# MULTISCALE HOMOGENIZATION AND ANALYSIS OF ANISOTROPIC ASSEMBLIES AS COSSERAT CONTINUA

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This work proposes a multiscale analysis of nanocomposites made of hexagonal assemblies. The present nanomaterial is made of irregular concave hexagonal shaped assemblies interacting with elastic interfaces. The homogenization of such irregular units results to have anisotropic constitutive properties by applying a homogenization method. The validity of the present homogenization and modeling is verified by comparing the continuum Cosserat model with a discrete model made of physical particles and elastic interfaces. Parametric investigation is also proposed by varying the geometric properties of the nanoparticles by showing the dynamic character of these materials by considering both Cosserat and Cauchy continuum models.

**KEY WORDS:** cosserat continua, anisotropic media, relative rotation, composites/masonry, finite element method

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### 1 1. INTRODUCTION

It is well known that multiscale methods have been introduced when continuum mechanics was developed. Since 2 mechanical properties introduced in the latter should have been determined for the solution of the formulated mathe-3 matical problem. The most compelling multiscale approaches are the ones that provide macroscale relations by taking 4 into consideration the underlying microscale. This connection is often provided by equivalence criteria (Trovalusci, 5 2014). Since originally elastic continua were modeled as interaction of particles/molecules depending on their mutual 6 distance, an approach based on mechanics was able to predict the macroscopic constitutive behavior using micro-7 scopic laws for systems of particles/molecules (also known as central-force scheme). The latter provided the basis of 8 the well-known Cauchy model of the elastic body where all particles/molecules are in contact in pairs. 9

The original definition provided by Cauchy has been extended by Voigt by introducing a continuum made of ori-10 ented rigid particles that interact among forces and couples. He was able to demonstrate that Navier-Cauchy molecular 11 theory was not correct due to the assumption of a central-force scheme, since orientation of the particles was not taken 12 into consideration (Trovalusci, 2014). The one that was able to overcome the limitations of molecular approaches in 13 elasticity was Poincaré (Trovalusci, 2014). Poincaré proposed a lattice model described by potential energy function 14 of point-like molecules which were able not only to interact in pairs, but also to give a multibody potential description 15 (Mariano and Trovalusci, 1999). It should be underlined that molecular mechanical theories were based on the discrete 16 nature of matter. The same was applied also in thermodynamics (Cimmelli et al., 2013; Li and Ostoja-Starzewski, 17 2011; Makowski and Stumpf, 2001)), electromagnetics and quantum mechanics too (Blanc et al., 2002; Curtin and 18 Miller, 2003). 19

As aforementioned, the mechanical properties of materials need a microstructure description in order to be accurately predicted and carried out by homogenization procedures (Budiansky, 1965; Nemat-Nasser et al., 1996). In particular, several length scales are often required, thus, discrete-continuous approaches are encountering a renewal. It is worth to mention that coarse–graining homogenizations exploit an explicit link between the fine and coarse scales, moreover, they keep memory of the microstructural origin of deformation mechanisms which is especially needed in novel custom-made materials (Sadowski et al., 2014).

Homogeneous deformations are considered in both Voigt's and Poincaré's models (in other words local actions are considered) and local angular potential are added to the local actions. At this stage, if no other constraint is applied the homogenized continua would exhibit its dependency on material length scales (Maugin, 2016). These models can be termed as 'implicit' non–local continua as described by Mindlin (1964) and Trovalusci (2014). On the contrary if not homogeneous deformations are taken into account the equivalent continua would be classified as 'explicit' non-local media such as by Eringen (1972) and Tuna et al. (2019). The aforementioned approach of Voigt related to
coarse-graining approach can be used in several composite material configurations such as fiber-reinforced materials,
microcracked solids (Greco et al., 2016a; Jain and Ghosh, 2009; Nguyen et al., 2012), voids and gaps (Pingaro et al.,
2019a) and dilatant materials (Shi et al., 2021). De Borst (1991) and Sluys et al. (1993) showed the advantages of
materials with microstructure when localization and discontinuities are introduced in the continuum.

As it has been demonstrated also by Kunin (2012), the description of materials with an internal microstructure 6 (e.g. materials made of constituents of significant size) must consider nonlocal modelling. The latter (also known as 7 microcontinua or complex continua as shown by Sadowski and Trovalusci (2014)) defines any continuum that keeps 8 memory of the internal microstructure by means of internal material lengths which often represent the distance be-9 tween particles in a lattice, grain or cell size, etc. as also discussed by Shaat et al. (2020). Nonlocal continua are known 10 to have dispersion properties which represent a dependency between wave-velocities and wave-length/frequency 11 (Cermelli and Pastrone, 2001; Kumar et al., 2008; Mondal et al., 2021; Oliveri and Speciale, 2008). Classical contin-12 uum modelling (also known as Grade 1 (Trovalusci, 2014) do not have the aforementioned properties. 13

It is noted that 'implicit' (weak) and 'explicit' (strong) nonlocal models both include internal length parameters in their mathematical formulation and their equations show dispersion properties (Eringen, 1983; Kröner, 1963)) and more recently by (Tuna et al., 2020; Tuna and Trovalusci, 2020). All these models are described by an extended virtual power framework, with classical and non-classical primary variables coupled with dual standard and/or non–standard fields (Trovalusci, 2014).

