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COARSE–GRAINING APPROACHES FOR PARTICULATE COMPOSITES AS MICROPOLAR CONTINUA

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Abstract. A multitude of composite materials ranging from polycrystals up to concrete and masonry–like materials overwhelmingly display random morphologies. In this work we propose a statistically–based multiscale procedure which allow us to simulate the actual microstructure of a two–dimensional and two–phase random medium and to estimate the elastic moduli of the energy equivalent homogeneous micropolar continuum. This procedure uses finite–size scaling of Statistical Volume Elements (SVEs) and approaches the so–called Representative Volume Element (RVE) through two hierarchies of constitutive bounds, respectively stemming from the numerical solution of Dirichlet and Neumann non-classical boundary value problems, set up on mesoscale material cells. The results of the performed numerical simulations point out the worthiness of accounting spatial randomness as well as the additional degrees of freedom of the Cosserat continuum.

1 INTRODUCTION

Several composite materials, extensively adopted in many engineering fields, are characterized by particulate random microstructures. Examples are polymer, ceramic, metal matrix composites or also concrete, granular materials and porous rocks (Figure 1).

A key issue in mechanics of materials characterized by microstructural randomness is that the classical concept of the Representative Volume Element (RVE), well established in periodicity based homogenization techniques since many years [16, 9], loses its validity [11]. In the last few years, various procedures based on the solution of specific Boundary Value Problems (BVPs) have been proposed to perform classical homogenization for non–periodic assemblies [17, 3, 14, 1, 15]. In order to account for the effects of

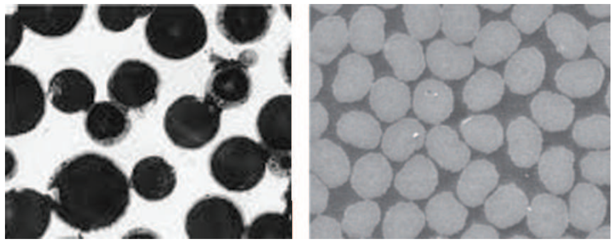

Figure 1: Examples of particulate composites.

the microstructural size, heterogeneous non–periodic materials have been also studied by extending the homogenization schemes to gradient–enhanced continua, although applied to a single fixed mesoscale [5, 6]. Stocastic approaches based on finite–size scaling homogenization have proved to be among the most effective for individuating the RVE size and the overall constitutive moduli in the linear elastic and thermoelastic, as well as in the non–linear and non–elastic, frame [10, 4, 12].

In this paper we adopt the statistically–based scale–dependent homogenization procedure developed in [18], which enables to simulate the actual microstructure of a simplified two–phase random media and to estimate the constitutive moduli of energy equivalent micropolar continua. This procedure uses finite–size scaling of Statistical Volume Elements (SVEs) and approaches the so–called Representative Volume Element (RVE) through two hierarchies of constitutive bounds, respectively stemming from the numerical solution of Dirichlet and Neumann non classical boundary value problems, set up on mesoscale material cells. For defining these problems we use a generalized macro-homogeneity (Hill–Mandel type [2]) condition, which accounts for non–symmetric stress and strain as well as couple–stress and curvature tensors. In particular, for a two–dimensional elastic medium made of a base matrix and a random distribution of disk–shaped inclusions of given density, two hierarchies of constitutive bounds are obtained by considering mesoscale test–windows of different sizes supposed placed anywhere in a random material domain. Under the hypotheses of statistical homogeneity and mean–ergodicity of the medium: the convergence trend of the bounds is detected as function of the SVE size; the RVE size is attained on the basis of a statistical criterion; the average homogenized, classical and micropolar, elastic moduli are estimated.

The results of the simulations performed point out the importance of taking into account the spatial randomness of the medium, and in particular the presence of inclusions that intersect the edges of the test windows. The worthiness of accounting the additional stress and strain measures of the Cosserat continuum is also discussed.

