THE OVERALL ELASTIC RESPONSE OF MATERIALS CONTAINING SPHERICAL INHOMOGENEITIES

GREGORY J. RODIN

Department of Aerospace Engineering and Engineering Mechanics, The University of Texas at Austin, TX 78712, U.S.A.

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Abstract—It is proposed to determine the overall response of linear elastic materials containing non-intersecting spherical inhomogeneities without altering the microscopic geometry of a given representative volume element. In the proposed method, a system of integral equations formulated for such an element is accurately approximated by a system of linear algebraic equations.

1. INTRODUCTION

In this paper, we are concerned with the overall response of linear elastic materials composed of an isotropic matrix filled with non-intersecting spherical inhomogeneities. Since this is an open problem and its complete solution is virtually impossible, a large number of approximate approaches have been proposed. The approaches accepted in the solid mechanics community can be divided into two groups. The first group includes rigorous approaches such as variational bounds [see reviews by Milton and Kohn (1988) and Torquato (1991)] and asymptotic expansions in powers of the volume fraction of inhomogeneities (Chen and Acrivos, 1978; O'Brien, 1979). However, the usefulness of the rigorous approaches is limited. Variational bounds work well only for composites with relatively small contrast between the phases, and asymptotic expansions may not be applicable to composites with high volume fractions of inhomogeneities. The second group of approaches includes approximations such as self-consistent schemes, Mori-Tanaka theory, and other effective medium theories [see reviews by Hashin (1983) and Mura (1982)]. In a typical approximation, the elasticity problem for a given representative volume element (RVE) is substituted by a problem(s) which involves an effective homogeneous matrix containing only one inhomogeneity. The validity of such a substitution is difficult to verify analytically, since it is unclear how to choose a benchmark solution. Existing experimental verifications are unsatisfactory as well: In each of four papers (Christensen, 1990; Cleary et al., 1980; Weng, 1984; Zimmerman, 1991), experimental data were presented in support of a different approximation. Following Christensen (1990), this situation may be explained by the fact that all approximations lead to somewhat similar predictions for dilute concentrations of inhomogeneities, so that only experiments on densly concentrated composites can identify a relevant approximation(s). Accordingly, Christensen (1990) demonstrates that the preference should be given to the generalized self-consistent technique.

In this paper, an approach which does not alter the microscopic geometry of the RVE is pursued. As explained in the next two sections, the proposed method of analysis is based on an assumption which allows us to reduce a rigorous integral equation formulation of the linear elasticity problem for N inhomogeneities inside the RVE to a system of 6N linear algebraic equations. Since in the proposed method the microscopic geometry can be unambiguously specified, the introduced assumption can be tested by applying the method to simple RVEs for which solutions can be obtained with more involved numerical techniques such as the finite element or boundary element methods. Accordingly, in Section 4, the method's predictions are compared with existing numerical solutions for basic cubic arrays of identical inhomogeneities.

As far as the solid mechanics literature is concerned, the proposed method can be viewed as a generalization of results due to Nemat-Nasser *et al.* (1982) and Rodin and Hwang (1991). In the former paper, simple cubic arrays of inhomogeneities are analysed

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using an assumption similar to the one adopted in this paper. However, because Nemat-Nasser *et al.* used very slowly converging series, their approach is hardly applicable to other arrays. The approach suggested by Rodin and Hwang is relevant only if there is a *finite* number of inhomogeneities contained in an *infinite* matrix. Other closely-related approaches are considered in Section 5.

In this paper, the focus is on the derivation of the method and verification of its accuracy; applications to random arrays of inhomogeneities will be presented elsewhere.

2. THE OVERALL RESPONSE

Consider a linear elastic RVE composed of an isotropic matrix and N non-intersecting spherical inhomogeneities. The stiffness tensors of the inhomogeneities are designated by C^{α} , $\alpha = 1, ..., N$; the matrix stiffness is C. The domains of the RVE and inhomogeneities are denoted respectively by V and V^{α} . For simplicity, V and V^{α} also designate the volumes of the corresponding domains.

For a statistically homogeneous material (Hashin, 1983), the overall response is established in terms of the macroscopic stress, $\bar{\sigma}$, and strain, $\bar{\epsilon}$. These quantities are defined as the volume averages over the RVE:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \int_{V} \boldsymbol{\sigma} \, \mathrm{d}V \tag{1}$$

and

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V} \int_{V} \boldsymbol{\varepsilon} \, \mathrm{d} V. \tag{2}$$

The macroscopic stress and strain are linearly related by

$$\bar{\sigma} = \mathbf{C}^* \bar{\varepsilon},\tag{3}$$

where C^* is termed the overall stiffness tensor. Also, a homogeneous material with stiffness tensor C^* is referred to as the effective matrix.

The tensor C* can be related to an average over the inhomogeneities:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \int_{V \to \Sigma V^{\alpha}} \boldsymbol{\sigma} \, \mathrm{d}V + \frac{1}{V} \sum_{\alpha} \int_{V^{\alpha}} \boldsymbol{\sigma} \, \mathrm{d}V = \frac{1}{V} \int_{V \to \Sigma V^{\alpha}} \mathbf{C} \boldsymbol{\epsilon} \, \mathrm{d}V + \frac{1}{V} \sum_{\alpha} \int_{V^{\alpha}} \mathbf{C}^{\alpha} \boldsymbol{\epsilon} \, \mathrm{d}V$$
$$= \frac{1}{V} \int_{V \to \Sigma V^{\alpha}} \mathbf{C} \boldsymbol{\epsilon} \, \mathrm{d}V + \frac{1}{V} \sum_{\alpha} \int_{V^{\alpha}} \mathbf{C} (\boldsymbol{\epsilon} - \boldsymbol{\beta}^{\alpha}) \, \mathrm{d}V = \mathbf{C} (\bar{\boldsymbol{\epsilon}} - \omega \bar{\boldsymbol{\gamma}}). \tag{4}$$

In this equation, the equivalent inclusion method is used (Eshelby, 1957; Mura, 1982), so that the inhomogeneities are simulated by inclusions with transformation strains, $\beta^{\alpha}(\mathbf{x})$. The quantity \bar{y} , termed the average "polarization strain", is defined as

$$\bar{\gamma} = \frac{1}{N} \sum_{\alpha} \gamma^{\alpha} = \frac{1}{N} \sum_{\alpha} \int_{V^{\alpha}} \boldsymbol{\beta}^{\alpha} \,\mathrm{d}V, \tag{5}$$

where γ^{α} is the polarization strain of V^{α} ; $\omega = N/V$. In the remainder of the paper, it is considered that the overall response is determined once the polarization strains are calculated.

Let us remark that the assumption of statistical homogeneity is of paramount importance because it implies that no length scale can enter the constitutive equations. As a result, the following simplifications are allowed :

- (1) The overall response is defined only in terms of the unweighted volume averages $\bar{\sigma}$ and $\bar{\varepsilon}$ because any other weight is associated with a length scale.
- (2) As far as the overall response is concerned, it is immaterial whether the microscopic fields are induced by uniform surface tractions or linear displacements. Thus, without any loss of generality, it is supposed that the RVE is subjected to surface displacements $\varepsilon^0 x$, where x is a point on the surface of the RVE. In this case, $\overline{\varepsilon} = \varepsilon^0$.
- (3) The macroscopic geometry of the RVE can be chosen as desired, as long as the RVE contains a sufficiently large number of inhomogeneities. In the sequel, the RVE is a cube.

