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HIGHER-ORDER ASYMPTOTIC HOMOGENIZATION OF PERIODIC MATERIALS WITH LOW SCALE SEPARATION

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Abstract. *In this work, we investigate the limits of classical homogenization theories pertaining to homogenization of periodic linear elastic composite materials at low scale separations and demonstrate the effectiveness of higher-order periodic homogenization in alleviating this limitation. Classical homogenization techniques are known to be very effective for materials with large scale separation between the scale of the heterogeneity and the macro-scale dimension, but inaccurate at low scale separations. Literature suggests that asymptotic homogenization is capable of pushing the limit to smaller scale separation by taking on board higher-order terms of the asymptotic expansion. We studied infinite two-dimensional elastic two-phase composite materials consisting of stiff inclusions in a soft matrix, subjected to a periodic body force, for various scale ratios between the period of the body force and that of the inclusions. We created reference solution using direct numerical simulation and used ensemble averaging for the complete family of all possible microstructures to obtain the reference homogenized solution. We show that the response predicted using zeroth order classical homogenization deviates from this reference homogenized solution for scale ratios below 10. The higher-order asymptotic homogenization solution still gives a very good approximation even in the low scale separation regime and it becomes better as more higher-order terms are included. The higher-order theory results in a size-dependent macroscopic model, which indeed allows one to push the limitations of homogenization in the direction of less scale separation.*

1 INTRODUCTION

All matter is heterogeneous at some scale, but frequently it is convenient to treat it as homogeneous. Some of the well-known examples are metal alloys, concrete, porous structures and fibrous composites. The distinct features of their microstructures respond quite differently to mechanical loading and hence their deformation is heterogeneously distributed at the scale of that microstructure. It is the combination of the different microstructural features which governs the overall response of the material to the loading.

Homogenization is a mathematical technique for studying partial differential equations with rapidly oscillating coefficients, which are typical of the equations that govern the physics of heterogeneous materials. An important aspect in the analysis of multiphase materials is to deduce their effective behavior (e.g. mechanical stiffness, thermal expansion properties, etc.) from the corresponding single-phase behaviors and the geometrical arrangement of the phases. This concept of rendering "homogeneous" a heterogeneous material is what we call homogenization.

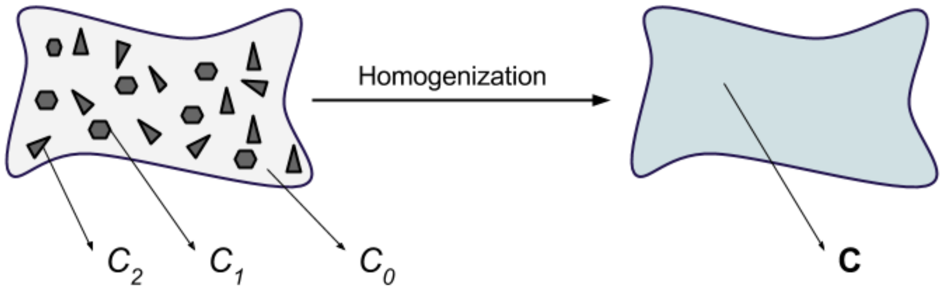

Figure 1: Homogenization: schematic

Conventional homogenization methods are based on *a separation of scales*, given by: $l << L$, where l is the size of the heterogeneity and L represents the macroscopic length scale. However, if the microstructural size is not much smaller, or even of the same order as the macroscopic length scale, then most of the classical homogenization schemes break down. Literature [1-4] suggests that the asymptotic homogenization method is capable of pushing the limit to smaller scale separation, by generating a hierarchy of problems which can be solved sequentially to generate a solution that asymptotically converges to the exact (homogenized) solution.

The present work investigates the scale separation limits of classical homogenization theories and demonstrates the effectiveness of higher order periodic homogenization for small scale separation. A qualitative and quantitative assessment of the scale separation limits of the classical and the higher order periodic homogenization methods is performed on two-dimensional elastic two-phase composites. The details of the problem are described in Section 2. We study the limits of classical homogenization and look into the contribution of each higher order term in rectifying this limitation.

