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POLARIZATION VERSUS MORI–TANAKA APPROXIMATIONS FOR EFFECTIVE CONDUCTIVITY OF ISOTROPIC COMPOSITES

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Abstract. Our polarization approximations for the effective conductivity of isotropic multicomponent materials, constructed recently as approximate solutions to the minimum energy principles, are compared with the widely used Mori–Tanaka approximation, derived as an approximate solution of the field equations. The similarities and differences, advantages and disadvantages of both approaches are analysed with illustrating numerical examples.

Keywords: Effective conductivity, isotropic composite material, polarization approximation, Mori–Tanaka approximation.

1. INTRODUCTION

Many practical composites, though having irregular microgeometries, often have relatively definite isotropic macroscopic properties, because the inhomogeneities do not have preference direction distribution in the material space and share some common specific feature. Hence various approximate formulae have been developed to estimate the effective properties, from the simplest volume arithmetic and harmonic averages to the more-advanced effective medium approximations (EMA) [1, 2]. One of the most notable EMAs applied to matrix composites is the Mori–Tanaka one, which has been used widely in applications [3–6]. Likes many other EMAs, the Mori–Tanaka approximation has been derived from the field equations using analytical dilute solution results for ellipsoidal inclusions suspended in a major matrix. Alternatively, polarization approximations have been constructed from a variational approach [7, 8]. Both approximations will be analysed and compared in this study.

2. MORI–TANAKA AND POLARIZATION APPROXIMATIONS

Let us consider an isotropic multicomponent material that consists of n components of volume proportions v_α having conductivities c_α ($\alpha = 1, \ldots, n$) in 3-dimensional Euclidean space.

Specifically, Mori–Tanaka approximation (MTA) applies to a matrix composite, which is composed of the matrix phase having the characteristics v_1, c_1, and ellipsoidal inclusions of aspect ratios $a_1^{(\alpha)} : a_2^{(\alpha)} : a_3^{(\alpha)}$ from the α-inclusion phases having the characteristics v_α, c_α, $\alpha = 2, \ldots, n$.

The Mori–Tanaka approximation c_{MTA}, derived as an approximate solution to the field equations for the composite, has the particular expression [3]

$$\begin{aligned} c_{MTA} = \quad & \left\{ v_1 c_1 + \sum_{\alpha=2}^{n} \frac{v_\alpha c_\alpha}{3} \sum_{i=1}^{3} \left[1 + \frac{p_i^{(\alpha)} (c_\alpha - c_1)}{c_1} \right]^{-1} \right\} \\ & \cdot \left\{ v_1 + \sum_{\alpha=2}^{n} \frac{v_\alpha}{3} \sum_{i=1}^{3} \left[1 + \frac{p_i^{(\alpha)} (c_\alpha - c_1)}{c_1} \right]^{-1} \right\}^{-1} , \end{aligned} \tag{1}$$

where $\mathbf{p}^{(\alpha)}$ is the symmetric depolarization tensor of the ellipsoids from the α-inclusion phase, which in the principal axes frame has the diagonal components or eigenvalues (called also the depolarization factors) given by elliptic integrals

$$p_i^{(\alpha)} = \frac{1}{2} \prod_{k=1}^{3} a_k^{(\alpha)} \int_0^\infty \frac{\mathrm{d}t}{\left[t + \left(a_i^{(\alpha)}\right)^2 \right] \sqrt{\prod_{j=1}^{3} \left[t + \left(a_j^{(\alpha)}\right)^2 \right]}} , \quad i = 1, 2, 3 ; \tag{2}$$

$a_i^{(\alpha)}$ is the semiaxis of the ellipsoid along the x_i direction; Trace $\mathbf{p}^{(\alpha)} = \sum_{i=1}^{3} p_i^{(\alpha)} = 1,\ 0 \leq p_i^{(\alpha)} \leq 1$. For examples,

- For the sphere $p_i^{(\alpha)} = \dfrac{1}{3}$.
- For the platelet $p_1^{(\alpha)} = 1; p_2^{(\alpha)} = p_3^{(\alpha)} = 0$.
- For the fiber $p_1^{(\alpha)} = p_2^{(\alpha)} = \dfrac{1}{2}; p_3^{(\alpha)} = 0$.