3. THE METHOD

3.1. Overview

In principle, the RVE described in the previous section can be analysed directly, using, for example, the finite element method. Indeed this approach has been proven useful for 2-D problems (Brockenbrough *et al.*, 1991), but 3-D problems which involve many spheres per RVE cannot be handled in this manner. Also, since the RVE occupies a finite domain it is difficult to take advantage of classical techniques because fundamental solutions are generally available only for infinite domains. This obstacle is eliminated if the RVE is replicated so that an infinite periodic array is formed with the RVE as the unit cell. In order to determine the overall response using this array, three steps are undertaken.

Step 1. An auxiliary boundary-value problem is formulated for the RVE imbedded into an infinite body of the matrix material (Rodin and Hwang, 1991). Based on this problem, it is demonstrated how a rigorous integral equation formulation for the transformation strains is approximated by a system of linear algebraic equations for the polarization strains. Since the auxiliary problem is stated for a finite number of inhomogeneities in an infinite matrix, it is free of the well-known convergence difficulties associated with an infinite number of inhomogeneities [see O'Brien (1979) for references].

Step 2. Following O'Brien (1979), we consider a limit as the number of inhomogeneities and the volume occupied by the composite material *simultaneously* tend to infinity.

Step 3. The limit is attained by replicating the RVE so that the periodic array is formed. Algebraic equations for the periodic array are derived with the aid of Ewald's technique as suggested by Beenakker (1986) and Brady *et al.* (1988).

3.2. The auxiliary problem

Let the RVE, described in Section 2, be imbedded into an infinite matrix with stiffness tensor C. The infinite body is subjected to remote boundary conditions so that the remote uniform strain field is ε^0 . The polarization strains induced by ε^0 are determined by the equivalent inclusion method (Eshelby, 1957; Mura, 1982), and it is supposed that the reader is familiar with its basics.

For a reference inhomogeneity V^{α} , the equivalence between the inhomogeneity and the inclusion is established if the condition

$$\mathbf{C}^{\alpha}(\boldsymbol{\varepsilon}^{0} + \boldsymbol{\varepsilon}^{\alpha}) = \mathbf{C}(\boldsymbol{\varepsilon}^{0} + \boldsymbol{\varepsilon}^{\alpha} - \boldsymbol{\beta}^{\alpha})$$
(6)

holds for any point inside V^{α} . In this equation, ε^{α} is the strain field in the domain V^{α} induced by the inhomogeneities. This field can be written in the form

$$\varepsilon^{\alpha}(\mathbf{x}) = \int_{\mathcal{V}^{\alpha}} \mathbf{K}(\mathbf{x}, \mathbf{y}) \boldsymbol{\beta}^{\alpha}(\mathbf{y}) \, \mathrm{d}\mathbf{y} + \sum_{\eta \neq \alpha} \int_{\mathcal{V}^{\eta}} \mathbf{K}(\mathbf{x}, \mathbf{y}) \boldsymbol{\beta}^{\eta}(\mathbf{y}) \, \mathrm{d}\mathbf{y}.$$
(7)

In this equation, dy denotes an infinitesimal volume centered at the point y. The components of the kernel K(x, y) are (Mura, 1982)

$$K_{ijkl}(\mathbf{x}, \mathbf{y}) = -\frac{1}{2}C_{pqkl}[G_{ip,qj}(\mathbf{x}, \mathbf{y}) + G_{jp,qi}(\mathbf{x}, \mathbf{y})], \qquad (8)$$

where

$$G_{ij}(\mathbf{x}, \mathbf{y}) = \frac{1}{16\pi\mu(1-\nu)} \left[\frac{(3-4\nu)\delta_{ij}}{|\mathbf{x}-\mathbf{y}|} + \frac{(x_i - y_i)(x_j - y_j)}{|\mathbf{x}-\mathbf{y}|^3} \right]$$
(9)

is the fundamental solution of linear elasticity. In (8), the standard index notation is adopted, and the derivatives can be evaluated with respect to either x or y. In (9), μ is the shear modulus, ν is Poisson's ratio, δ_{ij} is the Kronecker symbol, and $|\mathbf{x} - \mathbf{y}|$ is the distance between x and y. As the index α runs from 1 to N, (6)–(9) form a system of linear integral equations for $\boldsymbol{\beta}^{\alpha}(\mathbf{x})$.

Eshelby (1957) proved that the integral of the kernel K(x, y) is a constant if x and y belong to the same inhomogeneity:

$$S_{ijkl} \stackrel{\text{def}}{=} \int_{V^{\alpha}} K_{ijkl}(\mathbf{x}, \mathbf{y}) \, \mathrm{d}\mathbf{y} = \frac{5\nu - 1}{15(1 - \nu)} \, \delta_{ij} \delta_{kl} + \frac{4 - 5\nu}{15(1 - \nu)} \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right), \quad \mathbf{x} \in V^{\alpha}.$$
(10)

With this result, (7) is integrated over V^{α} (Rodin and Hwang, 1991):

$$\int_{\nu^{\alpha}} \varepsilon^{\alpha}(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \mathbf{S} \gamma^{\alpha} + \sum_{\eta \neq \alpha} \int_{\nu^{\alpha}} \int_{\nu^{\eta}} \mathbf{K}(\mathbf{x}, \mathbf{y}) \boldsymbol{\beta}^{\eta}(\mathbf{y}) \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{x}.$$
(11)

A particular approximation which reduces integral equations (6)–(9) to an algebraic form is obtained as follows. Let us decompose the transformation strain of a neighbor V^{η} into its uniform and non-uniform parts,

$$\boldsymbol{\beta}^{\eta}(\mathbf{x}) = \langle \boldsymbol{\beta}^{\eta} \rangle + \boldsymbol{\tilde{\beta}}^{\eta}(\mathbf{x}), \tag{12}$$

with the uniform part

$$\langle \boldsymbol{\beta}^{\eta} \rangle = \frac{1}{V^{\eta}} \, \boldsymbol{\gamma}^{\eta}. \tag{13}$$

If we neglect the effect of $\tilde{\beta}^{\eta}(\mathbf{x})$ on elastic interactions, i.e assume that

$$\sum_{\eta\neq\alpha}\int_{V^{\alpha}}\int_{V^{\eta}}\mathbf{K}(\mathbf{x},\mathbf{y})\widetilde{\boldsymbol{\beta}}^{\eta}(\mathbf{y})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{x}$$

is small, a combination of (6)-(13) leads to an algebraic system of equations for the polarization strains:

$$\mathbf{C}^{\alpha}\left[\boldsymbol{\varepsilon}^{0} + \frac{1}{V^{\alpha}}\mathbf{S}\boldsymbol{\gamma}^{\alpha} + \sum_{\eta\neq\alpha}\mathbf{T}(\mathbf{r}^{\alpha\eta})\boldsymbol{\gamma}^{\eta}\right] = \mathbf{C}\left[\boldsymbol{\varepsilon}^{0} + \frac{1}{V^{\alpha}}\mathbf{S}\boldsymbol{\gamma}^{\alpha} + \sum_{\eta\neq\alpha}\mathbf{T}(\mathbf{r}^{\alpha\eta})\boldsymbol{\gamma}^{\eta} - \frac{1}{V^{\alpha}}\boldsymbol{\gamma}^{\alpha}\right].$$
(14)

