# Homogenized tangent moduli for heterogeneous materials

**A. J. Carneiro Molina, E. A. de Souza Neto & D. Peric**
*School of Engineering*
*University of Wales Swansea*
*SA2 8PP*
egmolina@swansea.ac.uk

## 1. Introduction

This paper describes homogenization, procedures required for computation of effective tangent moduli of linear elastic microstructures undergoing small strain deformation, see [2]. Such procedures are important for computer modelling of heterogeneous materials when the length-scale of heterogeneities is small compared to dimensions of the body. In this instance applying a single mesh becomes too costly. This problem was elaborated in [1] with AEH (asymptotic expansion homogenization) theory. AEH is a perturbation technique based on the asymptotic series expansion, in a scale parameter, of a primary variable such as displacement. In recent years an alternative approach for homogenization has been developed, commonly denoted the multiscale computational homogenization. This work belongs to this class of numerical techniques with specific focus on deformation-driven microstructures [3]. The approach consists of imposing a macroscopic strain on the discretised unit cell, representing the microstructure, and then computing the macroscopic stress as a function of the strain.

The microstructures define representative volume elements (RVE) $\mathscr{V}$ of heterogeneous materials such as elastic composites. The homogenization procedure is based on the standard Finite Element discretisation of the microstructure. Tangent modulus $\overline{\boldsymbol{\mathcal{C}}}$ is then obtained as a function of stiffness, material properties of the components and geometrical distribution of heterogeneities. In this work two dimensional macro and micro structures have been studied. In Figure 1, a transition from the micro-scale to the macro-scale is sketched. This transition from microstructure RVE $\mathscr{V}$ to the macrostructure body $\overline{\mathscr{B}}$ is performed at integration Gauss point level to obtain the overall tangent moduli.

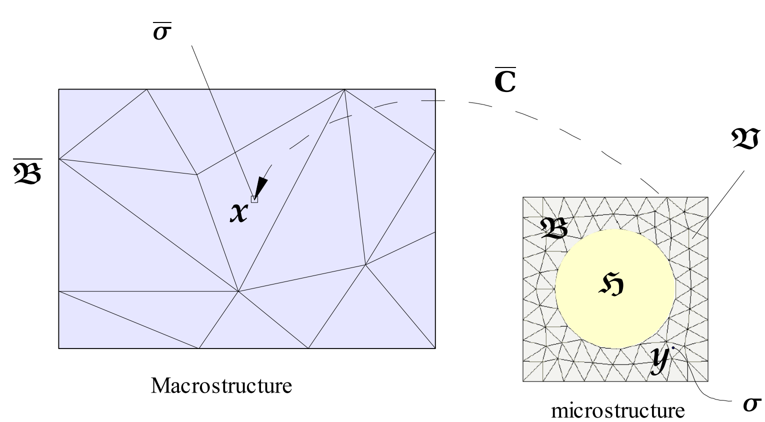


FIGURE 1. Micro to macro transition for obtaining overall tangent modulus $\overline{\boldsymbol{\mathcal{C}}}$ at macro-scale level.

## 2. continuum model

Overall macrostress $\overline{\boldsymbol{\sigma}}$ and overall macrostrain $\overline{\boldsymbol{\epsilon}}$ of microstructure $\mathscr{B}$ are defined as averages of the microstresses and microstrains over the unit cell respectively. They are expressed as

$$\overline{\boldsymbol{\sigma}} \equiv \frac{1}{|\mathscr{V}|}\int_{\partial\mathscr{V}} \mathrm{sym}[\mathbf{t}\otimes\mathbf{y}]\ \mathrm{dA} \qquad \overline{\boldsymbol{\epsilon}} \equiv \frac{1}{|\mathscr{V}|}\int_{\partial\mathscr{V}} \mathrm{sym}[\mathbf{u}\otimes\mathbf{n}]\ \mathrm{dA} \tag{1}$$

