Fast and accurate calculations of structural parameters for suspensions†

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The calculation of effective properties of periodic suspensions is often problematic. Particularly difficult are calculations involving unit cells with many, close to touching, inclusions and high desired accuracy. In this paper we apply the conjugate gradient method and the fast multipole method to simplify calculations of this kind. We show how to dramatically speed up the computation of the effective conductivities and structural parameters for suspensions of disks and spheres. This enables accurate treatment of unit cells with thousands of inclusions. Direct estimates of the effective conductivity are compared with estimates via bounds. Accuracy of twelve digits is obtained for a suspension of disks which has been studied previously, but for which no accurate digit has been determined.

1. Introduction

The calculation of the effective conductivity of two-component composites is a subject which has attracted interest over many years. Important theoretical progress includes the establishment of series of progressively tighter upper and lower bounds on this quantity (Hashin & Shtrikman 1962; Beran 1965; Prager 1969; Baker 1975; Bergman 1978; Milton 1981; Milton & McPhedran 1982). Bounds are constructed from known values of the effective conductivity and from coefficients in its perturbation expansion, so called structural parameters. Once some of these numbers are known for a material, the corresponding bounds can swiftly be evaluated for any component conductivities $\sigma_1$ and $\sigma_2$.

Attempts to do calculations of structural parameters have focused on periodic materials with unit cells consisting of inclusions in matrices. The parameters have been calculated for different volume fractions of the inclusions. Moderately accurate results are available for unit cells with one or two inclusions in the shape of disks, spheres (Bergman 1979; McPhedran & Milton 1981), and cubes (Helsing 1993).

Numerical calculations for unit cells with more than two inclusions, resembling random materials, have proven to be problematic (Kantor & Bergman 1982; Sangani & Yao 1988a,b; Durand & Ungar 1988; Miller & Torquato 1990; Bonnecaze & Brady 1991; Hinsen & Felderhof 1992). Difficulties include generation of the actual materials, storage of intermediary results, and evaluation of slowly con-

† This paper was produced from the author's disk by using the TeX typesetting system.
verging sums. More theoretical approaches invoke superposition approximations (Torquato & Lado 1988) and are, as a consequence, only valid when these approximations apply.

In this paper we show how to eliminate the difficulty of slowly converging sums and reduce the difficulty of handling large unit cells in the calculation of effective conductivities and structural parameters for suspensions of disks and spheres. The key feature is the use of the fast multipole method (Greengard & Rokhlin 1987) and the conjugate gradient method to solve variants of the well established equations for these problems (Rayleigh 1892; Mcphedran & McKenzie 1978; McPhedran & Milton 1981; Milton 1987). In two dimensions, our scheme allows for calculation of the effective conductivity of unit cells with up to $10^3$ disks and some structural parameters for unit cells with up to $10^5$ disks. In §2, we present bounds involving structural parameters only. In §3, we state what quantities are to be calculated for disks and how this may be done quickly and accurately. In §4, we calculate the lattice sums of Rayleigh (1892) with a simplified version of the fast multipole method. This enables us to calculate virtually any parameter for unit cells with only a few disks. In §5, we treat the square array of disks and get good results up to the regime where an asymptotic expression (McPhedran, Poladian & Milton 1988) becomes valid. For a unit cell of 16 nearly touching disks we get twelve digits of accuracy where previously no digit has been achieved. In §6, the formalism is extended to suspensions where the inclusions are objects of arbitrary shape. Calculations are presented for a dilute suspension of squares.

2. Higher-order bounds on the effective conductivity

Assume that the suspension is periodic with a unit cell of volume $V$. The local conductivity $\sigma(r)$ at position $r$ is

$$\sigma(r) = \chi_1(r)\sigma_1 + \chi_2(r)\sigma_2,$$  \hspace{1cm} (2.1)

where $\chi_a(r)$ is the indicator function and $\sigma_a$ is the conductivity of component $a$, ($a = 1, 2$). Let component 1 denote the matrix, let component 2 denote the inclusions, and let the volume fractions of the two components be $f_1$ and $f_2$, respectively.

The effective conductivity tensor $\sigma_{\text{eff}}$ of a composite can be defined by

$$\langle E^1, \sigma_{\text{eff}} E^1 \rangle \equiv \inf_\phi \langle E^1 + \nabla \phi, \sigma (E^1 + \nabla \phi) \rangle,$$  \hspace{1cm} (2.2)

where $E^1$ is a constant field of unit strength and $\phi$ ranges over functions with the same periodicity as the composite. The inner product in (2.2) is the usual for two vector fields $\mathbf{F}, \mathbf{G}$

$$\langle \mathbf{F}, \mathbf{G} \rangle = \frac{1}{V} \int_V \mathbf{F}(r) \cdot \mathbf{G}(r) dr.$$  \hspace{1cm} (2.3)

The tensor $\sigma_{\text{eff}}$ of (2.2) is symmetric (Bensoussan, Lions & Papanicolaou 1978). In the sequel we will refer to the left hand side of (2.2) as the (scalar) effective conductivity $\sigma_{\text{eff}}$. For an anisotropic composite $\sigma_{\text{eff}}$ will depend on the direction of the unit field $E^1$.

