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A COMPARISON OF HOMOGENIZATION, HASHIN-SHTRIKMAN BOUNDS AND THE HALPIN-TSAI EQUATIONS

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Abstract. In this paper we study a unidirectional and elastic fiber composite. We use the homogenization method to obtain numerical results of the plane strain bulk modulus and the transverse shear modulus. The results are compared with the Hashin-Shtrikman bounds and are found to be close to the lower bounds in both cases. This indicates that the lower bounds might be used as a first approximation of the plane strain bulk modulus and the transverse shear modulus. We also point out the connection with the Hashin-Shtrikman bounds and the Halpin-Tsai equations. Optimal bounds on the fitting parameters in the Halpin-Tsai equations have been formulated.

Keywords: Composite materials, homogenization, Hashin-Shtrikman bounds, Halpin-Tsai equations, effective properties

MSC 2000: 35B27, 73B27, 73K20

1. INTRODUCTION

Fiber reinforced composite materials have become an important class of engineering materials. A common feature for such materials is that the locally heterogeneous material behaves like a homogeneous one when the characteristic sizes of the inclusions are much smaller than the whole sample. A multiphase material of this type can be described by the effective properties which are obtained by some type of averaging. One way to proceed is to use the so called homogenization theory, developed in the studies of partial differential equations. Another way is to find bounds for the effective properties.

For design purposes, it is often desirable to have simple and rapid computational procedures for estimating the effective properties. Halpin and Tsai have suggested simple equations for this. These equations depend on a parameter which must be estimated.

In this paper we compare results obtained by the homogenization method with the Hashin-Shtrikman bounds. We will also point out the close connection between the Hashin-Shtrikman bounds and the Halpin-Tsai equations, see Section 2. Furthermore we formulate bounds on the fitting parameter in the Halpin-Tsai equations, see Section 3.

We start by considering a body which occupies a region Ω in \mathbb{R}^3 . We introduce a Cartesian coordinate system (x_i) . Moreover, let us introduce $\sigma = (\sigma_{ij})$, $e = (e_{ij})$, $f = (f_i)$, $t = (t_i)$, $u = (u_i)$ and $n = (n_i)$ as the stress tensor, the strain tensor, the internal force field, the surface force field, the displacement field and the outer unit normal to the boundary $\partial\Omega$ of Ω , respectively.

The governing equilibrium equations are

$$\begin{cases} -\frac{\partial}{\partial x_j} C_{ijkl} e_{kl}(u) = f_i \text{ in } \Omega, \\ u_i = 0 \text{ on } \Gamma_1 \text{ and } C_{ijkl} e_{kl}(u) n_j = t_i \text{ on } \Gamma_2, \end{cases}$$

where $\Gamma_1 \cup \Gamma_2 = \partial\Omega$.

Let us now assume that the body consists of two or more different linear elastic materials which are periodically distributed in the sense that we can define a unit cell (Y) which is periodically repeated. We introduce a local variable $y = \frac{x}{\varepsilon}$. Assume that $C_{ijkl}^\varepsilon = C_{ijkl}(\frac{x}{\varepsilon}) = C_{ijkl}(y)$ is Y-periodic. By Y-periodic we mean that $C_{ijkl}(y_1) = C_{ijkl}(y_2)$ whenever y_1 and y_2 have the same positions in the corresponding cells. This means that ε is a parameter for varying the fineness of the cell structure. We also assume that the functions C_{ijkl} are real-valued, measurable and satisfy the coercivity and boundedness conditions

$$\lambda \xi_{ij} \xi_{ij} \leq C_{ijkl}^\varepsilon \xi_{kl} \xi_{ij} \leq \beta \xi_{ij} \xi_{ij}$$

for every symmetric real-valued tensors ξ_{ij} where $0 < \lambda \leq \beta < \infty$. Physically this means that the strain energy is positive and bounded.

Now we study the following class of problems:

$$(1) \quad \begin{cases} -\frac{\partial}{\partial x_j} C_{ijkl}^\varepsilon e_{kl}(u^\varepsilon) = f_i^\varepsilon \text{ in } \Omega, \\ u_i^\varepsilon = 0 \text{ on } \Gamma_1 \text{ and } C_{ijkl}^\varepsilon e_{kl}(u^\varepsilon) n_j = t_i \text{ on } \Gamma_2. \end{cases}$$

We emphasize that if ε is small, i.e., if we have a fine microstructure, then the functions C_{ijkl}^ε will oscillate very rapidly. Therefore a direct numerical treatment is impossible and we have to attack the problem by making some average or by using the homogenization procedure.

