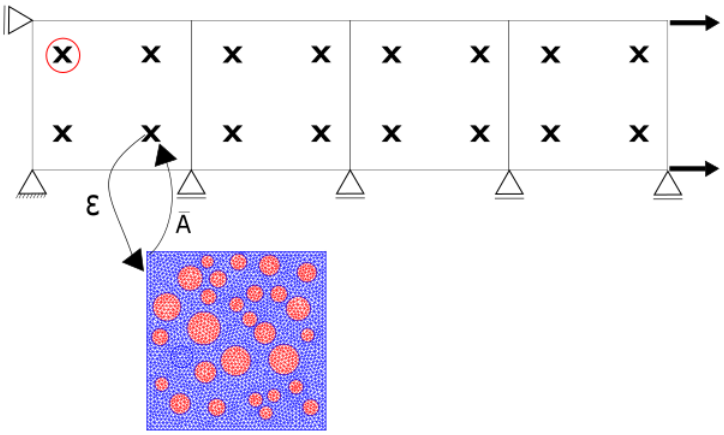
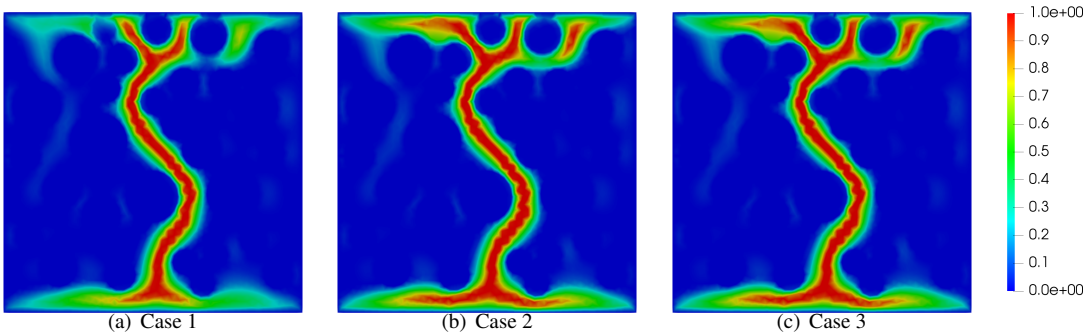


Figure 1. Scheme of the multiscale problem, where each Gauss point of the macro-structure is associated with an RVE that resolves the micro-structural characteristics.

The scheme shown in Fig. 2 illustrate the final distribution of the phase field ϕ in the Representative Volume Element (RVE) for three distinct scenarios studied. In all three cases, the formation of a main "S" - shaped fracture trajectory is observed, extending from one end of the RVE to the other. Figures 2a and 2c represent homogenization based on the Taylor assumption, which, as the literature points out, tends to overestimate the material's stiffness. In contrast, Figure 2b corresponds to the approach that includes the fluctuation term in the homogenized constitutive tensor formulation, correcting the stiffness overestimation and providing a more accurate representation of the material's mechanical behavior. The visual similarity in the fracture patterns suggests that crack evolution in this RVE model is robust with respect to the different homogenization choices, although the accuracy of the overall mechanical response fundamentally depends on the formulation used for the scale transition.



(a) Case 1 (b) Case 2 (c) Case 3

Figure 2. Phase-field contour plot at the final step of the analysis for an RVE of the first macroelement.

