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MULTISCALE ANALYSIS OF MATERIALS WITH ANISOTROPIC MICROSTRUCTURE AS MICROPOLAR CONTINUA

Nicholas Fantuzzi[1] **and Patrizia Trovalusci**[2]

[1]DICAM Department, University of Bologna, Italy
Viale del Risorgimento 2, 40136, Bologna, Italy
e-mail: nicholas.fantuzzi@unibo.it

[2] DISG Department, Sapienza University of Rome, Italy
Via Gramsci 53, 00197, Rome, Italy
e-mail: patrizia.trovalusci@uniroma1.it

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Abstract. *Multiscale procedures are often adopted for the continuum modeling of materials composed of a specific micro-structure. Generally, in mechanics of materials only two-scales are linked. In this work the original (fine) micro-scale description, thought as a composite material made of matrix and fibers/particles/crystals which can interact among them, and a scale-dependent continuum (coarse) macro-scale are linked via an energy equivalence criterion. In particular the multiscale strategy is proposed for deriving the constitutive relations of anisotropic composites with periodic microstructure and allows us to reduce the typically high computational cost of fully microscopic numerical analyses. At the microscopic level the material is described as a lattice system while at the macroscopic level the continuum is a micropolar continuum, whose material particles are endowed with orientation besides position. The derived constitutive relations account for shape, texture and orientation of inclusions as well as internal scale parameters, which account for size effects even in the elastic regime in the presence of geometrical and/or load singularities. Applications of this procedure concern polycrystals, wherein an important descriptor of the underlying microstructure gives the orientation of the crystal lattice of each grain, fiber reinforced composites, as well as masonry-like materials. In order to investigate the effects of micropolar constants in the presence of material non central symmetries, some numerical finite element simulations, with elements specifically formulated for micropolar media, are presented. The performed simulations, which extend several parametric analyses earlier performed [1], involve two-dimensional media, in the linear framework, subjected to compression loads distributed in a small portion of the medium.*

1 INTRODUCTION

The classical Cauchy theory of elasticity is not always suitable when solids with microstructure are taken into consideration, in particular when the microstructural length scale is compatible to the macroscopic one (e.g. [2]). In the presence of material heterogenities, discrete approaches have been often utilized when periodic micro-structure is present [3, 4, 5, 6]. These approaches due to their mathematical complexity exploit numerical methods that often involve high computational effort. An alternative way of modelling complex materials with microstructure is to consider generalized continua [7, 8, 9] that, when derived on the basis of homogenization procedures, provide accurate material description accounting for the size of heterogeneities as well as dispersion properties in wave propagation [2].Within this framework, the micropolar theory, including the constrained case of couple-stress theory, [10, 11, 12], supported by the experimental work by Lakes and co-workers [13, 14, 15, 16, 17], has been widely adopted over years and proves effective in several material applications [2, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27].

In the present work the mechanical behavior of panels, described as anisotropic micropolar two-dimensional continua, under loads distributed on a small portion of the boundary is presented, focusing on classical and micro-polar quantities coupled at the constitutive level. Different levels of coupling are considered according to the ratio between the correspondent elastic properties.

The numerical solution is obtained using an in-house finite element implementation with quadratic interpolation functions for the displacements and linear ones for the micro-rotations. In this way, strains result of the same order in the numerical solution. Results are given in graphical form as contour plots of vertical displacements, stresses and relative rotation. This latter is a strain measure, related to the skew part of the strain, peculiar of the micropolar model, suitable to well represent the anisotropic material response. [1].

2 ANISOTROPIC THEORY OF MICROPOLAR ELASTICITY

The micropolar continuum is a well-known model equipped by theoretical, numerical and experimental studies in the literature [10, 11, 12, 15, 16, 17, 18, 19, 20]. This continuum is made of particles which can displace and rotate at the same time so the kinematics of the continuum is non-classical. Reducing the description to two-dimensional (2D) media, kinematics is described by displacements components, u_1, u_2 (macro-displacements), and rotation, ϕ_3 (micro-rotation). Hence, each material particle in the 2D frame has 3 degrees of freedom. The local linearized kinematic compatibility relations take the form