The tensor $T(r^{\alpha\eta})$, introduced in (14), is defined as

$$\mathbf{T}(r^{\alpha\eta}) = \frac{1}{V^{\alpha}V^{\eta}} \int_{V^{\alpha}} \int_{V^{\eta}} \mathbf{K}(\mathbf{x}, \mathbf{y}) \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{x}, \tag{15}$$

where $\mathbf{r}^{\alpha\eta}$ is the vector connecting the centers of V^{α} and V^{η} . The components of $\mathbf{T}(\mathbf{r}^{\alpha\eta})$ are given by (Willis and Acton, 1976; O'Brien, 1979; Rodin and Hwang, 1991)

$$T_{ijkl}(\mathbf{r}^{a\eta}) = \frac{1}{8\pi(1-\nu)} [\psi_{,ijkl} - 2\nu\delta_{kl}\phi_{,ij} - (1-\nu)(\phi_{,ik}\delta_{jl} + \phi_{,il}\delta_{jk} + \phi_{,jk}\delta_{il} + \phi_{,jl}\delta_{ik})], \quad (16)$$

with

$$\phi = \frac{1}{r^{\alpha\eta}}$$
 and $\psi = r^{\alpha\eta} + \frac{(a^{\alpha})^2 + (a^{\eta})^2}{5r^{\alpha\eta}}$. (17)

In (17), a^{α} and a^{η} are the radii of V^{α} and V^{η} , and $r^{\alpha\eta} = |\mathbf{r}^{\alpha\eta}|$.

Let us mention two interesting features of the adopted approximation. First, since $T(r^{\alpha\eta}) = T(r^{\eta\alpha})$, algebraic equations (14) are characterized by a symmetric $6N \times 6N$ matrix as long as all inhomogeneities have the same stiffness. Second, the introduced assumption does not involve the reference inhomogeneity. This important distinction between the reference inhomogeneity and its neighbors was pointed out by Kachanov (1985, 1987) for cracks, and by Rodin and Hwang (1991) for ellipsoidal inhomogeneities. In contrast, Nemat-Nasser *et al.* (1982) did not make the distinction, and as a result adopted an unnecessary assumption.

3.3. O'Brien's method

In order to determine the overall response using the formalism developed in Section 3.2, it is necessary to consider a limit as the number of inhomogeneities tends to infinity. This limit has to be evaluated with care, since the tensor $T(r^{\alpha \eta})$ decays as $(r^{\alpha \eta})^{-3}$ so that the sum in (14) is only conditionally convergent. Perhaps the most compelling explanation of this paradox is due to O'Brien (1979). In that paper, it is shown that the convergence difficulty does not arise if the limit is evaluated so that the number of inhomogeneities and the volume occupied by the composite material tend to infinity *simultaneously*.

The limit involves a sequence of finite-size composite material cores imbedded into an infinite effective matrix with stiffness C^* ; in the limit, Γ , the surface bounding the core, tends to infinity. The key to O'Brien's analysis is a proper assessment of the displacement and traction fields on Γ induced by the remote strain field ε_0 in the effective matrix. The argument is that the majority of the inhomogeneities inside Γ , except for those located in a boundary layer, do not "realize" that there is the material transition across Γ . As a result, it is possible to substitute the microscopic fields on Γ with their macroscopic counterparts. Accordingly, on Γ , both the traction and displacement vectors can be specified :

$$\mathbf{u}(\mathbf{y}) = \bar{\boldsymbol{\varepsilon}}\mathbf{y} = \boldsymbol{\varepsilon}^0 \mathbf{y} \text{ and } \mathbf{t}(\mathbf{y}) = \bar{\boldsymbol{\sigma}}\mathbf{n}(\mathbf{y}) = (\mathbf{C}\boldsymbol{\varepsilon}^0 - \boldsymbol{\omega}\mathbf{C}\bar{\boldsymbol{y}})\mathbf{n}(\mathbf{y}); \quad \mathbf{y}\in\Gamma.$$
 (18)

Here, **n** is the outward normal to Γ . The displacement field in the core, $\mathbf{u}'(\mathbf{x})$, induced by the boundary data on Γ is derived from Somigliana's formula (Gurtin, 1972):

$$u_i'(\mathbf{x}) = -\int_{\Gamma} \left[G_{ij}(\mathbf{x}, \mathbf{y}) t_j(\mathbf{y}) - C_{ijkl} G_{km,l}(\mathbf{x}, \mathbf{y}) n_j(\mathbf{y}) u_m(\mathbf{y}) \right] d\Gamma(\mathbf{y}).$$
(19)

The corresponding strain field, $\varepsilon'(\mathbf{x})$, is derived from (19) in two steps. First, $\mathbf{u}'(\mathbf{x})$ is differentiated, and, second, the singularity for small $|\mathbf{x}-\mathbf{y}|$ is resolved. The latter step is accomplished with the aid of the divergence theorem applied to a domain V' which is bounded by the surface Γ and the surface of a small sphere centered at \mathbf{x} :

$$\boldsymbol{\varepsilon}'(\mathbf{x}) = \boldsymbol{\varepsilon}^0 - \boldsymbol{\omega} \mathbf{S} \bar{\boldsymbol{\gamma}} - \boldsymbol{\omega} \int_{V'} \mathbf{K}(\mathbf{x}, \mathbf{y}) \bar{\boldsymbol{\gamma}} \, \mathrm{d} \mathbf{y}.$$
(20)

Thus, in the limit as the composite material fully replaces the effective matrix, $\varepsilon'(\mathbf{x})$ must be used instead of ε^0 in integral equations (6)–(9). Accordingly, in (14), ε^0 must be substituted by the average of $\varepsilon'(\mathbf{x})$ evaluated over the domain V^{α} :

$$\langle \boldsymbol{\epsilon}' \rangle^{z} = \boldsymbol{\epsilon}^{0} - \omega \mathbf{S} \boldsymbol{\tilde{y}} - \frac{\omega}{V^{z}} \int_{V^{z}} \int_{V} \mathbf{K}(\mathbf{x}, \mathbf{y}) \boldsymbol{\tilde{y}} \, \mathrm{d} \mathbf{y} \, \mathrm{d} \mathbf{x}.$$
 (21)

In Section 3.4, it is shown that the integral in (21) combined with the sum in (14) leads to an absolutely convergent formulation. This formulation, however, is still unsuitable for computations due to extremely slow convergence.

3.4. The periodic array

Equations (14) and (21) can be recast into a form suitable for computations if the limit is attained by replicating the RVE so that an infinite periodic array is formed. In this case, it is possible to take advantage of Ewald's technique as suggested by Beenakker (1986) and Brady *et al.* (1988).

