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Local Homogenization of Composite Materials

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Abstract. The homogenization process has as its basic premise to change multiphase materials into a single material with a representative phase, regardless of which model is being used, whether based on the theory of elasticity, solid mechanics, or the mean-fields micromechanics models. These models, however sophisticated they may be, takes into account the interaction between the inclusions, the geometry of the inclusion up to the physical nonlinearity of the problem, which is always associated with the geometric limitation of the global model. To circumvent the geometric problem, it is proposed the development of a homogenization process that takes into account the geometry of the problem, in addition to the volumetric fractions and properties of each phase. This consideration is given by the generation of a quadtree recursive spatial subdivision, where the mesh nodes represent the inclusions and the elements connected to the nodes represent the matrix. With this, it can be shown the reduction of the global problem to a local problem of the Eshelby equivalent inclusion and homogenize of the mesh node by node. The obtained results are a map of properties homogenized locally since each node has different volumetric fractions for each problem of equivalent inclusion. This procedure opens a range of different possibilities of materials, including the application in multiphase cementitious composite materials.

Keywords: composite materials, local homogenization.

1 Introduction

The need to obtain new materials arose from the beginning of civil construction and continues to be researched fit to the present day, where there is a continuous effort for the improvement of several properties, highlighting: mechanical, thermal, optical, piezoelectric, chemical, magnetic properties, among others. One of the main ways to improve materials is by combining them in order to maximize their qualities and prolong their useful life.

Given a body is assumed to be homogeneous and continuous in its macrostructure when reduced to a sufficiently small scale, it does not behave as a homogeneous material, but as a heterogeneous material, in addition to presenting discontinuities and inhomogeneities. The literature brings several definitions about which volume will be representative of its macroscale in its microscale.

Drugan and Willis [1] indicate that the Representative Volume Element (RVE) is associated with the smallest volume that can represent the average properties of the composite. Stroven et al [2] discuss several definitions regarding the RVE), even proposing a way of measuring it.

Drago and Pindera [3] define the RVE as being a heterogeneous system in its microstructure, where applying the specific boundary conditions for each representative volume, the response does not differ from the material in its macroscale. Picheler and Hellmich [4] define a representative volume element as a function of the scales of analysis, and the same definitions mentioned above can be applied to multiscale systems.

In fact, there is an open discussion about the geometry of the representative volume element, however, despite homogenizing the representative volume, its geometry has no relevance in this process and is discarded from the analysis. A different proposal is to punctually homogenize any geometry from the generation of a regular or non-regular quadtree mesh.

The proposal was called local homogenization and will be described below. Illustrating the problem, take as a reference a concrete specimen, where it can be characterized as a composite material, initially by two distinct phases in its macroscale, namely the mortar (matrix) and the coarse aggregates (inclusions) (Figure 1).

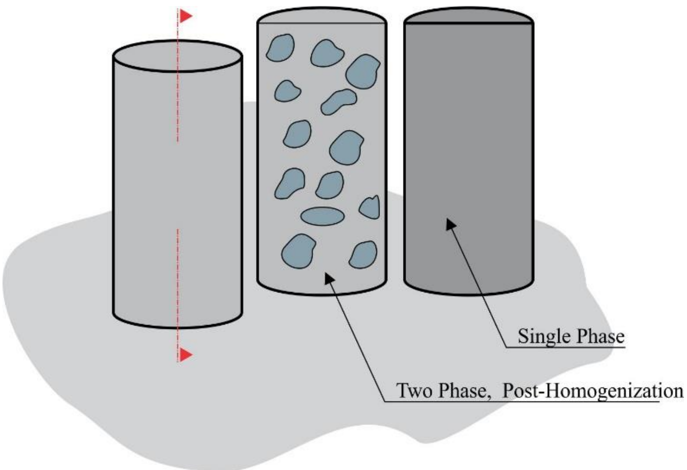

Figure 1. Concrete specimen.

Fig. 1, shows the homogenization of the concrete specimen, where the result would be just a representative phase, leaving the idea that the inclusions were diluted in the matrix, which does not represent reality. In the specific case of concrete, the inclusions will never be incorporated into the matrix, however, there is an influence of the closest materials, which is the premise of local homogenization.