Explicit nonlocal models are higher grade theories where the equations of motions contain derivatives in space 19 or time of the standard primal field (macrovelocity) of order different than the second as in the works by Bassani 20 et al. (2001); De Borst and Mühlhaus (1992); Mühlhaus and Aifantis (1991); Needleman (1988) among others. In this 21 regard, it is worth to cite also the contributions by Bažant et al. (1984); Pijaudier-Cabot and Bazant (1987). Regarding 22 the other set of equations of motion that contain non-standard primal fields can be divided into two further classes. 23 Firstly, the ones that can be derived from the standard frame invariance axioms, as in the classical case (Green and 24 Rivlin, 1997; Podio-Guidugli and Vianello, 2010). Secondly, additional degrees of freedom are considered which 25 contain non standard primal fields and – eventually – their derivatives. The latter set of equations are derived using a 26 different axiomatic framework as discussed by Gurtin and Podio-Guidugli (1992); Yavari and Marsden (2009) 27

The modern concept of material theories with additional degrees of freedom has been provided in the 50s by Ericksen and Truesdell (1957); Mindlin (2021), however, the seminal work by Mindlin (1964) shed the light on continua with additional degrees of freedom which were able to keep memory of the material microstructure. In order to provide such information microstructure is identified by a unit cell (also known as reference volume element)
as a portion of polycrystal or granular material as in Gerolymatou (2014); Luding (2005); Settimi et al. (2019).
Cosserat theory became very popular since the 70s due to the introduction of composite materials in most engineering
practices since most application have geometric and/or load discontinuities, both conditions wherein Cosserat models
work better than classical continuum (Cowin, 1970; Luciano and Barbero, 1995). In the same context the multiscale
homogenization of random composites is worth to be mentioned for its applicability (Luciano and Willis, 2000, 2003, 2005, 2006; Pingaro et al., 2019b).

The present work lays in the field of molecular-multifield models for composite materials. The procedure here 8 considered takes the advantage of an enriched macroscopic multifield model which is able to consider the description 9 of the material at the microscopic level (Trovalusci and Masiani, 1999). The material is considered here as a set of 10 rigid particles with a deformable matrix and their interaction depends only on their assemblage where also particle 11 orientation is taken into consideration. Material porosity can be also considered since it has an important role. It has 12 been demonstrated in the recent literature that the present model is able to analyze fibre-reinforced ceramics, porous 13 ceramic composites or metal-ceramic composites but also geomaterials or jointed rocks (Adhikary and Dyskin, 1997; 14 Adhikary et al., 1999; Li et al., 2009; Lu et al., 2020)) and masonry (Greco et al., 2016b, 2017; Pepe et al., 2019, 15 2020). 16

In the present work the focus is on anisotropic media and related simulations (Eremeyev and Pietraszkiewicz, 2016; Hasanyan and Waas, 2018). The interest on anisttropic media has been increasing in the recent years due to technology advancedments on industrial production and subsequent investigation (Eremeyev and Konopińska-Zmysłowska, 2020; Fahmy, 2021; Fahmy et al., 2021). Material characterization has been recently focused also on beams (structures where one dimension is larger than the other two) using nonlocal models (Apuzzo et al., 2019; Barretta et al., 2020; Taliercio and Veber, 2016). Nonlocal models demonstrated to be very effective in the analysis of nanostructures and nano composites (Acierno et al., 2017).

The present work considers previous knowledge of the authors on hexagonal assemblies with anisotropic nature as in Fantuzzi et al. (2019, 2020b) where novel material symmetries (Fantuzzi et al., 2020a) are analyzed. The aim of the work is to investigate the dynamic behavior of composite assemblies made of hexagonal particles as in Colatosti et al. (2021a) but by considering non-convex hexagonal shapes. This choice prove a fully anisotropic consitutive behavior of the equivalent material for a special selection of the geometric parameters. The validity of the homogenization procedure taken from the work by Trovalusci and Masiani (1999) is proven by considering a discrete finite element model and subsequently a parametric investigation is shown in order to demonstrated the peculiarity of 1 Cosserat modeling with respect to Cauchy when dynamics of these materials is under investigation.

The main structure of this work is listed below. After the introductory section, Cosserat theory is shortly detailed and main equations are reported together with the present finite element implementation considered in the following simulations. Numerical applications are detailed with reference to the present multiscale strategy and microscopic unit cell of the considered anisotropic class of materials. Discussions and conclusions are drawn at the end of the work.

### 7 2. COSSERAT CONTINUUM

8 As throughly discussed in the introductory section, many researchers showed that Cosserat theory can accurately 9 model materials with microstructure (or materials with internal length) Forest et al. (1999); Leonetti et al. (2019); 10 Trovalusci and Masiani (2003). In this work the analysis is restricted to the 2D framework, therefore the Cosserat 11 model considers two displacements and one rotation (microrotation) as free parameters, whereas the classical Cauchy 12 continuum has only two displacements. The linearized kinematic compatibility equations of the Cosserat model can 13 be written as:

$$\varepsilon_{11} = u_{1,1}, \quad \varepsilon_{22} = u_{2,2}, \quad \varepsilon_{12} = u_{1,2} + \omega, \quad \varepsilon_{21} = u_{2,1} - \omega, \quad \chi_1 = \omega_{,1}, \quad \chi_2 = \omega_{,2}$$
(1)

where  $u_1$  and  $u_2$  are macro displacements components and  $\omega$  is the microrotation.  $\omega \neq \vartheta = 0.5(u_{2,1} - u_{1,2})$ , thus relative rotation  $\vartheta - \omega$  represents an interesting strain measure for checking the micropolar effect.  $\varepsilon_{ij}$  (i, j = 1, 2)are the strain components and  $\chi_i$  (i = 1, 2) are curvatures in the Cosserat model and  $\varepsilon_{12} \neq \varepsilon_{21}$ . Subscripts  $_{,1}$  and  $_{,2}$ stand for the partial derivatives with respect to  $x_1$  and  $x_2$ .