2 MICROPOLAR CONTINUUM

A material point of a micropolar continuum is characterized by a position and an orientation; the kinematical descriptors are displacements and rotations, represented by the vectors (u_i) and (φ_i), respectively. Within the framework of a linearized theory, in which displacements and rotations stand for velocities and angular velocities, respectively, and works for rate of works, the kinematics of the continuum is governed by the following relations:

$$\begin{aligned} \gamma_{ij} &= u_{i,j} - e_{kij}\varphi_k, \\ \kappa_{ij} &= \varphi_{i,j}. \end{aligned} \tag{1}$$

where (γ_{ij}) and (κ_{ij}) are the generally asymmetric strain and curvature tensors, respectively, and where e_{ijk} is the Levi–Civita tensor, with $i, j, k = 1, 3$. The balance equations in the absence of body forces and couples are:

$$\begin{aligned} &\tau_{ij,j} = 0, \\ &\mu_{kj,j} + e_{kji}\tau_{ij} = 0\,, \end{aligned} \tag{2}$$

where (τ_{ij}) and (μ_{kj}) are respectively the generally asymmetric stress and couple stress tensors. Denoting with (t_i) and (m_i) the tractions and surface couples on the boundary of a control volume of outward normal (n_i), always with $i, j = 1, 3$, we also have:

$$\begin{aligned} t_i &= \tau_{ij}\, n_j\,, \\ m_i &= \mu_{ij}\, n_j\,. \end{aligned} \tag{3}$$

In order to separately investigate the classical and micropolar components we divide the strain and stress tensors in their symmetric and skew-symmetric part. That is:

$$\begin{aligned} \gamma_{ij} &= \varepsilon_{ij} + \alpha_{ij}\,, \\ \tau_{ij} &= \sigma_{ij} + \beta_{ij}\,. \end{aligned} \tag{4}$$

where (ε_{ij}) and (σ_{ij}) are the classical symmetric strain and stress tensors, while (α_{ji}) and (β_{ji}) are the skew–symmetric strain and stress tensors characterizing, together with the curvature and the couple stress tensor (κ_{ji}) and (μ_{ji}), a micropolar medium. In particular, $\alpha_{ji} = \frac{1}{2}(u_{i,j} - u_{j,i}) - e_{kji}\varphi_k$ is the relative rotation between the macrorotation and microrotation.

The constitutive relations in the linear elastic anisotropic case are:

$$\begin{aligned} \sigma_{ij} &= A^{YY}_{ijhk}\varepsilon_{hk} + A^{YK}_{ijhk}\alpha_{hk} + A^{YC}_{ijhk}k_{hk} \\ \beta_{ij} &= A^{KY}_{ijhk}\varepsilon_{hk} + A^{KK}_{ijhk}\alpha_{hk} + A^{KC}_{ijhk}k_{hk} \\ \mu_{ij} &= A^{CY}_{ijhk}\varepsilon_{hk} + A^{CK}_{ijhk}\alpha_{hk} + A^{CC}_{ijhk}k_{hk}\,, \end{aligned} \tag{5}$$

where (A^{YY}_{ijhk}) is the classical constitutive tensor, while (A^{YK}_{ijhk}), (A^{KY}_{ijhk}), (A^{KK}_{ijhk}), (A^{YC}_{ijhk}), (A^{KC}_{ijhk}), (A^{CY}_{ijhk}), (A^{CK}_{ijhk}) and (A^{CC}_{ijhk}) are the micropolar constitutive tensors $(i,j,h,k = 1,3)$. For hyperelastic materials: $A^{YY}_{ijhk}= A^{YY}_{hkij}$, $A^{KK}_{ijhk}= A^{KK}_{hkij}$, $A^{CC}_{ijhk}= A^{CC}_{hkij}$, $A^{YK}_{ijhk}= A^{KY}_{hkij}$, $A^{YC}_{ijhk}= A^{CY}_{hkij}$ and $A^{KC}_{ijhk}= A^{CK}_{hkij}$.