The physical implications are that the particle sees a surrounding matrix as that with an average temperature gradient of the matrix. The approximation is given in an explicit form and well describes behaviour of many practical composites, however it may violate Hashin–Shtrikman (HS) bounds for isotropic multicomponent materials [9].

The polarization approximation c_{PA} for the effective conductivity of a general isotropic n-component material, constructed as an approximate solution from the minimum energy principles, has the particular form [8]

$$c_{PA} = P_c(c_*) = \left(\sum_{i=1}^{n} \frac{v_i}{c_i + c_*} \right)^{-1} - c_* , \tag{3}$$

where the reference parameter c_* should be determined from a reference dilute solution result, or reference effective conductivity of the composite at certain finite volume proportions of the components (obtained theoretically, numerically, or experimentally). Once the reference effective conductivity c^{eff} satisfies HS bounds, the respective reference parameter c_* should lie within the limits

$$2c_{\min} \leq c_* \leq 2c_{\max} \,, \tag{4}$$

where $c_{\min} = \min\{c_1, \ldots, c_n\}$, $c_{\max} = \max\{c_1, \ldots, c_n\}$; then the polarization approximation (3) would obey HS bounds [10] over all the volume proportions v_α of the component materials

$$P_c\left(2c_{\min}\right) \leq c_{PA} \leq P_c\left(2c_{\max}\right) \,. \tag{5}$$

Presume the dilute solution result for the suspension of the same-geometry inclusions with the properties c_α, volume fractions tv_α $(\alpha = 2, \ldots, n\ ;\ t \ll 1)$ in the predominant matrix of conductivity c_1 is

$$c^{eff} = c_1 + \sum_{\alpha=2}^{n} tv_\alpha (c_\alpha - c_1) D_\alpha(c_\alpha, c_1) \,, \quad t \ll 1 \,, \tag{6}$$

where D_α are some inclusion-functions, which are specific for every α-inclusion-component's geometry.

In the case of matrix composite with the matrix component v_1, c_1, the polarization approximation (3) using dilute solution reference (6) would have the reference parameter c_* to be the solution of the equation

$$\sum_{\alpha=2}^{n} v_\alpha (c_\alpha - c_1) \left(\frac{c_1 + c_*}{c_\alpha + c_*} - D_\alpha(c_\alpha, c_1) \right) = 0 \,. \tag{7}$$

The polarization approximation (3), (7) using the dilute solution reference will be referred to as PA0, while that using a reference effective conductivity of the composite at certain finite volume proportions of the components will be referred to as PA1.

In the case of two-component matrix composite the solution c_* of (7) is obtained explicitly

$$c_* = \frac{D(c_2, c_1) c_2 - c_1}{1 - D_2(c_2, c_1)} \,. \tag{8}$$

Explicit expression of inclusion-function $D_\alpha(c_\alpha, c_1)$ in the case of isotropically-distributed ellipsoidal inclusions is

$$D_\alpha(c_\alpha, c_1) = \frac{c_1}{3} \sum_{i=1}^{3} \frac{1}{c_\alpha p_i^{(\alpha)} + c_1\left(1 - p_i^{(\alpha)}\right)} \,, \tag{9}$$

where $p_i^{(\alpha)}$ is defined in (2). An analytical comparison (in the next section) will reveal that the PA0 from (3), (8) for the two-component matrix composites with ellipsoidal inclusions coincides with MTA from (1).

In the specific case of spherical (circular) inclusion, one has

$$D(c_I, c_M) = \frac{3c_M}{c_I + 2c_M} , \tag{10}$$

and according to (8), one finds

$$c_* = 2c_M . \tag{11}$$

PA0 for sphere-like inclusion composites from (3), (11) also appears to coincide with MTA from (1), and one of HS bounds.

However PA0 and MTA will differ in the more general cases, as will be considered in the next section.