For each inhomogeneity in the periodic array, it is appropriate to assign two indices. The first index, η , identifies the corresponding inhomogeneity within the original RVE, and the second index, λ , identifies the cube in which the designated inhomogeneity lies. Due to periodicity, such attributes as the polarization strain, volume, etc. can be unambiguously identified with only one index. Also, we make one exception : the single index α is assigned to the reference inhomogeneity, which is always inside the original cube. Following this convention, the sum in (14) is rewritten as a double sum :

$$\sum_{\eta \neq x} \mathbf{T}(\mathbf{r}^{z\eta}) \mathbf{y}^{\eta} = \sum_{\{\eta, \lambda\} \neq x} \mathbf{T}(\mathbf{r}^{z\eta\lambda}) \mathbf{y}^{\eta}.$$
(22)

In accordance with Ewald's technique, the potentials in (17) are split using the error function:

$$\phi(r) = \phi^{(1)}(r) + \phi^{(2)}(r), \quad \phi^{(1)}(r) = \operatorname{erfc}(\xi r)\phi(r), \quad \phi^{(2)}(r) = \operatorname{erf}(\xi r)\phi(r),$$

$$\psi(r) = \psi^{(1)}(r) + \psi^{(2)}(r), \quad \psi^{(1)}(r) = \operatorname{erfc}(\xi r)\psi(r), \quad \psi^{(2)}(r) = \operatorname{erf}(\xi r)\psi(r), \quad (23)$$

where ξ is a positive constant. The error function and its complement are given by

$$\operatorname{erf}(r) = \frac{2}{\sqrt{\pi}} \int_0^r \exp(-t^2) dt$$
 and $\operatorname{erfc}(r) = 1 - \operatorname{erf}(r)$.

The potentials $\{\phi^{(1)}(r), \psi^{(1)}(r)\}$ and $\{\phi^{(2)}(r), \psi^{(2)}(r)\}$ generate the tensors $\mathbf{T}^{(1)}(\mathbf{r})$ and $\mathbf{T}^{(2)}(\mathbf{r})$, as prescribed by (16). These tensors permit the following rearrangement of the double sum in (22):

$$\sum_{\{\eta,\lambda\}\neq\alpha} \mathbf{T}(\mathbf{r}^{\alpha\eta\lambda})\boldsymbol{\gamma}^{\eta} = \sum_{\{\eta,\lambda\}\neq\alpha} \mathbf{T}^{(1)}(\mathbf{r}^{\alpha\eta\lambda})\boldsymbol{\gamma}^{\eta} + \sum_{\boldsymbol{\gamma}} \mathbf{T}^{(2)}(\mathbf{r}^{\alpha\eta\lambda})\boldsymbol{\gamma}^{\eta} - \mathbf{T}^{(2)}(\mathbf{r}=\mathbf{o})\boldsymbol{\gamma}^{\boldsymbol{\gamma}}.$$
 (24)

In the right-hand side of this equation, the first sum converges exponentially as $r \to \infty$ due to the presence of erfc (ζr), however the second sum is only conditionally convergent. The second sum is evaluated in two steps. First, it is shown that $\sum \sum \mathbf{T}^{(2)}(\mathbf{r}^{\alpha\eta\lambda})\gamma^{\eta}$ becomes absolutely convergent if it is combined with a conditionally convergent integral in (21). Second, the absolutely convergent sum is evaluated in a reciprocal Fourier space, where it converges exponentially.

The Fourier transform of a function $f(\mathbf{r})$ is defined as

$$f(\mathbf{s}) = \int_{\mathcal{R}^3} f(\mathbf{r}) \exp(i\mathbf{s} \cdot \mathbf{r}) \, \mathrm{d}\mathbf{r}, \quad i = \sqrt{-1},$$

where R^3 designates the entire three-dimensional space. The argument r is associated with position vectors in the physical space, and the argument s with those in the reciprocal space.

For an infinite periodic lattice in the physical space, one can construct the reciprocal lattice according to the equation

$$\exp\left(\mathrm{i}\mathbf{r}^{\lambda}\cdot\mathbf{s}^{\rho}\right)=1,$$

where \mathbf{r}^{λ} and \mathbf{s}^{ρ} are the lattice points. The period of the lattice in the physical space is the cube size L.

The transformation of $\sum \sum T^{(2)}(\mathbf{r}^{\alpha\eta\lambda})\gamma^{\eta}$ to the reciprocal space is accomplished with the aid of Poisson's sum formula (Morse and Feshbach, 1953):

$$\sum_{\lambda} \mathbf{T}^{(2)}(\mathbf{r}^{\lambda}) = \frac{1}{L^3} \sum_{\rho} \mathbf{T}^{(2)}(\mathbf{s}^{\rho}).$$
⁽²⁵⁾

From (25) we obtain

$$\sum \sum \mathbf{T}^{(2)}(\mathbf{r}^{\alpha\eta\lambda})\mathbf{y}^{\eta} = \frac{1}{L^{3}} \sum \sum \mathbf{T}^{(2)}(\mathbf{s}^{\rho})\mathbf{y}^{\eta} \exp\left(-\mathbf{i}\mathbf{s}^{\rho}\cdot\mathbf{r}^{\alpha\eta}\right)$$
$$= \frac{1}{L^{3}} \sum \sum \mathbf{T}^{(2)}(\mathbf{s}^{\rho})\mathbf{y}^{\eta} \cos\left(\mathbf{s}^{\rho}\cdot\mathbf{r}^{\alpha\eta}\right), \tag{26}$$

where the vector $\mathbf{r}^{\alpha\eta}$ is defined in the original RVE. The exponential and cosine factors reflect the shifted position of the simple cubic lattice generated by V^{η} with respect to the lattice generated by V^{α} . The tensor $\mathbf{T}^{(2)}(\mathbf{s})$ is evaluated directly from (16) and (17) (see the Appendix):

$$T_{ijkl}^{(2)}(\mathbf{s}) = \frac{1}{2(1-\nu)} \exp\left(-\frac{s^2}{4\xi^2}\right) \times \left\{ \left[-\frac{2}{s^4} - \frac{1}{2s^2\xi^2} - \frac{1}{4\xi^4} + \frac{(a^{\alpha})^2 + (a^{\eta})^2}{5s^2}\right] s_i s_j s_k s_l + \frac{1}{s^2} [2\nu s_i s_j \delta_{kl} + (1-\nu)(s_i s_k \delta_{jl} + s_i s_l \delta_{jk} + s_j s_k \delta_{il} + s_j s_l \delta_{ik})] \right\}.$$
 (27)

