Numerical analysis of strain gradient effects in periodic media

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Abstract. Standard effective properties of heterogeneous materials can no longer be used when strain gradients become large with respect to the scale of heterogeneity. The effective modelling can be improved in such cases by including higher-order deformation gradients. For the case of a periodic, linear elastic medium effective relations are derived directly from the properties of the microstructure. The coefficients in these relations can be computed by solving a set of boundary value problems for the periodic cell. This has been done numerically for a fibre-reinforced composite, showing that higher-order terms become more important as the stiffness contrast between fibre and matrix increases.

1. INTRODUCTION

Damage and fracture processes in engineering materials are accompanied by highly localised deformations and stresses. In these circumstances, standard continuum models cease to be meaningful representations of the actual material behaviour. Not only do they become inaccurate when the scale at which the continuum fields vary approaches that of the microstructure, but they may also suffer from mathematical difficulties and cease to be physically meaningful. Continuum models which remain mathematically and physically consistent for high-strain gradients can be obtained if nonlocal or gradient terms are included in the constitutive modelling. These terms represent the influence of microstructure and microstructural processes on the effective behaviour of the material.

Although often motivated from specific physical processes, most of the existing nonlocal and gradient models are largely phenomenological. The parameters featuring in them would therefore have to be determined from experiments. A more appealing way to arrive at enriched effective relations is to derive these relations directly from the behaviour of the microstructural constituents and their geometric arrangement. Such direct relations between microstructure and macroscopic behaviour, however, are generally difficult to obtain. A class for which this direct link can be made is purely elastic behaviour. A nonlocal effective representation of random, linear elastic composites has been developed by Willis and co-workers [1–3] by formally solving the equilibrium equations in terms of a stress polarisation and subsequent ensemble averaging. For a random composite, statistical properties of the microstructure are needed, but the method can also be applied to deterministic problems, where this information is readily available. Higher-order gradient theories have been developed by Boutin [4] and Triantafyllidis & Bardenhagen [5] for periodic, linear elastic media using an asymptotic solution of the microstructural problem. Based on the properties and morphology of the phases, effective moduli can be determined up to an arbitrary order. Smyshlyaev & Cherednichenko [6] have refined this approach by introducing variational arguments, which ensures that
the difference between real and homogenised behaviour is minimised and that the homogenised equilibrium equations are elliptic. The same authors have also extended the theory to the case of nonlinear elasticity [7]. Applications of the higher-order homogenisation methods have been limited to relatively simple morphologies. Boutin [4] has derived closed-form expressions for higher-order moduli (up to order two) for a two-phase laminate. The slightly further simplified case where forces vary only in the direction on lamina- tion has been considered by Luciano & Willis [3], resulting in a local effective stress-strain relation. For the full three-dimensional problem, i.e., with force variations also in the plane of the laminae, the relevant equations cannot be solved analytically. For this case bounds have been obtained for the Fourier transform of the effective nonlocal elasticity operator [3]. In order to obtain estimates of the effective relations for this and more complex arrangements, a numerical approach is necessary.

In the present paper such a computational strategy for higher-order homogenisation is developed on the basis of Smyshlyaev & Cherednichenko’s method for periodic, linear elastic media [6]. This theory is first extended to the full three-dimensional case. It requires a set of boundary value problems to be solved on the periodic cell. For this purpose, the boundary value problems are cast in a weak form and solved by the finite element method. Effective higher-order moduli can be computed as weighted averages of the resulting functions and their derivatives. The method has been applied to a fibre-matrix system, for which the influence of the ratio of the elastic moduli of the fibre and matrix on the effective behaviour has been examined.

2. ASYMPTOTICS OF THE HETEROGENEOUS PROBLEM

Following Smyshlyaev & Cherednichenko [6], we assume the elasticity problem to be doubly periodic; see Figure 1 for a one-dimensional graphical representation. The microstructure is constructed from a unit cell \( Q = [0, 1] \times [0, 1] \times [0, 1] \) by re-scaling by a small parameter \( \varepsilon \) and repetition. As a result, the microstructure is periodic with period \( \varepsilon Q \) and the small parameter \( \varepsilon \) appears as the natural length scale of the material. The body force vector \( f(x) \) is periodic with period \( T = [0, T] \times [0, T] \times [0, T] \), where \( T \) is of the order of 1 and \( T / \varepsilon \) is an integer. Assuming this periodicity of the body force, and therefore of the entire problem, allows us to concentrate on the behaviour of the bulk material, without any influence of boundary conditions or conditions at infinity. It also implies that the displacement \( u(x) \) is \( T \)-periodic. As a result, the elasticity problem need only be solved on one period \( T \), after which the solution on the entire domain can be obtained by repetition.

