ON THE RESPECT TO THE HASHIN-SHTRIKMAN BOUNDS OF SOME ANALYTICAL METHODS APPLYING TO POROUS MEDIA FOR ESTIMATING ELASTIC MODULI

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\textbf{Abstract}
In this work, some popular analytic formulas such as Maxwell (MA), Mori-Tanaka approximation (MTA), and a recent method, named the Polarization approximation (PA) will be applied to estimate the elastic moduli for some porous media. These approximations are simple and robust but can be lack reliability in many cases. The Hashin-Shtrikman (H-S) bounds do not supply an exact value but a range that has been admitted by researchers in material science. Meanwhile, the effective properties by unit cell method using the finite element method (FEM) are considered accurate. Different shapes of void inclusions in two or three dimensions are employed to investigate. Results generated by H-S bounds and FEM will be utilized as references. The comparison suggests that the method constructed from the minimum energy principle PA can give a better estimation in some cases. The discussion gives out some remarks which are helpful for the evaluation of effective elastic moduli.

\textbf{Keywords:} Maxwell approximation; polarization approximation; Mori-Tanaka approximation; effective elastic moduli; porous medium.

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1. Introduction

Most realistic materials, natural or man-made, such as rock, concrete, 3D printing materials contain several phases including pores inside their micro-structures. Modern technologies allow the description of unit cell materials in detail which facilitates extremely convincing results of the effective properties by using computational homogenization [1–8]. In practical engineering, an "instant"estimation, which does not depend too much on resources, is expected. As the distribution of material is random, it is supposed that the possible effective moduli vary in a range. This promoted analytical methods [9–13], which have developed formulas to construct the upper and lower bounds for this effective coefficient. Unfortunately, these formulas may give a large range of effective values, especially in the case of the high contrast between the properties of the matrix and the inclusion. The effective medium approximations (EMA) [14–17] have developed to avoids this drawback, such as

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the self-consistent, differential, correlation approximation [18–22], the Maxwell approximation (MA) [23, 24], the Mori-Tanaka approximations (MTA) [25], and the recent Polarization approximation (PA) [26]. These approximations are applicable for only limited types of inclusions. To overcome this drawback, the equivalent-inclusion approach using artificial neural network has been proposed in [27]. Several works studying PAs have clarified the advantages of this method applying for composite materials. This work will study the application of MA, MTA, and PA to compute effective elastic moduli of some porous microstructures. In the next section, we will review the Maxwell, Mori-Tanaka, and Polarization approximations. After that, numerical examples will be presented to compare the results of MA, MTA, and PA with Hashin-Shtrikman bounds (H-S bounds) and the finite element method (FEM). Finally, some discussion will be presented in the last section.

2. Briefly review of MA, MTA and PA predicting the effective elastic moduli

In this section, we briefly review some analytical approximations which have been used in a wide range of composite materials to estimate the elastic moduli. Considering an isotropic multicomponent material in \( d \)-dimensional space \( (d = 2, 3) \) consisting of \( n \) isotropic components. The matrix phase has the volume fraction \( v_{Ia} \) and the \( \alpha \)-inclusion has the volume fraction \( v_{I\alpha} \). The bulk modulus and shear modulus of the matrix are \( K_M \) and \( \mu_M \), respectively. Those of the \( \alpha \) inclusion phases are \( K_{I\alpha} \) and \( \mu_{I\alpha} \).

2.1. Maxwell approximation

Maxwell Approximations, also called as Maxwell-Garnett or Clausius Mossotti approximations [23, 24], for predicting effective elastic moduli of 2-phase materials are written as:

\[
K_{\text{eff}} = \left( \frac{v_I}{K_I + (d-1)K_{*M}} + \frac{v_M}{K_M + K_{*M}} \right)^{-1} - K_{*M}
\]

where

\[
K_{*M} = K_M \frac{2(d - 1)\mu_M}{d}
\]

and

\[
\mu_{\text{eff}} = \left( \frac{v_I}{\mu_I + \mu_{*M}} + \frac{v_M}{\mu_M + \mu_{*M}} \right)^{-1} - \mu_{*M}
\]

where

\[
\mu_{*M} = \mu_M \frac{d^2 K_M + 2(d + 1)(d - 2)\mu_M}{2dK_M + 4d\mu_M}
\]