$$\varepsilon_{11} = u_{1,1}, \quad \varepsilon_{22} = u_{2,2}, \quad \varepsilon_{12} = u_{1,2} + \phi_3, \quad \varepsilon_{21} = u_{2,1} - \phi_3, \quad \chi_{31} = \phi_{3,1}, \quad \chi_{32} = \phi_{3,2} \tag{1}$$

where ε_{ij} $(i, j = 1, 2)$ indicate the components of the strain tensor, while χ_{31}, χ_{32} indicate the only independent components of the curvature tensor. Comma notation has been used here for the partial derivative with respect to x_1 and x_2. The term $\theta = (u_{2,1} - u_{1,2})/2$ is the local rigid rotation (macro-rotation). Interaction among particles is described by stresses and micro-couples as

$$t_i = \sigma_{ij} n_j, \quad m_3 = \mu_{3j} n_j \tag{2}$$

where σ_{ij} and μ_{3j} are the components of the non-symmetric stress and couple-stress tensors, respectively. Equilibrium equations can be carried out in case body micro-couple forces are neglected (body forces b_i are present)

$$\sigma_{ij,j} + b_i = 0, \quad \mu_{3j,j} - e_{ij3}\sigma_{ij} = 0 \tag{3}$$

Linearly anisotropic stress-strain relations of the micropolar two-dimensional continuum assume the following matrix form

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ \sigma_{21} \\ \mu_{31} \\ \mu_{32} \end{Bmatrix} = \begin{bmatrix} A_{1111} & A_{1122} & A_{1112} & A_{1121} & B_{1131} & B_{1132} \\ A_{2211} & A_{2222} & A_{2212} & A_{2221} & B_{2231} & B_{2232} \\ A_{1211} & A_{1222} & A_{1212} & A_{1221} & B_{1231} & B_{1232} \\ A_{2111} & A_{2122} & A_{2112} & A_{2121} & B_{2131} & B_{2132} \\ B_{1131} & B_{2231} & B_{1231} & B_{2131} & D_{3131} & D_{3132} \\ B_{1132} & B_{2232} & B_{1232} & B_{2132} & D_{3231} & D_{3232} \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{12} \\ \varepsilon_{21} \\ \chi_{31} \\ \chi_{32} \end{Bmatrix} \tag{4}$$

where A_{ijhk}, B_{ij3k}, D_{3j3k}, $(i,j,h,k=1,2)$ are the constitutive components that for hyperelastic materials have the major symmetries.

3 FINITE ELEMENT FORMULATION

The two-dimensional (2D) problem of micropolar continua is solved through a finite element implementation wherein stress and strain vectors are defined as

$$\begin{aligned} \{\sigma\} = \begin{Bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{12} & \sigma_{21} \end{Bmatrix}^T, \{\mu\} = \begin{Bmatrix} \mu_{31} & \mu_{32} \end{Bmatrix}^T \\ \{\varepsilon\} = \begin{Bmatrix} \varepsilon_{11} & \varepsilon_{22} & \varepsilon_{12} & \varepsilon_{21} \end{Bmatrix}^T, \{\chi\} = \begin{Bmatrix} \chi_{31} & \chi_{32} \end{Bmatrix}^T \end{aligned} \tag{5}$$

The 2D weak form of the present problem has to be formulated in order to carry out the finite element implementation. Once displacement vectors are identified as

$$\{u\} = \begin{Bmatrix} u_1 & u_2 \end{Bmatrix}^T, \phi = \phi_3 \tag{6}$$

where the latter is a scalar quantity because only one rotation is present in 2D frame. The principle of virtual work reads

$$\int_\Omega \Big(\{\sigma\}\{\delta\varepsilon\}^T + \{\mu\}\{\delta\chi\}^T \Big) d\Omega = \int_\Omega \{b\}\{\delta u\}^T d\Omega + \int_\Gamma \Big(\{t\}\{\delta u\}^T + m\,\delta\phi \Big) d\Gamma \tag{7}$$

with δ denoting the variation operator, $\{b\}$ the body force vector, $\{t\}$ and $\{m\}$ the traction and couple-traction vectors applied on the boundary Γ. Note that, the curvature vector $\{\chi\}$ is due to the first-order partial derivatives of the micro-rotation, thus C^0 finite elements are adopted. Finite element approximation though interpolation functions $[N_u]$ and $[N_\phi]$ is given by