The three-dimensional equilibrium problem on the period \( T \) can be written as

\[
\frac{\partial \sigma_{ij}}{\partial x_i} + f_j(x) = 0, \quad j = 1, 2, 3, \tag{1}
\]

where the Cauchy stress tensor is given by

\[
\sigma_{ij} = C_{ijkl}(x/\varepsilon) e_{kl}, \quad e_{kl} = \frac{1}{2} \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \tag{2}
\]

and summation is implied over the repeated indices \( i, k, l = 1, 2, 3 \). The elasticity tensor \( C_{ijkl}(\xi) \) satisfies the usual symmetries \( C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij} \) and is assumed to be positive-definite and piecewise smooth; the appropriate weak conditions must be applied at discontinuity surfaces. Substitution of relations (2) in the set of equilibrium equations (1) results in a set of partial differential equations in terms of the displacement components \( u_k \). It proves to be useful to rewrite this set of equations in the vector form

\[
\frac{\partial}{\partial x_i} \left( A_{ij}(x/\varepsilon) \frac{\partial u}{\partial x_i} \right) + f(x) = 0, \tag{3}
\]

where the matrix-valued functions \( A_{ij}(\xi) \) are defined by \( A_{ij}^k(\xi) = C_{ijkl}(\xi) \). In addition to the requirement of periodicity of the displacement field \( u(x) \), the mean displacement on the period \( T \) is required to be zero in order to guarantee a unique solution of the equilibrium problem.
An asymptotic solution of equation (3) is now sought by separating the influence of the microscopic and macroscopic coordinates:

\[ u(x) = \sum_{m=1}^{\infty} \epsilon^m u_m(x, x/\epsilon), \]  

(4)

where the functions \( u_m(x, \xi) \) are Q-periodic with respect to the microstructural coordinates \( \xi \) and T-periodic with respect to the macroscopic coordinates \( x \). Straightforward substitution of (4) in (3) and requiring that the resulting equation is satisfied at each order of \( \epsilon \) shows that the asymptotic expansion (4) must be of the form [4, 8]:

\[ u(x) = v(x) + \sum_{m=1}^{\infty} \epsilon^m \sum_{|n|=m} N_n(x/\epsilon) D^n v(x). \]  

(5)

Here \( n = n_1 n_2 \ldots n_m \) is a multi-index with ‘length’ \( |n| = m \) in which each of \( n_1, n_2, \ldots, n_m \) adopts the values 1, 2, 3. \( D^n \) denotes differentiation with respect to \( x_{n_1}, x_{n_2}, \ldots \) etc.: \( D^n = \partial^n / \partial x_{n_1} \partial x_{n_2} \ldots \partial x_{n_m} \).

Reference is made to Bakhvalov & Panasenko [8] for the formal justification of (5).

The matrix-valued functions \( N_n(\xi) \) in (5) are the solutions of the following problems on the periodic cell:

\[ \frac{\partial}{\partial \xi_i} \left( A_{ji}(\xi) \frac{\partial N_n}{\partial \xi_j} \right) + T_n(\xi) = H_n, \quad |n| = m = 1, 2, 3, \ldots, \]  

(6)

where

\[ T_{n_1}(\xi) = \frac{\partial A_{jn_1}}{\partial \xi_i}, \quad m = 1, \]  

(7)

\[ T_{n_1 n_2}(\xi) = \frac{\partial}{\partial \xi_i} \left( A_{j n_1} n_2 + A_{j n_1} n_2 + A_{j n_2} n_2 \right), \quad m = 2, \]  

(8)

\[ T_n(\xi) = \frac{\partial}{\partial \xi_i} \left( A_{j n_1} n_{n_2} \ldots n_m \right) + A_{j n_1} \frac{\partial N_{n_2} \ldots n_m}{\partial \xi_i} + A_{j n_2} n_3 \ldots n_m, \quad m \geq 3 \]  

(9)
and

\[ H_n = (T_n) = \int_Q T_n(\xi) \, d\xi. \quad (10) \]

Note that \( H_{n1} = 0 \) because of periodicity. The functions \( N_n(\xi) \) are uniquely defined by the additional requirements that they are \( Q \)-periodic and that their mean on the periodic cell vanishes, i.e., \( (N_n) = 0 \). Problems (6) depend only on the microstructural stiffness distribution given by \( A_{ii}(\xi) \) and can therefore be solved independently of the macroscopic problem (in particular: independently of the distribution of body force \( f(x) \)). Since for values of \( m \geq 2 \) equations (6) depend on functions \( N_n(\xi) \) with \( |n| < m \), these problems have to be solved sequentially, for increasing \( m \) and starting at \( m = 1 \).