3 COMPUTATIONAL HOMOGENIZATION FOR RANDOM COMPOSITES

We study the scale-dependent effective response of heterogeneous random materials described as two–dimensional and two–phase composites, under the assumption that the medium is characterized by statistical homogeneity and mean–ergodicity.

We consider a simplified model made of a base matrix with randomly distributed disk–shaped inclusions of fixed radius $d= 10^{-3}$ $[mm]$ and nominal volume fraction $\rho= 40\%$. Two material cases represented in Figure 2 are considered: (a) stiff inclusions in a soft matrix and (b) soft inclusions in a stiff matrix. For instance, the former case can be considered representative of Metal Ceramic Composites (MCC) materials, while the latter can be considered representative of porous Ceramic Matrix Composites (CMC).

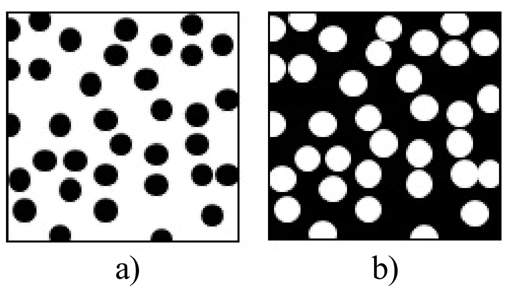

Figure 2: Scheme of material case studies

In the heterogeneous medium both phases are linear elastic and isotropic characterized by the stress–strain relations:

$$\begin{aligned} \sigma_{ij} &= \lambda\varepsilon_{ii}\delta_{ij} + 2\mu\varepsilon_{ij} \\ \beta_{ij} &= 2\mu_c\alpha_{ij} \\ \mu_{3j} &= 2\mu_c l_c^2 k_{3j} \end{aligned} \tag{6}$$

$(i, j= 1{,}2)$ where λ and μ are the Lamé constants, μ_c is the micropolar shear modulus, and l_c is the so–called characteristic length, responsible for the rotational stiffness. The adopted material parameters are reported in Table 1.

Material		Parameters			
		$\lambda[GPa]$	$\mu[GPa]$	$\mu_c[GPa]$	$l_c[mm]$
a	matrix	9.31	21.74	21.74	10^{-5}
	particles	428.5	107.4	107.4	10^{-4}
b	matrix	428.5	107.4	107.4	10^{-4}
	particles	9.31	21.74	21.74	10^{-5}

Table 1: Material parameters.

To determine the components of the homogenenized continuum constitutive tensors and to detect the RVE size, we follow the statistical procedure presented in [18].

Let us introduce a mesoscale window $\mathcal{B}_\delta$ of size L and characterize this by a dimensionless parameter:

$$\delta = \frac{L}{d}\,.$$

For each δ we generate particle distribution by a hard–core Poisson point field (not allowing for disks' overlaps): we determine the number of disks and simulate (uniform) random dispositions of disks' centers; that is the realizations of portions of random medium sampled in a Monte–Carlo sense.

For each realization of $\mathcal{B}_\delta$ we solve Dirichlet and Neumann classical and micropolar Boundary Value Problems (BVPs), consistently with a generalized macrohomogeneity condition which account for the presence of infinitesimal deformation gradients and curvatures:

$$\frac{1}{V}\int_{\mathcal{B}_\delta}(\sigma_{ij}\varepsilon_{ij}+\beta_{ij}\alpha_{ij}+\mu_{ij}\kappa_{ij})dV=\overline{\sigma}_{ij}\overline{\varepsilon}_{ij}+\overline{\beta}_{ij}\overline{\alpha}_{ij}+\overline{\mu}_{ij}\overline{\kappa}_{ij}\,, \tag{7}$$

where V is the volume of $\mathcal{B}_\delta$ and the overlined symbols define homogenized macroscopic measures, with the meaning of volume average quantities. The condition (7), in which the contributions of the classical and micropolar variables are considered separately, establishes a correspondence between the average internal work over a mesoscale window and the mechanical internal work density of the macromodel, expressed in terms of homogenized stress and strain measures.

