Elastic properties of two phase composites from optimal Neumann series and structure factors

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Résumé :

Dans ce papier, nous proposons une procédure pour estimer les propriétés élastiques des composites constitués de deux phases, matrice et inclusion. Une classe d'équation intégrale basée sur polarization a été construite. Chaque équation intégrale de cette classe peut produire une estimation du tenseur effectif par developpement de series de Neumann. La meilleure estimation est choisie en se basant sur la critere de convergence, c.a.d le rayon spectral doit être minimisé. La série optimisée converge pour tout rapport de contrast et l'application à différentes microstructures donne les résultats satisfaisants.

Abstract :

In this paper, we propose a new systematic procedure of estimating elastic properties of composites constituted of two phases, matrix and inclusions. A class of integral equations based on eigenstrain (or eigenstress) with the matrix as reference material is constructed with an explicit form in Fourier space. Each integral equation belonging to this class can yield estimates of the overall elastic tensor via Neumann series expansion. The best estimates and series are selected based on the convergence rate criteria of the series, i.e the spectral radius must be minimized. The optimized series is convergent for any finite contrast between inclusions and matrix. Applying the optimized series and the associated estimates to different microstructures yields very satisfying results when compared with the related full solution. For the case of a random distribution of spherical inclusions, exact relations between the elastic tensor and $n-th$ order structure factors are demonstrated.

Mots clefs : Strong contrast expansion, optimally convergent Neumann series, effective elastic tensors

1 Introduction

We consider the problem of finding the effective stiffness tensor $\mathbb{C}^e$ of periodic heterogeneous martrix-inclusion materials. Given the distribution of the constituents, the cell problem must be solved first and the linear relation between average stress and strain is then established. Estimates can be obtained by making relevant approximation to the ingredients constituting the effective tensor. Although the present contribution concerns the theory of optimally estimating $\mathbb{C}^e$ from the microstructure, it is closely related to FFT numerical homogenization methods.

By introducing a reference material $\mathbb{C}^0$, the heterogeneity effect can be viewed as a distribution of eigenstrains within an homogeneous material. Using the related Green tensor, our problem can be formulated as a Lippmann-Schwinger equation for eigenstrain. The integral equation is the origin of resolution methods based on iteration and Fast Fourier Transform (FFT) techniques [1,6]. Significant progresses have been made regarding the improvement of convergence rate [3, 4, 6–8]. The study of convergence rate in those works will be extended in the present contribution in the case of new integral equations. The iteration scheme used to solve the Lippmann-Schwinger equation corresponds to the Neumann series summation. The latter can be used to derive exact theoretical relations and estimates. In this paper, we propose a new estimate based on series expansion that works at all contrast ratio, while using the matrix as a reference material. Additionally, we can control and optimize the convergence rate so that the series converges in the quickest way, and therefore produces the best estimates when using a finite sum in the series expansion. A class of integral equations for eigenstrain is derived and the spectral radius and norm of the corresponding operators are estimated. Different optimization methods are proposed to find the fastest series convergence and the associated estimates.

Similarly to the estimations of the effective elasticity tensor using correlation functions, the new method presented in this paper allows to estimate the effective elasticity tensor using the $n-$ order structure factors, which represent the counterpart in Fourier space of correlation functions. As an example, a direct connection of the effective elasticity tensor to $n-$th order structure factors is given in the case of randomly distributed spheres. Numerical applications for cubic arrays and random distribution of spheres yield very good results in comparison with FFT based methods and other results from the literature.

2 Theoretical formulation

2.1 Notations and mathematical preliminaries

Most of our calculations involve symmetric second order tensors and fourth order tensors with minor symmetries. Unless specified, two tensors standing next to each other implies their double contraction product. We are also dealing with periodic functions using Fourier analysis. Any $V(a_1, a_2, a_3)-$periodic tensor field $\boldsymbol{u}$, function of coordinate $\boldsymbol{x}(x_1, x_2, x_3)$ can be expressed as an infinite Fourier series

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{\boldsymbol{\xi}} \boldsymbol{u}(\boldsymbol{\xi}) e^{i\boldsymbol{\xi}.\boldsymbol{x}}, \quad \boldsymbol{u}(\boldsymbol{\xi}) = \frac{1}{V}\int_V \boldsymbol{u}(\boldsymbol{x}) e^{-i\boldsymbol{\xi}.\boldsymbol{x}} d\boldsymbol{x} \tag{1}$$

with $\boldsymbol{u}(\boldsymbol{\xi})$ being the Fourier transform of $\boldsymbol{u}(\boldsymbol{x})$ and $\boldsymbol{\xi}(\xi_1, \xi_2, \xi_3)$ the wave vector

$$\xi_i = \frac{2\pi n_i}{a_i}, \quad i = 1, 2, 3, \quad n_1, n_2, n_3 \in \mathbb{Z} \tag{2}$$

