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A direct FEM approach for particulate reinforced elastic solids

Rodrigo Ribeiro Paccola *, Humberto Breves Coda

São Carlos School of Engineering, University of São Paulo, Av Trabalhador São Carlense, 400, ZIP-13560-590 SãoCarlos, SP, Brazil

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ABSTRACT

In this work we are interested to provide an alternative way to model particulate composites by the Finite Element Method. Our proposal allows the inclusion of particles with any geometry, quantity and any regular or random arrangement in continuous matrix. Accordingly, the main feature of the formulation is: maintaining the geometry and the discretization of the matrix, to introduce a given distribution of particles without increasing the number of degrees of freedom or change the initial mesh of the problem. In this sense a direct FEM approach for particulate composites arise.

Here, both the matrix and particles are considered elastic and totally connected, i.e., degeneration of the involved materials is not allowed and perfect adherence between matrix and particles phases is adopted, thus the interface or the transition zone between phases is not modeled.

The proposed formulation already includes geometrically exact description allowing the development of large displacements and moderate strains. Examples are presented to validate the formulation confronting it with usual techniques of homogenization and laboratory experiments. Furthermore, the possibilities of the proposed technique are shown in an original example.

1. Introduction

It is well known the fact that composites mix two or more materials in order to obtain, for a given application, a new material with physical and economic properties better than those presented separately by each constituent material. Composite materials are used in both traditional applications such as reinforced concrete and in recent applications such as lightweight composite materials of carbon fibers embedded in epoxy matrix.

Although we are always admitting approximations, we can divide composites into four categories, particulate, reinforced by fibers, laminated and combined composites [1]. The latter combines any of the three basic arrangements with each other in any proportion. It should be clarified that in this study we assume an extended definition given by [2] that composite materials are those whose predominant phases can be distinguished in macroscopic or microscopic forms, since the continuum mechanics can be applied in the solution of each phase of the material.

A recent and complete review of several aspects of the evolution of research on composite materials can be seen in [3].

Limiting the discussion to the mechanical behavior of materials, object of this study, the challenges associated with the development and application of composite materials are, as for any other material, associated to aspects of physical characterization and development of rheological/mathematical models which can predict its behavior [4–9]. In this sense the studies related to composite materials are divided into three ranges: the macro-scale, meso-scale and nano-scale. The first is concerned with the overall behavior of the structural components, even though the geometric size of stages is very small. The meso-scale addresses the interdependent behavior of the reinforcement and the matrix, i.e., the interface stress and its relative detachment. Finally, the nano-scale is interested in setting up the materials on its molecular and atomic level, and its influence on the behavior of the material in their meso and macro-level.

The interest of this study is to contribute in the modeling of the macro-mechanical behavior of composite materials through the FEM regardless particle size [10–18]. More specifically, it seeks to provide an alternative way (called here direct) to model composite particulate materials by Finite Element Method based on positions [19–23]. Our proposal enables the inclusion of a very large number of particles with any geometry, quantity and with any regular or random arrangement in continuous. In this sense, maintaining the geometry and the continuous matrix, defined for convenience of the examined solid boundary conditions, the main feature of the proposed formulation is to introduce a given distribution of particles into the system without increasing the number of degrees of freedom or change the initial mesh of the problem.

* Corresponding author.
E-mail addresses: rpaccola@sc.usp.br (R.R. Paccola), hbcoda@sc.usp.br (H.B. Coda).

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It is noteworthy that the proposed technique differs from those based on the partition of the unit, widely used in procedures related to the inclusion of fiber in volumes [24–26], because the inclusion of particulate reinforcement is made here directly by kinematic relationships between nodes that represent the particles and the degrees of freedom which represent the matrix. The latter are the only ones to be considered in the solution of the numerical system, such that the order of the system is not affected by the number of particles considered.

It is also worth noting that in the proposed technique it is not required the coincidence of the nodal positions, even of surfaces or interface zones. Thus, the macroscopic behavior of the material will be simulated from the basic properties of the constituents, without the need of developing numerical or analytical homogenization techniques like the ones present in the literature [7,8,27,28]. In this sense a direct FEM approach for particulate composites arise, i.e., it is possible to analyze a general structure or body without using homogenized material characteristics. However, if it is of interest, our formulation can be used to numerically extract homogenized elastic properties of particulate composite reducing the necessity of laboratory experiments and also used to perform indirect applications, using the extract homogenized properties.

This work is original and intends to publish the proposed formulation so that other researchers can take advantage of its unique features and improve it to covers more complex applications. Here, both the matrix and particles are considered elastic and totally connected, i.e., it will not be allowed degeneration of the involved materials and perfect adherence between matrix and particles is adopted. Thus the interface or transition zone between phases is not modeled. It is important to stress that a numerical strategy (deterministic and aleatory) of mesh and particles position generation is used in order to allow more general applications. One basic computational code for particle generation is available at Appendix A.

The proposed formulation already includes geometrically exact description allowing the development of large displacements and moderate strains. Examples are presented to validate the formulation confronting it with usual techniques of homogenization and laboratory experiments. Furthermore, the possibilities of the proposed technique are shown in an original example.