The Dirichlet boundary conditions (D–BCs) consistent with the condition (7), can be written:

$$u_i=\overline{\varepsilon_{ij}}x_j,\qquad \varphi_i=\frac{1}{2}e_{kji}\overline{\alpha}_{kj}+\overline{\kappa_{ij}}x_j\qquad \text{on }\partial\mathcal{B}_\delta\,. \tag{8}$$

And the Neumann boundary conditions (N–BCs):

$$t_i = (\overline{\sigma}_{ij} + \overline{\beta}_{ij})n_j, \qquad m_i = m_i^o + \overline{\mu}_{ji} n_j \qquad \text{on } \partial\mathcal{B}_\delta\,, \tag{9}$$

where $m_i^o = -\int_{\partial\mathcal{B}} e_{ijl} x_j \overline{\beta}_{kl} n_k$ is the moment imposed to ensure the moment balance in the presence of skew–symmetric shear.

The realizations of $\mathcal{B}_\delta$ and the BVPs solutions are repeated until the confidence interval of the average homogenized constitutive parameters set at 95%, evaluated over a normal standard distribution, is less than a small desired value. Then we increase δ and repeat the previous simulations.

The procedure stops when the number of realizations necessary for ensuring the requirement of the confidence interval is not greater than 5. This means that the values of the homogenized constitutive coefficients are distributed around their average with a vanishing coefficient of variation and that the RVE size (δ_{RVE}) is achieved. The RVE corresponds to the minimum window size at which estimate the homogenized material moduli with a tolerance interval less than 0.5%.

The BVPs are numerically solved using COMSOL Multiphysics®, a finite element code that enables one to directly implement the partial differential equations for the specific problem to investigate. Unstructured meshes of quadratic Lagrangian triangular Finite Elements are adopted.

The homogenized model is generally anisotropic and the constitutive coefficients are those reported in Equation (5). In the following we focus our attention on the most significant components of $(\overline{A}_{ijhk}^{YY})$, $(\overline{A}_{ijhk}^{KK})$ and $(\overline{A}_{ijhk}^{CC})$ and consider the elastic coefficients: $\overline{A}^{YY} = (\overline{A}_{1111} + \overline{A}_{2222})/2$, classical; $\overline{A}^{KK} = \overline{A}_{1212}^{KK}$ and $\overline{A}^{CC} = tr\overline{A}^{CC}$, micropolar.

The mesoscale window $\mathcal{B}_\delta$ ideally corresponds to a portion of the actual random medium in which inclusions are not prevented from intersecting the window edges. Thus, the numerical simulations are performed by taking into account non-homogeneous boundaries (crossing inclusions). We also consider the less realistic case of homogeneous boundaries (non–crossing inclusions). The comparison between the homogenized responses obtained by performing numerical simulations for the two cases, either applying Dirichlet and Neumann boundary conditions, allows us to emphasize the influence of positions of the inclusions with respect to the window's boundary.

Figure 3 reports the average of the classical coefficient $\overline{A}^{YY}$ versus the scale parameter δ, for both materials (a) and (b). This value is normalized to the average of the convergence coefficient evaluated in the case of crossing inclusions, $\overline{A}_{RVE}^{YY}$. It can be noticed the convergence trend in the case of inclusions that cross or do not cross the window boundary. In particular, for the material (a) δ_{RVE} is equal to 20 in the case of crossing inclusions, while it is $\delta_{RVE} = 25$ in the case of non–crossing inclusions. The material (b) shows a slower convergence trend. Accordingly, the RVE is attained for $\delta_{RVE} = 25$ in the case of crossing inclusions, while in the case of non–crossing inclusions $\delta_{RVE} > 25$.