2.2. Mori–Tanaka approximation

The MTA, derived as an approximate solution to the field equations for the composite to compute the elastic moduli \( C_{MTA} \), has the expression:

\[
C_{MTA} = \frac{v_M C_M + \sum_{a=2}^{n} v_{Ia} C_{Ia} : D^0_a}{v_M I + \sum_{a=2}^{n} v_{Ia} D^0_a}
\]
where

\[ D_0^\alpha = \left[ I + P_\alpha : C_M^{-1} : (C_{I\alpha} - C_M)^{-1} \right] \]  

(6)

In (5)–(6), \( C_{I\alpha}, C_M \) are elastic moduli of the \( \alpha \)-inclusion and the matrix; \( I \) is quadratic unit tensor. The Eshelby tensor \( P \) in the 2D case is the symmetric depolarization tensor of the ellipsoids from the \( \alpha \)-inclusion phase, determined according to [12]:

\[ P_{1111} = \frac{K_M}{K_M + \mu_M} \left( \frac{a_1^2 + 2a_1a_2}{(a_1 + a_2)^2} + \frac{\mu_M}{K_M} \cdot \frac{a_2}{a_1 + a_2} \right) \]  

(7)

\[ P_{2222} = \frac{K_M}{K_M + \mu_M} \left( \frac{a_1^2 + 2a_1a_2}{(a_1 + a_2)^2} + \frac{\mu_M}{K_M} \cdot \frac{a_1}{a_1 + a_2} \right) \]  

(8)

\[ P_{1122} = \frac{K_M}{K_M + \mu_M} \left( \frac{a_2^2}{(a_1 + a_2)^2} - \frac{\mu_M}{K_M} \cdot \frac{a_2}{a_1 + a_2} \right) \]  

(9)

\[ P_{2211} = \frac{K_M}{K_M + \mu_M} \left( \frac{a_2^2}{(a_1 + a_2)^2} - \frac{\mu_M}{K_M} \cdot \frac{a_1}{a_1 + a_2} \right) \]  

(10)

\[ P_{1212} = \frac{K_M}{K_M + \mu_M} \left( \frac{a_1^2 + a_2^2}{2(a_1 + a_2)^2} + \frac{\mu_M}{2K_M} \right) \]  

(11)

where \( a_1, a_2 \) are the semi axes of the ellipse. For the 3-D case, the formula of Eshelby tensor is more complicated, we refer to [28] for more details.

From (5), the bulk modulus \( K \) and the elastic shear modulus \( \mu \) formula of Mori-Tanaka approximation can be written as:

\[ K_{MTA} = \frac{\nu_M K_M + \sum_{\alpha=2}^{n} \nu_{I\alpha} K_{I\alpha} D_{K\alpha}}{\nu_M + \sum_{\alpha=2}^{n} \nu_{I\alpha} D_{K\alpha}} \]  

(12)

and

\[ \mu_{MTA} = \frac{\nu_M \mu_M + \sum_{\alpha=2}^{n} \nu_{I\alpha} \mu_{I\alpha} D_{\mu\alpha}}{\nu_M + \sum_{\alpha=2}^{n} \nu_{I\alpha} D_{\mu\alpha}} \]  

(13)

\( D_{K\alpha}, D_{\mu\alpha} \) are functions depending on the inclusion-shape, \( D_{K\alpha}, D_{\mu\alpha} \) with \( \alpha \)-ellipsoid inclusion phases, are specified:

\[ D_{K\alpha} = \frac{\alpha_{\mu} (P_{1111} - P_{1122} - P_{2211} + P_{2222}) + 2}{\hat{P}} \]  

(14)

\[ D_{\mu\alpha} = \frac{\alpha_{K} (P_{1111} + P_{1122} + P_{2211} + P_{2222}) + 2}{2\hat{P}} + \frac{1}{2(2\alpha_{\mu} P_{1212} + 1)} \]  

(15)

\[ \hat{P} = 2\alpha_M \alpha_K (P_{1111} P_{2222} - P_{2211} P_{1122}) + (\alpha_K + \alpha_{\mu}) (P_{1111} + P_{2222}) + (\alpha_K - \alpha_{\mu}) + 2 \]  

(16)

\[ \alpha_K = \frac{K_I}{K_M} - 1, \quad \alpha_{\mu} = \frac{\mu_I}{\mu_M} - 1 \]  