3. COMPARISONS

Consider firstly the case of two-component matrix composite. (1) is simplified as

$$\begin{aligned} c_{MTA} = & \left\{ v_1 c_1 + \frac{v_2 c_2}{3} \sum_{i=1}^{3} \left[1 + \frac{p_i^{(2)}(c_2 - c_1)}{c_1} \right]^{-1} \right\} \\ & \cdot \left\{ v_1 + \frac{v_2}{3} \sum_{i=1}^{3} \left[1 + \frac{p_i^{(2)}(c_2 - c_1)}{c_1} \right]^{-1} \right\}^{-1} , \end{aligned} \tag{12}$$

or

$$c_{MTA} = \frac{v_1 c_1 + v_2 c_2 D(c_2, c_1)}{v_1 + v_2 D(c_2, c_1)} . \tag{13}$$

In the mean time, the polarization approximation (3) can be rewritten as

$$c_{PA} = \left(\frac{v_1}{c_1 + c_*} + \frac{v_2}{c_2 + c_*} \right)^{-1} - c_* . \tag{14}$$

Substituting (8) into (14), after some manipulation, one obtains

$$c_{PA0} = \frac{v_1 c_1 + v_2 c_2 D(c_2, c_1)}{v_1 + v_2 D(c_2, c_1)} . \tag{15}$$

From (13) and (15), one can see that two approximations coincide.

However such agreement has not been observed in the general case of multi-component matrix composite ($n > 2$). For example, let us consider a composite which consists of 3 phases: the matrix phase having the characteristics v_1, c_1; the second phase is from the spherical inclusions with conductivity c_2 and volume fraction v_2; the third phase is from the platelet inclusions with conductivity c_3 and volume fraction v_3.

In this case, Mori–Tanaka approximation is determined by the following equation

$$c_{MTA} = \frac{v_1 c_1 + v_2 c_2 D(c_2, c_1) + v_3 c_3 D(c_3, c_1)}{v_1 + v_2 D(c_2, c_1) + v_3 D(c_3, c_1)} , \tag{16}$$

in which

$$D(c_2, c_1) = \frac{3c_1}{2c_1 + c_2}; \quad D(c_3, c_1) = \frac{c_1 + 2c_3}{3c_3} . \tag{17}$$

The polarization approximation has the form:

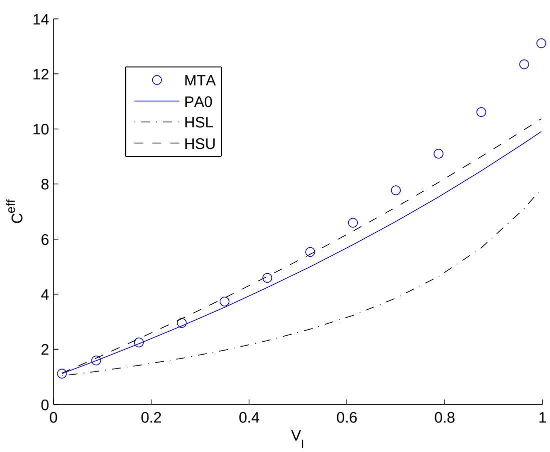
$$c_{PA0} = \left(\frac{v_1}{c_1 + c_*} + \frac{v_2}{c_2 + c_*} + \frac{v_3}{c_3 + c_*} \right)^{-1} - c_* \,, \tag{18}$$

with c_* is the solution of the following equation:

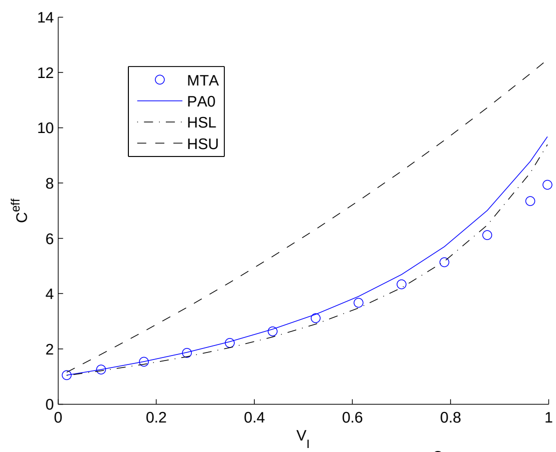
$$v_2(c_2 - c_1)\left(\frac{c_1 + c_*}{c_2 + c_*} - \frac{3c_1}{2c_1 + c_2} \right) + v_3(c_3 - c_1)\left(\frac{c_1 + c_*}{c_3 + c_*} - \frac{c_1 + 2c_3}{3c_3} \right) = 0 \,. \tag{19}$$

For illustrations, consider 2 sets of component conductivities:

- Set 1: $c_1 = 1, c_2 = 5, c_3 = 20$.
- Set 2: $c_1 = 1, c_2 = 20, c_3 = 5$.