$$\{u\} = [N_u]\{u^e\}, \quad \phi = [N_\phi]\{\phi^e\} \tag{8}$$

where the apex ^{e} indicates nodal parameters of the correspondent vectors. Quadratic interpolation functions for the displacements and linear ones for the rotations. Thus, displacements are modelled with eight nodes, whereas micro-rotation are related to the four corner nodes. Interpolation function vectors are given in matrix form as

$$[N_u] = \begin{bmatrix} N_{u1} & N_{u2} & \dots & N_{u8} & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & N_{u1} & N_{u2} & \dots & N_{u8} \end{bmatrix}, \quad [N_\phi] = \begin{bmatrix} N_{\phi1} & N_{\phi2} & \dots & N_{\phi4} \end{bmatrix} \tag{9}$$

Thus, the micropolar strains given by Eq. (1) can be written in matrix form as

$$\{\varepsilon\} = [D_u]\{u\} + [D_\phi]\,\phi, \quad \{\chi\} = [\hat{D}_\phi]\,\phi \tag{10}$$

where the operators $[D_u]$ and $[D_\phi]$ are defined as

$$[D_u] = \begin{bmatrix} \partial_1 & 0 \\ 0 & \partial_2 \\ \partial_2 & 0 \\ 0 & \partial_1 \end{bmatrix}, \quad [D_\phi] = \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \quad [\hat{D}_\phi] = \begin{bmatrix} \partial_1 \\ \partial_2 \end{bmatrix} \tag{11}$$

where ∂_i, for $i = 1, 2$ represents the partial derivative with respect to x_1 or x_2. By including the finite element approximation (9) into the linear strains definitions (10) the following is carried out

$$\begin{aligned} \{\varepsilon\} = [D_u][N_u]\{u^e\} + [D_\phi][N_\phi]\{\phi^e\} = \big[[D_u][N_u] \quad [D_\phi][N_\phi]\big] \begin{Bmatrix} \{u^e\} \\ \{\phi^e\} \end{Bmatrix} = [B_\varepsilon]\{d^e\} \\ \{\chi\} = [\hat{D}_\phi][N_\phi]\{\phi^e\} = \big[[0] \quad [\hat{D}_\phi][N_\phi]\big] \begin{Bmatrix} \{u^e\} \\ \{\phi^e\} \end{Bmatrix} = [B_\chi]\{d^e\} \end{aligned} \tag{12}$$

where $\{d^e\}$ indicates the unknown vector of nodal displacements. The matrices $[B_\varepsilon]$ and $[B_\chi]$ collect the derivatives of the interpolation functions. Therefore, the constitutive relations (4) become

$$\{\sigma\} = ([D_{\varepsilon\varepsilon}][B_\varepsilon] + [D_{\varepsilon\chi}][B_\chi])\,\{d^e\}, \quad \{\mu\} = \big([D_{\varepsilon\chi}]^T[B_\varepsilon] + [D_{\chi\chi}][B_\chi]\big)\,\{d^e\} \tag{13}$$

where

$$\begin{aligned} [D_{\varepsilon\varepsilon}] = \begin{bmatrix} A_{1111} & A_{1122} & A_{1112} & A_{1121} \\ A_{2211} & A_{2222} & A_{2212} & A_{2221} \\ A_{1211} & A_{1222} & A_{1212} & A_{1221} \\ A_{2111} & A_{2122} & A_{2112} & A_{2121} \end{bmatrix}, \\ [D_{\chi\chi}] = \begin{bmatrix} D_{3131} & D_{3132} \\ D_{3231} & D_{3232} \end{bmatrix}, \; B_{\varepsilon\chi} = \begin{bmatrix} B_{1131} & B_{1132} \\ B_{2231} & B_{2232} \\ B_{1231} & B_{1232} \\ B_{2131} & B_{2132} \end{bmatrix} \end{aligned} \tag{14}$$