The vector-valued function \( v(x) \) in (5) formally satisfies

\[ \sum_{m=2}^{\infty} \varepsilon^{m-2} \sum_{|n|=m} H_n D^n v(x) + f(x) = 0, \quad (11) \]

where \( H_n \) are the constant matrices defined by (10). Only macroscopic quantities appear in equation (11), the connection with the microstructure being provided by the matrices \( H_n \). This equation is therefore referred to as 'homogenised equation of infinite order' [8]; this nomenclature will be further substantiated in the next section.

The equilibrium problem (3) can be rephrased in a variational form by considering the energy functional

\[ E[u^*] = \int_T \left[ \frac{1}{2} \left( \frac{\partial u^*}{\partial x_i} \right)^T A_{ii} \frac{\partial u^*}{\partial x_i} - f^T u^* \right] \, dx, \quad (12) \]

where \( u^*(x) \) is \( T \)-periodic and has average zero. The equilibrium solution \( u \), the asymptotics of which are given by (5), minimises this functional. The elastic energy in one period \( T \) is therefore given by

\[ I = E[u] = \min_{u^*(x)} E[u^*]. \quad (13) \]

3. HOMOGENISATION BY ENSEMBLE AVERAGING

The averaged behaviour of the heterogeneous material is now determined based on the argument that the 'phase' of the microstructure with respect to the macroscopic body force is unknown. A family of problems is therefore considered, in which the microstructure is translated by a vector \( \varepsilon \zeta \), while the body force is kept fixed:

\[ \frac{\partial}{\partial x_i} \left( A_{ii}^\varepsilon(x/\varepsilon) \frac{\partial u_i^\varepsilon}{\partial x_i} \right) + f(x) = 0, \quad (14) \]

with \( A_{ii}^\varepsilon(\xi) = A_{ii}(\xi + \zeta) \) and \( \zeta \in Q \). The homogenised equilibrium equations should provide the best possible fit to the ensemble average of the solutions to each of these problems [6].

Following the same arguments that led to relation (5), it can easily be seen that the solution to each of the problems (14) is given by

\[ u_i^\varepsilon(x) = v(x) + \sum_{m=1}^{\infty} \varepsilon^m \sum_{|n|=m} N_n^\varepsilon(x/\varepsilon) D^n v(x), \quad (15) \]
with \( N_h(\xi) = N_n(\xi + \zeta) \). The ensemble average of the family of solutions \( u^\xi \) follows as
\[
\bar{u}(x) = \frac{1}{Q} \int_Q u^\xi(x) \, d\zeta = v(x).
\] (16)

As a result of the fact that \( \langle N_n \rangle = 0 \), the higher-order contributions vanish and only \( v(x) \) survives the averaging. The true homogenised solution therefore follows as the solution of the ‘homogenised equation of infinite order’ (11).

For practical applications, the infinite-order homogenised equation (11) must somehow be approximated by an equation of finite order. It has been argued by Smyshlyaev & Cherndnichenko [6] that simply truncating (11) at some order of \( \varepsilon \) may not be a good idea because ellipticity of the resulting equation cannot be guaranteed. Instead, they propose to derive the finite-order homogenised equation from a variational formulation of the averaged problem. In this way, ellipticity of the resulting equation is guaranteed in a natural way. Moreover, the resulting homogenised solution is the best possible fit to \( \bar{u}(x) \) in terms of elastic energy.

The energy in one realisation of the translated problem is given by (cf. (13))
\[
I^\xi = E^\xi[u^\xi] = \min_{u^\star(x)} E^\xi[u^\star],
\] (17)

with \( E^\xi[u^\star] \) defined analogous to (12). The ensemble average of the energy can therefore be written as
\[
\bar{I} = \int_Q I^\xi \, d\zeta = \frac{1}{Q} \int_Q \min_{u^\star(x)} E^\xi[u^\star] \, d\zeta = \min_{u^\star(x,\zeta)} \frac{1}{Q} \int_Q E^\xi[u^\star] \, d\zeta = \min_{u^\star(x,\zeta)} \bar{E}[u^\star],
\] (18)