2 Methodology

Figure 2 illustrates the process of local homogenization, where it is assumed that composite has its distinct phases, but the influence is local. With the global geometry, a quadtree mesh is created, verifying the connectivity of each node to each element. For the modeling methodology, the elements will be the composite matrix and the nodes will be the inclusions, respectively.

Each node in the mesh can be attached to a single element or to several elements simultaneously, however in a regular mesh, as shown in Fig. 2, each node can only be connected to a maximum of four elements.

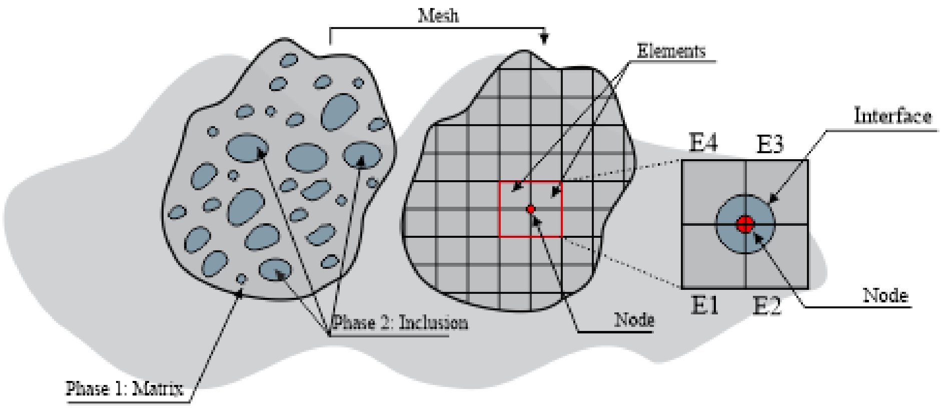

Figure 2. Local homogenization strategy.

The next step consists of evaluating the local volumetric fractions of each node and the respective elements that are in connectivity with it to establish the local problem. To measure the volumetric fraction of inclusions (nodes), one can choose a random statistical distribution or define the fractions of each node individually.

When the problem is randomic, one can choose to define the fractions statistically, taking into account three probability density functions, namely: Normal (standard curve), Gamma distribution (curves with concentration of inclusions of larger volumes), extreme value, or Gumbel (curves with concentration of inclusions of smaller volumes).

Mathematically, the normal distribution function model can be expressed as a continuous random variable X with mean μ and standard deviation σ, being:

$$\begin{gathered} -\infty < x < \infty \\ \sigma > 0 \end{gathered} \tag{1}$$

The probability density function (PDF) will be given by (CASELLA, et al., [5]), (MONTGOMERY, et al., [6]), (ARAÚJO, et al., [7]).

$$f_x(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{2}\right)^2} \tag{2}$$

With expected value $E(X) = \mu$ e variance $V(X) = \sigma^2$.

Extreme value functions, widely applied to maximum and minimum problems, establish in this problem the idea of building curves from the accumulation of values at the most extreme points of the distribution. The extreme functions depend on shape parameters, in addition to the mean of the data studied, however, it is possible to approximate the shape values for the deviation, with good distribution results.

The PDF for Gumbel is given by [5], [6] e [7]:

$$f_x(x) = \frac{1}{\beta} e^{\left(\frac{x-\alpha}{\beta}\right)^2} - e^{-e^{-\left(\frac{x-\alpha}{\beta}\right)}} \tag{3}$$

Where α is the position parameter and β is the scale parameter. It is possible to generate maximum and minimum events by controlling the positive or negative sign of the second exponent of the aforementioned equation. Another extreme function is the Gamma function, its PDF being given by

$$f_x(x) = \frac{1}{\beta^{\alpha}\Gamma(\alpha)} x^{(\alpha-1)} e^{-\frac{x}{\beta}} \tag{4}$$

where:

$$\Gamma(\alpha) = (\alpha - 1)! \tag{5}$$

For all positive integers, with expected values $E(X) = \alpha\beta$ and $V(X) = \alpha\beta^2$. In this process, it is essential to define the extreme and minimum value so that the fractions are properly attributed to each inclusion (node) of the mesh.