Finally, the algebraic finite element problem (without body actions) reads

$$\begin{aligned} \int_\Omega \Big([B_\varepsilon]^T[D_{\varepsilon\varepsilon}][B_\varepsilon] + [B_\varepsilon]^T[D_{\varepsilon\chi}][B_\chi] + [B_\chi]^T[D_{\varepsilon\chi}]^T[B_\varepsilon] + \\ [B_\chi]^T[D_{\chi\chi}][B_\chi] \Big) d\Omega\,\{d^e\} = \int_\Gamma \begin{bmatrix} [N_u]^T\{\bar{t}\} \\ [N_\phi]^T\{\bar{m}\} \end{bmatrix} d\Gamma \end{aligned} \tag{15}$$

where the stiffness matrix and force vector are respectively defined as

$$\begin{aligned} [K] = \int_\Omega \Big([B_\varepsilon]^T[D_{\varepsilon\varepsilon}][B_\varepsilon] + [B_\varepsilon]^T[D_{\varepsilon\chi}][B_\chi] \\ + [B_\chi]^T[D_{\varepsilon\chi}]^T[B_\varepsilon] + [B_\chi]^T[D_{\chi\chi}][B_\chi] \Big) d\Omega \end{aligned} \tag{16}$$

$$\{f\} = \int_\Gamma \begin{bmatrix} [N_u]^T\{\bar{t}\} \\ [N_\phi]^T\{\bar{m}\} \end{bmatrix} d\Gamma \tag{17}$$

A classical Gauss-Legendre full integration is considered for computing the integral terms appearing in Eq. (15). The present FE model passes the tests provided in [28] and has been implemented in MATLAB© environment.

4 NUMERICAL APPLICATIONS

This paper aims to investigate the mechanical behavior of 2D Cosserat solids when coupling effects between classical and micropolar components are present in the constitutive model. The material constants are determined using an homogenization procedure, considering at the micro-level anisotropic discrete assemblies, with particular reference to non-centrosymmetric materials. The basic configuration for the submatrix $[D_{\varepsilon\varepsilon}]$ (Eq. 14) is the orthotropic one without Poisson effect as listed in Table 1 .

A parametric study is presented in order to point out the physical meaning of some elastic coupling constants between classical and micropolar stresses/strains in the presence of non central material symmetries.

A_{1111}	$3.75 \cdot 10^{10}$ Pa	D_{11}	$1.125 \cdot 10^{6}$ N
A_{2222}	$1.5 \cdot 10^{10}$ Pa	D_{22}	$0.3750 \cdot 10^{6}$ N
A_{1212}	$0.75 \cdot 10^{10}$ Pa		
A_{2121}	$3.00 \cdot 10^{10}$ Pa		

Table 1: Material properties for all configurations.

Two configurations are taken into account.

Configuration 1 considers the coupling between normal stresses σ_{11}, σ_{22} and curvatures χ_{31}, χ_{32} respectively. At the same time, due to hyperelasticity, coupling is set between micro-couples μ_{31}, μ_{32} and normal strains ε_{11}, ε_{22}. The constitutive elastic coefficients responsible of the coupling are B_{1131} and B_{2232}. They take values according to the following relations

$$B_{1131} = c_1 \frac{A_{1111}}{D_{3131}} = c_1 3.33 \cdot 10^4, \quad B_{2232} = c_1 \frac{A_{2222}}{D_{3232}} = c_1 4.00 \cdot 10^4 \tag{18}$$

where $c_1 = 1,\ 10^2,\ 10^4$ and 10^6. It has been observed by previous studies [1] and also confirmed by classical material configurations such as classical isotropic or orthotropic materials that elastic constants on the main diagonal are generally predominant, with respect to the out-of-diagonal terms.

Configuration 2 considers the coupling between shear stresses σ_{12}, σ_{21} and curvatures χ_{31}, χ_{32}, respectively. At the same time, due to hyperelasticity, coupling is set between micro-couples μ_{31}, μ_{32} and shear strains ε_{12}, ε_{21}, respectively. The constitutive elastic coefficients responsible of the coupling are B_{1231} and B_{2132}. They take values according to the following relations

$$B_{1132} = c_2 \frac{A_{1111}}{D_{3232}} = c_2 1.00 \cdot 10^5, \quad B_{2132} = c_2 \frac{A_{2222}}{D_{3131}} = c_2 1.33 \cdot 10^4 \tag{19}$$

where $c_2 = c_1$ take the same values as above.

All the other unmentioned coefficients of the matrices in Eq. (14) are considered null.

The geometry of the present problem is a square domain of width $L = 4$ m, fixed at the bottom edge and subjected to a top load acting on length size $a/L = 0.25$ (Figure 1a) and pressure $q = 10$ MPa. The two configurations illustrated above are considered in the simulations.