where the average energy functional \( \bar{E}[u^\star] \) has been defined as
\[
\bar{E}[u^\star] = \int_Q E^\xi[u^\star] \, d\zeta
\] (19)

and the test function \( u^\star(x, \zeta) \) must be \( T \)-periodic in its first argument and \( Q \)-periodic in its second argument. The minimiser of \( \bar{E}[u^\star] \) is \( u^\star(x, \zeta) = u^\xi(x) \), the asymptotics of which are given by (15). The crux of the method proposed by Smyshlyaev & Cherndnichenko [6] is now to restrict the set of test functions \( u^\star(x, \zeta) \) by truncating (15) after a finite number of terms. In the present three-dimensional case this means that we consider a class \( \bar{U} \) of test functions that can be written as
\[
u^\star(x, \zeta) = v^\star(x) + \sum_{m=1}^{K} \varepsilon^l \sum_{|n|=m} N^\xi_n(x/\varepsilon) \, D^\theta v^\star(x),
\] (20)

where \( K \geq 1 \). A higher value of \( K \) implies that more detail of the microstructural fields is included and will result in a higher order of the resulting homogenised equations.

Straightforward substitution of (20) shows that the variational problem of order \( K \) can now be written as:
\[
\bar{I} = \min_{u^\star(x,\zeta) \in \bar{U}} \bar{E}[u^\star] = \min_{v^\star(x)} \bar{E}[v^\star].
\] (21)

Here the functional \( \bar{E}[v^\star] \) has been defined as
\[
\bar{E}[v^\star] = \int_T \left[ \sum_{r,s=1}^{K+1} \varepsilon^{r+s-2} \sum_{|p|=r,|q|=s} \frac{1}{2} (D^p v^\star)^T \mathbf{H}_{pq} \varepsilon^{r+s-2} D^q v^\star - f^T v^\star \right] \, dx,
\] (22)
with
\[
\hat{H}_{r,s}^\ast = \int_0^1 \left( N_p \frac{\partial}{\partial x_i} + \delta_{p1} N_{p2} \cdots \delta_{p_r} \right) A_{il} \left( N_q \frac{\partial}{\partial x_l} + \delta_{q1} N_{q2} \cdots \delta_{q_s} \right) \, d\xi, \quad r, s = 2, \ldots, K. \tag{23}
\]

For \( r = 1 \) or \( s = 1 \) the factors \( N_{p2} \cdots N_{q2} \) in (23) must be replaced by the identity matrix \( I \); for \( r = K + 1 \) or \( s = K + 1 \) the terms \( \partial N_p / \partial x_i \) or \( \partial N_q / \partial x_i \), respectively, must be dropped.

The minimiser \( \hat{v}(x) \) of \( \hat{E}[^v] \) satisfies the Euler-Lagrange equation associated to \( \hat{E}[^v] \). Grouping terms of equal order this equation can be written as:
\[
2K + 2 \sum_{m=2}^{K+2} \delta^{m-2} \sum_{|n|=m} \hat{H}_n D^n \hat{v}(x) + \hat{f}(x) = 0, \tag{24}
\]

with
\[
\hat{H}_n = \min_{r=\max(1,m-K-1)}^{\min(K+1,m-1)} \left\{ \begin{array}{ll}
\frac{1}{2} (1)^r + (1)^{m-r} \hat{H}_{r_1 \cdots r_m} \end{array} \right. \tag{25}
\]

Equation (24) is referred to as homogenised equation of order \( 2K + 2 \). It can be rewritten in the classical strain-gradient format of a set of higher-order equilibrium equations involving higher-order stresses [6]. Alternatively, it can be regarded as a set of equilibrium equations of the standard type (1) where the stress tensor depends not only on the (first-order) strains associated to the average displacement \( \hat{v}(x) \), but also on (higher-order) gradients of these strains. The latter view will be taken here, because the influence of higher-order deformation gradients is slightly more transparent in it. The interpretation in terms of strain-gradient theory will be elaborated elsewhere. If we define the average stresses \( \hat{\sigma}_{ij} \) which must satisfy the equilibrium equations
\[
\frac{\partial \hat{\sigma}_{ij}}{\partial x_i} + f_j(x) = 0 \tag{26}
\]