In the paper, we will encounter frequently equations in the form

$$\boldsymbol{u} = \boldsymbol{U} + \mathbb{B}\boldsymbol{u}, \quad [\mathbb{B}\boldsymbol{u}](\boldsymbol{\xi}) = \mathbb{B}(\boldsymbol{\xi})\boldsymbol{u}(\boldsymbol{\xi}) \tag{3}$$

for a given second order tensorial function $\boldsymbol{U}(\boldsymbol{x})$ and fourth order tensorial operator $\mathbb{B}$. The solution $\boldsymbol{u}$ of the above equation is the following Neumann series

$$\boldsymbol{u} = \sum_{n=0}^{\infty} \mathbb{B}^n \boldsymbol{U}. \tag{4}$$

The convergence rate of the Neumann series (or the iterative scheme) can be estimated from the spectral radius or the norm of the associated operator $\mathbb{B}$. In the case where $\mathbb{A}(\boldsymbol{\xi})$ is a transverse isotropic tensor in Fourier space, it can be represented as

$$\mathbb{B} = b_1\mathbb{E}_1 + b_2\mathbb{E}_2 + b_3\mathbb{E}_3 + b_4\mathbb{E}_4 + b_5\mathbb{E}_5 + b_6\mathbb{E}_6, \tag{5}$$

with $\mathbb{E}_1, \mathbb{E}_2, .., \mathbb{E}_6$ being the Walpole base elements [13] defined as

$$\begin{aligned}
&\mathbb{E}_1 = \frac{1}{2}\boldsymbol{k}^\perp \otimes \boldsymbol{k}^\perp, \quad \mathbb{E}_2 = \boldsymbol{k} \otimes \boldsymbol{k}, \quad \mathbb{E}_3 = \boldsymbol{k}^\perp \overline{\underline{\otimes}} \boldsymbol{k}^\perp - \mathbb{E}_1, \\
&\mathbb{E}_4 = \boldsymbol{k}^\perp \overline{\underline{\otimes}} \boldsymbol{k} + \boldsymbol{k} \overline{\underline{\otimes}} \boldsymbol{k}^\perp, \quad \mathbb{E}_5 = \boldsymbol{k} \otimes \boldsymbol{k}^\perp, \quad \mathbb{E}_6 = \boldsymbol{k}^\perp \otimes \boldsymbol{k}, \\
&\boldsymbol{k} = \overline{\boldsymbol{\xi}} \otimes \overline{\boldsymbol{\xi}}, \quad \boldsymbol{k}^\perp = \boldsymbol{I} - \boldsymbol{k},
\end{aligned} \tag{6}$$

The spectral radius $\rho(\mathbb{B})$ and the norm $||\mathbb{B}||$ can now be computed with the formula

$$\begin{aligned}
&\rho(\mathbb{B}) = \max\left\{|b_3|, |b_4|, \frac{1}{2}|(b_1 + b_2) \pm \sqrt{(b_1 - b_2)^2 + 8b_5b_6}|\right\}. \\
&||\mathbb{B}|| = \sqrt{\rho(\mathbb{B}^\dagger\mathbb{B})} = \max\left\{|b_3|, |b_4|, \frac{1}{2}[\sqrt{(b_1 - b_2)^2 + 2(b_5 + b_6)^2} + \right. \\
&\left. + \sqrt{(b_1 + b_2)^2 + 2(b_5 - b_6)^2}]\right\}.
\end{aligned} \tag{7}$$

2.2 Integral equations for eigen stresses

We consider a heterogeneous two-phase material where the local isotropic stiffness is either matrix $\mathbb{C}^0$ (elastic constants κ_0 and μ_0, compliance $\mathbb{S}^0$) or inclusion $\mathbb{C}^i$ (elastic constants κ_i and μ_i, compliance $\mathbb{S}^i$) is a $V-$periodic function of the coordinates $\boldsymbol{x}$. Using the matrix $\mathbb{C}^0$ as reference material, we have

$$\boldsymbol{\sigma} = \mathbb{C}^0\boldsymbol{\epsilon} + \boldsymbol{\tau}, \quad \boldsymbol{\epsilon} = \mathbb{S}^0\boldsymbol{\sigma} + \boldsymbol{e}, \tag{8}$$