It is clear from (27), that $T^{(2)}(s)$ converges exponentially for large *s*, however there is a weak singularity at the point s = o. This is not surprising because the Fourier images of remote points of the physical space are concentrated at the origin of the reciprocal space, and as a result the divergence of $T^{(2)}(r)$ for large *r* translates into the divergence of $T^{(2)}(s)$ for small *s*. In order to demonstrate that the singularity of the double sums in (26) is exactly cancelled by the integrals appearing in (21), the following manipulations are performed :

$$\omega \mathbf{S} \bar{\mathbf{y}} + \frac{\omega}{V^{\alpha}} \int_{V^{\alpha}} \int_{V'} \mathbf{K}(\mathbf{x}, \mathbf{y}) \bar{\mathbf{y}} \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{x} = \frac{\omega}{V^{\alpha}} \int_{V^{\alpha}} \int_{R^{3}} \mathbf{K}(\mathbf{x}, \mathbf{y}) \bar{\mathbf{y}} \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{x}$$
$$= \frac{\omega}{V^{\alpha}} \int_{R^{3}} \mathbf{D}(\mathbf{r}) \bar{\mathbf{y}} \, \mathrm{d}\mathbf{r} = \frac{\omega}{V^{\alpha}} \lim_{s \to 0} \mathbf{D}(\mathbf{s}) \bar{\mathbf{y}} = \frac{1}{L^{3}} \lim_{s \to 0} \sum_{\eta} \mathbf{T}^{(2)}(\mathbf{s}) \mathbf{y}^{\eta}. \quad (28)$$

In this equation, $D(\mathbf{r})$ is the "exterior" Eshelby tensor of the inhomogeneity V^{α} [see Mura (1982)]. This tensor can be derived from (16) if one puts $\phi = V^{\alpha}/r$ and $\psi = V^{\alpha}r + 4\pi (a^{\alpha})^{5}/15r$. Equation (28) implies that the inhomogeneities lying inside the RVE containing the origin of the reciprocal space must be excluded from the last sum in (26).

The tensor $\mathbf{T}^{(2)}(\mathbf{r} = \mathbf{0})$ is evaluated with the aid of the Fourier transform of $\mathbf{T}^{(2)}(\mathbf{s})$ (see the Appendix):

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$$\mathbf{T}_{ijkl}^{(2)}(\mathbf{r}=\mathbf{o}) = \frac{3[(a^{\alpha})^{2} + (a^{\eta})^{2}]\xi^{5} - 25(1+\nu)\xi^{3}}{75\pi^{3/2}(1-\nu)} (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \frac{3[(a^{\alpha})^{2} + (a^{\eta})^{2}]\xi^{5} - 25(2-\nu)\xi^{3}}{75\pi^{3/2}(1-\nu)} \delta_{ij}\delta_{kl}.$$
 (29)

At this stage, the sum in (14) can be rewritten as

$$\sum_{\eta \neq \alpha} \mathbf{T}(\mathbf{r}^{\alpha\eta}) \boldsymbol{\gamma}^{\eta} = \sum_{\{\eta,\lambda\} \neq \alpha} \mathbf{T}^{(1)}(\mathbf{r}^{\alpha\eta\lambda}) \boldsymbol{\gamma}^{\eta} + \frac{1}{L^3} \sum_{\rho \neq 0} \mathbf{T}^{(2)}(\mathbf{s}^{\rho}) \boldsymbol{\gamma}^{\eta} \cos{(\mathbf{s}^{\rho} \cdot \mathbf{r}^{\alpha\eta})} - \mathbf{T}^{(2)}(\mathbf{r} = \mathbf{o}) \boldsymbol{\gamma}^{\alpha}.$$
(30)

Now (14) and (30) form a system of 6N algebraic equations for the polarization strains of the periodic array generated by the RVE. Finally, the parameter ξ is chosen so that the sums in the physical and reciprocal spaces have equal rates of convergence : $\xi = \sqrt{\pi}/L$.

4. TEST PROBLEMS

In this section, the method's predictions are compared with detailed numerical solutions and variational bounds for arrays of identical spherical inhomogeneities whose centers are located at the nodes of three basic cubic lattices : simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC). The inhomogeneities are isotropic and characterized by the elastic constants μ^{I} and v^{I} . The overall elastic response of the arrays is characterized by cubic symmetry (Nunan and Keller, 1984), so that only three material constants are required :

$$\kappa^{*} = \frac{1}{3}C_{111}^{*} + \frac{2}{3}C_{1122}^{*},$$

$$\mu^{*} = C_{1212}^{*},$$

$$\tilde{\mu}^{*} = \frac{1}{2}C_{1111}^{*} - \frac{1}{2}C_{1122}^{*}.$$
(31)

In this equation, the elastic stiffness components are given with respect to a coordinate system whose base vectors are normal to the faces of the unit cell.

So far, the most comprehensive compilation of benchmark numerical solutions for cubic arrays of spherical inhomogeneities was reported by Sangani and Lu (1987). Those authors extended a collocation technique employed by Nunan and Keller (1984) who considered only rigid inhomogeneities. Brockenbrough *et al.* (1992) provided finite element solutions for arrays of voids and rigid inhomogeneities. Their computations, however, are limited to small volume fractions of inhomogeneities, $c \le 0.3$. Also, finite element solutions for SC arrays of voids, including large volume fractions, were obtained by this author. Since the majority of solutions reported in the literature are for $v = v^{I} = 0.3$, all comparisons in this paper are limited to these cases as well.

The constants introduced in (31) must be within variational bounds, as determined for cubic materials (Avellaneda, 1987). These bounds are less restrictive than the original Hashin–Shtrikman bounds for the shear moduli μ^* and $\tilde{\mu}^*$, and coincide with the Hashin–Shtrikman bounds for κ^* . In the sequel, we refer to the bounds only if they are violated.

Table 1 contains four sets of solutions for SC arrays of voids: by Sangani and Lu

Table 1. The overall elastic constants of SC arrays of voids: (SL) Sangani and Lu (1984), (B) Brockenbrough etal. (1992), (R) present finite element calculations, (M) the proposed method

	κ*/κ				μ * /μ				μ̃*/μ			
с	SL	В	R	М	SL	В	R	М	SL	В	R	М
0.10 0.20 0.30 0.40 0.50	0.774 0.602 0.464 0.363 0.242	0.778 0.605 0.468	0.603 0.466 0.351 0.245	0.774 0.604 0.471 0.364 0.276	0.817 0.665 0.554 0.470 0.375	0.814 0.642 0.494	0.642 0.492 0.365 0.256	0.812 0.641 0.496 0.379 0.288	0.841 0.718 0.608 0.504 0.394	0.847 0.724 0.616	0.720 0.610 0.506 0.373	0.841 0.719 0.612 0.512 0.413

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(1987) (SL), by Brockenbrough *et al.* (1992) (B), by this author obtained with the finite element method (R), and by the proposed method (M). The maximum porosity considered here, c = 0.5, is quite close to the maximum attainable, $c_{max} \approx 0.5236$. A remarkable feature of Table 1 is that the benchmark solutions exhibit considerable disagreement for the constant μ^* . In particular, for c = 0.5, the prediction of Sangani and Lu exceeds author's finite element prediction by 46%. This disagreement is particularly disconcerting because in both cases convergent numerical procedures were used. The two sets of finite element solutions are quite close to each other for all three constants, there is, however, one important detail. The predictions of Brockenbrough *et al.* for κ^* , for c = 0.1 and c = 0.2, do exceed the corresponding upper bounds in the third digit. According to Brockenbrough (1992), this is due to incomplete convergence of coarse meshes employed by Brockenbrough *et al.* (1992). Overall, the proposed method agrees better with the finite element solutions are not considerably different from the benchmark solutions.