Due to the symmetry of the problem only half of the domain is numerically studied and the correspondent finite element mesh is depicted in Figure 1b.

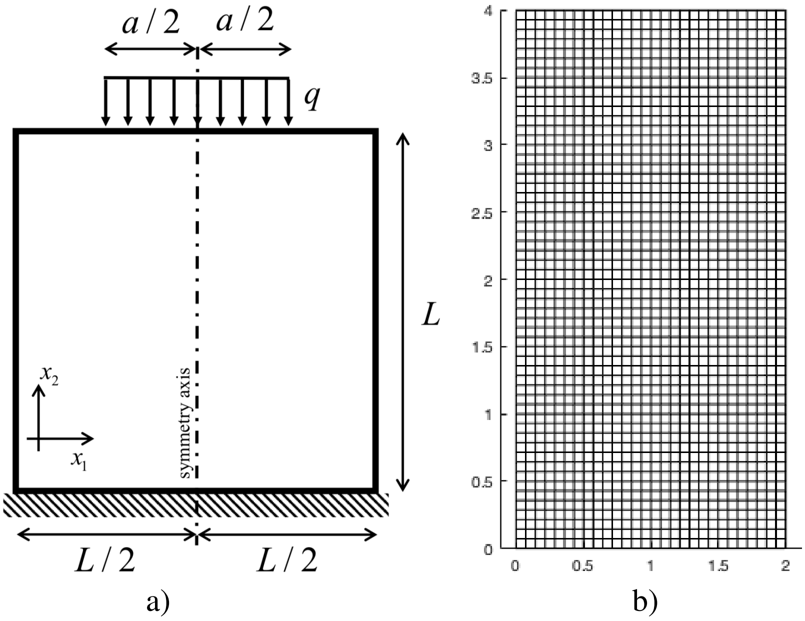

Figure 1: a) Structural scheme considered in the numerical applications, b) mesh considered in the computations.

The aim is to show the capability of the micropolar model to retain memory of the original composite behavior under the action of a load applied on a limited portion of the boundary of the body, as well as to numerically investigate the related mechanism of strain/stress diffusion according to the constitutive relations considered. Simulations underline the coupling effect of classical and micro-polar stresses/strain in the presence of non-centrosymmetric material symmetries under concentrated pressures.

Figures 2-4 represent the contour lines of the vertical displacement, u_2, the vertical stress, σ_{22}, and relative rotation, $\frac{1}{2}(u_{1,2} - u_{2,1}) - \phi$, for Configuration 1 in which the coupling occurs between normal stresses and the correspondent micro-couples and between curvatures and normal strains. Figures are placed so that the coupling effect, c_1 increases from left to right. So the first figure has $c_1 = 1$ and the last on the right side has $c_1 = 10^6$.

As expected by increasing c_1 the micropolar effect increases. In fact, the vertical displacement decreases evidently and there is a strong vertical stress redistribution which deviates from the vertical pattern shown for low values of c_1. Note that relative rotation changes sign from a positive value for $c_1 = 1$ to a negative one $c_1 = 10^6$ in the area below the applied load.

Figures 5-7 show the results obtained for Configuration 2, which considers the coupling between shear stresses and curvatures and at the same time between micro-couples and shear strains.

The same variation in terms of $c_2 = c_1$ is considered here. Vertical displacement u_2 is more distributed by increasing the micropolar effect through c_2; the displacement field within the solid changes strongly its patterns and the vertical displacement tends to be linearly uniform with along the wall height. Similar behavior occurs for the vertical stress σ_{22} which tends to be uniform (since the vertical displacement is becoming linear) in almost all the wall expect in the area close to the applied pressure where a strong relative rotation is measured and this demonstrate the high micro-polarity coupling effect of this medium. Once again relative rotation changes its sign by increasing c_2.

The first three sub-plots in all given figures (Figures 2-7) seems to be very similar while the fourth shows a relevant change because the coupling terms in all numerical simulations are defined as a function of c_1 and c_2 (where $c_1 = c_2$) which multiply the ratio between A_{iiii} and D_{ii}. It is observed that, due to the chosen values of the coefficients A_{ijkl} and D_{ij} such coupling terms become relevant only for large values of c_1.