(17)

We list in Table 1 the function \( D_{K\alpha}, D_{\mu\alpha} \) for several types of inclusion [? ]:
The effective elastic moduli $C_{\text{eff}}$ ($K_{\text{eff}}, \mu_{\text{eff}}$) of the isotropic composite may be defined via the minimum energy principle:

\[
\varepsilon^0 : C_{\text{eff}} : \varepsilon^0 = \inf_{\langle \varepsilon \rangle = \varepsilon^0} I(\varepsilon), \quad I(\varepsilon) = \int_V \varepsilon : C : \varepsilon dV
\]

for all macroscopic constant strain tensor $\varepsilon^0$ where $\varepsilon$ is expressed through the displacement field $u$, written as $\varepsilon = \frac{1}{2} \left( \nabla u + (\nabla u)^T \right)$. $C$ is fourth rank material stiffness tensor and $\langle . \rangle$ denotes the average over the volume $V$ or via the minimum complementary energy principle:

\[
\sigma^0 : C_{\text{eff}}^{-1} : \sigma^0 = \inf_{\langle \sigma \rangle = \sigma^0} \int_V \sigma : C^{-1} : \sigma dV
\]

for all macroscopic constant stress tensor $\sigma^0$ where the trial stress field $\sigma$ should satisfy $\nabla \cdot \sigma = 0$.

Avoiding the complicated problem of (18), $I(\varepsilon)$ is reformulated using polarization, then, minimizing only principal part of the formula yields the following trial strain field:

\[
\varepsilon_{ij} = \varepsilon_{ij}^0 + \frac{3K_0 + \mu_0}{\mu_0 (3K_0 + 4\mu_0)} \sum_{a=1}^n p_{ij}^a \varphi_{a,ijkl} - \frac{1}{2\mu_0} \sum_{a=1}^n \left( p_{ai}^a \varphi_{ajm} + p_{aj}^a \varphi_{aim} \right)
\]

where $(K_0, \mu_0)$ are elastic moduli of the reference material, $p_{ij}^a$ is the component $ij$ of the polarization field of the second order tensor $p^a, \varphi^a, \psi^a$ are harmonic and biharmonic potentials, see [26, 29, 30] for more details. There are several ways to determine the free reference parameters $K_0, \mu_0$. In this paper, the PA uses dilute solution reference, as most of other EMAs use this solution as the starting point.

By using (20) as the optimal polarization trial fields, the PA for the macroscopic elasticity of a general isotropic $n$-component material has the particular form:

\[
K_{PA} = \left( \sum_{a=1}^n \frac{v_a}{K_a + K_*} \right)^{-1} - K_*
\]

\[
\mu_{PA} = \left( \sum_{a=1}^n \frac{v_a}{\mu_a + \mu_*} \right)^{-1} - \mu_*
\]
where \( K_s \) and \( \mu_s \) are solutions of the following equations:

\[
\sum_{a=2}^{n} v_a \left( K_a - K_M \right) \left( \frac{K_M + K_s}{K_a + K_s} - D_{K_a} \right) = 0
\]

\[
\sum_{a=2}^{n} v_a \left( \mu_a - \mu_M \right) \left( \frac{\mu_M + \mu_s}{\mu_a + \mu_s} - D_{\mu_a} \right) = 0
\]

Note that using a suitable trial stress tensor to solve problem (18) came to the same results as (21) and (22) interestingly [29].

3. Numerical examples

In this section, we will examine some micro-structures using MA, PA, and MTA in 2D and 3D cases. Several shapes of inclusions will be considered: circle, ellipse (2D) and platelet, spherical, needle (3D).

3.1. 2D porous examples

We consider a sample of the size \( 1 \times \sqrt{3} \) mm in two cases of porous medium: (i) void circular inclusions (I1) and (ii) void ellipse inclusions (I2). The axis ratio of ellipse inclusion \( a/b \) equals 1/2. The distribution of inclusions is shown in Fig. 2 in which the nearest distance between the center of inclusions is 0.5 mm. The bulk modulus \( K_M \) and the shear modulus \( \mu_M \) of the matrix are 1 kN/mm\(^2\) and 0.4 kN/mm\(^2\), respectively.