A compact way of expressing bounds on the effective conductivity is to intro-
duce the variable $\rho \in [-1, 1]$

$$\rho = \frac{\sigma_2 - \sigma_1}{\sigma_2 + \sigma_1},$$  (2.4)

and to write

$$\sigma_{\text{eff}} = \sigma_1 \sum_{i=0}^{\infty} q_i \rho^i.$$  (2.5)

The Taylor coefficients $q_i$ of (2.5) are called structural parameters. A lower bound on the conductivity of order $M = 2L$ is the one-point Padé approximant (Milton & McPhedran 1982)

$$\sigma^- = \sigma_1 \frac{1 + \sum_{n=1}^{L} a_n \rho^n}{1 + \sum_{n=1}^{L} b_n \rho^n}$$  (2.6)

that coincides with the Taylor series for $\sigma_{\text{eff}}$ to order $M$ at $\rho=0$. An upper bound on the conductivity of order $M = 2L$ is the three-point Padé approximant

$$\sigma^+ = \sigma_1 \frac{1 + \sum_{n=1}^{L+1} a_n^+ \rho^n}{1 + \sum_{n=1}^{L+1} b_n^+ \rho^n}$$  (2.7)

that coincides with the Taylor series for $\sigma_{\text{eff}}$ to order $M$ at $\rho=0$ and in addition passes through the points $\left(\rho, \sigma_{\text{eff}}\right) = (-1, 0)$ and $(1, \infty)$.

The $2L$ coefficients $a_n^-$, $b_n^-$ of (2.6) can be determined by solving (Milton & McPhedran 1982; Sangani & Yao 1988a)

$$\gamma(n, L) a_n^--\sum_{m=1}^{\min \{n, L\}} q_{n-m} b_m^- = q_n, \quad n = 1, 2, \ldots, 2L$$  (2.8)

where $\gamma(n, L)$ is unity for $n \leq L$ and zero for $n > L$. The $2L + 2$ coefficients $a_n^+$, $b_n^+$ of (2.7) can, similarly, be determined from

$$\gamma(n, L+1) a_n^+ - \sum_{m=1}^{\min \{n, L+1\}} q_{n-m} b_m^+ = q_n, \quad n = 1, 2, \ldots, 2L,$$

$$\sum_{m=1}^{L+1} (-1)^m a_m^+ = -1, \quad \sum_{m=1}^{L+1} b_m^+ = -1.$$  (2.9)

The structural parameters $q_i$ can be found by differentiation of

$$\sigma_{\text{eff}} = \sigma_1 - 2\sigma_1 \langle \chi_2 \mathbf{E}^1, (1 - 2\chi_2 \Gamma_1 - 1/\rho)^{-1}\chi_2 \mathbf{E}^1 \rangle,$$  (2.10)

where the operator $\Gamma_1$ projects on zero-average curl-free fields. Equation (2.10) comes from simplification of equations in Milton (1987). We will refer to (2.10) as the direct method for the effective conductivity.

Differentiation of (2.10) and identification with (2.5) gives

$$q_i = \sum_{j=1}^{i} (-1)^{j-1} \binom{i-1}{j-1} 2^j \langle \chi_2 \mathbf{E}^1, (\chi_2 \Gamma_1)^{j-1}\chi_2 \mathbf{E}^1 \rangle.$$  (2.11)

The first structural parameter is trivially $q_1 = 2f_2$. For macroscopically isotropic
composites the second structural parameter can be evaluated with Fourier methods to (Phan-Thien & Milton 1982)

\[ q_2 = 2f_2 \left( 1 - \frac{2f_1}{d} \right), \tag{2.12} \]

where \( d = 2, 3 \) is the dimension. The calculation of higher-order structural parameters, generally, requires full knowledge of the material geometry.

3. Unit cell of \( N \) disks

In this section we show how to compute the \( q_i \) of (2.11) for a unit cell of \( N \) disks. Complex notation will be used with \( z = x + iy \). The complex field \( f(z) \) will represent the physical field \( (\text{Re}\ f(z), -\text{Im}\ f(z)) \) (Greengard & Rokhlin 1987), where \( \text{Re} \) and \( \text{Im} \) denote real and imaginary parts. The inner product of (2.3) between two physical fields becomes

\[ \langle f, g \rangle = \frac{1}{V} \int_V \text{Re} \left\{ f^*(z)g(z) \right\} dx dy, \tag{3.1} \]

where the asterisk denotes conjugation. For conjugation we will also use the operator \( K \) so that

\[ Kf = f^* \tag{3.2} \]