(a) $c_1 = 1, c_2 = 5, c_3 = 20, v_3 = \frac{3}{4}v_2$



(b) $c_1 = 1, c_2 = 20, c_3 = 5, v_3 = \frac{3}{4}v_2$

Fig. 1. Polarization (PA0) and Mori–Tanaka (MTA) approximations versus HS bounds for the three-component matrix composites having the spherical and platelet inclusion

Fig. 1(a) presents the polarization and Mori–Tanaka approximations for Set 1 (numerical results are presented in Tab. 1). HS bounds are included for comparisons. One can see that PA0 and MTA differ: while PA0 always obeys HS bounds, MTA violates HS upper bound at high volume proportion of inclusion ($v_I = v_2 + v_3 > 0.55$). The Fig. 1(b) presents the results for Set 2 (numerical results are presented in Tab. 2), where MTA violates HS lower bound. The violation of MTA also has been reported by Norris [9] for three-component composite with platelet inclusions at certain components' conductivity and volume fraction point.

Second example: A matrix composite consists of ellipsoidal (v_2, c_2) and platelet (v_3, c_3) inclusions, the conductivities of the component are:

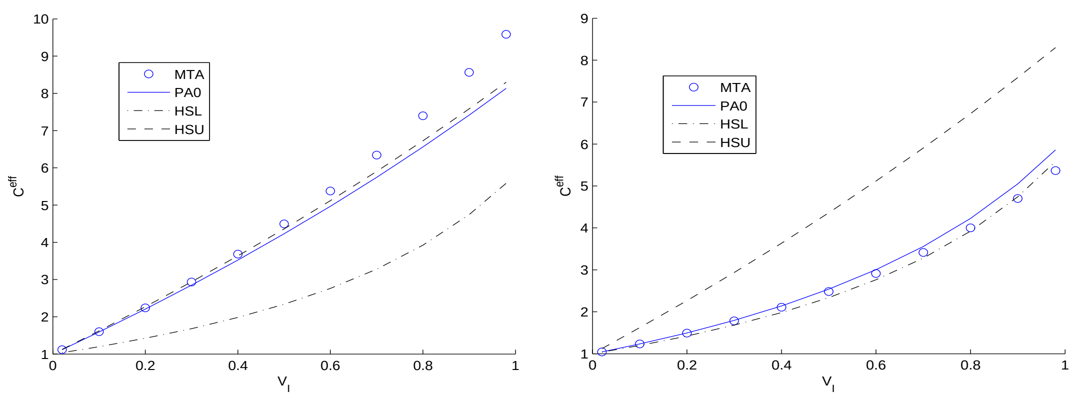
- Set 3: $c_1 = 1, c_2 = 3, c_3 = 16$.
- Set 4: $c_1 = 1, c_2 = 16, c_3 = 3$.

Table 1. Polarization versus Mori–Tanaka approximations for the three-component matrix composites having the spherical and platelet inclusions, with $c_1 = 1, c_2 = 5, c_3 = 20$, $v_3 = \frac{3}{4} v_2$

$v_I = v_2 + v_3$	MTA	PA0
0.0175	1.1155	1.1151
0.175	2.2460	2.2015
0.35	3.7324	3.5274
0.525	5.5364	4.9979
0.7	7.7719	6.6382
0.875	10.6147	8.4795
0.9975	13.1124	9.9086

Table 2. Polarization versus Mori–Tanaka approximations for the three-component matrix composites having the spherical and platelet inclusions, with $c_1 = 1, c_2 = 20, c_3 = 5$, $v_3 = \frac{3}{4} v_2$

$v_I = v_2 + v_3$	MTA	PA0
0.0175	1.0484	1.0485
0.175	1.5361	1.5446
0.35	2.2171	2.2616
0.525	3.1108	3.2482
0.7	4.3354	4,6920
0.875	6.1165	7.0064
0.9975	7.9358	9.6789



(a) $c_1 = 1, c_2 = 3, c_3 = 16, v_3 = v_2$ (b) $c_1 = 1, c_2 = 16, c_3 = 3, v_3 = v_2$

Fig. 2. Polarization (PA0) and Mori–Tanaka (MTA) approximations versus HS bounds for the three-component matrix composites having the ellipsoidal and platelet inclusions

The respective results for the matrix-composite are presented in Fig. 2 (numerical results are presented in Tabs. 3 and 4).