The main idea in the homogenization theory is to approximate the solutions u^ε of (1) by means of a function u which solves the so called *homogenized problem* corresponding to a homogeneous material, with the constant elasticity tensor \overline{C}_{ijkl} . The homogenized tensor \overline{C}_{ijkl} may be interpreted as the physical parameters of a homogeneous material, whose overall response is close to that of the heterogeneous periodic material, when the sizes of the cells tend to zero. The main problem is to find the homogenized tensor \overline{C}_{ijkl} .

The first step in this homogenization procedure is to assume a two scales expansion of $u^\varepsilon(x)$ and $f^\varepsilon(x)$ on the forms

$$u_i^\varepsilon(x) = u_i^{(0)}(x, y) + \varepsilon u_i^{(1)}(x, y) + \varepsilon^2 u_i^{(2)}(x, y) + \dots,$$

and

$$f_i^\varepsilon(x) = f_i^{(0)}(x, y) + \varepsilon f_i^{(1)}(x, y) + \varepsilon^2 f_i^{(2)}(x, y) + \dots,$$

where $u_i^{(n)}(x, y)$ and $f_i^{(n)}(x, y)$, $n = 0, 1, 2, \dots$, are Y -periodic in the variable y .

Next, we use the main homogenization theorem.

Theorem 1. Consider problem (1). Assume that $f_i^\varepsilon \in L^2(\Omega)$, $t_i \in L^2(\Gamma)$ and that C_{ijkl}^ε are Y -periodic. If $f_i^\varepsilon \rightarrow f_i^{(0)}$ in $L^2(\Omega)$, then, as $\varepsilon \rightarrow 0$,

$$u^\varepsilon \rightarrow u^{(0)} \text{ weakly in } [H_0^1(\Omega)]^n,$$

and

$$C_{ijkl}^\varepsilon e_{kl}(u^\varepsilon) \rightarrow \overline{C}_{ijkl} e_{kl}(u^{(0)}) \text{ weakly in } L^2(\Omega) \text{ for every } i \text{ and } j,$$

where

$$\overline{C}_{ijrs} = \frac{1}{|Y|} \int_Y (C_{ijrs} + C_{ijkl} e_{kl}(\chi^{rs})) \, dy,$$

where χ^{rs} is the solution of the cell problem

$$\begin{cases} -\frac{\partial}{\partial y_j} (C_{ijkl} e_{kl}(\chi^{rs})) = \frac{\partial}{\partial y_j} C_{ijrs} \text{ in } Y, \\ \chi^{rs} \text{ is } Y\text{-periodic.} \end{cases}$$

A proof of Theorem 1 can be found in e.g. [Jikov, Kozlov & Oleinik, 1994].

Theorem 1 yields that

$$\begin{cases} -\overline{C}_{ijkl} \frac{\partial}{\partial x_j} e_{kl}(u^{(0)}) = \frac{1}{|Y|} \int_Y f_i^{(0)} \, dy \text{ in } \Omega, \\ u_i^{(0)} = 0 \text{ on } \Gamma_1 \text{ and } \overline{C}_{ijkl} e_{kl}(u^{(0)}) n_j = t_i \text{ on } \Gamma_2. \end{cases}$$

It can also be proved, see e.g. [Persson, Persson, Svanstedt & Wyller, 1993] that the lowest order approximation of the stress field can be expressed as

$$\sigma_{ij}^{(0)}(x, y) = (C_{ijrs}(y) + C_{ijkl}e_{kly}(\chi^{rs}(y)))e_{rsx}(u^{(0)}),$$

where e_{klx} and e_{kly} are defined by

$$e_{klx}(\psi) = \frac{1}{2} \left(\frac{\partial \psi_k}{\partial x_l} + \frac{\partial \psi_l}{\partial x_k} \right) \text{ and } e_{kly}(\psi) = \frac{1}{2} \left(\frac{\partial \psi_k}{\partial y_l} + \frac{\partial \psi_l}{\partial y_k} \right).$$