Approximate solutions of Nemat-Nasser *et al.* (1982) for SC arrays of voids cannot be treated as benchmark solutions because their approach, as well as the proposed method, is not structured as a sequence of successive approximations which converges to the exact solution. Nevertheless, since Nemat-Nasser *et al.* adopted essentially the same assumption as we did, and managed to compute the series they used, their solutions are coincident with ours. Let us mention that, in the computations reported in this paper, the series in (30) was evaluated using $5^3 - 1 = 124$ replicas of the RVE; this guarantees at least four-digit accuracy. In the computations of Nemat-Nasser *et al.*, three-digit accuracy was obtained as a result of using $101^3 - 1 = 1,030,300$ replicas.

In Tables 2 and 3, the method's predictions are compared with the finite element solutions of Brockenbrough *et al.* for BCC and FCC arrays of voids. These cases were not considered by Sangani and Lu. As in Table 1, there is only minor disagreement between the two analyses. Again, for c = 0.1 and c = 0.2, Brockenbrough's predictions for κ^* exceed the corresponding upper bounds in the third digit.

In cases which involve elastic inhomogeneities, the method's predictions are compared with solutions of Sangani and Lu (Figs 1-3). These comparisons are presented only for the constant μ^* since the other two constants behave similarly. Figure 1 contains results for SC arrays for $\mu^{I}/\mu = 0.05$, 5, and 40; the curves correspond to the solutions of Sangani and Lu and the scattered symbols to those obtained by the method. The data is plotted for μ^*/μ versus c. Results for BCC ($c_{max} \approx 0.6802$) and FCC ($c_{max} \approx 0.7403$) arrays are presented in Figs 2 and 3, respectively. Figures 1-3 reveal that the method performs well for $\mu^{I}/\mu = 0.05$ and $\mu^{I}/\mu = 5$ even if c is close to c_{max} . There is, however, a clear divergence tendency for $\mu^{I}/\mu = 40$ as c approaches c_{max} . This tendency will persist further as the ratio μ^{I}/μ increases.

с	κ*/κ		μ*	'/μ	μ̃*/μ		
	В	М	В	М	В	М	
0.10	0.784	0.774	0.840	0.829	0.834	0.819	
0.20	0.604	0.604	0.684	0.686	0.660	0.662	
0.30	0.469	0.471	0.552	0.564	0.521	0.527	

Table 2. The overall elastic constants of BCC arrays of voids: (B) Brockenbrough et al. (1992), (M) the proposed method

 Table 3. The overall elastic constants of FCC arrays of voids: (B) Brockenbrough

 et al. (1992), (M) the proposed method

с	κ*	*/ĸ	μ*	*/μ	μ̃*/μ		
	B	М	В	M	В	М	
0.10	0.776	0.774	0.830	0.828	0.821	0.820	
0.20	0.611	0.604	0.695	0.686	0.675	0.662	
0.30	0.464	0.471	0.553	0.565	0.519	0.526	



Fig. 1. Normalized shear modulus, μ^*/μ , versus the volume fraction of spheres, c, for SC arrays of inhomogeneities. The lines designate results due to Sangani and Lu (1987): $-\mu^{l}/\mu = 0.05$, $-\mu^{l}/\mu = 5$, $-\mu^{l}/\mu = 40$. The scattered symbols designate results obtained by the proposed method: $\oplus \mu^{l}/\mu = 0.05$, $\mu^{l}/\mu = 5$, $\wedge \mu^{l}/\mu = 40$.



Fig. 2. Normalized shear modulus, μ^*/μ , versus the volume fraction of spheres, c, for BCC arrays of inhomogeneities. The lines designate results due to Sangani and Lu (1987: $\mu^{I}/\mu = 0.05, \dots, \mu^{I}/\mu = 5, \dots, \mu^{I}/\mu = 40$. The scattered symbols designate results obtained by the proposed method : $\Phi \mu^{I}/\mu = 0.05$, $\Pi \mu^{I}/\mu = 5$, $\Delta \mu^{I}/\mu = 40$.



Fig. 3. Normalized shear modulus, μ^*/μ , versus the volume fraction of spheres, c, for FCC arrays of inhomogeneities. The lines designate results due to Sangani and Lu (1987): $\mu^{I}/\mu = 0.05$, $\mu^{I}/\mu = 5$, $---\mu^{I}/\mu = 40$. The scattered symbols designate results obtained by the proposed method: $\Psi^{I}/\mu = 0.05$, $\Pi^{I}/\mu = 5$, $\Lambda^{I}/\mu = 40$.

Ultimately, for rigid inhomogeneities, the ratio μ^*/μ logarithmically diverges (Nunan and Keller, 1984) in the limit as $c \rightarrow c_{max}$. This feature cannot be captured by the proposed method. A modification which can remedy this problem is briefly discussed in Section 5.4. To this end, it is expedient to point out that the majority of composites encountered in structural applications are characterized by the μ^{I}/μ ratios which are less than 40. This is definitely true for metal- and ceramic-matrix composites. For polymer-matrix composites, typical values of $\mu = 2$ GPa (PMMA) and $\mu^{I} = 40$ GPa (glass) (Ashby and Jones, 1980) lead to $\mu^{I}/\mu = 20$. The ratio μ^{I}/μ can be very large for solid propellents, but these composites typically exhibit strongly inelastic response so that, in this case, the use of linear elasticity *per se* is questionable.

5. RELATED METHODS

In this section, we examine connections between the proposed method and closelyrelated methods which preserve the geometry of the RVE and approximate the rigorous problem formulation by a system of algebraic equations. For simplicity, the comparisons are based on the auxiliary problem stated for N identical inhomogeneities in an infinite matrix.

5.1. Multipole expansion

According to this method (Morse and Feshbach, 1953), integral equations (6)–(9) are approximated using Taylor's expansion. In particular, the external strain field induced by an inhomogeneity V^n is obtained upon expanding the kernel K(x, y) about the center r^n of V^n :

$$\int_{\mathcal{V}^{\eta}} K_{ijkl}(\mathbf{x}, \mathbf{y}) \beta_{kl}^{\eta}(\mathbf{y}) \, \mathrm{d}\mathbf{y} \approx K_{ijkl}(\mathbf{x}, \mathbf{r}^{\eta}) \int_{\mathcal{V}^{\eta}} \beta_{kl}^{\eta}(\mathbf{y}) \, \mathrm{d}\mathbf{y} + K_{ijkl,m}(\mathbf{x}, \mathbf{r}^{\eta}) \int_{\mathcal{V}^{\eta}} (y_m - r_m^{\eta}) \beta_{kl}^{\eta}(\mathbf{y}) \, \mathrm{d}\mathbf{y} + \frac{1}{2!} K_{ijkl,mn}(\mathbf{x}, \mathbf{r}^{\eta}) \int_{\mathcal{V}^{\eta}} (y_m - r_m^{\eta}) \beta_{kl}^{\eta}(\mathbf{y}) \, \mathrm{d}\mathbf{y} + \cdots$$
(32)

If only the leading term of this expansion is retained, (11) is approximated as

$$\int_{V^{\alpha}} \varepsilon^{\alpha}(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \mathbf{S} \mathbf{y}^{\alpha} + \sum_{\eta \neq \alpha} \left[\int_{V^{\alpha}} \mathbf{K}(\mathbf{x}, \mathbf{r}^{\eta}) \, \mathrm{d}\mathbf{x} \right] \mathbf{y}^{\eta}.$$
(33)

Thus, if integral equations (6)–(9) are reduced to an algebraic form according to (33), the tensor $T(\mathbf{r}^{z\eta})$ in (14) must be substituted by $(1/V^{\alpha}) \int_{V^{\alpha}} \mathbf{K}(\mathbf{x}, \mathbf{r}^{\eta}) d\mathbf{x}$. It is important to emphasize that the difference between these two tensors is of order $\mathcal{O}(d^{-5})$, where *d* is the distance between the centers normalized by the radius. Since the tensors themselves are $\mathcal{O}(d^{-3})$, the approximation of elastic interactions adopted in the proposed method is consistent with the one provided by the leading term of the multipole expansion.