where the eigenstress $\boldsymbol{\tau}$ and the eigenstrain $\boldsymbol{e}$ have been introduced. Using the characteristic function $\chi(\boldsymbol{x})$, $\chi = 1$ for matrix and $\chi = 0$ for inclusion, the integral equation for the eigenstress $\boldsymbol{\tau}$ may be expressed as :

$$\boldsymbol{\tau} = \chi\delta\mathbb{C}(\boldsymbol{E} - \boldsymbol{\Gamma}^0 * \boldsymbol{\tau}), \quad \delta\mathbb{C} = \mathbb{C}^i - \mathbb{C}^0 \tag{9}$$

and the dual integral equation for the eigenstrain $\boldsymbol{e}$

$$\boldsymbol{e} = \chi\delta\mathbb{S}(\boldsymbol{\Sigma} - \boldsymbol{\Delta}^0 * \boldsymbol{e}), \quad \delta\mathbb{S} = \mathbb{S}^i - \mathbb{S}^0. \tag{10}$$

The Green operators $\mathbf{\Gamma}^0$ and $\mathbf{\Delta}^0$ for strain and stress are defined in Fourier space by :

$$\mathbf{\Gamma}^0(\boldsymbol{\xi}) = \frac{3}{3\kappa_0 + 4\mu_0}\mathbb{E}_2 + \frac{1}{2\mu_0}\mathbb{E}_4 \quad \forall\boldsymbol{\xi} \neq \mathbf{0}, \quad \mathbf{\Gamma}^0(\mathbf{0}) = \mathbf{0},$$
$$\mathbf{\Delta}^0(\boldsymbol{\xi}) = \frac{18\mu_0\kappa_0}{3\kappa_0 + 4\mu_0}\mathbb{E}_1 + 2\mu_0\mathbb{E}_3 \quad \forall\boldsymbol{\xi} \neq \mathbf{0}, \quad \mathbf{\Delta}^0(\mathbf{0}) = \mathbf{0}, \tag{11}$$

where $\boldsymbol{\xi}$ is the wave vector and the tensors $\mathbb{E}_i$ are defined in Fourier space from the Walpole base. The elastic constants κ_0 and μ_0 appearing in (11) are respectively the bulk modulus and the shear modulus associated to the reference tensor $\mathbb{C}^0$.

From the two elementary integral equations, we can construct a family of integral equations for $\boldsymbol{\tau}$ (or $\boldsymbol{e}$ equivalently) by linear combination. Using two tensors $\mathbb{L}$ and $\mathbb{I} - \mathbb{L}$, we can obtain

$$\boldsymbol{\tau} = \chi\mathbb{A}\boldsymbol{E} + \chi\mathbb{B}\boldsymbol{\tau}, \tag{12}$$

in which

$$\mathbb{A} = ((\mathbb{I} - \mathbb{L})(\delta\mathbb{C}) - \mathbb{L}\mathbb{C}^0(\delta\mathbb{S})\mathbb{C}^e)$$
$$\mathbb{B} = -((\mathbb{I} - \mathbb{L})(\delta\mathbb{C})\mathbf{\Gamma}^0 + \mathbb{L}\mathbb{C}^0(\delta\mathbb{S})\mathbf{\Delta}^0\mathbb{S}^0). \tag{13}$$

The solution to the above equation is the Neumann series $\boldsymbol{\tau} = \chi\sum_{n=0}^{\infty}(\mathbb{B}\chi)^n\boldsymbol{E}$ and the convergence rate of Neumann series depend on the spectral radius of $\mathbb{B}\chi$. Next we are limited to the case where

$$\mathbb{L} = 2\alpha\mathbb{K} + 3\beta\mathbb{J} \tag{14}$$

where α and β are two constants. Noting that $\rho(\chi) = |\chi| = 1$ and that $\mathbb{B}$ is transversely isotropic tensor in Fourier space, we propose three methods of finding α, β to obtain the best convergence rate
- Optimizing the spectral radius of $\mathbb{B}$ (OR)
- Optimizing the norm of $\mathbb{B}$ (ON)
- Optimizing directly the spectral radius of $\mathbb{B}\chi$ (OD)
The first two methods can be done using the results on $\rho(\mathbb{B})$ and $|\mathbb{B}|$ in the previous sections. The final