If a complex number is viewed as an ordered pair of real numbers \( (\text{Re}\ f, \text{Im}\ f) \) conjugation becomes matrix vector multiplication

\[ Kf \sim \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \text{Re}\ f \\ \text{Im}\ f \end{pmatrix}, \tag{3.3} \]

as does multiplication of two complex numbers

\[ af \sim \begin{pmatrix} \text{Re}\ a & -\text{Im}\ a \\ \text{Im}\ a & \text{Re}\ a \end{pmatrix} \begin{pmatrix} \text{Re}\ f \\ \text{Im}\ f \end{pmatrix}. \tag{3.4} \]

For evaluation of (2.11) we want the action of \( \chi_2 \Gamma_1 \) when applied to a field \( \chi_2 \mathbf{E} \). First, write

\[ \chi_2 = \sum_{ik=1}^{N\infty} \chi_{2ik}. \tag{3.5} \]

In this double sum \( \chi_{2ik} \) is the indicator for disk \( i \) in unit cell \( k \), \( i \) runs over the \( N \) disks of the unit cell, and \( k \) runs over all unit cells. The unit cells are assumed to form a square array in the material \( \Omega \) and the unit cell volume is \( V = 1 \).

Next, approximate \( \chi_2 \mathbf{E} \) by its projection on the \( p \) first elements of orthonormal bases of harmonic functions

\[ \chi_2 \mathbf{E} = \sum_{imk=111}^{Np\infty} \chi_{2ik}c_{im} \sqrt{\frac{m}{\pi}} \frac{(z - z_{ik})^{m-1}}{(R_i)^m}. \tag{3.6} \]

Here \( z_{ik} \) is the center of disk \( i \) with radius \( R_i \) in unit cell \( k \). The field \( \chi_{2ik} \mathbf{E} \) can be decomposed into the electric field

\[ \chi_{2ik} \sum_{m=1}^{p} \frac{c_{im}}{2} \sqrt{\frac{m}{\pi}} \frac{(z - z_{ik})^{m-1}}{(R_i)^m} - (1 - \chi_{2ik}) \sum_{m=1}^{p} \frac{c_{im}^2}{2} \sqrt{\frac{m}{\pi}} \frac{(R_i)^m}{(z - z_{ik})^{m+1}}. \tag{3.7} \]
and the current density field
\[
\chi_{2i} \sum_{m=1}^{p} \frac{c_{im}}{2} \sqrt{\frac{m}{\pi}} \frac{(z - z_{ik})^{m-1}}{(R_{i})^{m}} + (1 - \chi_{2ik}) \sum_{m=1}^{p} \frac{c_{im}^{k}}{2} \sqrt{\frac{m}{\pi}} \frac{(R_{i})^{m}}{(z - z_{ik})^{m+1}}.
\] (3.8)

This means that inside unit cell \( k = 1 \) the field \( \chi_{2i} \Gamma_{1} \chi_{2} \mathbf{E} \) becomes
\[
\chi_{2i} \Gamma_{1} \chi_{2} \mathbf{E} = \sum_{i=1}^{N} \chi_{2i} \left\{ \sum_{m=1}^{p} \frac{c_{im}}{2} \sqrt{\frac{m}{\pi}} \frac{(z - z_{ii})^{m-1}}{(R_{i})^{m}} - \sum_{j=111}^{N \text{p}} \frac{c_{jm}}{2} \sqrt{\frac{m}{\pi}} \frac{(R_{j})^{n}}{(z - z_{j})^{m+n}} \right\}
\]
\[
= \sum_{m=11}^{N \text{p}} \chi_{2i} \left\{ \frac{c_{im}}{2} - \sum_{j=111}^{N \text{p}} \frac{\sqrt{m!n!(z - z_{j})^{m+n}}}{(R_{j})^{m+n}} \frac{(m + n - 1)!}{m!n!} \right\}
\]
\[
\quad \quad \quad \times \sqrt{\frac{m}{\pi}} \frac{(z - z_{i})^{m-1}}{(R_{i})^{m}},
\] (3.9)

where equality holds in the subspace of (3.6). Equation (3.9) describes the action of \( \chi_{2} \Gamma_{1} \).

Now represent the field \( \chi_{2} \mathbf{E} \) as a vector of length \( pN \) whose components are the coefficients of (3.6). The self-adjoint operator \( \chi_{2} \Gamma_{1} \) becomes a symmetric matrix on the form
\[
\chi_{2} \Gamma_{1} \sim \frac{1}{2} \{ \mathbf{I} - \mathbf{W} \},
\] (3.10)

where \( \mathbf{I} \) is a \( pN \times pN \) identity matrix and \( \mathbf{W} \) is a matrix with \( N^{2} \) blocks \( W_{ij} \) of size \( p \times p \). For equisized disks with \( R_{i} = R \) the elements of these blocks are
\[
W_{mn}^{ij} = V_{mn} S_{mn}^{ij} K_{i},
\] (3.11)

where
\[
V_{mn} = \frac{\sqrt{m!n!(m + n - 1)!}R^{m+n}(-1)^{n+1}}{m!n!},
\] (3.12)

and
\[
S_{mn}^{ij} = \sum_{j=1}^{\infty} \frac{1}{(z_{j} - z_{i})^{m+n}}.
\] (3.13)