It appears that the proposed method is more appealing than the multipole expansion. Indeed, in the multipole expansion, a neighbor is simulated by a singular source of the polarization strain located at the center, while, in the proposed method, the approximation is in the spirit of the Saint-Venant principle so that the polarization strain is uniformly distributed inside the inhomogeneity. As a result, the proposed method performs consistently better than the multipole expansion, at least for the test problems considered in Section 4.

5.2. Expansion of Moschovidis and Mura

In the approach of Moschovidis and Mura (1975), Taylor's expansion is applied twice. First, the transformation strain of each inhomogeneity is expanded about its center:

$$\beta_{ij}^{\alpha}(\mathbf{x}) = \beta_{ij}^{\alpha}(\mathbf{r}^{\alpha}) + (x_{k} - r_{k}^{\alpha})\beta_{ij,k}^{\alpha}(\mathbf{r}^{\alpha}) + \frac{1}{2}(x_{k} - r_{k}^{\alpha})(x_{l} - r_{l}^{\alpha})\beta_{ij,kl}^{\alpha}(\mathbf{r}^{\alpha}) + \cdots, \quad \alpha = 1, \dots, N.$$
(34)

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This approximation is exploited with the aid of Eshelby's polynomial theorem (Eshelby, 1961; Mura, 1982) which states that if $\mathbf{x} \in V^{\alpha}$ and $\mathbf{f}(\mathbf{x})$ is a polynomial transformation strain of degree *m*, then the integral $\int_{V^{\alpha}} \mathbf{K}(\mathbf{x}, \mathbf{y}) \mathbf{f}(\mathbf{y}) d\mathbf{y}$ is also a polynomial of degree *m*. Thus, in accordance with (34), the strain field induced by $\boldsymbol{\beta}^{\alpha}(\mathbf{x})$ inside the domain V^{α} is a polynomial. Of course, the strain fields induced by the neighbors are not polynomials inside V^{α} . At this stage, the second expansion is invoked, this time for the strain fields induced by the neighbors. If only the leading term in (34) is retained, the corresponding algebraic equations for $\alpha = 1, \ldots, N$ are

$$\mathbf{C}^{\alpha}\left\{\boldsymbol{\varepsilon}^{0}+\sum_{\eta=1}^{N}\left[\int_{\mathcal{V}^{\eta}}\mathbf{K}(\mathbf{x},\mathbf{r}^{\alpha})\,\mathrm{d}\mathbf{x}\right]\boldsymbol{\beta}^{\eta}(\mathbf{r}^{\eta})\right\}=\mathbf{C}\left\{\boldsymbol{\varepsilon}^{0}+\sum_{\eta=1}^{N}\left[\int_{\mathcal{V}^{\eta}}\mathbf{K}(\mathbf{x},\mathbf{r}^{\alpha})\,\mathrm{d}\mathbf{x}\right]\boldsymbol{\beta}^{\eta}(\mathbf{r}^{\eta})-\boldsymbol{\beta}^{\alpha}(\mathbf{r}^{\alpha})\right\}.$$
(35)

For this truncation, the polarization strains are related to the unknowns $\beta^{\alpha}(\mathbf{r}^{\alpha})$ by

$$\gamma^{\alpha} = V^{\alpha} \boldsymbol{\beta}^{\alpha}(\mathbf{r}^{\alpha}). \tag{36}$$

It is interesting that eqns (35) and (36) coincide with those derived from the leading term truncation of the multipole expansion. This is not the case, however, if higher order terms are included in both expansions. Furthermore, since Moschovidis and Mura employed Taylor's expansion twice, one should expect that the multipole expansion is a better choice between these two methods.

5.3. Method of reflections

This method, which was proposed by Smoluchowski (1911), is virtually unknown in the solid mechanics community. Numerous applications of the method of reflections to low-Reynolds-number hydrodynamic interactions can be found in Kim and Karrila (1991).

The method of reflections is an iterative procedure. It is initiated by assigning to each inhomogeneity the transformation strain induced by the remote field as if the neighbors were absent. The corresponding polarization strain is denoted by $\gamma^{\alpha 0}$, where the superscript 0 designates that this is the initial step. For the reference inhomogeneity V^{α} , the first iteration involves the equation

$$\mathbf{C}^{\alpha} \left[\boldsymbol{\varepsilon}^{0} + \frac{1}{V^{\alpha}} \mathbf{S} \boldsymbol{\gamma}^{\alpha 1} + \sum_{\eta \neq \alpha} \mathbf{T}(\mathbf{r}^{\alpha \eta}) \boldsymbol{\gamma}^{\eta 0} \right] = \mathbf{C} \left[\boldsymbol{\varepsilon}^{0} + \frac{1}{V^{\alpha}} \mathbf{S} \boldsymbol{\gamma}^{\alpha 1} + \sum_{\eta \neq \alpha} \mathbf{T}(\mathbf{r}^{\alpha \eta}) \boldsymbol{\gamma}^{\eta 0} - \frac{1}{V^{\alpha}} \boldsymbol{\gamma}^{\alpha 1} \right], \quad (37)$$

which implies that the strain field induced by the neighbors of V^{α} is determined in terms of $\gamma^{\eta 0}$. As α runs from 1 to N the first iteration is completed. For the second iteration, the strain field induced by the neighbors is determined in terms of $\gamma^{\eta 1}$, and so on. Thus the method of reflections does not require inversion of the large $6N \times 6N$ matrix, instead the many 6×6 matrices have to be inverted.

It is easy to demonstrate that, for identical inhomogeneities, a successive approximation $\gamma^{\alpha n}$ can be written in the form

$$\gamma^{\alpha n} = \left(\mathbf{I} + \mathbf{U}^{\alpha} + \mathbf{U}^{\alpha}\mathbf{U}^{\alpha} + \dots + \underbrace{\mathbf{U}^{\alpha}\mathbf{U}^{\alpha}\dots\mathbf{U}^{\alpha}}_{n}\right)\gamma^{\alpha 0}.$$
 (38)

In this equation, I is the fourth rank symmetric identity tensor, and U^{α} is a fourth rank tensor dependent on the geometry and elastic properties of the array. This series converges as long as the inhomogeneities do not intersect, and in the limit as $n \to \infty$, the polarization strain $\gamma^{\alpha n}$ coincides with that obtained with the proposed method (Durlofsky *et al.*, 1987).