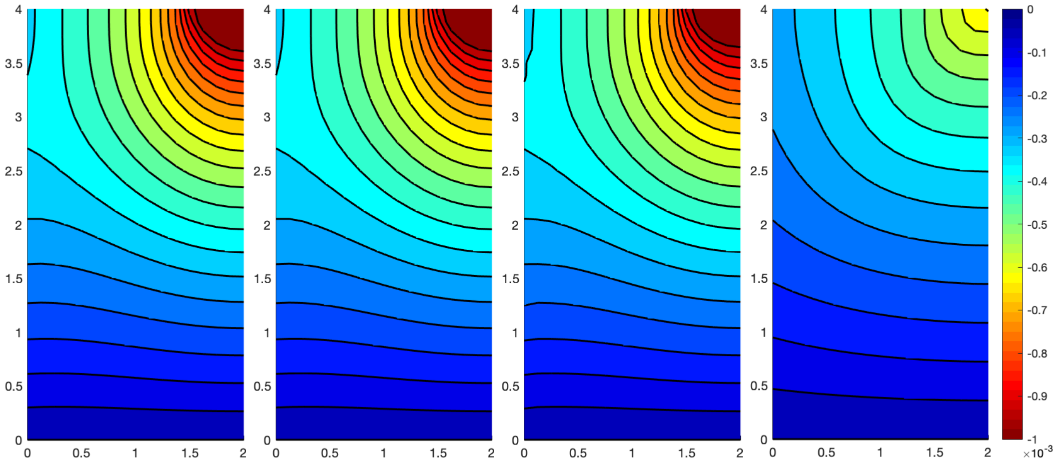

Figure 2: Configuration 1. $B_{1131} = c_1 \frac{A_{1111}}{D_{3131}}$, $B_{2232} = c_1 \frac{A_{2222}}{D_{3232}}$, $c_1 = 1$, 10^2, 10^4 and 10^6 increases from left to right. Vertical displacement field u_2.

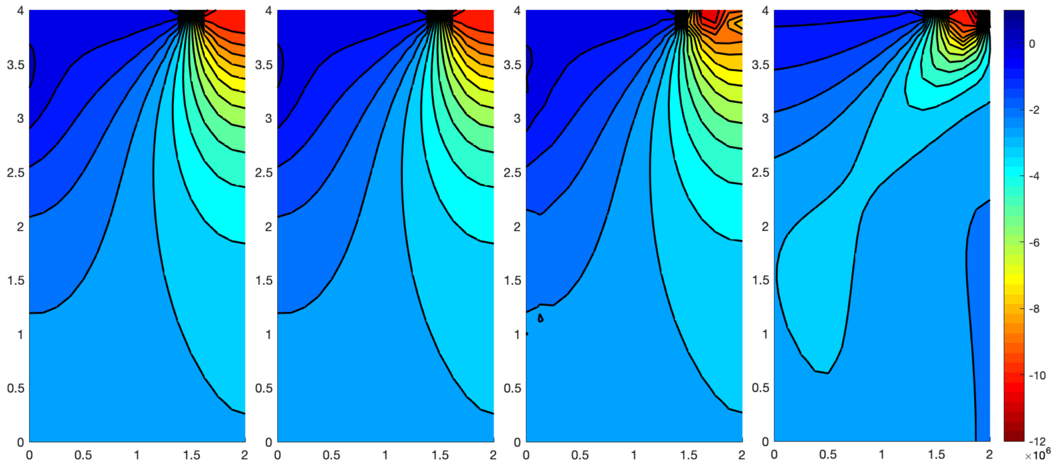

Figure 3: Configuration 1. $B_{1131} = c_1 \frac{A_{1111}}{D_{3131}}$, $B_{2232} = c_1 \frac{A_{2222}}{D_{3232}}$, $c_1 = 1$, 10^2, 10^4 and 10^6 increases from left to right. Vertical stress field σ_{22}.