In (3.13) the lattice sums with \( m = n = 1 \) are shape dependent. This reflects that for \( m = 1 \) the integral over \( \Omega \) of the second parts of (3.7) and (3.8) are indeterminate. As we shall see later, in our calculations the sum
\[
\sum_{i=2}^{\infty} \frac{1}{(z_{j} - z_{i})^{2}}
\] (3.14)

should be taken as \( \pi K \). The sum of (3.14) is referred to as \( S_{2} \) and is the first member in a series of lattice sums
\[
S_{n} = S_{n}^{I} + S_{n}^{II} = \sum_{i=2}^{9} \frac{1}{(z_{j} - z_{i})^{n}} + \sum_{j=10}^{\infty} \frac{1}{(z_{j} - z_{i})^{n}},
\] (3.15)

introduced in the composite literature by Rayleigh (1892). In the first of the

actually, only odd-order series expansion gives for the structural parameters of anisotropically isotropic composites (Milton 1981) where

\[ S^i_{m+n} = S_{m+n}, \quad \text{and for } j \neq i \text{ to double precision accuracy} \]

\[ S^i_{m+n} = \sum_{l=1}^{9} \frac{1}{(z_{jl} - z_{il})^{m+n}} + \sum_{q=0}^{100} \binom{m+n+q-1}{q} S_{m+n+q}^{i+q} (z_{il} - z_{jl})^q. \]

Once the lattice sums of (3.13) are determined the structural parameters \( q_i \) of (2.11) can be calculated. The field \( \chi_2 E^i \) is represented by a vector

\[ \chi_2 E^i = \sqrt{\pi} R u^1 = \sqrt{\pi} R (u, 0, 0, 0, u, 0, 0, 0, 0, 0, 0, 0, \ldots). \]

Here the unit vector \( u^1 \) has been introduced and \( u \) has magnitude one. With (3.10) the inner products of (2.11) become

\[ 2^j \langle \chi_2 E^i, (\chi_2 F_1)^{j-1} \chi_2 E^1 \rangle = 2\pi R^2 \text{Re} \left\{ u^{iT} (I - W)^{j-1} u^1 \right\}. \]

Series expansion gives for the structural parameters

\[ q_{2i-1} = 2\pi R^2 u^{iT} u^i, \]

\[ q_{2i} = 2\pi R^2 \text{Re} \left\{ u^{iT} u^{i+1} \right\}, \]

where

\[ u^i = (W)^{i-1} u^1. \]

Actually, only odd-order \( q_i \) need to be calculated since for two-dimensional macroscopically isotropic composites (Milton 1981)

\[ q_{2n} = \frac{1}{2} \sum_{u=1}^{2n-1} (-1)^{u+1} q_u q_{2n-u}. \]

A square array of disks has \( N=1 \) and \( f_2 = \pi R^2 \). Due to symmetries only \( m, n \) odd need to be considered. Equation (3.20) reduces to the expression of McPhedran & Milton (1981) and the direct method of (2.10) becomes the algorithm of McPhedran & McKenzie (1980). Comparison of (2.12) and (3.20) for \( i=1 \) with (3.11) gives \( S_2 = \pi K \), as claimed above.

The above scheme, which will be implemented in § 5, has similarities to those of Rayleigh (1982), McPhedran & Milton (1981), Poladian & McPhedran (1986), and Sangani & Yao (1988a, b). A drawback of these schemes is that for the matrix vector multiplications of (3.21) the \( pN^2 \) different lattice sums of (3.13) must be calculated and stored, or repeatedly calculated anew. Further, the work for matrix vector multiplication is proportional to \( p^2N^2 \). This limits the size of a unit cell that can be handled to approximately 50 disks.

There is, however, a faster way to evaluate the matrix vector multiplication above. Simultaneous multiplication of a vector \( u \) with every \( p:th \) row of \( W \), starting with the first row, amounts to summing multipole contributions from an
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infinite medium with unit cell of \( pN \) particles (\( p \) particles each at \( N \) sites) and evaluating the sums at each site. This can be done with the fast multipole method (Greengard & Rokhlin 1987) with work proportional only to \( p^{7/3}N \). Remaining row sums are obtained from

\[
\sum_{jn} W_{(m+1)n}^{ij} u_{jn} = \frac{R}{\sqrt{(m+1)m}} \frac{d}{dz_{i1}} \sum_{jn} W_{mn}^{ij} u_{jn},
\]

(3.23)

and from that the fast multipole method generates a power series in \( z_{i1} \) for the row sums. This means that the fast multipole method can be accurately determined for systems of thousands of disks. For an implementation of this fast multiplication, see Greengard & Helsing (1994).