2 PROBLEM DESCRIPTION

An infinite two-dimensional elastic two-phase composite material consisting of stiff circular inclusions in a soft matrix material, is subjected to anti-plane shear by means of a periodic body force. This anti-plane shear problem [1] can be described by the following partial differential equation:

$$\frac{\partial}{\partial x_1}\Big(G\frac{\partial u_3}{\partial x_1}\Big) + \frac{\partial}{\partial x_2}\Big(G\frac{\partial u_3}{\partial x_2}\Big) + F = 0 \tag{1}$$

where $u_3 = u(x_1, x_2)$ is the resulting out-of-plane displacement, $G(x_1, x_2)$ is the Shear Modulus distribution function, defined below, and $F(x_1, x_2)$ is a body force which we define here as $F = F_0 \sin\left(\frac{2\pi x_1}{L}\right) \sin\left(\frac{2\pi x_2}{L}\right)$.

The period of the material's microstructure is l and that of the body force is L, and the ratio L/l hence characterises the scale separation. The homogenized properties are defined not for a specific microstructural configuration with respect to a period of the body force, but for an ensemble averaged microstructural configuration as described in Section 3.

The microstructure consists of a matrix material having Shear Modulus G_m and a circular inclusion having radius r and Shear Modulus G_p. Rather than considering a sharp interface, we define the Shear Modulus function $G(x)$ such that it smoothly varies from G_m to G_p by a cubic distribution. For $a \leq x \leq b$, it is given by:

$$G(x) = \frac{(3a - b - 2x)(b - x)^2 G_m + (a - 3b + 2x)(a - x)^2 G_p}{(a - b)^3} \tag{2}$$

where a and b represents the interface boundaries such that the thickness of the interface is given by $(b - a)$. Fig.2 shows the Shear Modulus distribution for a microstructure having the following parameters: $G_m = 1$, $G_p = 20$, $r = 0.3$, $a = 0.25$ and $b = 0.35$. The amplitude of the body force, F_0, is taken as 1.

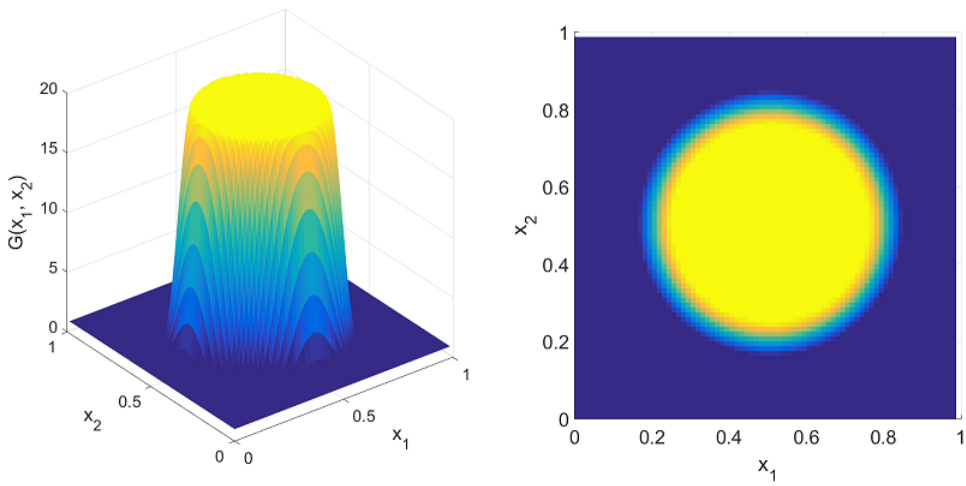

Figure 2: Shear Modulus distribution within a microstructure of size $l = 1$

3 METHODOLOGY

On the one hand, reference solutions are created using direct numerical simulation of a family of microstructural configurations for a range of scale ratios. On the other hand, asymptotic homogenization is used to obtain homogenized properties for zeroth order and higher-order effective continua. Predictions made using these homogenized properties are then compared against the reference solutions. Fig.3 shows a schematic of the methodology.

