Non-classical continuum modeling of materials with microstructure: a multiscale/multifield approach

P. Trovalusci

Department of Structural and Geotechnical Engineering, Sapienza University of Rome

patrizia.trovalusci@uniroma1.it

Abstract

The mechanical behavior of complex materials, characterized at finer scales by the presence of heterogeneities of significant size and texture, strongly depends on their microstructural features. By lacking in material internal scale parameters, the classical continuum does not always seem appropriate for describing the macroscopic behavior taking into account the size, orientation and disposition of the micro-heterogeneities. This calls for the need of non-classical continuum theories that can be constitutively characterized through multiscale approaches, which allow us to deduce material properties and relations at different levels of description by bridging information at proper underlying sub-levels.

In the framework of a multiscale modeling, aimed at deriving suitable homogeneous anisotropic continua for these materials, the non-local character of the description is crucial for avoiding physical inadequacies and theoretical computational problems. In particular, in problems in which a characteristic internal (material) length, l, is comparable to a macroscopic (structural) length, L. Among non-local theories, it is useful to distinguish between ‘explicit’ or ‘strong’ and ‘implicit’ or ‘weak’ non-locality, where implicit non-locality concerns continua with extra degrees of freedom [4, 10], such as the multifield continua here adopted. In this presentation, particular attention will be devoted to show the effectiveness of continua with local rigid and/or deformable microstructure (micropolar/ micromorphic or affine microstructure) [3, 4], here adopted for describing fiber reinforced/particle composites, such as: ceramic/metal/polymer matrix composites, i.e. polycrystals with interfaces (grain boundaries or thin/thick interfaces); short fiber-reinforced composites; masonry-like materials (brick/block masonry, roman concrete, rocks).

A two-step multiscale (three levels) procedure is developed for deriving the constitutive equations for special kinds of these materials. As an example, at the microscopic level the material is described as a lattice system, at the mesoscopic level as a two-phase micropolar continuum and at the macroscopic level as a homogeneous micropolar continuum. For the transition from the discrete micro-level to the two-phases meso-level (i) a coarse graining procedure based on a generalized Cauchy-Voigt correspondence maps and energy equivalence is adopted [5, 6, 11]. For the meso-macro level transition (ii), a statistical homogenization procedure is developed, basing on the solution of Boundary Value Problems (BVP) posed on Statistically Representative Elements (SVE), with Boundary Conditions (BC) derived from a generalized macrohomogeneous condition of Hill’s type [7, 8]. This procedure provides hierarchies of bonds and aims at estimating the size of the Representative Volume Element (RVE) to adopt for performing homogenization. In this framework, a new criterion of convergence introduced allow us to estimate the elastic, classical and micropolar, constitutive moduli for particular classes of particle composites. Finally, some applications of the mentioned approach to periodic as well as to random particle composite materials, by varying the material contrast between matrix and inclusions, will be reported and discussed.

Keywords: Composite materials, Continua with Microstructure, Homogenization,

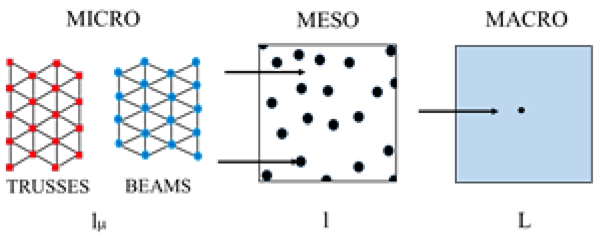

Figure 1. Schematic of the proposed multiscale procedure

Micro-Meso transition (i): coarse-graining procedure

Firstly, focus is on physically-based corpuscular-continuous models, as originated by the molecular models developed in the 19th century to give explanations 'per causas' of elasticity. In particular, a discrete-continuum deterministic approach, based on a generalization of the so-called Cauchy-Born, as well as Voigt-Poincaré, rule, used in crystal elasticity and in the classical molecular theory of elasticity [1, 9, 10], is adopted to derive a continuum equivalent in terms of energy to lattice models made of interacting 'structured' particles. This continuum retains memory of the fine organization of the material by means of additional field descriptors and is named multifield continuum. Once defined the lattice system, basing on such a rule and assuming proper response functions for the lattice interactions, the requirement of the preservation of the strain energy in the micro-meso transition - for any admissible deformation field over a REV - allow us to identify the (classical and non-classical) constitutive parameters of the macromodel, in terms of the geometry of the microstructure (shape, size, orientation, texture) [5, 6, 11].
With reference to a composite material made of particles embedded in a matrix with different material properties, we assume that each constituent is a material with microstructure that can be described as a lattice system (truss-like or beam-like network). The meso-scale is then perceived as the result of the above mentioned coarse-graining procedure from an underlying discrete level (micro-level), that in the former case leads to a classical continuum while in the latter case to a multifield continuum with rigid local structure (micropolar/Cosserat). The latter case is here considered, which is particularly suitable when microscopic bending deformation mechanisms are predominant, as in the case of polycrystals with stiff particles or fiber-beam networks, (fiber reinforced composites, cellular materials, etc.).