4. Numerical calculations of the lattice sums \( S_{4k} \)

Accurate calculation of structural parameters requires accurate values of Rayleigh’s lattice sums. In the past these sums have been evaluated by the method of Rayleigh (1892) to six digits (Perrins, McKenzie & McPhedran 1979). In this section we do double precision accurate evaluation of the slowly converging \( S_{4}^{ll} \) and \( S_{8}^{ll} \) with a simplified variant of the fast multipole method (Greengard & Rokhlin 1987). Rayleigh’s method, too, could achieve this but we prefer the fast multipole method since the decomposition of (3.15) is desired. Lattice sums with higher subscript we evaluate by direct summation.

We start with a square array of unit cells. Every unit cell has a site at its center. One of the sites coincides with the origin. At every site, except for the origin, there is a \( 4k \) pole of unit strength. We will evaluate \( S_{4k} \) of (3.15) with \( z_{i1} \) being the origin.

We first consider the \( 4k \) poles in the eight cells that are nearest neighbours to the cell containing the origin. Their contribution to the lattice sum is

\[
S_{4k}^{ll} = 4 + \frac{(-1)^k}{4^k - 1}.
\]

(4.1)

Then, taking \( k = 1 \) and as an intermediary step, we consider the field due to the quadrupoles in a 9-supercell of three times three unit cells. We express this field as a multipole expansions around the center of the 9-supercell. The expansion is valid outside a circle of radius \( \sqrt{2} \) from its center.

We now look at \( S_{4}^{ll} \) and the 72 quadrupoles of the eight 9-supercells that are the nearest neighbours to the 9-supercell containing the origin. We evaluate the contribution from these quadrupoles, nine at a time, to \( S_{4}^{ll} \). The evaluation is easy since the multipole expansion of a 9-supercell is known.

The next intermediary step is to form the multipole expansion for the field due to the quadrupoles in a 81-supercell of nine times nine unit cells. We form this expansion by shifting the centers of eight 9-supercell expansions and adding them together with one unshifted expansion.

The process of adding contributions to \( S_{4}^{ll} \) and forming multipole expansions for distant supercells of increasing size is continued until desired accuracy is achieved. In double precision, 17 iterations of this procedure were needed, summing contributions from multipoles in a medium of \( 10^7 \) times \( 10^7 \) disks. Expansions terms up

to \( p=60 \) were included. The computation took a few seconds on a workstation. The sum \( S_8 \) was treated analogously to \( S_4 \). All results are presented in table 1.

5. Numerical examples

First we take the square array of disks. Difficult calculations pertain to close to touching disks at high conductivity ratios. Following McPhedran, Poladian & Milton (1988) we introduce the parameter

\[
e = \frac{1}{\sqrt{1-4H^2}},
\]

characterizing disk separation. Previous investigators (Perrins, McKenzie & McPhedran 1979; McPhedran & Milton 1981) only had the lattice sums of (3.15) to six digits and bounds are calculated with this accuracy to order 16. Direct estimates of the effective conductivity seem to be computed with numerical methods of order \( p^5 \). For \( \min \{ c, \sigma_1/\sigma \} > 10^5 \) this gives no accurate digit at all.

With Eqs. (2.6-2.9) and (3.20), bounds of order \( M < 30 \), and \( p < 400 \) we get accurate effective conductivity for \( \min \{ c, \sigma_1/\sigma \} < 10^4 \). For higher values of \( \min \{ c, \sigma_1/\sigma \} \) progressively higher order bounds are needed for full accuracy. For \( M > 42 \) we observe an instability in the convergence due to finite precision. The

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### Table 1. Evaluation of the second part of Rayleigh’s lattice sum \( S_n^R \), as defined in (3.15). The operator \( K \) is defined in (3.2).

<table>
<thead>
<tr>
<th>( S_n^R )</th>
<th>( \pi K )</th>
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<tbody>
<tr>
<td>( S_{12} )</td>
<td>0.151212002153897</td>
</tr>
<tr>
<td>( S_{16} )</td>
<td>5.77303365189707D-003</td>
</tr>
<tr>
<td>( S_{20} )</td>
<td>1.349012827970373D-003</td>
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<tr>
<td>( S_{24} )</td>
<td>7.003302502485501D-005</td>
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<td>( S_{28} )</td>
<td>3.003176289539156D-006</td>
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<tr>
<td>( S_{36} )</td>
<td>1.60694099570086D-008</td>
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<td>( S_{40} )</td>
<td>8.975806666669377D-010</td>
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<td>( S_{44} )</td>
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<td>8.90971469335412D-016</td>
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<td>5.56538380974350D-017</td>
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<tr>
<td>( S_{96} )</td>
<td>1.2023200806001D-026</td>
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<td>( S_{100} )</td>
<td>8.07807173594912D-028</td>
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</table>

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Table 2. Effective conductivity of a square array of disks for different disk separation parameters $c$ of (5.1) and disk conductivities $\sigma$. The conductivity of the matrix is unity.