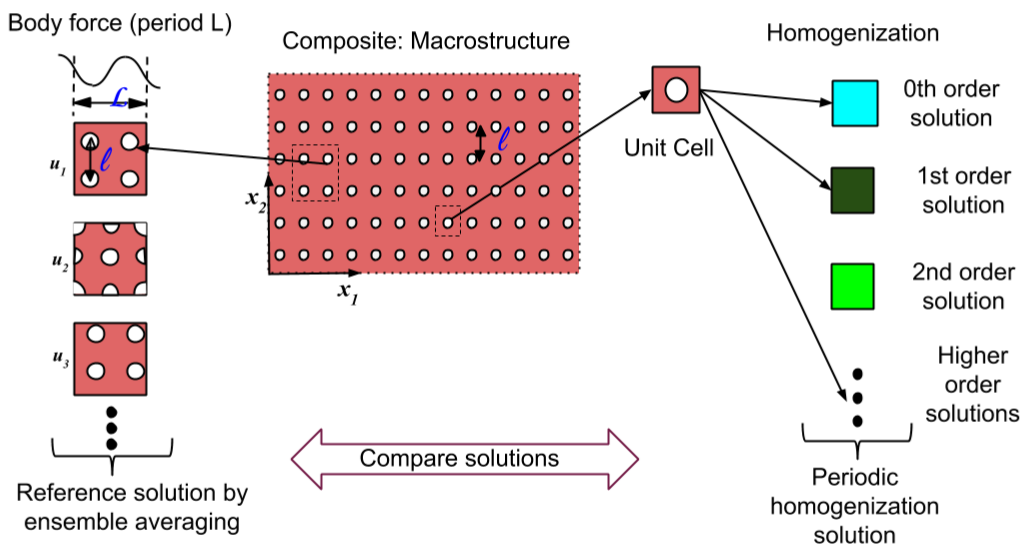

Figure 3: Schematic of the problem: Comparison of periodic homogenization solution with reference solution created by full-scale simulation for various scale ratios

Reference solutions are created using a brute force method, by performing a full-scale numerical simulation. Since the exact location of the microstructure with respect to that the body force is unknown, each relative position is assumed to have the same probability of occurrence. The homogenized response is defined not for a specific microstructural configuration with respect to a period of the body force, but by taking an ensemble average for the complete family of all possible microstructures i.e., by averaging the displacement solutions computed for all shifts. The result is plotted in Fig.4 in terms of the peak averaged displacement (infinity norm) versus the ratio *L/l* for circular inclusions. For scale ratios larger than 10, the curves would be horizontal as the particle sizes become very small relative to the period of the body force and hence do not cause any significant influence on the average displacement solution. As the scale ratio becomes smaller than 10, the relative size of particles becomes high enough to cause size effects, which is apparent in the plot. The curvature of these curves is dependent on the geometry of the microstructure and stiffness contrast.

Periodic homogenization is a rigorous method used to extract effective or homogenized properties from heterogeneous media. For our problem, we first analyze a representative unit cell and derive the effective Shear Moduli. This is then inserted into the macroscopic model to compute the displacement field of the homogenized material subjected to the antiplane shear load defined above.

The microscopic scale described by $\vec{y}$ is determined by the microstructure with a characteristic length l. The macroscopic length $\vec{x}$ described by the wavelength of the applied loading on the material (or the boundary conditions), has a characteristic length L. The small parameter η is defined as the ratio of the two length scales. Hence we have $\eta = l/L$ and $\vec{y} = \eta^{-1}\vec{x}$.

The equilibrium equation can be written in terms of $\vec{x}$ and $\vec{y}$:

$$\vec{\nabla} \cdot (\mathbf{G}(\vec{y}) : \vec{\nabla} u) + \vec{f}(\vec{x}) = 0 \tag{3}$$

Periodic homogenization makes use of an asymptotic expansion of the unknown variable in terms of the powers of the small parameter η:

$$u(\vec{x}) = u_0(\vec{x}, \vec{x}/\eta) + \eta u_1(\vec{x}, \vec{x}/\eta) + \eta^2 u_2(\vec{x}, \vec{x}/\eta) + \mathcal{O}(\eta^3) \tag{4}$$