Measuring the fractions of the matrix, once the entire mesh is known, it is verified which elements are connected to each node and defines the fraction as the sum of the areas of each connected element.

In this methodological step, it is worth mentioning that the study scale is macroscopic, and the geometry of the problem and the mesh are important for the measurement of local fractions. Finally, each local problem will be treated as an Eshelby equivalent inclusion problem. Depending on the model to be used, it is possible to introduce a third phase referring to the matrix-inclusion interface, quite common in some composite materials.

The formulation of the local homogenization process is generalized for any composite, as well as the methods to be used can be based on any premise: theory of elasticity, solid mechanics or the mean-fields micromechanics, since the idea starts exactly from the problem the equivalent inclusion of Eshelby (BENVENISTE, [8]) on which these models are based.

It is emphasized that some composites are suitable for certain models (Table 1). That means, for example, that the concrete, which is known to have a transition phase, is not suitable for modeling with only two phases.to find out the effective properties

Table 1. Characteristics of homogenization models.

Models	Characteristics
Reuss	Its limitation is the imposition of a constant state of tension, in addition to not evaluating the interaction between inclusions (REUSS, [9]) $\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m : \mathbb{C}_i : [\mathbb{C}_i(1 - f_i) + \mathbb{C}_m f_i]^{-1}$
Voigt	Its limitation is the imposition of a constant deformation state, in addition to not evaluating the interaction between the inclusions (VOIGT,[10]), (KAW, [11]) $\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m(1 - f_i) + \mathbb{C}_i f_i$
Hashin	It does not estimate constant stress and strain fields, instead of it estimates auxiliary fields representing a variation of the reference solution. When the formulation of the energy obtained is maximized, the upper limit is found and when it is minimized, the lower limit is found. (HASHIN, et al., [12]) $E_c{}^{+} = \left[\frac{9k^{+}G^{+}}{3k^{+} + G^{+}}\right]$ $E_c{}^{-} = \left[\frac{9k^{-}G^{-}}{3k^{-} + G^{-}}\right]$
Mori-Tanaka	It is the most used model for homogenization of composites, it considers the interaction between the particles and can be used with larger volumetric fractions. (MORI, et al., [13])