5 CONCLUSIONS

This work addresses a numerical finite element solution of an anisotropic, non-centrosymmetric, micropolar panel subjected to a force acting on a small portion at the top of the given domain. Two coupling effects are discussed. The first regards the effect between normal stresses σ_{11}, σ_{22} and curvatures and χ_{31}, χ_{32} and, due to hyperelasticity, micro-couples μ_{31}, μ_{32} and, normal strains ε_{11}, ε_{22}. The second one is between shear stresses σ_{12}, σ_{21} and curvatures χ_{31}, χ_{32} and, due to hyperelasticity, micro-couples μ_{31}, μ_{32} and shear strains ε_{12}, ε_{21}.

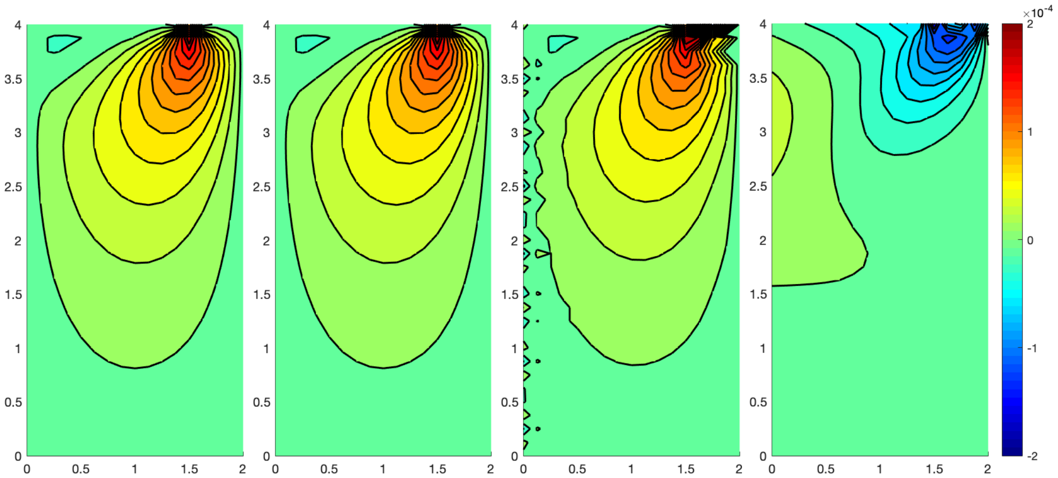

Figure 4: Configuration 1. $B_{1131} = c_1 \frac{A_{1111}}{D_{3131}}$, $B_{2232} = c_1 \frac{A_{2222}}{D_{3232}}$, $c_1 = 1$, 10^2, 10^4 and 10^6 increases from left to right. Relative rotation field $\frac{1}{2}(u_{1,2} - u_{2,1}) - \phi$.

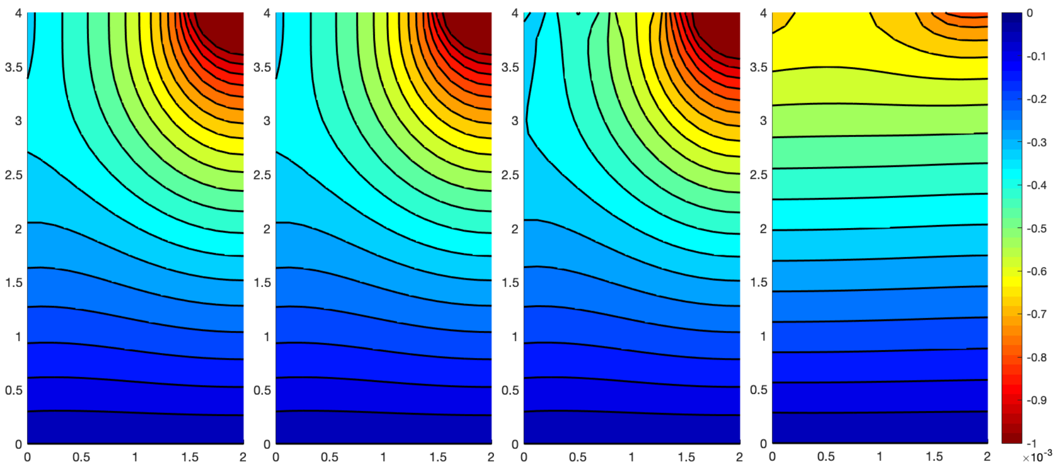

Figure 5: Configuration 2. $B_{1132} = c_2 \frac{A_{1111}}{D_{3232}}$, $B_{2132} = c_2 \frac{A_{2222}}{D_{3131}}$. Vertical displacement field u_2.