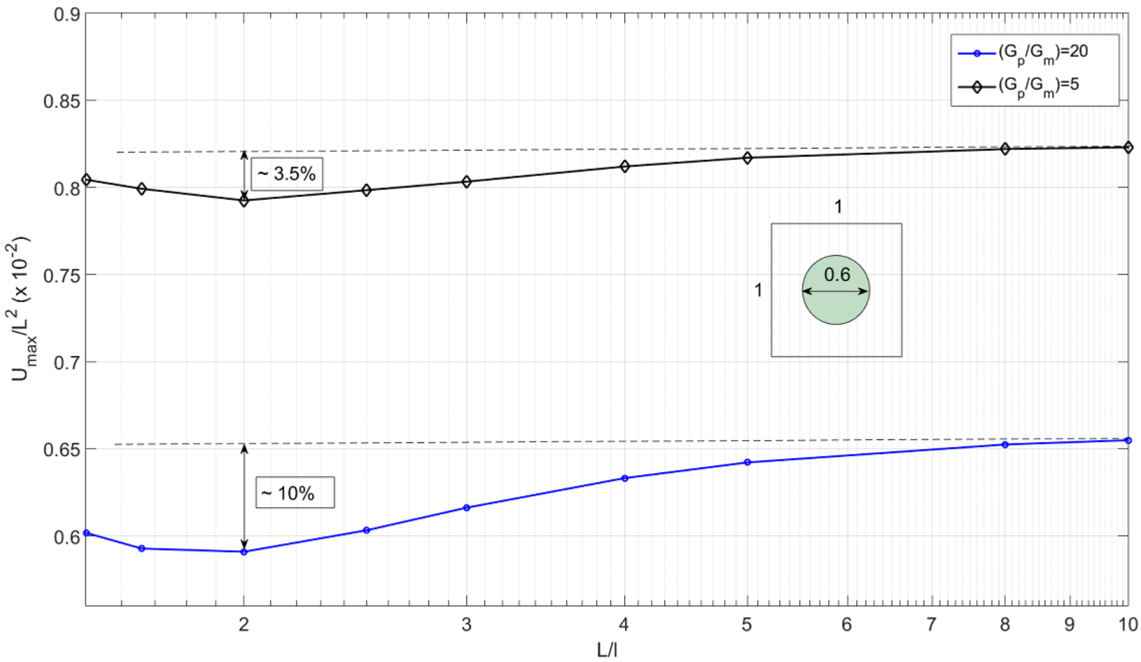

Figure 4: Peak average displacement versus scale ratio for circular inclusions with different stiffness contrast

where the functions $u_i(\vec{x}, \vec{x}/\eta)$ have to be determined and must be periodic in $\vec{y}$. This periodic dependence introduces the fast displacement fluctuations (*microfluctuations*) at the microscale η, while the dependence on $\vec{x}$ is slow. For small η, the equation can be regarded as consisting of a leading term $u_0(\vec{x}, \vec{x}/\eta)$, followed by a series of rapidly diminishing correction terms. As η increases, the contributions from the higher order terms increase and are not negligible anymore.

The essence of this asymptotic method lies in requiring the new equilibrium equation ((3) after replacing u with (4)) to be satisfied at each order of η separately and for independent $\vec{x}$ and $\vec{y}$. Thus, we generate a hierarchy of problems which needs to be solved sequentially to compute the unknown functions u_i. One can show that the result must be of the form [2]:

$$u(\vec{x}) = v_0(\vec{x}) + \eta(v_1(\vec{x}) + N_1(\vec{y}) : \vec{\nabla} v_0) + \eta^2(v_2(\vec{x}) + N_1(\vec{y}) : \vec{\nabla} v_1 + N_2(\vec{y}) \vdots (\vec{\nabla}\vec{\nabla} v_0)^T) + \mathcal{O}(\eta^3) \tag{5}$$

where $N_i(\vec{y})$ is called the microfluctuation function of $(i-1)^{th}$ order, which can be obtained by solving a unit cell problem for each order of η. Here we solve this problem numerically, using a finite difference discretization Fig.5 shows some of the microfluctuation functions computed. Note that the order of magnitude of these fluctuation functions decreases for higher order solutions.

Once the microfluctuation functions are computed, the effective constants of the corresponding order can be calculated. These homogenized constants are then passed on to the macroscale in order to compute the variables v_i.

4 RESULTS

The results obtained using periodic homogenization solution are now compared with the reference solution obtained using direct numerical simulation. Fig.6 shows the average peak displacement, normalized by that predicted by the classically homogenized solution, as a function of the scale ratio $\eta^{-1} = L/l$. Shown are the reference solution, the classical homogenization