More information about how to apply the homogenization method to elasticity problems can be found in [Lukkasen, Persson & Wall, 1995]

2. A COMPARISON BETWEEN THE HOMOGENIZED COEFFICIENTS AND THE HASHIN-SHTRIKMAN BOUNDS

Background: There have been intensive studies on how to find bounds on the effective properties of multiphase materials. One of the best known results are the Hashin-Shtrikman bounds. Originally, the Hashin-Shtrikman bounds were formulated for isotropic three dimensional mixtures with arbitrary phase geometry, see [Hashin & Shtrikman, 1963]. In [Hashin, 1965] bounds were derived for transversely isotropic composites with arbitrary phase geometry. The bounds we consider here are those for the plane strain bulk modulus \bar{k} and the transverse shear modulus $\bar{\mu}$ of a two-phase composite. When x_1 and x_2 are in the transverse plane and x_3 is in the fiber direction, \bar{k} and $\bar{\mu}$ are defined by

$$\bar{k} = \frac{1}{2}(\bar{C}_{1111} + \bar{C}_{1122}) \text{ and } \bar{\mu} = \frac{1}{2}(\bar{C}_{1111} - \bar{C}_{1122}).$$

It is also assumed that the composite is well ordered in the sense that both the plane strain bulk modulus k_1 and the transverse shear modulus μ_1 of the first material are bigger than those for the second material, i.e., $k_1 \geq k_2$ and $\mu_1 \geq \mu_2$, where the indices refer to the material number.

Theorem 2. *For a transversely isotropic and well ordered composite the plane strain bulk modulus \bar{k} and the transverse shear modulus $\bar{\mu}$ satisfy*

$$k_l \leq \bar{k} \leq k_u \text{ and } \mu_l \leq \bar{\mu} \leq \mu_u,$$

where

$$k_l = k_2 + \frac{m_1}{\frac{1}{k_1 - k_2} + \frac{m_2}{k_2 + \mu_2}}, \quad k_u = k_1 + \frac{m_2}{\frac{1}{k_2 - k_1} + \frac{m_1}{k_1 + \mu_1}},$$

$$\mu_l = \mu_2 + \frac{m_1}{\frac{1}{\mu_1 - \mu_2} + \frac{m_2(k_2 + 2\mu_2)}{2\mu_2(k_2 + \mu_2)}}, \quad \mu_u = \mu_1 + \frac{m_2}{\frac{1}{\mu_2 - \mu_1} + \frac{m_1(k_1 + 2\mu_1)}{2\mu_1(k_1 + \mu_1)}},$$

and m_i is the volume fraction of material i , $i = 1, 2$.

For a proof see the original paper [Hashin, 1965].

Sharpness: The bounds in Theorem 2 are the best possible in the sense that we can find phase geometries such that they are attained. For the bulk modulus Hashin and Rosen, [Hashin & Rosen, 1964] showed that the lower bound is obtained in the limit, if we fill the space with composite cylinders that consist of a cylindrical core of material 1 surrounded by a cylinder of material 2, see Figure 1. Each composite cylinder is assumed to have the same volume fraction of material 1. The upper bound is attained by switching the place of the materials.

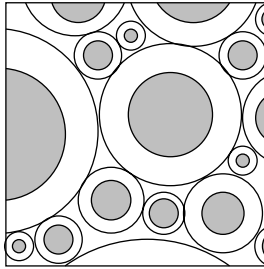


Fig. 1. Hashin-Shtrikman structure

The optimality of the transverse shear modulus remained open for a long time. However, Milton and Kohn, [Milton & Kohn, 1988] used the Hashin-Shtrikman variational principles, see [Hashin & Shtrikman, 1963] or [Hashin, 1983], to derive a tensor inequality on the effective elasticity tensor of a two-phase composite. Lipton used this result to obtain an optimal tensor inequality, see [Lipton, 1991]. The tensor inequality includes the bounds originally derived by Hashin (1965). Moreover, it follows that Hashin's bounds on the transverse shear modulus are attained by rank 3 laminar microgeometries. For more information about bounds we also refer to [Cherkaev & Gibiansky, 1993], [Milton, 1990] and [Lukkasen, Persson & Wall, 1995].