5.4. Stokesian dynamics

Stokesian dynamics (Durlofsky et al., 1987; Brady and Bossis, 1988; Brady et al., 1988) is intended for dynamic simulations of low-Reynolds-number suspensions of rigid spherical particles. The governing equations for such suspensions are parallel to those for rigid particles imbedded into an incompressible elastic matrix. The proposed method is not restricted to this particular class of problems, thus it is more general than Stokesian dynamics. However, as far as this particular class of problem is concerned, Stokesian dynamics is the better method.

In Stokesian dynamics, two types of hydrodynamic interactions are identified: longrange and short-range. The former are determined exactly as it is done in the proposed method. The latter are pair-wise interactions due to singular lubrication forces in the ligament between closely positioned inhomogeneities. These interactions become dominant in arrays with high volume fractions, and they guarantee correct asymptotic behavior for the overall viscosity in the limit as $c \rightarrow c_{max}$. Thus, in *Stokesian dynamics*, both limits for small and large c are properly incorporated, and therefore the method is capable of handling both dilute and concentrated suspensions. The short-range interactions are calibrated using solutions for two rigid inhomogeneities (Kim and Karrila, 1991). For further details the reader is refered to the original papers.

In solid mechanics, the nature of short-range interactions is much more complex. Of course, following Brady and co-workers, one can simply take advantage of asymptotic solutions for two rigid inhomogeneities in the elastic matrix (Nunan and Keller, 1984). This extension, however, does not reflect two important physical factors. First, two identical inhomogeneities do not interact as rigid inhomogeneities unless their Young's modulus exceeds that of the matrix by about three orders of magnitude (Yeh, 1992). This estimate was obtained as a result of numerical experiments with the conduction problem which exhibits the same singularity in the ligament as the elasticity problem (Batchelor and O'Brien, 1977; Nunan and Keller, 1984). Since solid composite materials are characterized by much lower ratios of the Young's moduli, the inhomogeneities cannot be treated as rigid and the asymptotic solution becomes considerably more complicated. The second factor is related to the probable onset of inelastic deformation in the ligament in the form of yielding or debonding. This consideration is particularly important if one realizes that the asymptotic elastic solution for rigid inhomogeneities predicts the stress in the ligament to be proportional to χ^{-1} and the polarization strain only proportional to $\ln \chi$, where χ is the ligament thickness normalized by the radius. Thus, before the short-range interactions can significantly influence the overall response, they must induce very high stress concentrations which should lead to inelasticity.

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APPENDIX

According to (16), (17) and (23), the Fourier transform of the tensor $T^{(2)}(\mathbf{r})$ can be written as

$$T_{ijkl}^{(2)}(\mathbf{s}) = \frac{1}{8\pi(1-\nu)} \left\{ \psi^{(2)}(\mathbf{s})s_i s_j s_k s_l + \phi^{(2)}(\mathbf{s}) [2\nu s_i s_j \delta_{kl} + (1-\nu)(s_i s_k \delta_{jl} + s_i s_l \delta_{jk} + s_j s_k \delta_{il} + s_j s_l \delta_{ik})] \right\},$$
(A1)

with the potentials

$$\phi^{(2)}(\mathbf{s}) = \int_{\mathbb{R}^3} \frac{\operatorname{erf}\left(\xi r\right)}{r} \exp\left(\mathbf{s} \cdot \mathbf{r}\right) d\mathbf{r}$$
(A2)

and

$$\psi^{(2)}(\mathbf{s}) = \int_{\mathbb{R}^3} \operatorname{erf}\left(\xi r\right) r \exp\left(\mathbf{s} \cdot \mathbf{r}\right) d\mathbf{r} + \frac{(a^x)^2 + (a^y)^2}{5} \int_{\mathbb{R}^3} \frac{\operatorname{erf}\left(\xi r\right)}{r} \exp\left(\mathbf{s} \cdot \mathbf{r}\right) d\mathbf{r}.$$
 (A3)

Since the pre-exponential factors of the integrands in (A2) and (A3) depend only on r, the expressions for the potentials can be simplified as follows:

$$\phi^{(2)}(\mathbf{s}) = \int_0^\infty \frac{\text{erf}(\zeta r)}{r} \, 4\pi r^2 \frac{\sin(sr)}{sr} \, \mathrm{d}r \tag{A4}$$

and

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$$\psi^{(2)}(\mathbf{s}) = \int_0^\infty \operatorname{erf}\left(\xi r\right) r 4\pi r^2 \frac{\sin\left(sr\right)}{sr} \, \mathrm{d}r + \frac{(a^s)^2 + (a^\eta)^2}{5} \int_0^\infty \frac{\operatorname{erf}\left(\xi r\right)}{r} \, 4\pi r^2 \frac{\sin\left(sr\right)}{sr} \, \mathrm{d}r. \tag{A5}$$

With the introduction of the integral (Gradshteyn and Ryzhik, 1980)

$$I(s) = 4\pi \int_0^\infty \operatorname{erf}(\xi r) \sin(sr) \, \mathrm{d}r = \frac{4\pi}{s} \exp\left(-\frac{s^2}{4\xi^2}\right),\tag{A6}$$

the potentials can be calculated from

$$\phi^{(2)}(\mathbf{s}) = \frac{1}{s} I(s)$$
 (A7)

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$$\psi^{(2)}(\mathbf{s}) = -\frac{1}{s} \frac{d^2 I(s)}{ds^2} + \frac{(a^n)^2 + (a^n)^2}{5s} I(s).$$
(A8)

The tensor $T^{(2)}(\mathbf{r} = \mathbf{0})$ in (27) is evaluated in terms of the inverse Fourier transform of $T^{(2)}(\mathbf{s})$:

$$\mathbf{T}^{(2)}(\mathbf{r}=\mathbf{o}) = \frac{1}{8\pi^3} \int_{\mathcal{R}^3} \mathbf{T}^{(2)}(\mathbf{s}) \, \mathrm{d}\mathbf{s}. \tag{A9}$$

This integral is written as

$$\mathbf{T}^{(2)}(\mathbf{r}=\mathbf{0}) = \frac{1}{8\pi^3} \int_{\mathbb{R}^3} \mathbf{T}^{(2)}(\mathbf{s}) \, \mathrm{d}\mathbf{s} = \frac{1}{8\pi^3} \int_0^\infty \int_{\Omega(s)} \mathbf{T}^{(2)}(\mathbf{s}) \, \mathrm{d}\Omega \, \mathrm{d}s, \tag{A10}$$

where $\Omega(s)$ is the surface of a sphere with radius s. The surface integral can be calculated using simple symmetry arguments,

$$\int_{\Omega(s)} s_i s_j \, \mathrm{d}\Omega = \frac{4\pi}{3} \, s^4 \delta_{ij} \quad \text{and} \quad \int_{\Omega(s)} s_i s_j s_k s_l \, \mathrm{d}\Omega = \frac{4\pi}{15} \, s^6 (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \tag{A11}$$

and the integral with respect to s is an elementary combination based on the integral (Gradshteyn and Ryzhik, 1980),

$$\int_{0}^{\infty} s^{2n} \exp\left(-\frac{s^{2}}{4\xi^{2}}\right) \mathrm{d}s = 2^{n}(2n-1)!!\xi^{2n+1}.$$
 (A12)