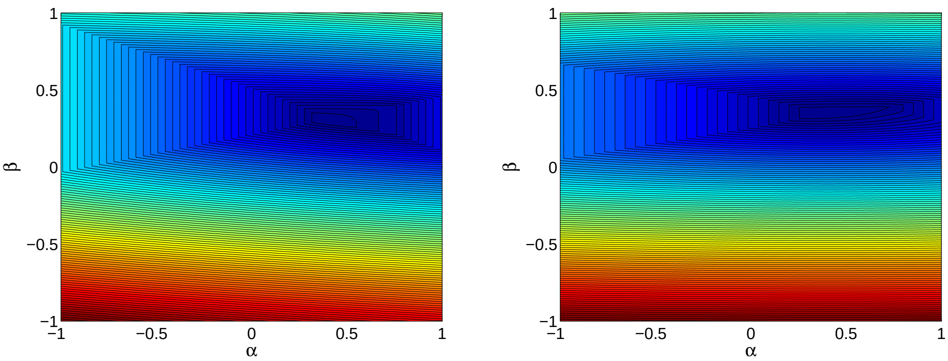

FIGURE 1 – Isolines of spectral radius $\rho(\mathbb{B})$ (left) and norm $||\mathbb{B}||$ (right) as functions of α and β. The results are obtained for two materials with the following parameters $\nu_1 = 0.4, \nu_0 = 0.3, \mu_1/\mu_0 = 3$. The optimal values by the two methods are respectively $(\alpha, \beta) = (0.355, 0.298)$ and $(\alpha, \beta) = (0.309, 0.349)$

method leads to the result

$$2\alpha = \varepsilon_m/(\varepsilon_m + 1), \quad 3\beta = \varepsilon_k/(\varepsilon_k + 1), \quad \varepsilon_m = \mu_i/\mu_0, \quad \varepsilon_k = \kappa_i/\kappa_0 \tag{15}$$

and the expressions for $\mathbb{A}$ and $\mathbb{B}$ as follows

$$\begin{aligned}\mathbb{A} &= \left[\left(3\frac{\varepsilon_k - 1}{\varepsilon_k + 1}\kappa_0\mathbb{J} + 2\frac{\varepsilon_m - 1}{\varepsilon_m + 1}\mu_0\mathbb{K}\right) + \left(\frac{\varepsilon_k - 1}{\varepsilon_k + 1}\mathbb{J} + \frac{\varepsilon_m - 1}{\varepsilon_m + 1}\mathbb{K}\right)\mathbb{C}^e\right], \\ \mathbb{B} &= \left(\frac{\varepsilon_k - 1}{\varepsilon_k + 1}\mathbb{J} + \frac{\varepsilon_m - 1}{\varepsilon_m + 1}\mathbb{K}\right)\left(\mathbb{E}_1 - \mathbb{E}_2 + \mathbb{E}_3 - \mathbb{E}_4 - \frac{2(3\kappa_0 - 2\mu_0)}{3\kappa_0 + 4\mu_0}\mathbb{E}_6\right).\end{aligned} \tag{16}$$

It can be shown that using the OD method, we can guarantee that

$$\rho(\mathbb{B}\chi) \leq \max\left\{\left|\frac{\varepsilon_m - 1}{\varepsilon_m + 1}\right|, \left|\frac{\varepsilon_k - 1}{\varepsilon_k + 1}\right|\right\} \tag{17}$$

Case	α			β		
	OR	ON	OD	OR	ON	OD
$\nu_1 = \nu_0 = 0.3$, $\mu_1/\mu_0 = 0.01$	0.0040	- 0.0031	0.0050	0.0027	-0.0012	0.0033
$\nu_1 = 0.1, \nu_0 = 0.3$, $\mu_1/\mu_0 = 0.1$	0.0525	-0.0215	0.0528	0.0430	0.0037	0.0159
$\nu_1 = 0.4, \nu_0 = 0.3$, $\mu_1/\mu_0 = 1$	0.923	-1.000	0.250	0.259	0.353	0.228
$\nu_1 = 0.4, \nu_0 = 0.3$, $\mu_1/\mu_0 = 3$	0.355	0.309	0.375	0.298	0.349	0.289
$\nu_1 = 0.2, \nu_0 = 0.3$, $\mu_1/\mu_0 = 10$	0.455	0.453	0.454	0.281	0.347	0.287
$\nu_1 = 0.1, \nu_0 = 0.3$, $\mu_1/\mu_0 = 100$	0.496	0.496	0.495	0.325	0.337	0.326
$\nu_1 = 0.1, \nu_0 = 0.3$, $\mu_1/\mu_0 = 1000$	0.500	0.500	0.499	0.333	0.334	0.332

TABLE 1 – Comparison of the results α, β issued from three methods of optimization. Notations : OR for optimization based on spectral radius of $\mathbb{B}$, ON for optimization based on norm of $\mathbb{B}$ and OD for optimization based on the direct estimation of spectral radius of $\mathbb{B}\chi$.