Figure 4 reports the micropolar results in terms of the average of the coefficient $\overline{A}^{KK}$ (normalized to the average convergence value $< \overline{A}^{KK}_{RVE} >$) versus the scale parameter δ, always for both materials (a) and (b). The two materials exhibit convergence trends similar to the coefficient $\overline{A}^{YY}$. It can be also referred that $\overline{A}^{KK}_{RVE}$ does not vanish as δ increases, pointing out that this micropolar moduli is significant also in the presence of inclusions of small size.

Figure 5 shows the micropolar results in terms of the average of the homogenized characteristic length parameter $\overline{l}_c = \sqrt{\overline{A}^{CC}/\overline{A}^{KK}}$ (normalized to the average convergence value $< \overline{l}_{cRVE} >$) versus the scale parameter δ. Both materials exhibit differences between the curves obtained in the case of crossing and non–crossing inclusions greater than in the classical case. For the material (a) the RVE is attained at $\delta_{RVE} = 15$ in the case of crossing inclusions and at $\delta_{RVE} = 20$ in the case of non–crossing inclusions. For the material (b) the RVE is attained at $\delta_{RVE} = 20$ in the case of crossing inclusions and at $\delta_{RVE} = 25$ in the case of non–crossing inclusions. In can be referred moreover, that for both materials $< \overline{l}_c >$, when δ increases, tends to the value of the characteristic length l_c of the matrix: material (a) $< l_{cRVE} >= 0.1$); material (b) $< l_{cRVE} >= 1$. This shows micropolar bending effects weaker in the medium (a) than in the medium (b). These findings are in agreement with some experimental and analytical results [7, 8].

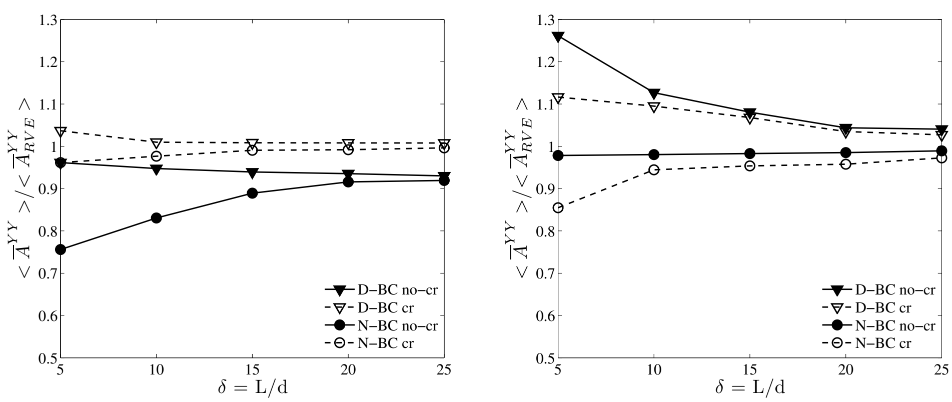

Figure 3: Effective average classical constitutive parameters $< \overline{A}^{YY} >$ (normalized to $< \overline{A}^{YY}_{RVE} >$) versus the scale parameter δ. Material (a) (left side); material (b) (right side). D–BC (Dirichlet BC), N–BC (Neumann BC), cr (crossing inclusions), n–cr (non crossing inclusions).