A striking numerical experiment: Now we consider a unidirectional fiber composite consisting of carbon and epoxy. For the sake of simplicity we just compute

the transversal effective components. To compute the effective plane strain bulk modulus \bar{k} and the effective transverse shear modulus $\bar{\mu}$ we use the homogenization method, described in Section 1. We use the following data on k_i and μ_i :

$$(2) \quad \begin{array}{l} \text{Carbon: } k_1 = 10.42 \text{ GPa} \quad \mu_1 = 6.25 \text{ GPa}, \\ \text{Epoxy: } k_2 = 3.70 \text{ GPa} \quad \mu_2 = 1.11 \text{ GPa}. \end{array}$$

In our numerical calculations we model the composite by a hexagonal fiber array, this fiberpacking is known to be transversely isotropic. Note that the materials considered are well ordered. The effective moduli were computed for six different volume fractions of fibers (m_1). The results of these calculations are presented in Table 1.

m_1	0.35	0.45	0.55	0.65	0.75	0.85
\bar{k} (GPa)	4.94	5.41	5.97	6.64	7.46	8.50
$\bar{\mu}$ (GPa)	1.75	2.04	2.42	2.91	3.54	4.38

Table 1.

Now we want to compare these results with the Hashin-Shtrikman bounds, see Theorem 2. In Figures 2 and 3 below the numerical results and the Hashin-Shtrikman bounds are plotted.

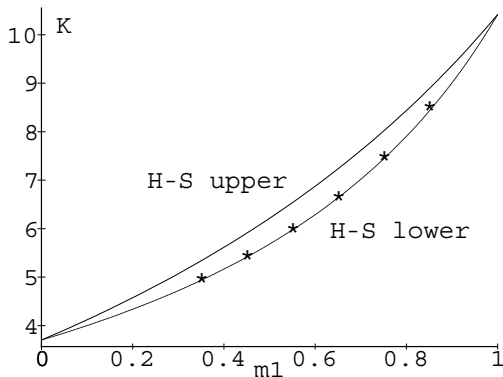


Fig. 2. Numerical results and Hashin-Shtrikman bounds for the bulk modulus.

A physical explanation: We observe that the numerical results are close to the lower bounds. A physical explanation of this can be given for the plane strain bulk modulus. As previously mentioned the bounds were optimal. For \bar{k} the lower bound was reached by filling the body with coated cylinders with material 1 inside. In the

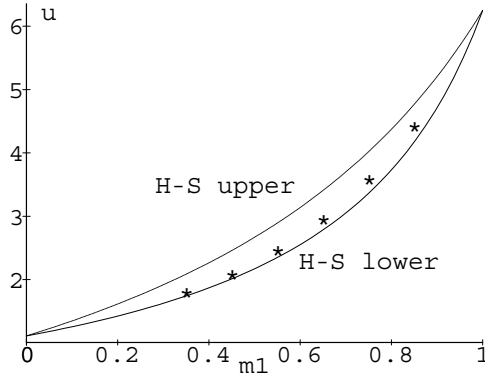


Fig. 3. Numerical results and Hashin-Shtrikman bounds for the shear modulus.

numerical calculations we used a hexagonal fiber array which means that instead of cylinders the body was filled with regular hexagons with a circular inclusion of material 1. Due to the similar geometries, see Figure 4, it is reasonable to believe that the results for these structures would be close to each other.

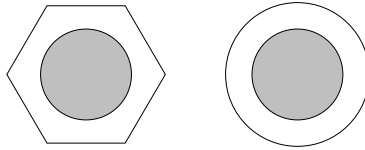


Fig. 4. Coated regular hexagon and coated cylinder.

The numerical results indicate that the lower bounds k_l and μ_l could be used to obtain good approximations of \bar{k} and $\bar{\mu}$. In the next section we discuss the connection between the Hashin-Shtrikman lower bounds and the Halpin-Tsai equations.