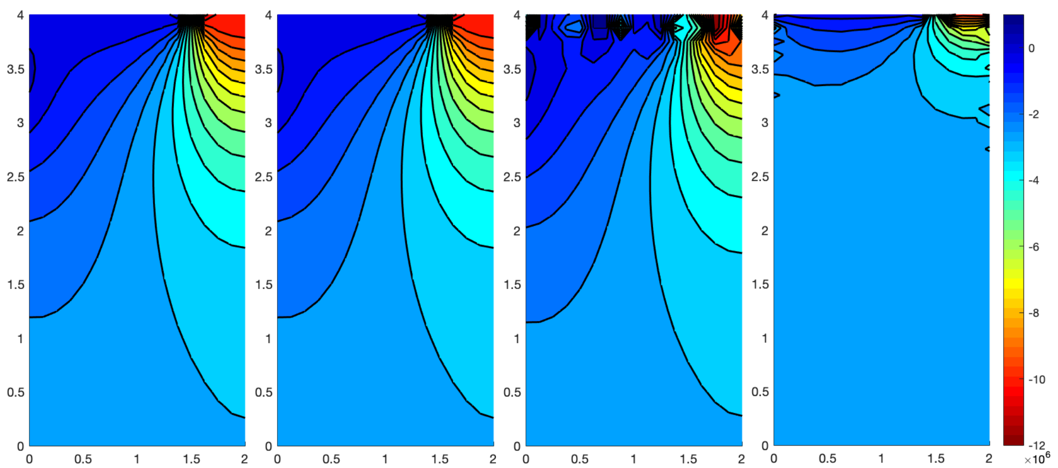

Figure 6: Configuration 2. $B_{1132} = c_2 \frac{A_{1111}}{D_{3232}}$, $B_{2132} = c_2 \frac{A_{2222}}{D_{3131}}$. Vertical stress field σ_{22}.

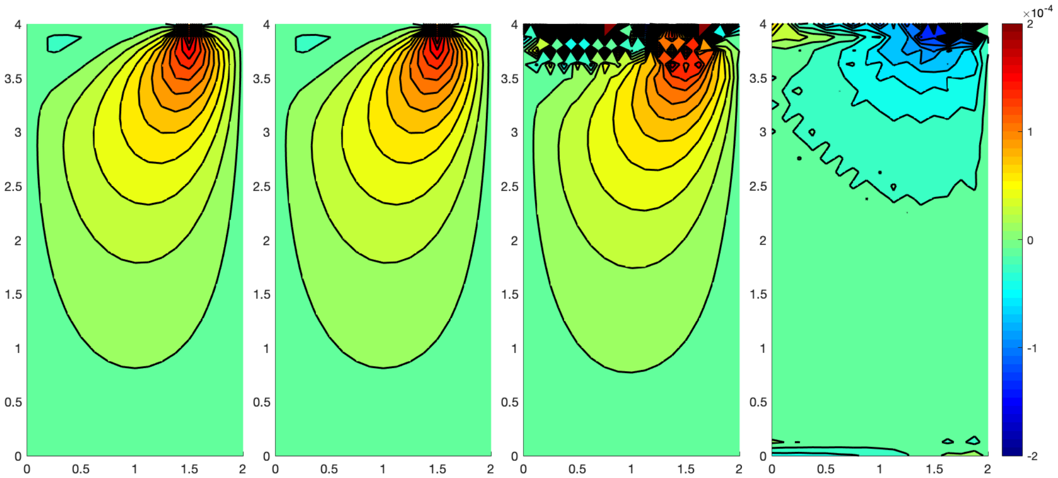

Figure 7: Configuration 2. $B_{1132} = c_2 \frac{A_{1111}}{D_{3232}}$, $B_{2132} = c_2 \frac{A_{2222}}{D_{3131}}$. Relative rotation field $\frac{1}{2}(u_{1,2} - u_{2,1}) - \phi$

Emphasis has been given to the strain measure of the relative rotation $\theta - \omega$ which is a peculiar character of micro-polar models [2, 25]. Numerical simulations proved that coupling coefficients strongly change the behavior of orthotropic micro-polar solids.

6 ACKNOWLEDGMENTS

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