Meso-Macro transition (ii): homogenization procedure

The second step concerns a different homogenization method based on the solution of BVP, defined at the meso-level under Dirichlet and Neumann BC and derived from a macrohomogeneity condition of Hill's type, here generalized in order to take into account the additional degrees of freedom of a micropolar continuum, namely the relative rotation and curvature [7, 8].
At the meso-level the material is perceived as a random aggregate of inclusions embedded in a matrix, either softer or stiffer. As a result of the coarse graining procedure (i), both the inclusions and the matrix are described as isotropic micropolar continua. The macroscopic continuum is also supposed to be micropolar, able to naturally account for scale and skew–symmetric shear effects [5, 11]. In this framework, the adopted generalized macrohomogeneity condition ensures a one-to-one correspondence between the two scales, avoiding the introduction of kind of internal constraints for the deformation mechanisms as occurs in the case of continua of different type.
With the aim of investigating the gross mechanical response of this special class of random composites, we adopt a statistically-based multiscale procedure which allow us to detect the size of the RVE, unknown in the case of random media, and to estimate the constitutive moduli of an energy equivalent homogeneous micropolar continuum [12]. The RVE is obtained by increasing a scale factor, representing the ratio between the size of a control window (SVE) and the particle size, until the statistical convergence, defined adopting a specifically conceived criterion, is reached. The results obtained for different kind of composites - ranging from metal or ceramic matrix composites up to concrete, masonry-like and geo-materials - highlight the importance of taking into account the spatial randomness of inclusions in identifying the bulk, shear and bending behavior of composites as well as the effectiveness of the micropolar continuum modelling.

Final remarks

In the modeling of materials with microstructure, such as particle composites, the discrete and heterogeneous nature of the matter must be taken into account, because interfaces and/or material phases dominate the gross behavior. And this is definitely ascertained. What is not completely recognized instead, is the possibility of preserving memory of the microstructure, and in particular of the presence of material length scales, without resorting to the discrete modelling, that can often be cumbersome. The proposed three-steps procedure moves from a physically-based discrete description at the micro-level, on the tracks of the classical molecular theory of elasticity [1, 10], and allow us to rationally derive the material constants that are generally difficult to obtain resorting to standard experimental results [2]. Moreover the procedure provides an appropriate base framework for future investigations concerning the non-linear behavior of microstructured materials, on the basis of some convincing results already obtained for periodic media [5, 13].

Acknowledgments: MIUR, Sapienza University Grant 2015

References

[1] Ericksen, J.L. (1977) Special Topics in Elastostatics, in Yih, C.-S. (ed.) *Advances in Applied Mechanics*, **17**, 189–241, Academic Press, New York.

[2] Lakes R.S. (1986) Experimental microelasticity of two porous solids, *International Journal of Solids and Structures*, **22**(1):55–63

[3] Capriz, G., *Continua with Microstructure* (1989), Springer, Berlin (1989)

[4] Eringen, A.C., Microcontinuum Field Theories (1999), Springer, New York (1999)

[5] Trovalusci, P., Masiani, R. (2003) Non-linear micropolar and classical continua for anisotropic discontinuous materials", *International Journal of Solids and Structures*, **40**(5), 1281-1297.

[6] Trovalusci, P., Varano, V., Rega, G. (2010) A generalized continuum formulation for composite materials and wave propagation in a microcracked bar, *Journal of Applied Mechanics*, **77**(6), 061002/1-11.

[7] Li, X., Liu, Q. (2009) A version of Hill's lemma for Cosserat continuum, *Acta Mechanica Sinica*, 25, 499-506.

[8] Ostoja-Starzewski, M. (2011). Macrohomogeneity condition in dynamics of micropolar media. *Archives of Applied Mechanics*, **81**, 899-906.

[9] Capecchi D., Ruta G., Trovalusci P. (2011) Voigt and Poincaré's mechanistic–energetic approaches to linear elasticity and suggestions for multiscale modelling, *Archive of Applied Mechanics*, **81**(11), 1573-584.

[10] Trovalusci, P. (2014), Molecular approaches for multifield continua: origins and current developments, in Sadowski T., Trovalusci P. (Eds.), *Multiscale Modeling of Complex Materials: Phenomenological, Theoretical and Computational Aspects*, CISM (Int Center for Mechanical Sciences) Series, 556, Springer, Berlin, 211-278.

[11] Trovalusci, P., Pau, A. (2014), Derivation of microstructured continua from lattice systems via principle of virtual works. The case of masonry-like materials as micropolar, second gradient and classical continua. *Acta Mechanica*, **225**(1), 157-177.

[12] Trovalusci, P., Ostoja-Starzewski, M., De Bellis, M.L, Murrali, A. (2015) Scale--dependent homogenization of random composites as micropolar continua", *European Journal of Mechanics A/Solids*, 49, 396–407.

[13] Greco, F., Leonetti, L., Luciano, R., Trovalusci, P. (2017) Multiscale failure analysis of periodic masonry structures with traditional and fiber-reinforced mortar joints (2017), *Composites Part B:Engineering*, **118**, 75-95.