The comparative results between Case 2 (with the fluctuation tensor) and Case 3 (with the Taylor term only) indicate that the gain in theoretical accuracy is accompanied by a high computational cost. As can be observed in Fig. 3, the stress versus strain curves for both cases is minor and is practically the same, suggesting that the absence of the fluctuation tensor did not significantly impact the mechanical response of the RVE for this configuration. Similarly, the load factor versus displacement curves (Fig. 4) shows a correponding behavior for the two scenarios, with very similar load peaks and softening stages. However, when analyzing the computational costs, the difference becomes evident. Fig. 5 illustrates that Case 2, which includes the calculation of the fluctuation tensor, demands a considerably longer processing time, despite exhibiting a lower total number of iterations, as shown in Figure 5a. This can be justified by the fact that considering the fluctuation term produces a better initial approximation of the real tangent constitutive tensor, requiring fewer iterations to reach the equilibrium point of the analysis. However, even so, the analysis time is longer than that of case 3 (only with the Taylor tensor), as highlighted in Figure 5b. This occurs due to the complexity of the inversion of the stiffness matrix at the microscale, a calculation intrinsic to the formulation of the fluctuation term. The analysis therefore suggests that, although the fluctuation tensor is crucial for theoretical consistency and for correcting the overestimation of stiffness, its impact on computational cost may be disproportionate to the variation in the stress-strain response in certain scenarios.

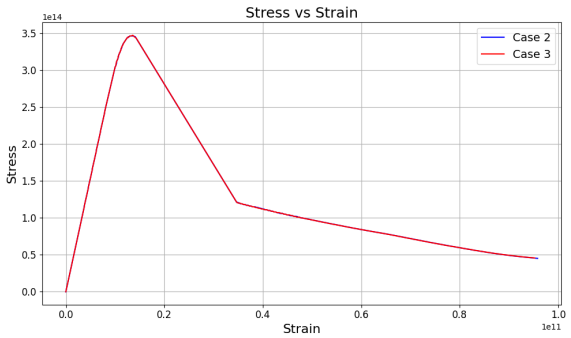


Figure 3. Stress versus strain curves for the integration point highlighted in the first macroelement.

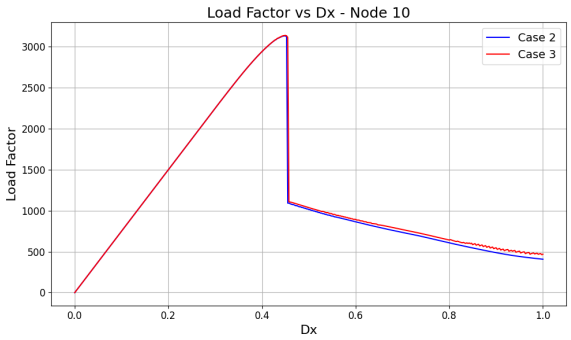
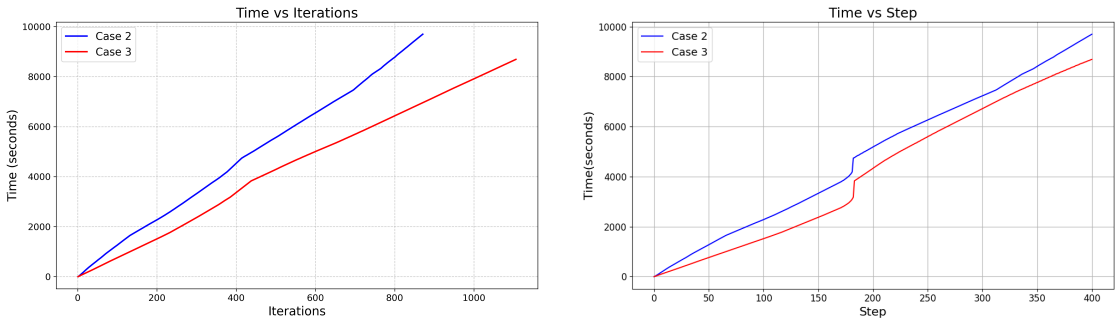


Figure 4. Load factor versus displacement curves for the different analysis cases.