3. BOUNDS ON THE FITTING PARAMETER IN THE HALPIN-TSAI EQUATIONS FOR $\bar{\mu}$ AND \bar{k}

For design purposes, it is often desirable to have simple and rapid computational procedures for estimating composite properties. Halpin and Tsai have developed simple equations for this purpose, see e.g. [Halpin & Kardos, 1976] or [Agarwal & Broutman, 1990]. The equations are based on a micromechanics analysis where the composite is assumed to consist of composite cylinders. Let \bar{p} be an effective composite property. The Halpin-Tsai equation for \bar{p} has the form

$$(3) \quad \frac{\bar{p}}{p_2} = \frac{1 + \xi_p \eta m_1}{1 - \eta m_1}, \quad \text{where } \eta = \frac{\frac{p_1}{p_2} - 1}{\frac{p_1}{p_2} + \xi_p},$$

and ξ_p is a fitting parameter, in this paper $\bar{p} = \bar{\mu}$ or $\bar{p} = \bar{k}$.

Remark 1. It was suggested by Halpin and Tsai [Halpin & Kardos, 1976] that the fitting parameter for $\bar{\mu}$ and \bar{k} may be chosen as

$$\xi_\mu = \frac{k_2}{k_2 + 2\mu_2} \quad \text{and} \quad \xi_k = \frac{\mu_2}{k_2},$$

respectively.

The equation (3) motivates that we study the function \bar{p} defined by

$$\bar{p}(\xi_p, m_1) = p_2 \frac{1 + \xi_p \eta m_1}{1 - \eta m_1}, \quad \text{where } \eta = \frac{\frac{p_1}{p_2} - 1}{\frac{p_1}{p_2} + \xi_p} \quad \text{and} \quad 0 \leq \xi_p < \infty, \quad 0 \leq m_1 \leq 1.$$

The function \bar{p} has the following properties:

(i) \bar{p} is an increasing function in m_1 for every fixed ξ_p and

$$\bar{p}(\xi_p, 0) = p_2 \quad \text{and} \quad \bar{p}(\xi_p, 1) = p_1;$$

(ii) \bar{p} is an increasing function in ξ_p for every fixed m_1 ;

(iii)

$$(4) \quad \bar{p}(0, m_1) = \frac{1}{\frac{m_1}{p_1} + \frac{1 - m_1}{p_2}}.$$

This is the harmonic mean also known as the lower Reuss-Voigt bound, see Figures 5 and 7.

(iv)

$$(5) \quad \bar{p}(\xi_p, m_1) \longrightarrow m_1 k_1 + m_2 k_2 \quad \text{as } \xi_p \longrightarrow \infty.$$

This is the arithmetic mean also known as the upper Reuss-Voigt bound, see Figures 5 and 7.

Theorem 3. *The approximation of $\bar{\mu}$ by the Halpin-Tsai equation (3) is equal to the lower Hashin-Shtrikman bound for $\xi_\mu = \frac{k_2}{k_2 + 2\mu_2}$ and to the upper Hashin-Shtrikman bound for $\xi_\mu = \frac{\mu_1 k_1}{\mu_2(k_1 + 2\mu_1)}$.*

Proof. We note that

$$\begin{aligned} \bar{\mu}(\xi_\mu, m_1) &= \mu_2 \frac{1 + \frac{k_2}{k_2 + 2\mu_2} \frac{\frac{\mu_1}{\mu_2} - 1}{\frac{\mu_1}{\mu_2} + \frac{k_2}{k_2 + 2\mu_2}} m_1}{1 - \frac{\frac{\mu_1}{\mu_2} - 1}{\frac{\mu_1}{\mu_2} + \frac{k_2}{k_2 + 2\mu_2}} m_1} \\ &= \frac{\mu_1 \mu_2 (k_2 + 2\mu_2) + k_2 \mu_2^2 + k_2 \mu_2 (\mu_1 - \mu_2) m_1}{\mu_1 (k_2 + 2\mu_2) + k_2 \mu_2 - (k_2 + 2\mu_2) (\mu_1 - \mu_2) m_1}. \end{aligned}$$