in terms of the traction $\mathbf{t}$ at $\mathbf{y} \in \partial\mathscr{V}$ and the displacement $\mathbf{u}$ at $\mathbf{y} \in \partial\mathscr{V}$, where $\mathbf{n}$ is the outward normal unit vector at $\mathbf{y} \in \partial\mathscr{V}$. Expressions (1) have been derived assuming the absence of body forces.
The overall tangent modulus $\overline{\boldsymbol{\mathcal{C}}}$ in linear elasticity relates the overall macrostress $\overline{\boldsymbol{\sigma}}$ and the macrostrain $\overline{\boldsymbol{\epsilon}}$ in a linear relation form

$$\overline{\boldsymbol{\sigma}} = \overline{\boldsymbol{\mathcal{C}}} : \overline{\boldsymbol{\epsilon}} \qquad \text{with} \quad \overline{\boldsymbol{\mathcal{C}}} \equiv \frac{\mathrm{d}\overline{\boldsymbol{\sigma}}}{\mathrm{d}\overline{\boldsymbol{\epsilon}}} \tag{2}$$

In order to compute the above-mentioned tangent modulus $\overline{\boldsymbol{\mathcal{C}}}$ and then to obtain effective elastic properties, two types of boundary conditions are imposed over the unit cell: (a) Linear displacements on the boundary and (b) periodic displacements and antiperiodic tractions on the boundary. These boundary conditions satisfy the averaging condition [4], which equates microscopic virtual work with the macroscopic one. These boundary conditions, in general, generate two different values of the overall tangent moduli.

2.1. **Linear displacements on the boundary.** In this state, the definition of the deformation boundary constraint applied on the boundary of RVE, in terms of the macroscopic strain $\overline{\boldsymbol{\epsilon}}$, assumes the form: $\mathbf{u}(\mathbf{y}) = \overline{\boldsymbol{\epsilon}}\,\mathbf{y}$ at $\mathbf{y}$ on $\partial\mathscr{V}$.

2.2. **Periodic deformation and antiperiodic traction on the boundary.** Another possibility to satisfy the averaging theorem on the boundary of the RVE $\partial\mathscr{V}$, is to prescribe the two following conditions: $\mathbf{u}(\mathbf{y}^+) - \mathbf{u}(\mathbf{y}^-) = \overline{\boldsymbol{\epsilon}}\,(\mathbf{y}^+ - \mathbf{y}^-)$ and $\mathbf{t}(\mathbf{y}^+) + \mathbf{t}(\mathbf{y}^-) = \mathbf{0}$ representing periodic deformation and antiperiodic traction at $\mathbf{y}^+$ and $\mathbf{y}^-$ on the opposite faces of $\partial\mathscr{V}$.

## 3. Discrete model

The displacement field $\mathbf{u}$ is divided in two parts: $\mathbf{u} = \mathbf{u}^* + \widetilde{\mathbf{u}}$, where $\mathbf{u}^*$ is the *Taylor displacement*, which defines a constant deformation $\overline{\boldsymbol{\epsilon}}$ over the unit cell and it takes the following form: $\mathbf{u}^*_{\mathrm{j}} \equiv \overline{\boldsymbol{\epsilon}}\,\mathbf{y}_{\mathrm{j}}$ for every node j of the microstructure. Moreover, the component $\widetilde{\mathbf{u}}$ is known as *displacement fluctuation*, which is the unknown quantity of the displacement field $\mathbf{u}$. Furthermore, we note that the periodic part $\widetilde{\mathbf{u}}$ gives no contribution to the average deformation. Average stress is computed by discretising and expressing in matrix formulation the expression (1), as

$$\overline{\boldsymbol{\sigma}} = \frac{1}{|\mathscr{V}|}\,\mathbb{D}_{\mathrm{b}}\ \mathbf{f}_{\mathrm{b}}^{ext} \tag{3}$$

where $\mathbb{D}_{\mathrm{b}}$ is the *boundary coordinate matrix* and $\mathbf{f}_{\mathrm{b}}^{ext}$ is the *external boundary force vector.* The homogenized tangent modulus (2) is then calculated in its discrete form as

$$\overline{\boldsymbol{\mathcal{C}}} = \frac{\mathrm{d}\overline{\boldsymbol{\sigma}}}{\mathrm{d}\overline{\boldsymbol{\epsilon}}} = \frac{1}{|\mathscr{V}|}\,\mathbb{D}_{\mathrm{b}}\,\frac{\mathrm{d}\mathbf{f}_{\mathrm{b}}^{ext}}{\mathrm{d}\overline{\boldsymbol{\epsilon}}} \tag{4}$$