	$\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m : \{\mathbb{I} + f_i(\mathbb{S} - \mathbb{I}) : [(\mathbb{C}_m - \mathbb{C}_i)^{-1} : \mathbb{C}_m - \mathbb{S}]^{-1}\} : \{\mathbb{I} + f_i \mathbb{S} : [(\mathbb{C}_m - \mathbb{C}_i)^{-1} : \mathbb{C}_m - \mathbb{S}]^{-1}\}^{-1}$
Dilute Suspension	It is limited by the amount of volumetric fraction of inclusion in the homogenization process, and can only be applied to low inclusion rates $\mathbb{C}^{\mathrm{H}} = \mathbb{C}_m + f_i(\mathbb{C}_i - \mathbb{C}_m) : \mathbb{A}_i$ $\mathbb{A}_i = [\mathbb{I} - \mathbb{S} : \mathbb{C}_m : (\mathbb{C}_m - \mathbb{C}_i)]$
Self-Consistent	Evaluates interaction between particles, however, cannot differentiate between matrix and inclusion in the analysis, it is an implicit method requiring an initial estimate (HILL, [14]) $\mathbb{C}^{\mathrm{H}}{}_{n+1} = \mathbb{C}_m + f_i(\mathbb{C}_i - \mathbb{C}_m) : [\mathbb{I} - \mathbb{S}^{\mathrm{H}}{}_n : \mathbb{C}^{\mathrm{H}^{-1}}{}_n : (\mathbb{C}^{\mathrm{H}}{}_n - \mathbb{C}_i)]^{-1}$
Generalized Self-Consistent	Based on the theory of elasticity, it manages to evaluate the interaction between inclusions being developed as a three-phase model, essentially it only evaluates two phases. It takes into account the inclusion-matrix interaction between inclusions (CHRISTENSEN, et al., [15]) $A\left[\frac{G^H}{G_m}\right]^2 + B\left[\frac{G^H}{G_m}\right] + C$ $K^H = \left[K_m + \frac{f_i(K_i - K_m)(3K_m + 4G_m)}{3K_m + 4G_m + 3(1 - f_i)(K_i - K_m)}\right]$ $E^H = \left[\frac{9K^H G^H}{G^H + 3K^H}\right]$
Differential Scheme	It is different from the others that suppose a inclusion embedded in a infinite matrix. This one considers incremental dosis of inclusions. Diferente dos demais métodos que pressupõe uma inclusão imersa em uma matriz infinita, o esquema diferencial trabalha com doses incrementais de inclusões (HASHIN, [16]) $\mathbb{C}^{\mathrm{H}}{}_{n+1} = \mathbb{C}^{\mathrm{H}}{}_n + \frac{\Delta f_i}{1 - f_i}(\mathbb{C}_i - \mathbb{C}^{\mathrm{H}}{}_n) : \mathbb{A}_i{}^{\mathrm{D}}$ $\mathbb{A}_i{}^{\mathrm{D}} = [\mathbb{I} - \mathbb{S}^{\mathrm{H}}{}_n : \mathbb{C}^{\mathrm{H}}{}_n{}^{-1} : (\mathbb{C}^{\mathrm{H}}{}_n - \mathbb{C}_i)]^{-1}$ $\mathbb{S}^{\mathrm{H}} = \mathbb{S}$ $\mathbb{C}^{\mathrm{H}}{}_n = \mathbb{C}_m$
Four-phase	The four-phase or double-inclusion model manages to measure beyond the above-mentioned basic models as it evaluates the matrix-inclusion interface (LI, et al., [17]), Generalized Self-Consistent + "Composite Sphere Assemblage (CSA)" [16] ou "Composite Cylinder Assemblage (CCA)" (HASHIN, et al., [18])
Multi-phase	The multi-phase model has the same premise as the four-phase model, but it has in its formulation the mean-fields micromechanics, which differs from the four-phase model which is based on the theory of elasticity. (SHI, et al., [19]) $\mathbb{A}_i{}^D = \mathbb{I} + \mathbb{S}_i : \Phi_i + \Delta\mathbb{S} : \Phi_r$ $\mathbb{A}_r{}^D = \mathbb{I} + \mathbb{S}_r : \Phi_r + \frac{f_i}{f_r}\Delta\mathbb{S} : (\Phi_i - \Phi_r)$ $\Delta\mathbb{S} = \mathbb{S}_i - \mathbb{S}_r$ $\Phi_i = -\left[(\mathbb{S}_i + \mathbb{A}_i) + \Delta\mathbb{S} : \left(\mathbb{S}_i + \mathbb{A}_i - \frac{f_i}{f_r}\Delta\mathbb{S}\right) : \left(\mathbb{S}_r + \mathbb{A}_r - \frac{f_i}{f_i}\Delta\mathbb{S}\right)^{-1}\right]^{-1}$ $\Phi_r = -\left[\Delta\mathbb{S} + (\mathbb{S}_i + \mathbb{A}_i) : \left(\mathbb{S}_i + \mathbb{A}_i - \frac{f_i}{f_r}\Delta\mathbb{S}\right)^{-1} : \left(\mathbb{S}_r + \mathbb{A}_r - \frac{f_i}{f_i}\Delta\mathbb{S}\right)\right]^{-1}$ $\mathbb{A}_i = (\mathbb{C}_i - \mathbb{C}_m)^{-1} : \mathbb{C}_m$ $\mathbb{A}_r = (\mathbb{C}_r - \mathbb{C}_m)^{-1} : \mathbb{C}_m$ $\mathbb{C}^H = \mathbb{C}_m + \left[f_r(\mathbb{C}_r - \mathbb{C}_m) : \mathbb{A}_r{}^D + f_i(\mathbb{C}_i - \mathbb{C}_m) : \mathbb{A}_i{}^D\right]$

Legend:

$\mathbb{C}$ - Constitutive tensor; $\mathbb{S}$ – Eshelby Tensor; $\mathbb{A}$ – Concentration Tensor; $\mathbb{I}$ – Identity Tensor; f – volumetric fraction, E – Young modulus, K – volumetric modulus; G – Shear modulus; Φ – Fourth-order tensor.