and average strains
\[
\hat{\epsilon}_{kl} = \frac{1}{2} \left( \frac{\partial \hat{v}_k}{\partial x_l} + \frac{\partial \hat{v}_l}{\partial x_k} \right), \tag{27}
\]
equation (24) can be recovered from (26) by defining the constitutive relations
\[
\hat{\sigma}_{ij} = \hat{C}_{ijkl} \hat{\epsilon}_{kl} + \sum_{r=1}^{K} \sum_{|p|=2r} \hat{C}_{ijpkl} D^p \hat{\epsilon}_{kl}, \tag{28}
\]

with
\[
\hat{C}_{ijkl} = \hat{H}_{ijl}^{\ast} \quad \text{and} \quad \hat{C}_{ijpkl} = \frac{1}{|p|!} \sum_{q=\mathcal{P}(p)} \hat{H}_{ijq}^l, \tag{29}
\]

where \( \mathcal{P}(p) \) denotes permutation of the indices \( p \). Note that the constitutive relations have been symmetrised with respect to \( p \) and that use has been made of the fact that \( \hat{H}_{ijq} \) vanishes for odd \( |q| \) (cf. (25)). The stresses \( \hat{\sigma}_{ij} \) thus depend on \( \hat{\epsilon}_{kl} \) and gradients of \( \hat{\epsilon}_{kl} \) of even order up to \( 2K \). The influence of these higher-order gradients, however, decreases as \( e^{2r} \).
4. PRELIMINARY RESULTS

The moduli $\hat{C}_{ijkl}$ and $\hat{C}_{ijkp}$, which appear in the averaged constitutive relations (28) depend on the microstructural functions $N_n(\xi)$ via (23), (25) and (29). In order to obtain these moduli, the boundary value problems (6) on the periodic cell must therefore be solved for all $n$ for which $|n| \leq K$. This has been done numerically for a microstructure consisting of regularly stacked circular fibres embedded in a homogeneous matrix. The periodic cell which has been used in these analyses is shown in Figure 2(a). The diameter of the fibre has been selected such that the fibre volume fraction equals 0.25. Isotropic linear elastic behaviour is assumed for the fibre and matrix material, with respective Young’s moduli $E_f$, $E_m$ and Poisson’s ratios $\nu_f$, $\nu_m$. Only in-plane deformations are considered and a plane strain state is assumed in the fibre direction. Equations (6) have been cast in a weak form and discretised by finite elements (Figure 2(b)). Higher-order terms up to order $K = 3$ have been taken into account. Effective moduli which have thus been obtained have been plotted versus the contrast in elastic moduli $E_f/E_m$ in Figure 3; a value of $\nu_f = \nu_m = \frac{1}{3}$ was used for Poisson’s ratio of the fibre as well as the matrix.

Figure 3(a) shows the moduli $\hat{C}_{ijkl}$ of the standard order. Only the components $\hat{C}_{1111}$, $\hat{C}_{1122}$, $\hat{C}_{1212}$ are given; the other components follow from symmetry properties of $\hat{C}_{ijkl}$ and of the periodic cell. For increasing stiffness of the fibre, the moduli increase from the homogeneous values at $E_f = E_m$ to horizontal asymptotes in the limit of a rigid fibre. The second-order moduli $\hat{C}_{ijklp}$, the unique values of which have been plotted in Figure 3(b), vanish for the homogeneous material ($E_f = E_m$). As the degree of

![Figure 2](image1.png)

(a) (b)

Figure 2. Periodic cell of the fibre-matrix system: (a) geometry and (b) finite element discretisation.

![Figure 3](image2.png)

(a) (b)

Figure 3. Effective moduli: (a) standard, zeroth-order ($\hat{C}_{ijkl}$) and (b) second-order ($\hat{C}_{ijklp}$) versus Young’s modulus of the fibre; both axes have been normalised by Young’s modulus of the matrix.
heterogeneity increases, however, these higher-order terms become more important. It is interesting to note that the second-order moduli asymptote to a finite value for a rigid fibre. The same trend is observed for terms of order higher than two.

5. CONCLUDING REMARKS

The higher-order moduli computed for the fibre-matrix system largely show the behaviour that would be expected on the basis of heuristic arguments. The advantage of the method followed here, however, is that the effective behaviour is computed directly from the properties of the microstructure without any assumptions a priori about the form of the average constitutive relations. It is emphasised that, although a periodic body force has been assumed in deriving the effective constitutive model, its application is by no means limited to this case. The effective moduli are properties of the material and can therefore also be used for non-periodic problems. Periodicity of the microstructure, on the other hand, is an essential condition, which often will not be met for real materials. It is believed, however, that the method may still provide valuable insight and estimates in such cases.

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References