 $\sigma_{ij}$  and  $\mu_i$  (i, j = 1, 2) are the work conjugated stress and microcouple measurements for  $\varepsilon_{ij}$  and  $\chi_i$ , respectively, and  $\sigma_{12} \neq \sigma_{21}$ . Current notation for stress and strain measures are depicted in Fig. 1 (Tejchman and Górski (2006)).  $\sigma_{ij}$  and  $\mu_i$  should satisfy the equilibrium at external boundary as  $t_i = \sigma_{ij}n_j$  and  $m_i = \mu_j n_j$ , where  $t_i$  and  $m_i$  are the surface traction and moment traction,  $n_j$  collects the components of the outward normal to the boundary. Balance equations can be obtained from the virtual work principle (Trovalusci and Masiani (1999)):

$$\sigma_{ij,j} + b_i = 0, \quad \mu_{j,j} - e_{ij3}\sigma_{ij} = 0$$
 (2)

where  $b_i$  are the body force components,  $e_{ij3}$  is the permutation tensor (in the present case specified for the 2D framework).



FIG. 1: Plane differential elements of the Cosserat continuum.

1 Linear stress-strain relations for the Cosserat model can be written as:

$$\begin{cases} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ \sigma_{21} \\ \mu_1 \\ \mu_2 \end{cases} = \begin{bmatrix} A_{1111} & A_{1122} & A_{1112} & A_{1121} & B_{111} & B_{112} \\ A_{2211} & A_{2222} & A_{2212} & A_{2221} & B_{221} & B_{222} \\ A_{1211} & A_{1222} & A_{1212} & A_{1221} & B_{121} & B_{122} \\ A_{2111} & A_{2122} & A_{2112} & A_{2121} & B_{211} & B_{212} \\ B_{111} & B_{122} & B_{112} & B_{121} & D_{11} & D_{12} \\ B_{211} & B_{222} & B_{212} & B_{221} & D_{21} & D_{22} \end{bmatrix} \begin{cases} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{12} \\ \varepsilon_{21} \\ \chi_{1} \\ \chi_{2} \end{cases}$$
(3)

where the constitutive matrix shows major symmetries if considering hyperelastic materials, i.e.  $A_{ijhk} = A_{hkij}$ ,  $B_{ijh} = B_{hij}$ ,  $D_{ij} = D_{ji}$  (*i*, *j*, *h*, *k* = 1, 2). The same matrices can be represented in matrix form by using the symbols  $\mathbb{A}$ ,  $\mathbb{B}$ , and  $\mathbb{D}$ .

#### 5 3. FINITE ELEMENT METHOD

6 A 2D displacement-based finite element method is considered. For Cosserat continua, the vector of model parameters 7 is indicated as d which includes the displacement vector u and the microrotation vector  $\omega$  (that in the 2D case is a 8 scalar, but it will be presented as in Leonetti et al. (2019)):

$$\boldsymbol{u}^{\top} = \left\{ u_1 \quad u_2 \right\}, \quad \boldsymbol{\omega} = \left\{ \boldsymbol{\omega} \right\}, \quad \boldsymbol{d}^{\top} = \left\{ \boldsymbol{u}^{\top} \quad \boldsymbol{\omega} \right\}$$
 (4)

9 Considering a domain A and boundary  $\Gamma$ , the weak form of the current problem (Leonetti et al. (2019); Shi et al.

(2021) can be written as:

$$\int_{\mathcal{A}} \delta \boldsymbol{\varepsilon}^{\top} \boldsymbol{\sigma} + \delta \boldsymbol{\chi}^{\top} \boldsymbol{\mu} \, d\mathcal{A} = \int_{\mathcal{A}} \delta \boldsymbol{u}^{\top} \mathbf{b} \, d\mathcal{A} + \int_{\Gamma} \delta \boldsymbol{u}^{\top} \overline{\boldsymbol{t}} + \delta \boldsymbol{\omega}^{\top} \overline{\boldsymbol{m}} \, d\Gamma \qquad \forall \delta \boldsymbol{u}, \delta \boldsymbol{\omega}$$
(5)

where δ is the variational operator, b is the body force vector. t and m are the traction and couple-traction vectors
applied on the boundary Γ. Different interpolating polynomials are used for the displacements and the microrotation.
In particular, bi-quadratic (N<sub>u</sub>) and bi-linear (N<sub>w</sub>) shape functions are considered to approximate the classical
displacements and microrotation respectively (Ferreira and Fantuzzi (2020); Leonetti et al. (2019)) as:

$$\boldsymbol{u} = N_{\boldsymbol{u}}\tilde{\boldsymbol{u}}, \quad \boldsymbol{\omega} = N_{\boldsymbol{\omega}}\tilde{\boldsymbol{\omega}}$$
 (6)

6 where  $\tilde{u}$  and  $\tilde{\omega}$  are nodal displacement and microrotation values of each element.