2.3 Overall elastic properties

Repeating the recurrence at step n we obtain an equation for $\boldsymbol{\tau}$

$$\boldsymbol{\tau} = \chi\sum_{j=0}^{n-1}(\mathbb{B}\chi)^j\mathbb{A}\boldsymbol{E} + (\chi\mathbb{B})^n\boldsymbol{\tau}. \tag{18}$$

Averaging both sides over the inclusion volume and making the approximation $\boldsymbol{\tau} \simeq \chi\langle\boldsymbol{\tau}\rangle_\Omega$, we obtain the following equation for $\langle\boldsymbol{\tau}\rangle_\Omega$

$$\langle\boldsymbol{\tau}\rangle_\Omega \simeq \sum_{j=0}^{n-1} \mathbb{D}^j \mathbb{A}\boldsymbol{E} + \mathbb{D}^n \langle\boldsymbol{\tau}\rangle_\Omega. \tag{19}$$

in which the tensors $\mathbb{D}^0, \mathbb{D}^1, ..$ are determined with the formulas

$$\begin{aligned}
&\mathbb{D}^0 = \langle(\mathbb{B}\chi)^0\rangle_\Omega = \mathbb{I}, \\
&\mathbb{D}^1 = \langle(\mathbb{B}\chi)^1\rangle_\Omega = f^{-1}\sum_{\boldsymbol{\xi}} \chi(-\boldsymbol{\xi})\mathbb{B}(\boldsymbol{\xi})\chi(\boldsymbol{\xi}), \\
&\mathbb{D}^2 = \langle(\mathbb{B}\chi)^2\rangle_\Omega = f^{-1}\sum_{\boldsymbol{\xi}} \chi(-\boldsymbol{\xi})\mathbb{B}(\boldsymbol{\xi})\sum_{\boldsymbol{\xi}'} \chi(\boldsymbol{\xi}-\boldsymbol{\xi}')\mathbb{B}(\boldsymbol{\xi}')\chi(\boldsymbol{\xi}'), \\
&\dots \\
&\mathbb{D}^j = \langle(\mathbb{B}\chi)^j\rangle_\Omega = f^{-1}\sum_{\boldsymbol{\xi}^1,\boldsymbol{\xi}^2,\dots,\boldsymbol{\xi}^n} \chi(-\boldsymbol{\xi}^1)\chi(\boldsymbol{\xi}^1-\boldsymbol{\xi}^2)...\chi(\boldsymbol{\xi}^{j-1}-\boldsymbol{\xi}^j)\chi(\boldsymbol{\xi}^1)\mathbb{B}(\boldsymbol{\xi}^1)...\mathbb{B}(\boldsymbol{\xi}^j).
\end{aligned} \tag{20}$$

We note that the average $\boldsymbol{\tau}$ over the inclusion domain $\langle\boldsymbol{\tau}\rangle_\Omega$ is connected to the effective stiffness tensor $\mathbb{C}^e$ via the relation

$$f\langle\boldsymbol{\tau}\rangle_\Omega = (\mathbb{C}^e - \mathbb{C}^0)\boldsymbol{E}. \tag{21}$$

Solving (19) for $\langle\boldsymbol{\tau}\rangle_\Omega$ and substituting back into (21), we obtain a new expression for $\mathbb{C}^e$

$$\mathbb{C}^e \simeq \left[(\mathbb{I}-\mathbb{D}^n) + f\sum_{j=0}^{n-1}\mathbb{D}^j\mathbb{L}\mathbb{C}^0(\delta\mathbb{S})\right]^{-1}\left[(\mathbb{I}-\mathbb{D}^n) + f\sum_{j=0}^{n-1}\mathbb{D}^j(\mathbb{I}-\mathbb{L})(\delta\mathbb{C})\mathbb{S}^0\right]\mathbb{C}^0. \tag{22}$$

In the case where the effective material is isotropic or at least cubic, we can extract the main shear modulus μ_e and the bulk modulus κ_e using the expressions

$$\begin{aligned}
&\frac{\mu_e}{\mu_0} \simeq 1 + f\frac{(1-2\alpha)\delta\mu/\mu_0 + 2\alpha\delta\mu/\mu_1}{\frac{1-2\alpha_n}{\sum_{j=0}^{n-1}2\alpha_j} - 2\alpha f\delta\mu/\mu_1} \\
&\frac{\kappa_e}{\kappa_0} \simeq 1 + f\frac{(1-3\beta)\delta\kappa/\kappa_0 + 3\beta\delta\kappa/\kappa_1}{\frac{1-3\beta_n}{\sum_{j=0}^{n-1}3\beta_j} - 3\beta f\delta\kappa/\kappa_1}, \\
&\mu_e = C^e_{1212}, \quad 3\kappa_e = C^e_{1111} + 2C^e_{1122}, \\
&\alpha_j = D^j_{1212}, \quad 3\beta_j = D^j_{1111} + 2D^j_{1122},
\end{aligned} \tag{23}$$

From (23), it is interesting to remark that all the microstructure information is contained in the parameters $\frac{1-2\alpha_n}{\sum_{j=0}^{n-1}2\alpha_j}$ and $\frac{1-3\beta_n}{\sum_{j=0}^{n-1}3\beta_j}$.