Indexers:

i, m, r, n, H, D – Inclusion, Matrix, Coating (interface), Iteration Step, Homogenized, Dilute

3 Results and Discussion

Demonstrating the developed technique, it was considered as a composite to be analyzed the concrete that has unique characteristics such as interfacial transition zone, consideration of isotropy in the distribution of inclusions (large aggregates) in addition to having a great interest in civil engineering.

For this study, a standard rectangular specimen measuring 15 x 30 cm was modeled, creating a regular mesh of four-node quadrangular elements (Figure 3). It is important to emphasize that the mesh is not required to be regular or quadrangular, but the mesh refinement must be controlled since the inclusions have volumetric fractions that cannot exceed the total volume of the problem.

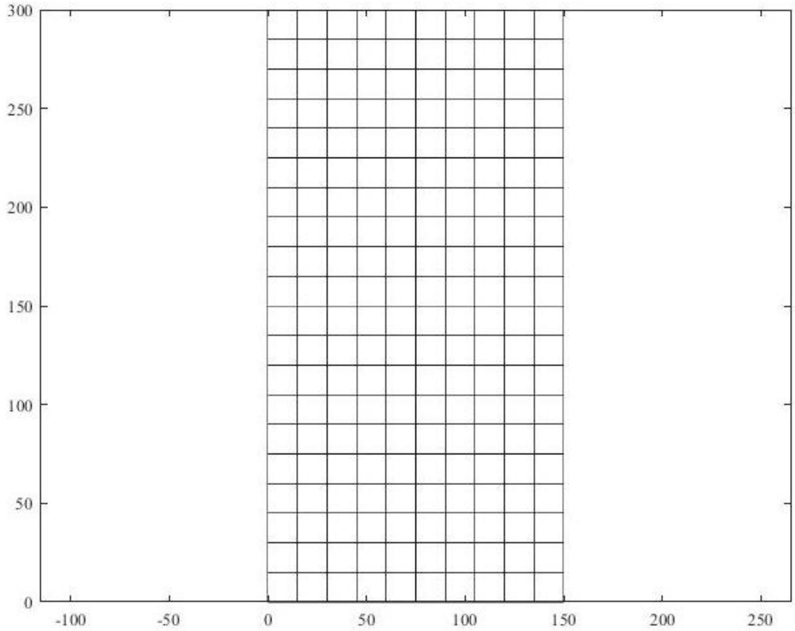

Figure 3. Quadtree recursive spatial subdivision mesh on a 15 x 30 specimen.

Table 2 shows information about the geometry, mesh and the homogenization process generated in the example.

Table 2. Analysis data.

Mesh			
Geometry	Elements	Nodes	Statistical distribution
15 x 30cm	200	231	Extreme value
Homogenization			
Models	Matrix	Interface	Inclusion
Four-phases	$E_m = 21{,}34$ GPa	$E_r = 80\% E_m$ GPa	$E_i = 77{,}60$ GPa
	$\nu_m = 0{,}15$	$\nu_r = 0{,}20$	$\nu_i = 0{,}25$

The granulometric distribution within the global geometry was generated randomly and can be seen in Figure 4.