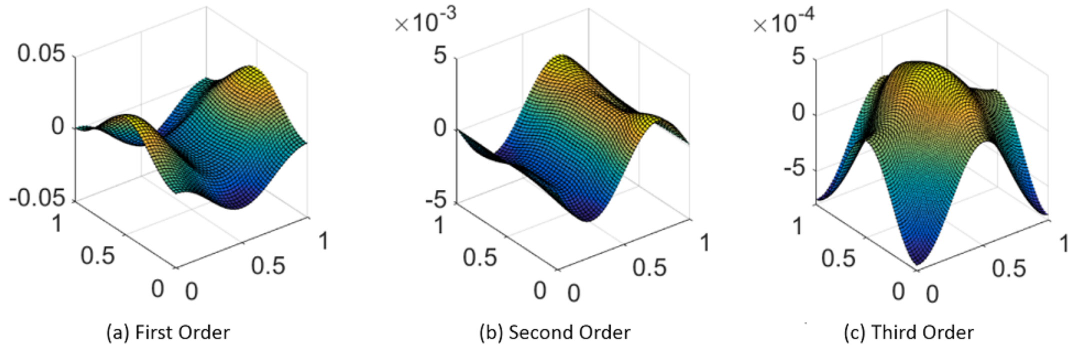

Figure 5: Microfluctuation functions of different orders

solution and higher order solutions, for a phase contrast of 20. The zeroth order classical homogenization solution is independent of the scale ratio and hence is a straight line as shown in the plot. For scale ratios $L/l > 10$, the reference solution converges to this constant value, but at low scale separations it deviates from it significantly. The higher order periodic homogenization solutions closely match with the reference solution even for low scale ratios. The second order solution starts to deviate from the reference solution at $L/l \approx 4.5$, while the fourth order solution can still give a good approximation for even lower scale ratios.

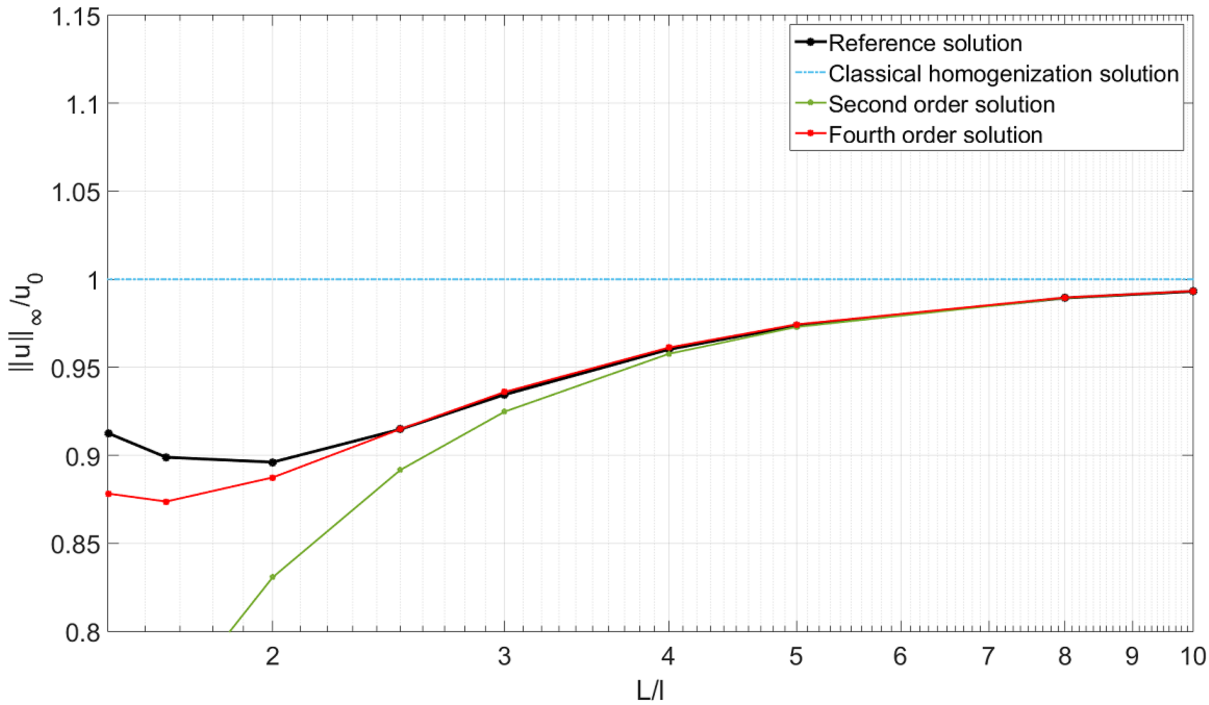

Figure 6: Scale separation plot: Norm of the displacement solution vs. scale separation, for various cases

5 CONCLUSIONS

The result gives a very good insight into the low scale separation regime of an elastic periodic two-phase composite. Some of the observations from this work are as follows:

- The classical homogenization solution is accurate only for cases where $l << L$. However, quantitatively it can still predict homogenized solution accurately for scale separations above $L/l = 10$.

- Higher order periodic homogenization is an accurate method for tackling problems in linear elasticity for the cases with low scale separation. The approximation in the low scale separation regime becomes better as more higher-order terms are included.

- We can conclude that higher order periodic homogenization is not constrained by the conventional separation of scales. It rather has a more flexible law $l < L$, where if the material property and geometry are specified, a clear criteria stating the order required for a certain accuracy can be made.

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