3 Numerical applications and analysis

Let us consider the application of our theory to a cubic array of spheres in comparison with FFT and some literature results. From Figs. 2, 3 and Tabs. 2, 3, we find that the second order estimates have improved significantly the Hashin Shtrikman estimate [5] which coincides with the first order estimates. The degree of improvement depends on the properties considered, estimation scheme, microstructure and the elastic properties of constituents. For BCC array with contrast ratio as high as 10 (see Fig 2, 3)), the second order estimates of the bulk modulus κ_e/κ_0 and the shear modulus μ_e/μ_0 issued from the three schemes are close to the FFT results at convergence. The agreement is good upto a very high volume fraction near the percolation limit.

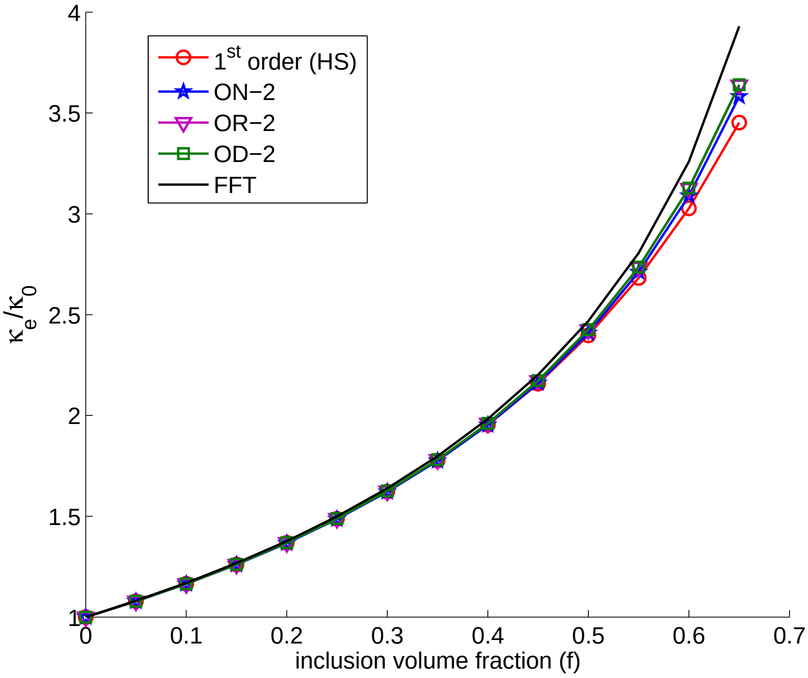

FIGURE 2 – Normalized effective bulk modulus κ_e/κ_0 vs inclusion volume fraction f of BCC array. Elastic properties of the constituents are $\nu_1 = 0.4, \nu_0 = 0.3, \mu_1/\mu_0 = 10$. The results are computed by first order estimates which all coincide with HS estimates, second order estimates of the three methods (OR,ON and OD) and the numerical method FFT at convergence.

Detailed results on FCC array also have the same trend as those for BCC cases. Tables 2 and 3 show that the two series OR and OD yield very good results while the series ON works less well. It is interesting to note that at volume fraction as large as 0.5 and the rigidity contrast ratio as high as 100, our three estimates perform well.

Next, we study microstructures constituted of randomly isotropic distribution of spheres. Two extreme cases of rigid spheres and voids will be considered. Fifty sample composed of 500 non overlapping spheres are prepared by standard Event Driven Molecular Dynamics [10]. To compute the effective properties of the material, we shall limit to OD based estimates and final results are obtained by averaging over the 50 samples. It may be noticed that, the iterative scheme is not theoretically convergent for fields in void or rigid inclusions but the effective properties exist for the considered microstructures. In this case, the expressions for μ_e and κ_e at first and second order can be used for infinite contrast. Simulations on the systems show that the OD-2 estimate is close to the estimate of Torquato [11, 12]. For spherical voids (see Fig. 5), our second order estimate again shows a significant improvement with respect to the first order (HS bound). The estimate is also close to Torquato's estimate [11,12] using three point parameters. Those results again confirm the robustness of our estimation scheme at high rigidity contrast and high volume fraction. We note that the good performance comes from the benefit of the fast