The bulk modulus and the shear modulus estimated by MA, PA, MTA are shown in Figs. 2 and 3 in the comparison with FEM and H-S bounds. We can see that: (i) with void circular inclusion, the results estimated by MA, PA, MTA coincide. Simultaneously, these moduli show a good agreement with the result from the unit-cell method (FEM); (ii) with void ellipse circular inclusions, the MA results coincide with the upper H-S bounds (HSU), which defer lightly from the results by MTA and PA. We note that in FEM implementation, 160000 regular tri-elements have been utilized. The material coefficients of the void phase are extremely small (1E-6). This is easy to learn when comparing the formula of these estimations. However, the agreement reduces remarkably between the results of analytic methods and FEM when the volume fraction of the void phase increases.
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3.2. 2D 3-component examples

This section employs some 3-component porous media to compare results generated by PA, MTA, and the H-S bounds. First, a square sample in 2D of the size 1 × 1 mm² as shown in Fig. 4 is employed to investigate.

The elastic properties of components are: (i) the matrix (\(K_M, \mu_M\)) = (1, 0.4) kN/mm², (ii) void ellipse inclusions (\(K_{11}, \mu_{11}\)) = (0, 0) kN/mm², (iii) circular inclusions (\(K_{12}, \mu_{12}\)) = (20, 12) kN /mm². The ellipse inclusions (in dark) have the volume fraction of 10.1% while that of circular inclusions (in white) varies. The ratio between radius of ellipse \(a/b = 1/5\). In FEM implementation, we used 180000 triangular elements, and the material properties of the voids phase are nearly zeros as they are in 2D 2-component examples.
Figure 4. A 2D 3-component unit cell with ellipse and circle inclusions

The elastic properties of components are: (i) void ellipse inclusions, whose properties of the matrix are larger than those of the inclusions. The properties of the matrix \((M_K, \mu_K)\), ellipse inclusions \((K_{11}, \mu_{11}) = (40, 20) \text{ kN/mm}^2\), ellipse inclusions \((K_{12}, \mu_{12}) = (10, 0.4) \text{ kN/mm}^2\). We consider another 2D 3-component sample in which the properties of the matrix are larger than those of the inclusions. The properties of the matrix \((M_K, \mu_K)\), ellipse inclusions \((K_{11}, \mu_{11}) = (0, 0) \text{ kN/mm}^2\), circular inclusions \((K_{12}, \mu_{12}) = (10, 0.4) \text{ kN/mm}^2\).

Fig. 5 plots the bulk modulus (a) and shear modulus (b). In this case, there is no significant discrepancy between MTA and PA estimation while the discrepancy between those and FEM increases in proportion to the volume fraction of inclusions.

We consider another 2D 3-component sample in which the properties of the matrix are larger than those of the inclusions. The properties of the matrix \((M_K, \mu_K)\), the ellipse inclusions \((K_{11}, \mu_{11})\) and circular inclusions \((K_{12}, \mu_{12})\) are \((1, 0.4)\), \((0, 0)\), \((20, 12) \text{ kN/mm}^2\), respectively. With this set of data, the MTA lightly violates the upper HS bound while those the PA is closely under the upper bounds as shown in Fig. 6.
the case of platelet and sphere inclusion. The MTA may invade but PA always respects the H-S bounds.

Note that, in these examples, ellipse inclusions $(I_{1K}, I_{1P}) = (1, 0.4)$, circular inclusions $(I_{2K}, I_{2P}) = (0, 0)$ kN/mm$^2$, and sphere inclusions $(I_{12K}, I_{12P}) = (0, 0)$ kN/mm$^2$. The bulk modulus $K_{11} = (10, 0.4)$ kN/mm$^2$, $K_{12} = (20, 12)$ kN/mm$^2$, $I_1$ and $I_2$.

3.3. 3D 3-component examples

Figure 6. Comparison of elastic modulus estimated by PA and MTA of a 2D 3-component unit cell: the matrix $(K_M, \mu_M) = (40, 20)$ kN/mm$^2$, ellipse inclusions $(K_{11}, \mu_{11}) = (1, 0.4)$ kN/mm$^2$, circular inclusions $(K_{12}, \mu_{12}) = (0, 0)$ kN/mm$^2$.