$$\boldsymbol{\varepsilon} = \boldsymbol{L}\boldsymbol{u} + \boldsymbol{M}\boldsymbol{\omega}, \quad \boldsymbol{\chi} = \nabla\boldsymbol{\omega} \tag{7}$$

7 where,  $\nabla$  is the gradient operator, L and M can be expressed as:

$$\boldsymbol{L} = \begin{bmatrix} \frac{\partial}{\partial x_1} & 0 & \frac{\partial}{\partial x_2} & 0\\ 0 & \frac{\partial}{\partial x_2} & 0 & \frac{\partial}{\partial x_1} \end{bmatrix}^{\top}, \quad \boldsymbol{M} = \begin{bmatrix} 0 & 0 & 1 & -1 \end{bmatrix}^{\top}$$
(8)

8 Substituting Eq. (6) into (7), the strain vectors become:

$$\varepsilon = B_{\varepsilon} \tilde{d}, \quad \chi = B_{\chi} \tilde{d}$$
 (9)

9 where  $B_{\varepsilon}$  and  $B_{\chi}$  are the derivatives of the shape functions.  $\tilde{d}$  is the unknown vector of nodal displacements that 10 follows the same order of d as indicated in eq. (4). Substituting Eq. (9) into Eq. (3), the constitutive relations become:

$$\boldsymbol{\sigma} = \mathbb{A}\boldsymbol{B}_{\varepsilon}\tilde{\boldsymbol{d}} + \mathbb{B}\boldsymbol{B}_{\chi}\tilde{\boldsymbol{d}}, \quad \boldsymbol{\mu} = \mathbb{B}^{\top}\boldsymbol{B}_{\varepsilon}\tilde{\boldsymbol{d}} + \mathbb{D}\boldsymbol{B}_{\chi}\tilde{\boldsymbol{d}}$$
(10)

11 By excluding body forces (only boundary loads will be considered in the following), the weak form Eq. (5) can be

1 expressed as:

$$\underbrace{\int_{\mathcal{A}^e} \left( \boldsymbol{B}_{\varepsilon}^{\top} \mathbb{A} \boldsymbol{B}_{\varepsilon} + \boldsymbol{B}_{\varepsilon}^{\top} \mathbb{B} \boldsymbol{B}_{\chi} + \boldsymbol{B}_{\chi}^{\top} \mathbb{B}^{\top} \boldsymbol{B}_{\varepsilon} + \boldsymbol{B}_{\chi}^{\top} \mathbb{D} \boldsymbol{B}_{\chi} \right) d\mathcal{A}^e}_{\boldsymbol{K}^e} \tilde{\boldsymbol{d}} = \underbrace{\int_{\Gamma^e} \left[ \begin{array}{c} \boldsymbol{N}_{\boldsymbol{u}}^{\top} \boldsymbol{\bar{t}} & \boldsymbol{N}_{\boldsymbol{\omega}}^{\top} \boldsymbol{\bar{m}} \end{array} \right]^{\top} d\Gamma^e}_{\boldsymbol{F}^e} \qquad (11)$$

where  $K^e$  and  $F^e$  are the stiffness matrix and the nodal force vector of the element. The integral terms in Eq. (11) are computed numerically by a classical Gauss-Legendre integration with  $3 \times 3$  grid.

### 4 4. NUMERICAL SIMULATIONS

- 5 In the following, a rectangular domain (fixed at the bottom edge and free on the other sides is considered) with width
- 6  $L_x = 8.5 \ \mu\text{m}$  and height  $L_y = 12.9375 \ \mu\text{m}$  is used to take numerical dynamic simulations. This rectangular domain
- 7 is considered to be made of microstructured material with a density of  $\rho = 10^{-6} \,\mu g/\mu m^3$ .



FIG. 2: a) General anisotropic assembly with RVE. b) Representative geometry of the anisotropic tile.

An assembly made of the irregular tiles organized according to the Representative Volume Element (RVE) given in Fig. 2a is considered in the following. A single tile, as shown in Fig. 2b, is defined by a parallelogram with a corner cutout. The geometry of the tile is determined by four parameters  $l_r$ ,  $\alpha$ , X, and Y, where  $l_r$  is the relative length defined as  $\frac{l_r}{100} = \frac{b}{a+b}$ , X and Y define the size of unfilled parallelogram corner, i.e.  $\frac{X}{100} = \frac{d}{b}$  and  $\frac{Y}{100} = \frac{e}{a}$ . And f = b - d, c = a - e. The size/scale of the tile is identified by the parameter b, thus, Cartesian coordinates of the tile 1 by considering the origin in the point  $A \equiv O$  they are given by:

$$A = (0; 0)$$

$$B = (b; 0)$$

$$C = b\left(1 + \left(\frac{100}{l_r} - 1\right)\left(1 - \frac{Y}{100}\right)\cos\alpha; \left(\frac{100}{l_r} - 1\right)\left(1 - \frac{Y}{100}\right)\sin\alpha\right)$$

$$D = b\left(1 - \frac{X}{100} + \left(\frac{100}{l_r} - 1\right)\left(1 - \frac{Y}{100}\right)\cos\alpha; \left(\frac{100}{l_r} - 1\right)\left(1 - \frac{Y}{100}\right)\sin\alpha\right)$$

$$E = b\left(\left(\frac{100}{l_r} - 1\right)\cos\alpha + \left(1 - \frac{X}{100}\right); \left(\frac{100}{l_r} - 1\right)\sin\alpha\right)$$

$$F = b\left(\left(\frac{100}{l_r} - 1\right)\cos\alpha; \left(\frac{100}{l_r} - 1\right)\sin\alpha\right)$$
(12)