<table>
<thead>
<tr>
<th>$\sigma_2$</th>
<th>$c$</th>
<th>Conductivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1000</td>
<td>35.957646297</td>
</tr>
<tr>
<td>1000</td>
<td>36.672577611</td>
<td>243.0059784</td>
</tr>
<tr>
<td>10000</td>
<td>36.680438632</td>
<td>245.9797711</td>
</tr>
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</table>

direct method of (2.10), which with (3.10) becomes

$$\sigma_{\text{eff}} = \sigma_1 + 2\sigma_1\pi R^2 u_1 (I/\rho - W)^{-1} u_1,$$

is stable and we resort to that. The linear equations of (5.2) are solved with the conjugate gradient method. This method is of order $p^2$ and can be accelerated from the observation that only elements within a distance $15\sqrt{p}$ from the diagonal of $W$ are important in the matrix vector multiplications. Results for $\min\{c, \sigma_2/\sigma_1\} > 10^2$ with multipoles up to $p = 4 \cdot 10^3$ are presented in table 2. We get good results in the regime $\min\{c, \sigma_2/\sigma_1\} > 10^3$ where the asymptotic expression of MePhedran, Poladian & Milton (1988)

$$\sigma_{\text{eff}} = \sigma_1 + \frac{\sigma_1\pi (c-1)}{1 + 2s[\ln(c) - \gamma - \Psi(1+s)]},$$

is accurate to at least 1%. In (5.3) $\gamma$ is Euler’s constant, $\Psi(x)$ is the psi function, and

$$s = \ln(\rho)/\ln[(c-1)/(c+1)].$$

Next we take the unit cell of $N=16$ disks with $f_2 = 0.7$ suggested and solved by Sangani (1993), seemingly with an order $p^3N^3$ method, as in Sangani & Yao (1988b). Coordinates for disks centers are presented in table 3. For $\sigma_2/\sigma_1 = \infty$ and $p=15$, corresponding to the largest $p$ used (Sangani & Yao 1988b; Sangani 1993), we get lower bounds that coincide with Sangani (1993) to six digits. However, no digit, or at most one digit, has converged. We continue with lower bounds, including multipoles up to $p=250$, and get convergence to five digits. To go beyond this we again use the direct method of (5.2) and solve the system of $16p$ linear equations with the order $p^2N^2$ conjugate gradient method. This method can be accelerated with the fast multipole method to become an order $p^2N$ method, similarly as in §3. The result converges at a rate of approximately one digit per 50 new multipoles. Accurate results with multipoles up to $p=650$, computed without acceleration, are presented in table 4.

The convergence of our calculations can be estimated by inspection and the accuracy by numerical perturbation experiments. The error of the structural parameters can also be estimated as follows; The operator $\chi_2 \Gamma_1$ of (3.10) has a spectrum in the interval $(0,1)$, which can be checked by Fourier decomposition. Thus $W$ has eigenvalues in the interval $(-1,1)$ in the limit $p \to \infty$. The infinite matrix, $W_\infty$, we can write as a sum of a truncated part $W_N$ of size $pN \times pN$, and a remainder $W_{\text{rem}}$

$$W_{pN} = W_\infty - W_{\text{rem}}.$$

Numaric tests indicate that $W_{pN}$ as well as $W_{\text{rem}}$ also have eigenvalues in $(-1,1)$.
Table 3. Position of centers of 16 disks as provided by Sangani (1993). All disks have radius one. Upon division of all coordinates and radii with 8.473950205308800 the disks centers fall in the square of unit length centered at the origin. Disk concentration is 0.7.

<table>
<thead>
<tr>
<th>disk</th>
<th>x-coordinate</th>
<th>y-coordinate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.43339682776082</td>
<td>-3.426031862515099</td>
</tr>
<tr>
<td>2</td>
<td>-0.2532362304577981</td>
<td>3.115007149779412</td>
</tr>
<tr>
<td>3</td>
<td>-2.33395488116567</td>
<td>-1.900065763678761</td>
</tr>
<tr>
<td>4</td>
<td>2.430690042206030</td>
<td>-3.035788795968029</td>
</tr>
<tr>
<td>5</td>
<td>-1.617714737177291</td>
<td>-3.873154789827250</td>
</tr>
<tr>
<td>6</td>
<td>-2.18920901000176</td>
<td>2.480777879379034</td>
</tr>
<tr>
<td>7</td>
<td>-2.023821933488570</td>
<td>0.4550470344004374</td>
</tr>
<tr>
<td>8</td>
<td>2.03957290295240</td>
<td>3.29080342033851</td>
</tr>
<tr>
<td>9</td>
<td>0.1166913475994012</td>
<td>1.10641618360710</td>
</tr>
<tr>
<td>10</td>
<td>-3.85396201888438</td>
<td>-3.987913396858088</td>
</tr>
<tr>
<td>11</td>
<td>2.432515622106518</td>
<td>1.328497205325373</td>
</tr>
<tr>
<td>12</td>
<td>4.16470727801518</td>
<td>0.234880088064994</td>
</tr>
<tr>
<td>13</td>
<td>4.227994046003651</td>
<td>2.32236063036797</td>
</tr>
<tr>
<td>14</td>
<td>4.09600335702866</td>
<td>-1.92609878025435</td>
</tr>
<tr>
<td>15</td>
<td>2.2113099023620173</td>
<td>-0.9900188297062963</td>
</tr>
<tr>
<td>16</td>
<td>-0.1882304178050852</td>
<td>-1.324673898607316</td>
</tr>
</tbody>
</table>