2. The Finite Element Method based on positions – 2D phases modeling

In this work any phase of the particulate composite is modeled using the Finite Element Method based on positions. Thus, it is important to provide a short description in order to enable its easy reproduction by other researchers interested in the subject. We started the description from the total energy stationary principle and describe the formulation of the FEM based on positions. In the absence of dissipative potentials and considering isothermal and static applications the total energy of any body, Fig. 1a, and its variation are written as.

$$\Pi = U + P \quad \delta\Pi = \delta U + \delta P = 0 \tag{1}$$

where U is the strain energy stored in all phases of the composite (matrix and particles) and P is the potential energy of external forces, see Fig. 1.

Bearing in mind that both particles and matrix are modeled here by two-dimensional finite elements, Fig. 1b, we describe the initial and final body configuration from the kinematic description of a generic two-dimensional solid finite element (membrane) as shown in Fig. 2. It should be noted that the approximation order of the finite element shown in Fig. 2 is merely illustrative and that the formulation is described for any element approximation order.

We propose the following guide to define the formulation. First we define the change of configuration function of a finite element by writing the associated Green strain. Next, we define the specific strain energy to be integrated in the finite element volume, resulting in the composite strain energy as a function of nodal positions. At this point it appears the novelty of the formulation, which is the inclusion of particles without the addition of new degrees of freedom in the discretization previously developed for the matrix. Then we include the potential of the external conservative forces and apply the total energy stationary principle resulting in the no linear equilibrium equations. Finally, the Newton–Raphson procedure is used to solve the nonlinear system achieving the searched solution.

2.1. Kinematics and strain energy

In Fig. 2 letter B_0 represents the initial configuration of a finite element of any phase of the composite and letter B represents its current configuration. The dimensionless space B_1 is used to generate the Lagrange polynomials ϕ_ℓ that compose the initial f_i^0 and final f_i^1 mappings as:

$$f_i^0 = x_i(\xi_1,\xi_2) = \phi_\ell(\xi_1,\xi_2)\cdot X_{\ell i} \quad \text{e} \quad f_i^1 = y_i(\xi_1,\xi_2) = \phi_\ell(\xi_1,\xi_2)\cdot Y_{\ell i} \tag{2}$$

in which index notation is applied, i.e., repeated indices represents summation. Both in Eq. (2) as in Fig. 2 x_i and y_i indicate coordinates at initial and current configurations, respectively. Index ℓ indicates a finite element node while $X_{\ell i}$ and $Y_{\ell i}$ represent, respectively, the initial and current nodal coordinates. To simplify the understanding we accept, in Eq. (2), the coordinates inside the continuum x_i as the mapping f_i^0 and the current coordinates y_i as the mapping f_i^1.

In order to assemble the method we are interested in the gradient of the change of configuration function (or deformation function) of a portion of any phase described by the FEM, i.e., [29]:

$$Grad\left(\vec{f}\right) = Grad\left(\vec{f}^1 \circ \left(\vec{f}^0\right)^{-1}\right) = Grad\left(\vec{f}^1\right)\cdot Grad\left(\left(\vec{f}^0\right)\right)^{-1} = A^1\cdot\left(A^0\right)^{-1} \tag{3}$$

The gradients of the mappings, i.e., A^0 and A^1 are easily determined, since we know the initial and current coordinates of the nodes of the finite element. The initial coordinates are known from the mesh generation process and, as the proposed formulation is geometrically non-linear, the current coordinates are known as a trial for the iterative process of solution. In the numerical process, the integration of the domain densities is accomplished by full Hammer quadrature and, therefore, A^0 and A^1 are numerical matrices of dimension 2. Thus, A^0 and A^1 are given by:

$$A_{ij}^0 = \frac{\partial f_i^0}{\partial \xi_j} = \phi_{\ell j} X_{\ell i} \quad \text{and} \quad A_{ij}^1 = \frac{\partial f_i^1}{\partial \xi_j} = \phi_{\ell j} Y_{\ell i} \tag{4}$$

From the gradients of the mappings, Eq. (4), and the deformation gradient, Eq. (3), one writes the Green strain $\boldsymbol{E}$ as:

$$\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{A}^t\cdot\boldsymbol{A} - \boldsymbol{I}\right) = \frac{1}{2}\left(\boldsymbol{C} - \boldsymbol{I}\right) \quad \text{or} \quad E_{k\ell} = \frac{1}{2}\left(A_{ik}A_{i\ell} - I_{k\ell}\right) \tag{5}$$

in which $\boldsymbol{C}$ is the well-known right Cauchy–Greeen stretch tensor.

From the Green strain one writes the expressions of the specific strain energy which defines, respectively, the plane stress or the plane strain Saint–Venant–Kirchhoff constitutive laws.

$$u^{PStress} = \frac{1}{2}\left\{K\left(E_{11}^2 + E_{22}^2\right) + 2\nu K(E_{11}E_{22}) + 2G\left(E_{12}^2 + E_{21}^2\right)\right\} \tag{6}$$