2 It is clear from Eq. (12) that *b* represents the tile size/scale since it multiplies all geometric components. For the sake
3 of clarity the following, *b* values for different scales *s* are defined as:

• 
$$s = 1$$
 corresponds to  $\frac{b}{L_x} \approx 0.0588$  (large tiles  $b = \frac{1}{2}$ );

5 • 
$$s = \frac{3}{4}$$
 corresponds to  $\frac{b}{L_x} \approx 0.04412$  (medium tiles  $b = \frac{3}{8}$ );

6 • 
$$s = \frac{1}{4}$$
 corresponds to  $\frac{b}{L_x} = 0.01471$  (small tiles  $b = \frac{1}{8}$ );

The tiles interact among elastic interfaces with normal component  $K_{11} = 0.785$  mN/ $\mu$ m and shear component  $K_{22} = 0.3925$  mN/ $\mu$ m. The homogenization approach by Trovalusci and Masiani (1999) can be applied by considering the RVE depicted in Figure 2.

### 10 4.1 Verification

In order to verify the present material modelling a simplified case is considered and then compared with a discrete model as in the previous works (Colatosti et al. (2021b)). The geometric parameters used in the present section are  $l_r = X = Y = 50$  and  $\alpha = 90^\circ$ . Thus, the Constitutive matrix (Eq. (3)) for the microstructure with s = 1 corresponds



Vibration modes: microstructure scale s = 1.

1 to:

$$\mathbf{C}_{s=1} = \begin{bmatrix} 1.5700 & 0 & -0.3925 & 0 & -0.0491 & 0.0327 \\ 0 & 1.5700 & 0 & -0.3925 & -0.0327 & 0.0491 \\ -0.3925 & 0 & 1.1775 & 0 & 0.0327 & -0.0327 \\ 0 & -0.3925 & 0 & 1.1775 & 0.0327 & -0.0327 \\ -0.0491 & -0.0327 & 0.0327 & 0.0327 & 0.1043 & -0.0429 \\ 0.0327 & 0.0491 & -0.0327 & -0.0327 & -0.0429 & 0.0981 \end{bmatrix}$$
(13)

2 It can be noted from Eq. (13) that the present microstructure does not present Poisson effect (e.g. transverse con-3 traction) but exhibits coupling between normal and shear components of stress/strains in A as well as full coupling 4 because  $\mathbb{B} \neq 0$  in all its components. The negligible Poisson effect is due to the chosen angle  $\alpha = 90^{\circ}$  which reports 5 horizontal and vertical geometric shape of each tile.

Results are depicted for the first 6 mode shapes in Figure 3 and frequency values are listed in Table 3 where
relative error with respect to the discrete model are presented.



Vibration modes: microstructure scale  $s = \frac{3}{4}$ .

For the case considered, both Cosserat and Cauchy models represent accurately the dynamic behavior of the discrete model. Cauchy model is analyzed using the constitutive law as detailed in the appendix. This is due to the selected regular geometry which appear to have a major symmetry and the coupling effect due to matrix  $\mathbb{B} \neq 0$  not relevant as well as scale matrix  $\mathbb{D} \neq 0$ . Therefore, it is expected to have similar behavior for the other smaller scales which generally tends to behave like a Cauchy continuum (Colatosti et al. (2021b)).

Mode	Discrete	Cosserat	Error	Cauchy (MH <sub>2</sub> )	Error
			(70)		(70)
1	8.0158	7.8223	2.4140	7.8542	2.0160
2	23.371	22.9166	1.9443	23.1925	0.7638
3	27.158	26.5713	2.1603	26.7215	1.6073
4	50.941	50.6451	0.9935	50.2650	1.3270
5	59.241	58.6451	1.0059	58.8080	-0.7309
6	64.253	63.2484	1.5635	64.7447	-0.7653

**TABLE 1:** Natural frequencies scale s = 1

## The Constitutive matrix (Eq. (3)) for the microstructure with $s = \frac{3}{4}$ corresponds to:

$$\mathbf{C}_{s=3/4} = \begin{bmatrix} 1.5700 & 0 & -0.3925 & 0 & -0.0368 & 0.0327 \\ 0 & 1.5700 & 0 & -0.3925 & -0.0245 & 0.0368 \\ -0.3925 & 0 & 1.1775 & 0 & 0.0245 & -0.0245 \\ 0 & -0.3925 & 0 & 1.1775 & 0.0245 & -0.0245 \\ -0.0368 & -0.0245 & 0.0245 & 0.0245 & 0.0586 & -0.0241 \\ 0.0245 & 0.0368 & -0.0245 & -0.0245 & -0.0241 & 0.0552 \end{bmatrix}$$
(14)

As mentioned in the previous works by Trovalusci and Masiani (1999); Trovalusci and Pau (2014). A change in the
scale results in a change of matrices B and D, whereas matrix A is unchanged.

scale results in a change of matrices  $\mathbb{B}$  and  $\mathbb{D}$ , whereas matrix  $\mathbb{A}$  is unchanged.

Comparison in terms of natural frequencies in depicted in Figure 4 for the first 6 mode shapes. The same in terms
of frequency is listed with the correspondent relative error in Table 2.