Moreover, add and subtract $k_2 \mu_2^2 + 2\mu_2^3 + m_1 \mu_2^2 (k_2 + 2\mu_2) + m_1 \mu_1 \mu_2 (k_2 + 2\mu_2)$ in the numerator, add and subtract $(1 - m_1)(k_2 + 2\mu_2)\mu_2$ in the denominator and use $1 - m_1 = m_2$. Then a straightforward calculation gives

$$\begin{aligned} \bar{\mu}_1(\xi_\mu, m_1) &= \frac{\mu_2 \{ 2\mu_2(k_2 + \mu_2) + (1 - m_1)(k_2 + 2\mu_2)(\mu_1 - \mu_2) \} + m_1 2\mu_2(\mu_1 - \mu_2)(k_2 + \mu_2)}{2\mu_2(k_2 + \mu_2) + (1 - m_1)(k_2 + 2\mu_2)(\mu_1 - \mu_2)} \\ &= \mu_2 + \frac{m_1}{\frac{1}{\mu_1 - \mu_2} + \frac{m_2(k_2 + 2\mu_2)}{2\mu_2(k_2 + \mu_2)}} = \mu_1. \end{aligned}$$

The result for the upper bound follows by a similar calculation. \square

By (4), (5), Theorem 3 and the fact that $\bar{\mu}$ is a continuously increasing function in ξ_μ we conclude that we have a continuous scale of functions. The “end point functions” correspond to the Reuss-Voigt bounds and there are intermediate states that correspond to the Hashin-Shtrikman bounds, see Figure 5.

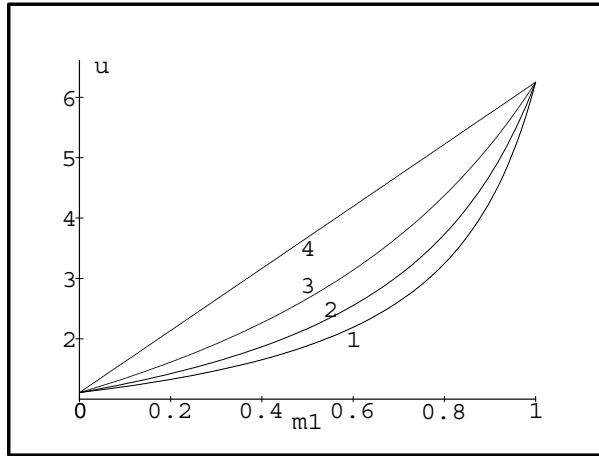


Fig. 5. 1. $\bar{\mu}(0, m_1)$, 2. $\bar{\mu}\left(\frac{k_2}{k_2 + 2\mu_2}, m_1\right)$, 3. $\bar{\mu}\left(\frac{\mu_1 k_1}{\mu_2(k_1 + 2\mu_1)}, m_1\right)$ and 4. $\bar{\mu}(\infty, m_1)$.

As a consequence we can formulate the following bounds on the fitting parameter in the Halpin-Tsai equation:

Corollary 4. *The fitting parameter ξ_μ in the Halpin-Tsai equation for the transverse shear modulus $\bar{\mu}$ must satisfy*

$$\frac{k_2}{k_2 + 2\mu_2} \leq \xi_\mu \leq \frac{\mu_1 k_1}{\mu_2(k_1 + 2\mu_1)}.$$

The numerical results indicate that $\bar{\mu}$ is close to, but above, the lower Hashin-Shtrikman bound, see Figure 3. This shows that the values on $\bar{\mu}$ obtained by using the suggested value on ξ_μ , see Remark 1, in the Halpin-Tsai equation are too low. By using Corollary 4 and the material data given in (2) we conclude that in our example ξ_μ has to satisfy the following condition:

$$0.6 \approx \frac{k_2}{k_2 + 2\mu_2} \leq \xi_\mu \leq \frac{\mu_1 k_1}{\mu_2(k_1 + 2\mu_1)} \approx 2.6.$$

In Figure 6 we have used $\xi_\mu = 0.9$ to fit the curve to the numerical results.