Figure 7. Comparison of Bulk modulus estimated by PA and MTA of a 3D material with the matrix $(K_M, \mu_M) = (40, 20)$ kN/mm$^2$, ellipsoid inclusions $(K_{11}, \mu_{11}) = (10, 0.4)$ kN/mm$^2$ and sphere inclusions $(K_{12}, \mu_{12}) = (0, 0)$ kN/mm$^2$, $v_1 = v_{11} + v_{12}$.
In this part, we apply MTA and PA for some 3D porous media with several types of inclusion, including platelet, needle, and sphere. In the following examples, the properties of the matrix \((K_M, \mu_M)\) are constant at \((40, 20) \text{kN/mm}^2\). The bulk modulus is taken into consideration in different cases of volume fraction from low to high.

Fig. 7 plots the estimation of MTA and PA for the case of ellipsoid inclusions \((K_{11}, \mu_{11}) = (10, 0.4) \text{kN/mm}^2\) and sphere voids \((K_{12}, \mu_{12}) = (0, 0) \text{kN/mm}^2\). We can observe that PA, MTA, and HSU nearly coincide when the volume fraction of needles is small \(\nu_{11} = 5\%\) and \(15\%\). Whereas, as can be seen in Fig. 7(c) when the volume fraction of needles is \(75\%\), the MTA estimation start to exceed the HSU and PA estimation still respect the upper of H-S bounds.

Fig. 8 plots the estimation of MTA and PA for the case when inclusions are platelets \((K_{11}, \mu_{11}) = (10, 0.4) \text{kN/mm}^2\) and sphere \((K_{12}, \mu_{12}) = (0, 0) \text{kN/mm}^2\). In this case, the violation of MTA is first observed in Fig. 8(b) when the platelet phase has a volume fraction of \(\nu_{11} = 15\%\). This is more obvious in Fig. 8(c) when the sample contains a high proportion of platelet \(\nu_{11} = 75\%\). Again, the violation to H-S bounds of PA is acknowledged.

![Diagram](image_url)

Figure 8. Comparison of elastic modulus estimated by PA and MTA of a 3D material with the matrix \((K_M, \mu_M) = (40, 20) \text{kN/mm}^2\), platelet inclusions \((K_{11}, \mu_{11}) = (10, 0.4) \text{kN/mm}^2\), spherical inclusions \((K_{12}, \mu_{12}) = (0, 0) \text{kN/mm}^2\)

Similarly, we consider the case when inclusions are platelets and ellipsoids (voids). Fig. 9 plots the estimation of MTA and PA in the three cases of platelet inclusion volume fraction \(5\%, 15\%, 75\%\)
respectively. The trend is not different from the case of platelet and sphere inclusion. The MTA may invade but PA always respects the H-S bounds.

Figure 8. Comparison of elastic modulus estimated by PA and MTA of a 3D material with the matrix \((K_M, \mu_M) = (40, 20)\) kN/mm\(^2\), platelet inclusions \((K_{I1}, \mu_{I1}) = (10, 0.4)\) kN/mm\(^2\), spherical inclusions \((K_{I2}, \mu_{I2}) = (0, 0)\) kN/mm\(^2\).

Figures (a) \(\nu_{I1} = 5\%\), (b) \(\nu_{I1} = 15\%\), (c) \(\nu_{I1} = 75\%\).

Figure 9. Comparison of elastic modulus estimated by PA and MTA of a 3D material with the matrix \((K_M, \mu_M) = (40, 20)\) kN/mm\(^2\), platelet inclusions \((K_{I1}, \mu_{I1}) = (10, 0.4)\) kN/mm\(^2\), ellipsoid inclusions \((K_{I2}, \mu_{I2}) = (0, 0)\) kN/mm\(^2\). 

Note that, in these examples, \(\nu_{I2}\) varies and \(\nu_I = \nu_{I1} + \nu_{I2}\).

4. Conclusions

This work has investigated the respect to H-S bounds of the MTA and PA0 of some porous media. The results reveal that: (i) in a 2D porous medium, in which the void inclusion is ideally circular, the estimation of MA, MTA, and PA coincide and agree with that of FEM while the deviation is clearly when the shape of inclusions changes to ellipses; (ii) The MTA estimation can violate the H-S bounds when the sample is highly porous in the case of 2D-3 phase composite; (iii) The influence of platelet inclusion is significant in the sense of the violation HS- bounds when estimating by MTA. In all the investigated example, the polarization approximation respects the H-S bounds which suggests that PA is a reliable method.
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References


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