As aforementioned, the results show good agreement between Cosserat and Cauchy models with respect to the
reference discrete one.

8 Finally, the constitutive matrix for the microstructure  $s = \frac{1}{4}$  is given:

$$\mathbf{C}_{s=1/4} = \begin{bmatrix} 1.5700 & 0 & -0.3925 & 0 & -0.0123 & 0.0082 \\ 0 & 1.5700 & 0 & -0.3925 & -0.0082 & 0.0123 \\ -0.3925 & 0 & 1.1775 & 0 & 0.0082 & -0.0082 \\ 0 & -0.3925 & 0 & 1.1775 & 0.0082 & -0.0082 \\ -0.0123 & -0.0082 & 0.0082 & 0.0082 & 0.0065 & -0.0027 \\ 0.0082 & 0.0123 & -0.0082 & -0.0082 & -0.0027 & 0.0061 \end{bmatrix}$$
(15)

9 The results in terms of mode shapes are depicted in Figure 5 and compared among discrete, Cosserat and Cauchy

Mode	Discrete	Cosserat	Error	Cauchy	Error		
	(MHz)	(MHz)	(%)	(MHz)	(%)		
1	8.0709	7.7939	3.4321	7.8542	2.6850		
2	23.39	22.8794	2.1997	23.1925	0.8613		
3	27.243	26.5317	2.6109	26.7215	1.9143		
4	51.023	50.3142	1.3892	50.2650	1.4856		
5	60.415	58.6227	2.9666	58.8080	2.6599		
6	66.454	63.4760	4.4813	64.7447	2.5722		

**TABLE 2:** Natural frequencies scale  $s = \frac{3}{4}$ 

1



Vibration modes: microstructure scale  $s = \frac{1}{4}$ .

1 models. The same in terms of vibration frequency is listed in Table 3. Once again the results all agree well with

2 respect to the discrete model.

### 3 4.2 Parametric investigation

4 In this section, a parametric investigation in order to analyze the effects of three parameters  $\alpha$ , X and Y are reported

5 according to the following three selections:

6 1. Effect of  $\alpha$ :  $l_r = 50, X = 50, Y = 50, \alpha = 30^\circ \sim 150^\circ$  with an interval of  $10^\circ$ .

		1	4			
Mode	Discrete	Cosserat Error		Cauchy	Error	
	(MHz)	(MHz)	(%)	(MHz)	(%)	
1	7.7780	7.7500	0.3600	7.8542	-0.9797	
2	22.646	22.7984	-0.6730	23.1925	-2.4132	
3	26.208	26.4477	-0.9146	26.7215	-1.9593	
4	48.934	50.0730	-2.3276	50.2650	-2.7200	
5	57.428	58.4539	-1.7864	58.8080	-2.4030	
6	62.581	63.6443	-1.6991	64.7447	-3.4574	

**TABLE 3:** Natural frequencies scale  $s = \frac{1}{4}$ 



**FIG. 6:** First 3 frequencies as a function of parameter  $\alpha$ .

1 2. Effect of X:  $l_r = 50, \alpha = 90^{\circ}, Y = 50, X = 20 \sim 80$  with an interval of 10.

2 3. Effect of Y:  $l_r = 50$ ,  $\alpha = 90^\circ$ , X = 50,  $Y = 20 \sim 80$  with an interval of 10.

Free vibration tests are performed on the rectangular domain mentioned above using both Cosserat and Cauchy
continua. The first 3 frequencies are used to evaluate the effects of the parameters.

Fig. 6 shows the first 3 frequencies as a function of the angle  $\alpha$ . Frequencies  $f_1$  and  $f_2$  have little difference between Cosserat and Cauchy continuum. These two frequencies firstly increase and then decrease with the  $\alpha$  for both models. The highest  $f_1$  and  $f_2$  can be found when  $\alpha = 80^\circ$ . Similar behavior can be also observed for  $f_3$ from the Cosserat continuum, whereas  $f_3$  from the Cauchy continuum has no obvious trend with  $\alpha$ , resulting in big difference in this frequencies between the two models. All 3 frequencies from the two continuum coincide well when  $\alpha$  is close to  $80^\circ$  (also also shown in the verification section more in detail) but show more or fewer differences as  $\alpha$ the departs from  $80^\circ$ .

Fig. 7 shows the effect of parameter X on the first 3 frequencies. All 3 frequencies from the two continuum coincide well when  $X \le 50$  (as shown also in the verification section), whereas when X > 50 the difference between two continuum become larger as X increases. Such differences are greater in  $f_2$  and  $f_3$  than that in  $f_1$ . Similar behavior can be also found when  $Y \le 50$  and Y > 50 (Fig. 8). However, these three frequencies behave differently as X and Y increase. Actually,  $f_1$  changes slightly with both X and Y.  $f_2$  from Cosserat and Cauchy continuum both increase slightly and then decrease with X, whereas they decrease monotonously with increasing Y.



FIG. 7: First 3 frequencies as a function of parameter X.

1  $f_3$  shows the highest difference between two continuum if X and Y have high values. As X increases,  $f_3$  of Cosserat 2 continuum increases firstly and then decreases, whereas that of Cauchy continuum keep increasing. As Y increases, 3  $f_3$  of Cosserat continuum changes slightly, whereas that of Cauchy continuum has a obvious increase trend when 4 Y > 50.