Table 3. Polarization versus Mori–Tanaka approximations for the three-component matrix composites having the ellipsoidal and platelet inclusions, with $c_1 = 1, c_2 = 3, c_3 = 16, v_3 = v_2$

$v_I = v_2 + v_3$	MTA	PA0
0.01	1.1163	1.1159
0.1	1.5981	1.5898
0.2	2.2409	2.2055
0.3	2.9337	2.8491
0.4	3.6825	3.5224
0.5	4.4943	4,2276
0.6	5.3776	4.9668
0.7	6.3421	5.7428
0.8	7.3995	6.5582
0.9	8.5641	7.4162
0.98	9.5844	8.1356

Table 4. Polarization versus Mori–Tanaka approximations for the three-component matrix composites having the ellipsoidal and platelet inclusions, with $c_1 = 1, c_2 = 16, c_3 = 3, v_3 = v_2$

$v_I = v_2 + v_3$	MTA	PA0
0.01	1.0445	1.0446
0.1	1.2323	1.2335
0.2	1.4913	1.4969
0.3	1.7819	1.7963
0.4	2.1104	2.1397
0.5	2.4845	2.5373
0.6	2.9146	3.0034
0.7	3.4142	3.5570
0.8	4.0016	4.2257
0.9	4.7022	5.0492
0.98	5.3681	5.8594

Third example: Consider a matrix-composite consisting of fiber (v_2, c_2) and platelet (v_3, c_3) inclusions with $c_2 = 2, c_3 = 14, v_3 = \frac{1}{2} v_2$ (the results are presented in Fig. 3 and Tab. 5).

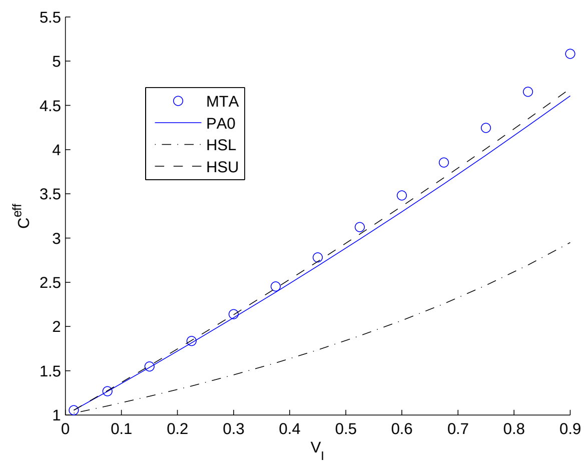


Fig. 3. Polarization (PA0) and Mori–Tanaka (MTA) approximations versus HS bounds for the three-component matrix composites having the fiber and platelet inclusions with $c_1 = 1, c_2 = 2, c_3 = 14,\ v_3 = \dfrac{1}{2}v_2$

Table 5. Polarization versus Mori–Tanaka approximations for the three-component matrix composites having the fiber and platelet inclusions, with $c_1 = 1, c_2 = 2, c_3 = 14,\ v_3 = \dfrac{1}{2}v_2$

$v_I = v_2 + v_3$	MTA	PA0
0.015	1.0529	1.0528
0.15	1.5472	1.5377
0.3	2.1391	2.0986
0.45	2.7812	2.6842
0.6	3.4804	3.2962
0.75	4.2445	3.9365
0.9	5.0831	4.6069

4. CONCLUSION

Comparisons between widely-used classical Mori–Tanaka approximation (MTA) and our newly-constructed polarization approximation using dilute solution reference (PA0), in applications to the conducting matrix composites, yield the following similarities:

- MTA and PA0 give the same result for two-component matrix composites with ellipsoidal inclusions,

- MTA and PA0 give the same result for multi-component matrix composites with spherical inclusions;

and differences:

- MTA has been constructed as an approximate solution to the conduction field equations, while PAs are formulated as approximate solutions of the minimum energy principles.

- MTA and PA0 differ for general *n*-component matrix composites with ellipsoidal inclusions. MTA may violate HS bounds, but PA0 (and generally PAs) always obey HS bounds.

- MTA for general *n*-component matrix composites with ellipsoidal inclusions has the explicit expression (1), while for PA0 one needs to solve the algebraic equation (7) for the approximation (3).

Else, PAs are more flexible. One can use not only the dilute solution reference, but also the references at finite volume proportions of the components, once the macroscopic conductivity of the composite is known at a point analytically, numerically, or experimentally.

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