Therefore, the following steps are required to compute the underlying modulus: $(i)$ First, a linear expression for $\mathbf{f}_{\mathrm{b}}^{ext}$ is obtained in terms of the macroscopic strain $\overline{\boldsymbol{\epsilon}}$. $(ii)$ Differentiate the expression with respect to $\overline{\boldsymbol{\epsilon}}$. $(iii)$ The resulting expression is then inserted into (4) to derive $\overline{\boldsymbol{\mathcal{C}}}$. The system, which supplies the algebraic expression for the external boundary force vector, comes from the establishment of the B.V.P in the microstructure level by F.E. discretisation. The B.V.P. is derived prescribing one of the two boundary conditions outlined in sections 2.1 and 2.2 in their discrete form. This procedure will be briefly described in the following.

3.1. **Linear displacements on the boundary in discrete form.** This constraint can be satisfied by imposing zero value to the boundary displacement fluctuation $\widetilde{\mathbf{u}}_{\mathrm{b}} = \mathbf{0}$ on the boundary of the RVE $\partial\mathscr{V}$. To carry out this task, a partitioning of the microstructure nodes is essential. This division is made in two groups as shown in Figure 2(a): $\mathrm{n_i}$ internal nodes and $\mathrm{n_b}$ boundary nodes.

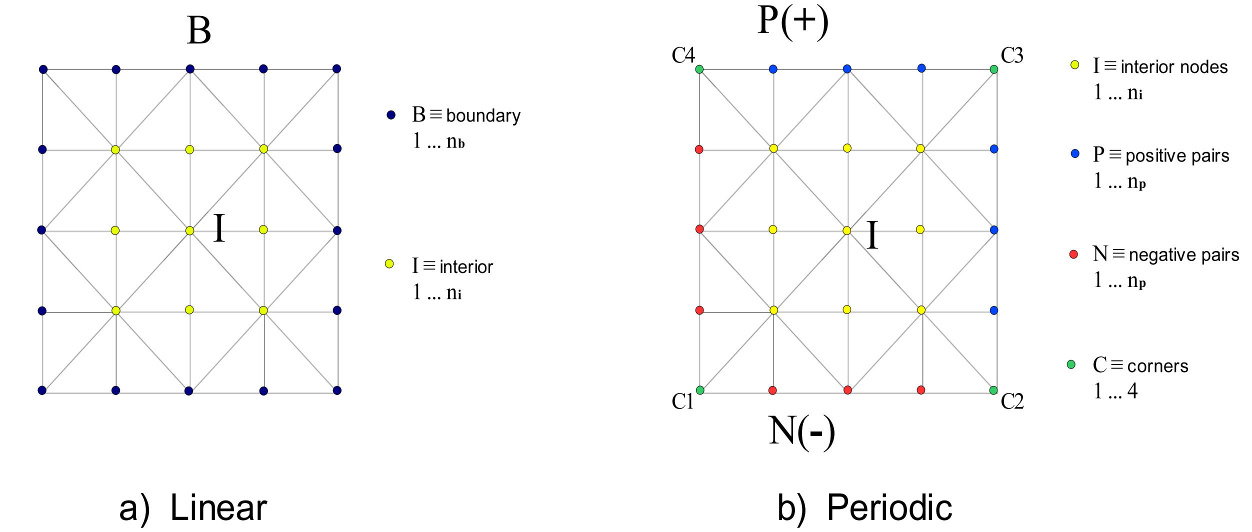


FIGURE 2. Partition of the mesh nodes for a) linear displacement and b) periodic displacement and antiperiodic traction, on the boundary of the microstructure RVE