Table 4. Effective conductivity of the unit cell whose disk centers are given in Table 3. $\sigma_{\text{eff},x}$ and $\sigma_{\text{eff},y}$ is the effective conductivity when the applied electric field is in the x-direction and the y-direction, respectively.

<table>
<thead>
<tr>
<th>$\sigma_{\text{eff},x}$</th>
<th>$\sigma_{\text{eff},y}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_2 = 10$</td>
<td>4.016405183005</td>
</tr>
<tr>
<td>$\sigma_2 = 100$</td>
<td>7.44445359175</td>
</tr>
<tr>
<td>$\sigma_2 = \infty$</td>
<td>8.50651253404</td>
</tr>
</tbody>
</table>

This means that matrix vector multiplication $W_{pN}u^j$, apart from introduces a truncation error, at most amplifies an existing error in $u^j$ with a factor of 2.

For the square array of disks the the norm of the first truncation error vector $e^1$ in the series

$$e^j = W_{\text{rem}}u^j,$$

(5.6)

can be estimated. Assuming $S_{m+n} = 4$ for $m > p$ and/or $n > p$ summation of a geometric series gives

$$||e^1||_2 = \frac{4\sqrt{p - p f_2}}{\pi} (\frac{f_2}{\pi})^{\frac{p+1}{2}}. \quad (5.7)$$

Taking this truncation error as a typical error an estimated upper bound on the error for parameter $q_n$ of (3.20) becomes

$$\Delta q_n \leq 2f_2 \sum_{i=1}^{n-2} ||e^i||_2 2^i \approx 2^m 2f_2 \sqrt{p} f_2 \left(\frac{f_2}{\pi}\right)^{\frac{p+1}{2}}. \quad (5.8)$$

Fast and accurate structural parameters

This approximation holds for low and moderate concentration of disks. For such composites the eigenvector of \( \mathbf{W} \) corresponding to the dominant eigenvalue has rapidly vanishing components and similar direction as \( \mathbf{u}^1 \). For high concentration of disks the error in the structural parameters \( q_n \), especially for high indices \( n \), could be much larger than predicted by (5.8).

6. Suspensions of arbitrary objects

In a general suspension the inclusions are objects of arbitrary shape. Assume that, for such a suspension, we know an electric field \( \mathbf{E}^1 \). In this section, just as in § 3, we will show how to calculate the action of the operator \( \chi_2 \Gamma_1 \), so that the inner products of (2.11) can be evaluated.

Denote, in the infinite medium \( \Omega \), the interior of the inclusions \( D \), and the boundary between inclusions and matrix \( B \). Write

\[
\mathbf{E}^i = \nabla u^i. \tag{6.1}
\]

Since \( \mathbf{E}^1 \), the first field of our scheme, is uniform, \( u^i \) is harmonic in \( \Omega/B \) and continuous in \( \Omega \).

Decompose \( \chi_2 \mathbf{E}^i \) into an average zero electric field, an average zero current density field, and a uniform field

\[
\chi_2 \mathbf{E}^i = \mathbf{E}^{i+1} + \mathbf{J}^{i+1} + \mathbf{U}^{i+1}. \tag{6.2}
\]

Introduce a charge density on \( B \)

\[
\rho^{i+1}(x_0) = \lim_{x \to x_0} \chi_2 \mathbf{E}^i(x) \cdot \mathbf{n}(x), \tag{6.3}
\]

where \( \mathbf{n}(x) \) is the outward normal vector on \( B \). From (6.3) and the harmonicity of \( u^i \) in \( D \) follows charge neutrality

\[
\int_{B_j} \rho^{i+1}(x_0(s))ds = 0, \tag{6.4}
\]

where \( B_j \) is any of the \( N \) disconnected boundaries in \( \Omega \).

Now we propose the single layer representation

\[
\mathbf{E}^{i+1} = \int_B \nabla x G_{xy} \rho^{i+1}(y_0(s))ds, \tag{6.5}
\]

which is the same as

\[
\chi_2 \Gamma_1 \chi_2 \mathbf{E}^i = -\frac{\chi_2}{2\pi} \int_B \nabla x \ln |x - y_0(s)| \lim_{y \to y_0(s)} \chi_2 \mathbf{E}^i(y) \cdot \mathbf{n}(y_0(s))ds. \tag{6.6}
\]

If the boundary is smooth this integral is finite even for \( x \in B \).