For better investigate the change in frequency as parameter varies, Tables 4-6 calculate the relative error of above frequencies with respect to a reference parameter configuration. The reference configurations has 90°, 50 and 50 for parameters  $\alpha$ , X and Y, respectively. It can be seen that  $\alpha$  has a greater effect on the relative change in the frequency than X and Y. By varying  $\alpha$  results in the highest relative error that near to -50%. Such a value is only -14.55% and -11.03% when changing X and Y, respectively. In general, for all the three parameters, as the configuration departs from its corresponding reference configuration, the relative error of frequency increases. Table. 4 indicates that the change in frequency as  $\alpha$  is more relevant in the Cosserat continuum than in the Cauchy one for all three frequencies.

**TABLE 4:** Effect of parameter  $\alpha$  on first 3 frequencies: relative error with respect to  $\alpha = 90^{\circ}$  (%).

					α			
Freq.	models	30°	50°	70°	90°	110°	130°	150°
£	Cosserat	-30.74	-10.47	0.87	0	-11.40	-27.74	-45.84
$J_1$	Cauchy	-23.04	-6.16	0.17	0	-5.89	-18.89	-38.95
$f_2$	Cosserat	-33.61	-13.08	2.50	0	-16.35	-33.49	-49.99
	Cauchy	-32.28	-10.66	2.07	0	-12.37	-29.91	-49.10
$f_3$	Cosserat	-27.87	-8.10	-0.90	0	-6.52	-22.53	-43.25
	Cauchy	-6.31	-0.51	-1.95	0	2.00	-2.13	-19.73



FIG. 8: First 3 frequencies as a function of parameter Y.

1  $f_2$  changes the most, followed by  $f_1$  and then  $f_3$ .

As for varying X (Table. 5), the highest relative error (-14.35%) is also observed for  $f_2$  when X = 80 using 2 Cosserat continuum. Only for  $f_3$ , it is shown that the relative error is greater in the Cauchy continuum than in the 3 Cosserat one for all configurations. Effect of continuum used on the relative error in  $f_1$  and  $f_2$  seems uncertain 4 for different configurations. On the contrary, Table 6 shows that for  $f_1$  and  $f_2$  the relative change in frequency is 5 significant in the Cosserat continuum than in the Cauchy one. And the effect of continuum is uncertain for  $f_3$  as Y 6 changes. In general, by varying Y can result in the most significant relative change in  $f_2$ , followed by  $f_1$  and then 7  $f_3$ . Exception is made in the Cauchy continuum when Y > 50, where the relative change in  $f_2$  is the greatest but 8 followed by  $f_3$  and then  $f_1$ . 9

- In conclusion, as the investigated parameters vary, there is small difference in low frequency  $(f_1)$  between the
- 11 Cosserat and Cauchy continuum, whereas such a difference become larger for high frequencies ( $f_2$  and  $f_3$ ) especially

X 50 70 80 Freq. models 20 30 40 60 Cosserat -4.51 -2.10 -0.51 0 -0.78 -2.95 -6.49  $f_1$ Cauchy -5.05 -3.04 -1.33 0.84 1.02 0.35 0 Cosserat -4.27 -0.86 0.81 0 -3.16 -8.18-14.55  $f_2$ -5.17 -1.94-0.11-3.76 -7.38 Cauchy 0 -1.30Cosserat -4.62 -3.29 -1.800 1.61 2.38 1.84  $f_3$ Cauchy -5.25 -4.52 -2.82 0 3.44 6.98 10.14

**TABLE 5:** Effect of parameter X on first 3 frequencies: relative error with respect to X = 50 (%).

1 when  $\alpha$  departs from 80°, X > 50, and Y > 50. The parameter  $\alpha$  has the highest effect on the relative change 2 in frequencies comparing with effects of X and Y, which means that  $\alpha$  also largely influence the tile's degree of 3 anisotropy. All three investigated parameters result in the highest effect on the relative change in  $f_2$ . Although  $f_1$  is 4 the smallest in value, the relative changes in  $f_1$  as parameters are comparable with other frequencies. Since the low 5 frequency plays an important role in dynamic analysis, such an effect of parameter on the change in  $f_1$  should be 6 noted.

### 7 5. CONCLUSIONS

8 This work presented a multiscale homogenization of anisotropic nanocomposites made of non-convex hexagonal 9 assemblies. Homogenized material properties are included in a continuum Cosserat model and compared with a clas-10 sical Cauchy model and a reference discrete configuration in free vibration. A parametric investigation is conducted 11 in order to provide details on how the material symmetries are influenced by the non-convex geometries considered. 12 Interlocking and tile distortion result to play a fundamental role in Cosserat media as previously discussed in previous 13 work, however, in this paper for the first time such aspects are demonstrated via numerical applications.