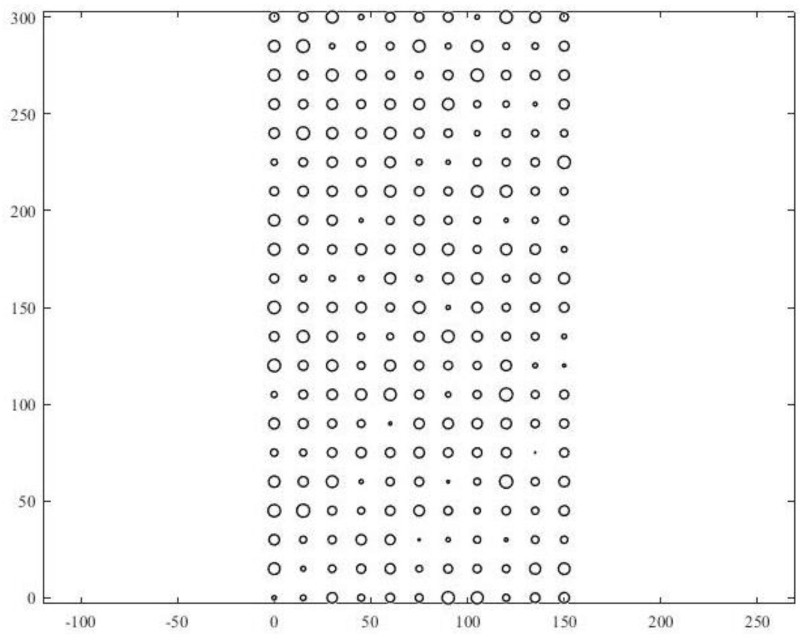

Figure 4. Size distribution of inclusions in the global geometry.

As a result of local homogenization, the distribution of elastic modulus is shown in Figure 5.

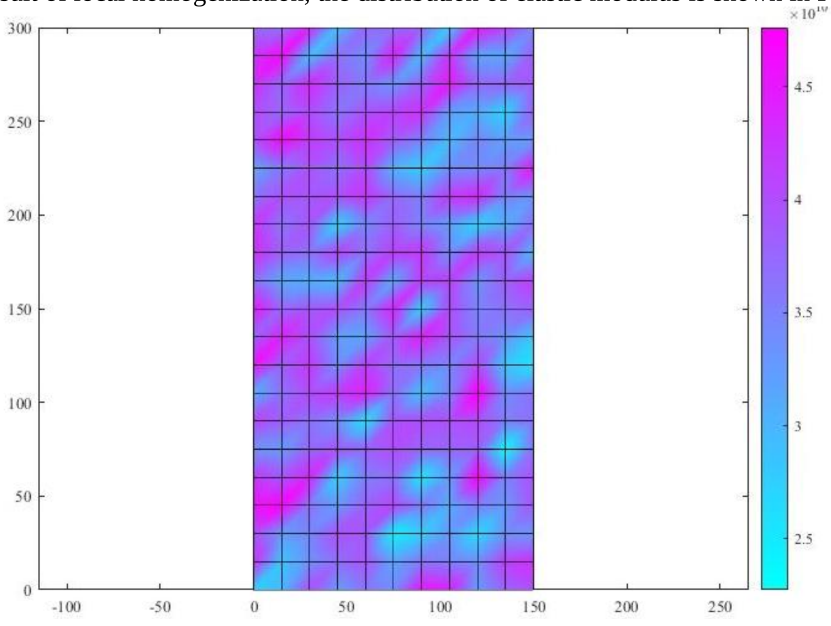

Figure 5. Local Young modulus.

The statistical random distribution brings the benefit of the analysis of the isotropy of the problem since the granulometry curves are generated randomly as well as the attribution of the fractions of each node, the only control being the concentration of diameters of the aggregates that can be defined.

4 Conclusions

The proposal of this paper is extremely new, initially observing some limitations, namely: the problem is dependent on the generated mesh, so that although the mesh is not obligatory to be regular, this factor minimizes the global influence of the mesh, being able to take advantage of local information.

A second important point is that the global module of the problem cannot be evaluated because it has been converted into multiple smaller problems. It is possible to control the mesh by refining it, but it must be controlled so that there is no contact between the inclusions.

In the aforementioned modeling, each node has a volumetric fraction associated with it, this leads to the consideration of the nodes that are in the geometry interface that must be analyzed separately since not every volumetric fraction of these nodes contributes to the analysis.

As stated in the case of a new study, it is important to verify the possibility of applications and adaptations for modeling, being able to highlight the problem of concrete that can be studied segregation, voids, possible crack openings etc.

If the local mapping comes together with mapping by finite elements in tension, the overlapping of the layers can generate useful information for concrete modeling.

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