Being the gradient of a single layer potential the field \( \mathbf{E}^{i+1} \) in (6.5) is an electric field. It contains the projection of \( \chi_2 \mathbf{E}^i \) onto the subspace of average zero electric fields since

\[
\nabla \cdot (\chi_2 \mathbf{E}^i - \mathbf{E}^{i+1}) = 0. \tag{6.7}
\]

Equation (6.7) clearly holds in \( \Omega/B \). Since \( \chi_2 \mathbf{E}^i \) and \( \mathbf{E}^{i+1} \) have identical jumps (Guenter & Lee 1988) their difference is divergence-free also on \( B \). The spatial average of \( \mathbf{E}^{i+1} \) is indeterminate, just as the integrals of the second part of the

fields of (3.7) and (3.8). This indetermination poses no problem since physically correct values of sums and fields can be found like in §3.

Equations (6.3) and (6.5) give any charge density $\rho_j$ by recursion. If we approximate these densities with their values at discrete boundary points it is easy to use the fast multipole method to speed up the recursion (Greengard & Rokhlin 1987). The inner products of (2.11) can be evaluated as discrete line integrals. An alternative to bounds is here the direct boundary integral method of Moura (1993).

For comparison with §3 we may consider disks. If the charge densities are represented with (6.3) in the approximation of (3.6) Fourier series expansion of the Green's function $G_{\text{xy}}$ gives that (6.6) can be written as (3.9).

For an application of (6.6) and (2.11) we look at $q_3$ for the square array of squares with $p_2 < \pi/4$. Let there be one square per unit cell and let one square, $Q$ say, have the origin at its center. $\chi_2 \Gamma_1 \chi_2$ acting on the constant unit field $E_1$ gives in $Q$

$$
E^2 = -\frac{f_2}{2} \left( 1 + 1 \frac{1}{\pi} \sum_{k=1}^{\infty} (4k - 1) S_{4k} z^{4k-2} \right)
$$

where $z_j$ is the corner of $Q$ lying in the $j$th quadrant. Equation (2.11) for $q_3$, with the definition of (3.1), is now easy to evaluate; some surface integrals can be evaluated analytically, while others can be converted into line integrals and evaluated numerically. We get to lowest order in $f_2$

$$
q_3 = Af_2 + O(f_2^2),
$$

(6.9)

where

$$
A = 0.16159123635089.
$$

(6.10)

This result coincides with the numeric calculation of Hetherington & Thorpe (1992) to the five digits presented therein. From (6.9) and the work of Miller (1969) we can also deduce

$$
q_3 = Af_2 + (2 - 3A)f_2^2 + 2Af_2^3,
$$

(6.11)

for any two-component symmetric cell composite with cells in the shape of squares. See Milton (1982) and Bruno (1990) for more recent discussions of structural parameters for symmetric cell materials.

7. Discussion

We have presented fast and accurate methods to calculate effective conductivities and structural parameters for periodic suspensions. Disks as well as general two-dimensional inclusions were treated. Roughly speaking, we combined the well established ideas of Rayleigh (1892), the formalism of Milton (1987), and contemporary numerical methods such as the conjugate gradient method and the fast multipole method (Greengard & Rokhlin 1987). Our calculations gave up to twelve digits more accuracy than previously achieved.

To be efficient for unit cells with many inclusions we must make full use of the
Fast and accurate structural parameters

As described in the last paragraph of §3, Programming of this kind is currently being undertaken, aiming at structural parameters for unit cells with thousands of disks (Greengard & Helsing 1994). We did not mention implementation of our methods for three-dimensional suspensions but, at least conceptually, the transition is quite straightforward. See Greengard & Rokhlin (1988) for relevant details on spherical harmonics.

For suspensions with a moderate number of disks per unit cell we can get virtually any structural parameter with double precision accuracy, including the effective conductivity at most ratios $\sigma_2/\sigma_1$. In §5 a standard algorithm to evaluate bounds from structural parameters only, was found to be unstable. Therefore, useful tight bounds should contain both structural parameters and known values of effective conductivities for different ratios $\sigma_2/\sigma_1$.

We emphasize that, for disks, calculation of higher-order structural parameters and determination of the effective conductivity with the direct method are problems of equal magnitude. Both problems involve similar repeated multiplications of a vector with a matrix of size $pN \times pN$, which can be accelerated with the fast multipole method.

I am indebted to Leslie Greengard, Robert Kohn, and Monique Moura for helpful discussions and suggestions. This work was prepared under partial support from grant AFOSR 90-0090 and from a Packard Foundation Fellowship to Leslie Greengard.

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Received 5 August 1993; accepted 4 November 1993.