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 $\overline{Y}$ 20 50 70 80 Freq. models 30 40 60 Cosserat 5.98 4.00 1.99 0 -1.97 -3.91 -5.82  $f_1$ 

2.80

7.36

6.32

0.96

-0.62

1.19

3.73

3.07

0.33

-0.73

0

0

0

0

0

-0.72

-3.73

-2.76

-0.05

1.55

-0.92

-7.41

-5.11

0.16

3.96

-0.57

-11.03

-7.00

0.59

7.19

<b>FABLE 6:</b> Effect of parameter Y on first 3 frequencies: relative error with respec	to	Y =	50 (%	%)	•
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4.79

10.71

9.50

2.02

0.42

 $f_2$ 

 $f_3$ 

Cauchy

Cosserat

Cauchy

Cosserat

Cauchy

### **APPENDIX A. CAUCHY CONSTITUTIVE MATRIX**

2 In this section the Cauchy constitutive matrix is derived from the Cosserat homogenized constitutive relation (Eq. (3))

3 according to the notation provided in the work by Trovalusci et al. (2015). Starting from the strain definitions in 2D:

$$\varepsilon_{ij} = u_{i,j} + e_{3ij}\omega, \quad \chi_3 j = \omega_{,j}$$
 (A.1)

4 where i, j = 1, 2 and  $e_{3ij}$  is the Levi-Civita symbol. If the classical and micropolar components are identified as

5 symmetric and antisymmetric parts of the strain and stress tensors as:

$$\varepsilon_{ij} = \varepsilon_{ij}^S + \varepsilon_{ij}^A, \quad \sigma_{ij} = \sigma_{ij}^S + \sigma_{ij}^A$$
(A.2)

6 where subscripts S and A indicate symmetric and skew-symmetric parts of the tensors and

7 from equation (A.3) with i = 1 and j = 2 the following can be carried out

$$u_{1,2} = 2\varepsilon_{12}^S - u_{2,1}, \quad \omega = -\frac{1}{2}(u_{1,2} - u_{2,1}) + \varepsilon_{12}^A$$
 (A.4)

8 by substituting definitions (A.4) in Eq. (3) it results:

$$\begin{aligned} \sigma_{11} &= A_{1111}\varepsilon_{11} + A_{1122}\varepsilon_{22} - A_{1121}(\varepsilon_{12}^{A} - \varepsilon_{12}^{S}) + A_{1112}(\varepsilon_{12}^{A} + \varepsilon_{12}^{S}) \\ \sigma_{22} &= A_{1122}\varepsilon_{11} + A_{2222}\varepsilon_{22} - A_{2221}(\varepsilon_{12}^{A} - \varepsilon_{12}^{S}) + A_{2212}(\varepsilon_{12}^{A} + \varepsilon_{12}^{S}) \\ \sigma_{12} &= A_{1112}\varepsilon_{11} + A_{2212}\varepsilon_{22} - A_{1221}(\varepsilon_{12}^{A} - \varepsilon_{12}^{S}) + A_{1212}(\varepsilon_{12}^{A} + \varepsilon_{12}^{S}) \\ \sigma_{21} &= A_{1121}\varepsilon_{11} + A_{2221}\varepsilon_{22} - A_{2121}(\varepsilon_{12}^{A} - \varepsilon_{12}^{S}) + A_{1221}(\varepsilon_{12}^{A} + \varepsilon_{12}^{S}) \end{aligned}$$
(A.5)

1 it is noted that  $\varepsilon_{ii} = \varepsilon_{ii}^S = u_{i,i}$ . Such relationships can be rewritten as:

$$\begin{aligned} \sigma_{11} &= A_{1111}\varepsilon_{11} + A_{1122}\varepsilon_{22} + (A_{1112} + A_{1121})\varepsilon_{12}^{S} + (A_{1112} - A_{1121})\varepsilon_{12}^{A} \\ \sigma_{22} &= A_{1122}\varepsilon_{11} + A_{2222}\varepsilon_{22} + (A_{2221} + A_{2212})\varepsilon_{12}^{S} + (A_{2212} - A_{2221})\varepsilon_{12}^{A} \\ \sigma_{12}^{S} &= \frac{A_{1112} + A_{1121}}{2}\varepsilon_{11} + \frac{A_{2212} + A_{2221}}{2}\varepsilon_{22} + \frac{A_{1212} + 2A_{1221} + A_{2121}}{2}\varepsilon_{12}^{S} + \frac{A_{1212} - A_{2121}}{2}\varepsilon_{12}^{S} + \frac{A_{1212} - A_{2121}}{2}\varepsilon_{12}^{A} \\ \sigma_{12}^{A} &= \frac{A_{1112} - A_{1121}}{2}\varepsilon_{11} + \frac{A_{2212} - A_{2221}}{2}\varepsilon_{22} + \frac{A_{1212} - A_{2121}}{2}\varepsilon_{12}^{S} + \frac{A_{1212} - 2A_{1221} + A_{2121}}{2}\varepsilon_{12}^{A} \end{aligned}$$
(A.6)

2 Since in the Cauchy continuum  $2\epsilon_{12}^S = \gamma_{12}$  and  $\epsilon_{12}^A = 0$  constitutive matrix for the Cauchy continuum can be derived:

$$\begin{cases} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12}^{S} \end{cases} = \begin{bmatrix} A_{1111} & A_{1122} & \frac{1}{2}(A_{1112} + A_{1121}) \\ A_{1122} & A_{2222} & \frac{1}{2}(A_{2221} + A_{2212}) \\ \frac{1}{2}(A_{1112} + A_{1121}) & \frac{1}{2}(A_{2212} + A_{2221}) & \frac{1}{4}(A_{1212} + 2A_{1221} + A_{2121}) \end{bmatrix} \begin{cases} \varepsilon_{11} \\ \varepsilon_{22} \\ \gamma_{12} \end{cases}$$
(A.7)

3 It is noted that the constitutive matrix is symmetric as it is expected from the theory. Constitutive matrix (A.7) is the

4 one used in the computations as Cauchy continuum.

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