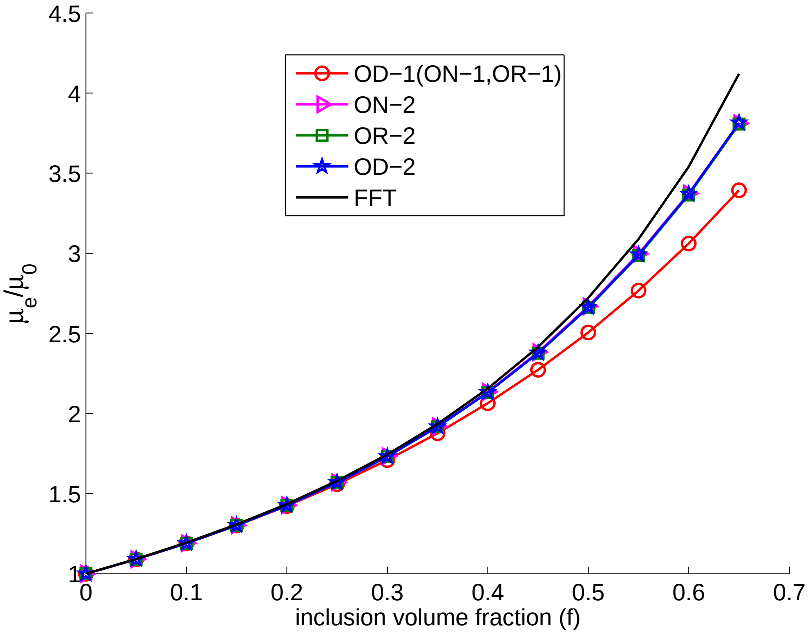

FIGURE 3 – Normalized effective shear moduli μ_e/μ_0 vs inclusion volume fraction f of BCC array. Elastic properties of the constituents are $\nu_1 = 0.4, \nu_0 = 0.3, \mu_1/\mu_0 = 10$. The results are computed by first order estimates, second order estimates of the three methods (OR,ON and OD) and the numerical method FFT at convergence.

convergence series and the high order correlation information.

4 Concluding remarks

In this paper, we have presented a new estimate of the overall stiffness tensor of elastic composites. Starting from a class of Lippmann-Schwinger integral equations for eigenstress (or eigenstrain), the optimization procedure is then carried out to find the best Neumann series, i.e those with the fastest convergence rate. To this end, we have introduced tools to bound the spectral radius and norm of fourth order operators in Fourier space and methods to obtain the optimal series. The series are then used to derive estimates at different order n.

We have also shown that $n-$ order statistical information on the microstructure, in this case corresponding to the structure factors, also appear in the estimates. Numerical applications of the procedure on some test cases show that our estimates perform very well in comparison with FFT results and those from the literature.

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f	Order 1	ON-2	OR-2	OD-2	FFT
0.10	1.1784	1.1754	1.1791	1.1795	1.1907
0.20	1.4009	1.3950	1.4024	1.4031	1.4254
0.30	1.6863	1.6769	1.6898	1.6911	1.7293
0.40	2.0659	2.0536	2.0758	2.0785	2.1424
0.50	2.5952	2.5872	2.6287	2.6357	2.7533
0.60	3.3850	3.4182	3.5059	3.5276	3.8286
0.70	4.6900	4.9483	5.1744	5.2562	7.2886

TABLE 2 – Normalized effective bulk modulus κ_e/κ_0 vs inclusion volume fraction f of FCC. Elastic properties of the constituents are $\nu_1 = 0.4, \nu_0 = 0.3, \mu_1/\mu_0 = 100$. The results are computed by first order estimates which coincide with HS estimates, second order estimates of the three methods (OR,ON and OD) and the numerical method FFT at convergence.

f	Order-1	ON-2	OR-2	OD-2	FFT
0.10	1.2338	1.2348	1.2350	1.2355	1.2523
0.20	1.5365	1.5433	1.5437	1.5457	1.5819
0.30	1.9347	1.9667	1.9675	1.9745	2.0417
0.40	2.4719	2.5742	2.5770	2.5970	2.7232
0.50	3.2230	3.4793	3.4896	3.5381	3.8078
0.60	4.3281	4.8812	4.9222	5.0277	5.5844
0.70	6.0830	7.2978	7.4748	7.7229	10.7332

TABLE 3 – Effective shear moduli μ_e/μ_0 vs inclusion volume fraction f of FCC. Elastic properties of the constituents are $\nu_1 = 0.4, \nu_0 = 0.3, \mu_1/\mu_0 = 100$. The results are computed by first order estimates, second order estimates of the three methods (OR,ON and OD) and the numerical method FFT at convergence.