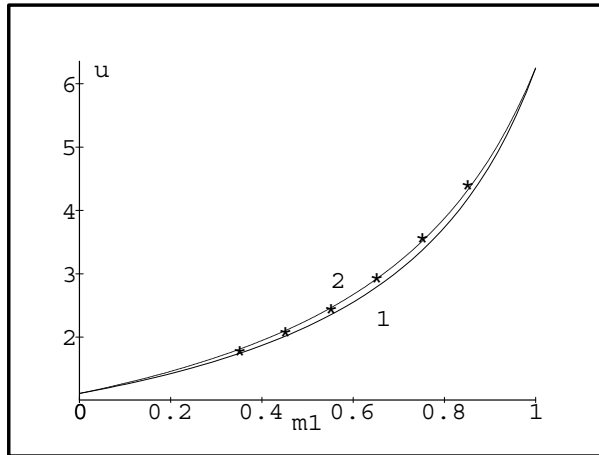


Fig. 6. 1. $\bar{\mu}(\frac{k_2}{k_2+2\mu_2}, m_1)$, 2. $\bar{\mu}(0.9, m_1)$.

Let us now study the corresponding problem for the plane strain bulk modulus \bar{k} .

Theorem 5. *The approximation of \bar{k} defined as in (3) is equal to the lower Hashin-Shtrikman bound for $\xi_k = \frac{\mu_2}{k_2}$ and to the Hashin-Shtrikman upper bound for $\xi_k = \frac{\mu_1}{k_2}$.*

Proof. The proof is similar to that of Theorem 3 so we leave the details to the reader. \square

By (4), (5), Theorem 5 and the fact that \bar{k} is a continuous increasing function in ξ_k we conclude that we have a continuous scale of functions. The “end point functions” correspond to the Reuss-Voigt bounds and there are intermediate states that correspond to the Hashin-Shtrikman bounds, see Figure 7.

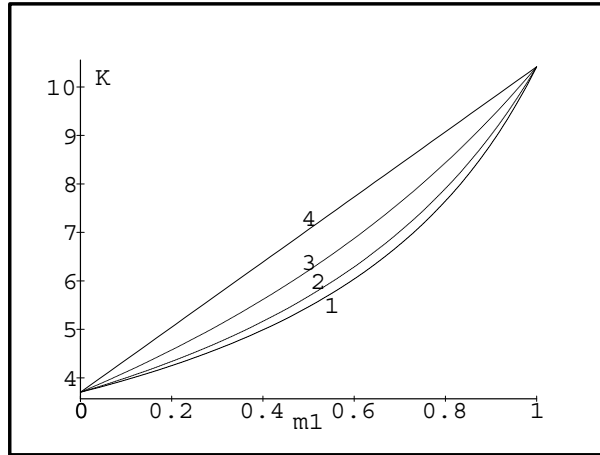


Fig. 7. 1. $\bar{k}(0, m_1)$, 2. $\bar{k}(\frac{\mu_2}{k_2}, m_1)$, 3. $\bar{k}(\frac{\mu_1}{k_2}, m_1)$ and 4. $\bar{k}(\infty, m_1)$.

We have deduced the following important information:

Corollary 6. *The fitting parameter ξ_k in the Halpin-Tsai equation for the plane strain bulk modulus \bar{k} must satisfy*

$$\frac{\mu_2}{k_2} \leq \xi_k \leq \frac{\mu_1}{k_2}.$$

Remark 2. If $\mu_1 = \mu_2$ the bounds coincide and we have an exact solution.

As the numerical results indicate the lower bound could be used as a first approximation of \bar{k} . This suggests that $\xi_k = \frac{\mu_2}{k_2}$ should be used in the Halpin-Tsai equation for \bar{k} . This is in good agreement with Halpin and Tsai’s suggestion, see Remark 1. It is nonetheless important to observe that it is a lower bound, see Corollary 6.

4. CONCLUDING REMARKS

Some supplementary information related to this paper can be found in [Wall, 1994]. In this work we use the homogenization theory to solve a linear elasticity problem. It is nonetheless important to observe that the method is not restricted to linear problems and can be applied to other partial differential equations as well. For other types of problems that have been studied by using this homogenization we refer to [Bakhvalov & Panasenko, 1989], [Dal Maso, 1993], [Jikov, Kozlov & Oleinik, 1994], [Persson, Persson, Svanstedt & Wyller, 1993] and [Sanchez-Palencia, 1980].

In this work we have formulated bounds on ξ_k and ξ_μ independently of each other. By using the results of Cherkaev and Gibiansky (1993) it is reasonable to believe that it is possible to characterize the set of all possible couples of the form (ξ_k, ξ_μ) . These ideas will be developed in a forthcoming paper.

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