The analysis of the evolution of the homogenized phase field, presented in Fig. 6, reveals notable differences between the three homogenization scenarios. The curves for Case 2 (without failure zone homogenization and with fluctuation) and Case 3 (without failure zone homogenization and with Taylor only) show an almost identical behavior, indicating that the consideration of the fluctuation tensor in the constitutive tensor does not significantly impact the evolution of the homogenized phase field for this problem. Both scenarios exhibit a gradual and small evolution of the phase field after a critical point, which represents the moment of greatest damage growth on the microscale. On the other hand, Case 1 (with failure zone homogenization and Taylor) exhibits a drastically different behavior. After the same critical point, where a higher value is already observed in the homogenized phase-field, this variable continues to grow continuously and considerably. This difference suggests that the use of failure zone homogenization leads to higher values in the phase field visualized at the macroscale, since the average of the phase field variable calculated at the microscale is taken only in a selected region that accompanies the crack and regions in imminent damage growth. It is worth noting that this variable is calculated based on the value of the micro-scale phase-field variable, but is used only for visualization at the macro-scale.



(a) Time vs. Iterations

(b) Time vs. Step

Figure 5. Comparative analysis of computational cost for different cases.

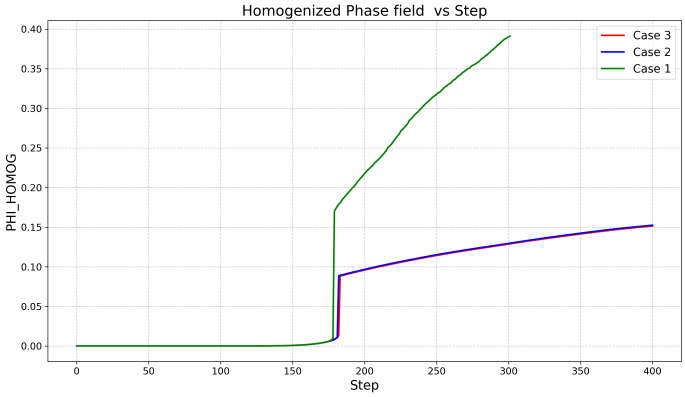


Figure 6. Evolution of the homogenized phase field as a function of the time step for the different cases.

5 Conclusions

This work explored the application of the multilevel finite element method (FE^2) for phase-field fracture analysis in heterogeneous materials, with a focus on comparing different homogenization strategies. The results obtained reveal crucial information about the impact of modeling choices on both the mechanical response and the computational performance of the method.

The visual analysis of the fracture patterns in the RVE, illustrated in Fig. 2, showed that the morphology of the main crack was remarkably similar in the three scenarios investigated, with the formation of a robust "S" - shaped path. This finding suggests that, for this type of microstructure, the fundamental failure mechanism is consistent, regardless of how the homogenization is conducted.

However, the comparison between Case 2 (with fluctuation) and Case 3 (with Taylor only) demonstrated an important trade-off between theoretical accuracy and computational cost. While the stress-strain and load factor versus displacement curves (Figs. 3 and 4) were practically indistinguishable for both scenarios, Case 2, which incorporates the fluctuation term, required a longer processing time although it requires fewer total iterations for convergence of the analysis, as evidenced in Fig. 5. This result indicates that, under certain conditions, the computational cost of the more refined homogenization may not translate into a substantial difference in the observed mechanical response.

The comparison with Case 1 (selective homogenization) highlights the influence of the upscaling strategy on damage representation. The evolution of the homogenized phase field (Fig. 6) was substantially more pronounced in Case 1, where the homogenized phase-field variable is obtained as the average of a selected region and not of the entire RVE, where some elements are in a unloading regime, for example. This initial result shows the importance of selecting an appropriate region in defining the averaging zone that accurately represents the behavior of the material. A natural development of this research is to conduct the same investigation in structural models with more complex behavior and that have experimental results for validating the multiscale implementation, such as L-shaped panels and beams in 3- and 4-point bending.

In conclusion, this study validates the applicability of the FE^2 method for modeling phase-field fractures,

demonstrating that different homogenization choices can distinctly influence computational efficiency and damage representation at the macroscale. A further study should be conducted to verify whether the findings presented here are also valid in more complex stress states.

Acknowledgements. The authors gratefully acknowledge the support from the Brazilian research agencies CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior), FAPEMIG (Fundação de Amparo à Pesquisa do Estado de Minas Gerais; Grant PPM-00747-18) and CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico; Grant 316240/2021-4).

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