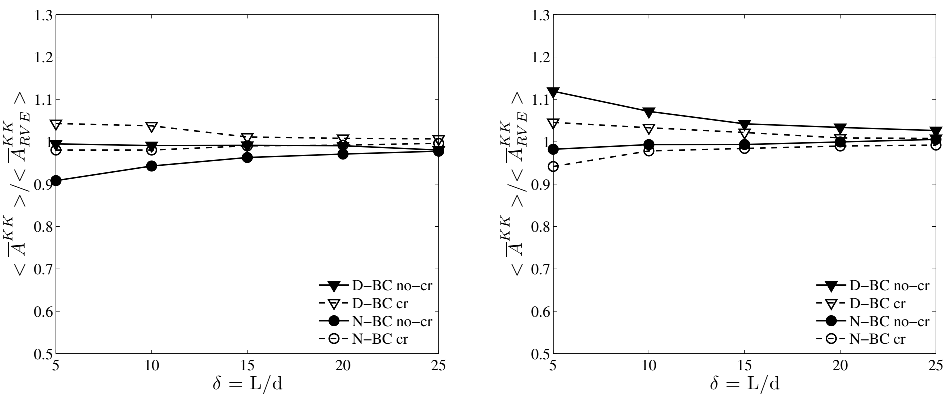

Figure 4: Effective average micropolar constitutive parameters $< \overline{A}^{KK} >$ (normalized to $< \overline{A}^{KK}_{RVE} >$) versus the scale parameter δ. Material (a) (left side); material (b) (right side). D–BC (Dirichlet BC), N–BC (Neumann BC), cr (crossing inclusions), n–cr (non crossing inclusions).

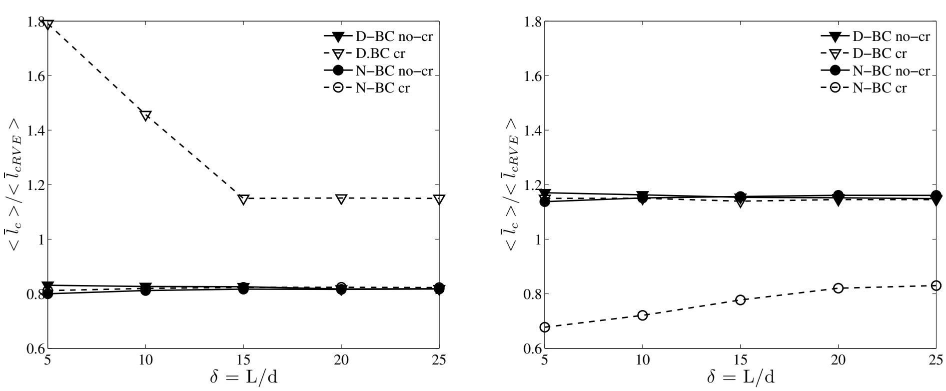

Figure 5: Effective average micropolar constitutive parameters $< \bar{l}_c > = < \sqrt{\overline{A}^{CC} / \overline{A}^{KK}} >$ (normalized to $< \bar{l}_{cRVE} >$) versus the scale parameter δ. Material (a) (left side); material (b) (right side).

D–BC (Dirichlet BC), N–BC (Neumann BC), cr (crossing inclusions), n–cr (non crossing inclusions).

4 FINAL REMARKS

In this work we study the scale–dependent homogenization of composite materials made of random distribution of inclusions in a matrix. Two sample cases are studied: (a) stiff inclusions embedded in a soft matrix; and (b) soft inclusions in a stiff matrix. For the numerical simulations we consider two cases: windows with inclusions intersecting the edges and windows with inclusions which do not intersect the edges (homogeneous boundary). The simulations in the two cases yield different convergence trends and values, both for the classical and mainly for the micropolar constitutive coefficients. These results indicates that the true random case of heterogeneous boundary should be accounted for in the homogenization processes.

The RVE size obtained in the micropolar material is smaller than the RVE size of a classical material. Moreover, the curvature effects show to be less significant in the case of material (a), with inclusions stiffer than matrix, than in the case of material (b), with inclusions softer than the matrix. Nevertheless, the elastic moduli relating the relative rotation to the skew–symmetric part of the shear stress, never vanishes as the window size increases. This entails that the micropolar effects cannot be neglected in the presence of non–symmetric strain and shear effects. Like in the in the widely investigated case of anisotropic periodic materials [13, 19]. Further confirmations of the suitability of micropolar model are expected with the investigation of media with particles of different shapes and also with the investigation of non–linear constitutive behaviour.

ACKNOWLEDGMENTS
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