3.1.1. *Homogenized Tangent modulus.* The linear algebraic F.E. system is partitioned, according to Figure 2(a), in the following way:

$$\begin{bmatrix} \mathbf{k}_{\mathrm{ii}} & \mathbf{k}_{\mathrm{ib}} \\ \mathbf{k}_{\mathrm{bi}} & \mathbf{k}_{\mathrm{bb}} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_{\mathrm{i}} \\ \mathbf{u}_{\mathrm{b}} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_{\mathrm{i}}^{ext} \\ \mathbf{f}_{\mathrm{b}}^{ext} \end{Bmatrix} \quad \equiv \quad \mathbf{K}\ \mathbf{u} = \mathbf{f}^{ext} \tag{5}$$

where the external force vector corresponding to the internal nodes satisfies $\mathbf{f}_{\mathrm{i}}^{ext} = \mathbf{0}$. Then the constraint $\widetilde{\mathbf{u}}_{\mathrm{b}} = \mathbf{0}$ is applied to the system, which gives an expression for the external boundary force vector. Finally, the $\mathbf{f}_{\mathrm{b}}^{ext}$ is differentiated with respect to $\bar{\boldsymbol{\epsilon}}$ and then inserted into (4), to obtain a tangent modulus expression.

3.2. **Periodic displacements and antiperiodic traction on the boundary in discrete form.** This periodicity assumption, with continuum form outlined in Section 2.2, can be obtained by prescribing the following conditions on $\partial\mathscr{V}$: (*i*) equating the positive (+) and negative (−) displacement fluctuations: $\widetilde{\mathbf{u}}_{\mathrm{p}} = \widetilde{\mathbf{u}}_{\mathrm{n}}$, (*ii*) prescribing zero value at the node corners displacement fluctuation: $\widetilde{\mathbf{u}}_{\mathrm{c}} = \mathbf{0}$ and (*iii*) prescribing the same module value with opposite sign for the positive and negative external force: $\mathbf{f}_{\mathrm{p}} = -\mathbf{f}_{\mathrm{n}}$. In Figure 2(b) a partition of the microstructure RVE nodes in four different groups is sketched: a) $\mathrm{n_i}$ internal nodes, b) $\mathrm{n_p}$ positive boundary nodes c) $\mathrm{n_p}$ negative boundary nodes, and finally d) 4 nodes at the corners.

3.2.1. *Homogenized Tangent modulus.* Similarly to the procedure in Section 3.1.1, the F.E. system is partitioned, according to Figure 2(b),

$$\begin{bmatrix} \mathbf{k}_{\mathrm{ii}} & \mathbf{k}_{\mathrm{ip}} & \mathbf{k}_{\mathrm{in}} & \mathbf{k}_{\mathrm{ic}} \\ \mathbf{k}_{\mathrm{pi}} & \mathbf{k}_{\mathrm{pp}} & \mathbf{k}_{\mathrm{pn}} & \mathbf{k}_{\mathrm{pc}} \\ \mathbf{k}_{\mathrm{ni}} & \mathbf{k}_{\mathrm{np}} & \mathbf{k}_{\mathrm{nn}} & \mathbf{k}_{\mathrm{nc}} \\ \mathbf{k}_{\mathrm{ci}} & \mathbf{k}_{\mathrm{cp}} & \mathbf{k}_{\mathrm{cn}} & \mathbf{k}_{\mathrm{cc}} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_{\mathrm{i}} \\ \mathbf{u}_{\mathrm{p}} \\ \mathbf{u}_{\mathrm{n}} \\ \mathbf{u}_{\mathrm{c}} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_{\mathrm{i}}^{ext} \\ \mathbf{f}_{\mathrm{p}}^{ext} \\ \mathbf{f}_{\mathrm{n}}^{ext} \\ \mathbf{f}_{\mathrm{c}}^{ext} \end{Bmatrix} \quad \equiv \quad \mathbf{K}\ \mathbf{u} = \mathbf{f}^{ext} \tag{6}$$

where the external force vector corresponding to the internal nodes satisfies $\mathbf{f}_{\mathrm{i}}^{ext} = \mathbf{0}$. We then, apply the conditions described in Section 3.2, along the boundary of the microstructure: $\widetilde{\mathbf{u}}_{\mathrm{p}} = \widetilde{\mathbf{u}}_{\mathrm{n}}$, $\widetilde{\mathbf{u}}_{\mathrm{c}} = \mathbf{0}$ and $\mathbf{f}_{\mathrm{p}} = -\mathbf{f}_{\mathrm{n}}$. The rest of procedure is similar to the tangent modulus calculation described in Section 3.1.1.