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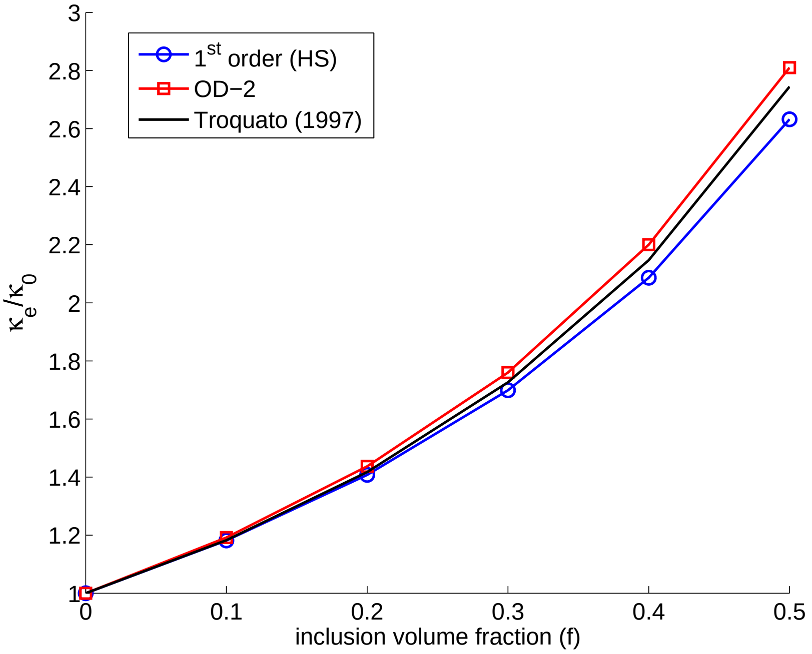

FIGURE 4 – Normalized effective bulk modulus κ_e/κ_0 vs inclusion volume fraction f for random distribution of rigid spheres ($\mu_1/\mu_0 = \kappa_1/\kappa_0 = \infty$). The solutions of the present work (OD-1, OD-2) are compared with the results of [11, 12]. The first order estimates coincide with HS estimates.

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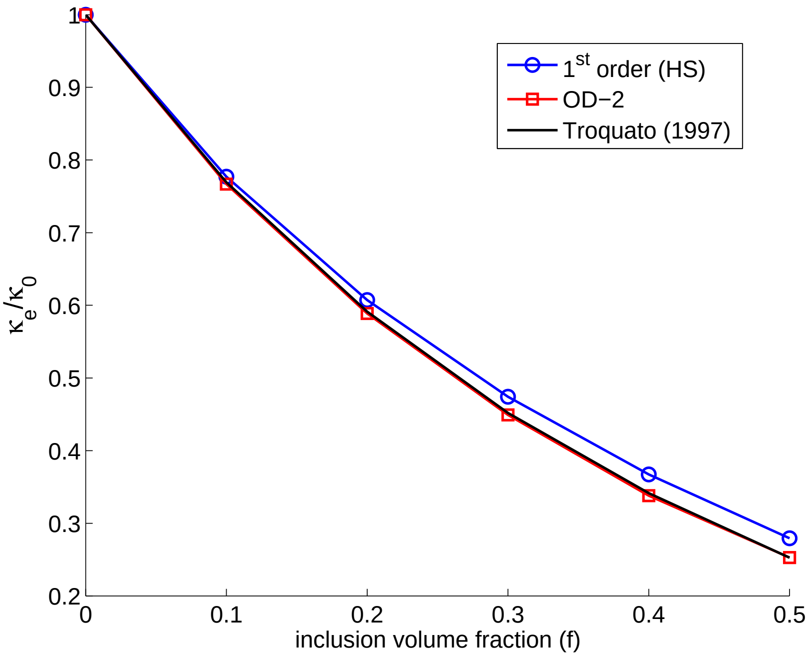

FIGURE 5 – Normalized effective bulk modulus κ_e/κ_0 vs inclusion volume fraction f with random distributions of spherical voids ($\mu_1/\mu_0 = \kappa_1/\kappa_0 = 0$). The solutions of the present work (OD-1, OD-2) are compared with the results of [11, 12]. The first order estimates coincide with HS estimates.