## 4. Numerical Results

Numerical tests under plane strain conditions have been performed for squared microcells composed of Epoxy matrix with Young's modulus $E = 3.13\ GPa$ and Poisson ratio $\nu = 0.34$. Glass fiber is embedded in the matrix is the second material with Young's modulus $E = 73\ GPa$ and Poisson ratio $\nu = 0.2$. In Figure 3 values of the effective shear modulus over the matrix modulus ratio $\overline{\mathrm{G}}/\mathrm{G}_{matrix}$ are compared with analytically obtained properties following Nemat-Nasser [5]. A very similar response can be observed for less than 20% of the inclusion volume fraction. Especially, the Periodic assumption seems to be the very accurate. Note that the Nemat-Nasser's analytical model is effective in predicting equivalent material properties for a low volume fraction of the second phase inclusion.

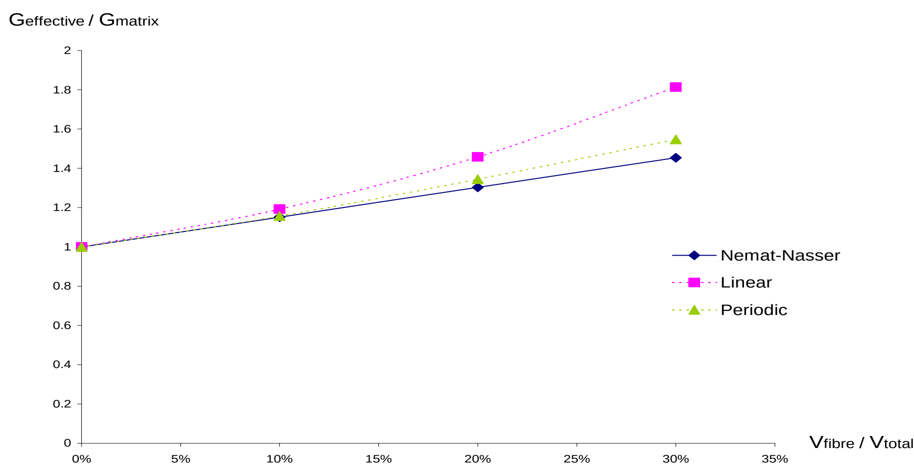


Figure 3. Comparative of $\frac{\overline{\mathrm{G}}}{\mathrm{G}_{matrix}}$ between analytically solution of Nemat-Naseer and Numerically obtained results

## 5. Remarks

Periodic boundary condition has been shown to be more accurate than the Linear assumption for the general tangent modulus computation. Numerical computed values for a standard composite microcell have been compared with analytically calculated properties, and good correlation has been found.

## References


[1] E. Sanchez-Palencia Non-homogeneous media and vibration theory. *Springer-Verlag, Berlin*, **1980**.

[2] C. Miehe and A. Koch, Computational micro-to-macro transitions of discretized microstructures undergoing small strains, *Archive of Applied Mechanics*, 72, **2002**, 300-31.

[3] C. C. Swan, Techniques for stress- and strain-controlled homogenization of inelastic periodic composites, *Computer methods in applied mechanics and engineering*, 117, **1994**, 249-267.

[4] R. Hill, On constitutive macro-variables for heterogeneous solids at finite strain, *Proc. R. Soc. Lond.*, 326, **1972**, 131-147.

[5] S. Nemat-Nasser and M. Hori, Micromechanics: overall properties of heterogeneous materials, *Elsevier*, **1999**.