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On the numerical evaluation of electrostatic fields in composite materials

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A classical problem in electrostatics is the determination of the effective electrical conductivity in a composite material consisting of a collection of piecewise homogeneous inclusions embedded in a uniform background. We discuss recently developed fast algorithms for the evaluation of the potential and electrostatic fields induced in multiphase composites by an applied potential, from which the desired effective properties may be easily obtained. The schemes are based on combining a suitable boundary integral equation with the Fast Multipole Method and the GMRES iterative method; the CPU time required grows linearly with the number of points in the discretization of the interface between the inclusions and the background material.

A variety of other questions in electrostatics, magnetostatics and diffusion can be formulated in terms of interface problems. These include the evaluation of electrostatic fields in the presence of dielectric inclusions, the determination of magnetostatic fields in media with variable magnetic permeability, and the calculation of the effective thermal conductivity of a composite material. The methods presented here apply with minor modification to these other situations as well.

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1. Introduction

Interface problems arise in a wide variety of areas of applied mathematics, including the determination of the electrostatic and magnetostatic fields in heterogeneous media, the calculation of effective transport properties, and the motion of multiphase fluids. The governing equation common to each of these problems is often the second-order elliptic partial differential equation

$$\nabla(\sigma \nabla u) = 0, \tag{1.1}$$

where σ is piecewise constant, subject to some appropriate boundary condition on u. In many situations, the dynamic range of σ can vary enormously and the geometry can be very complex. The reason for the use of the phrase 'interface' problem is that the differential equation (1.1) is often reformulated as follows: find a continuous function u which satisfies the Laplace equation in each phase (where σ is constant), and whose flux $\sigma \partial u/\partial n$ is continuous across each interface.

Definition 1.1 A function u which satisfies the above conditions will be referred to as a *total potential.*

For the sake of clarity, we will focus our attention on questions of electrical conductivity and leave the translation of our results to other application areas to the reader. We will restrict our attention for the most part to two-dimensional problems and consider primarily two issues. One is the determination of the electric field in the vicinity of a collection of inclusions in free space; the other is the determination of the effective conductivity of a composite material.

1.1. Inclusions in free space

The simplest problem of the first type is probably the determination of the electric field in an infinite plane with conductivity σ_e in which is embedded a disk D of conductivity σ_d. In the presence of a uniform applied field

$$\mathbf{E} = (E_a, 0),$$

corresponding to an applied potential $\Psi_a = -E_a x$, the interface problem takes the form

$$\begin{aligned} \Delta u_e &= 0 \quad \text{in } \mathbb{R}^2 \setminus D \\ \Delta u_d &= 0 \quad \text{in } D \\ u_e &= u_d \quad \text{on } \partial D \qquad (1.2) \\ \sigma_e \frac{\partial u_e}{\partial \nu} &= \sigma_d \frac{\partial u_d}{\partial \nu} \quad \text{on } \partial D, \qquad (1.3) \end{aligned}$$

where u_d denotes the restriction of the total potential u to D, u_e denotes the restriction of u to $\mathbb{R}^2 \setminus D$, and ν denotes the outward normal to ∂D. We

also have the far field boundary condition

$$u_e(x,y) \to \Psi_a(x,y) \quad \text{as} \quad |(x,y)| \to \infty.$$

Without loss of generality, let us assume that the disk is of radius one, centred at the origin. The standard approach to solving this problem (Van Bladel, 1964; Jackson, 1975) is based on Fourier analysis. Making use of symmetry, we seek a solution of the form

$$\begin{aligned} u_d(r,\theta) &= \sum_{k=0}^{\infty} \alpha_k r^k \cos k\theta \\ u_e(r,\theta) &= -E_a r \cos\theta + \sum_{k=1}^{\infty} A_k r^{-k} \cos k\theta, \end{aligned}$$

where (r,θ) are the polar coordinates of a point in the plane. Imposition of the interface conditions (1.2) and (1.3) and a straightforward calculation yield

$$\begin{aligned} u_d(r,\theta) &= E_a \lambda r \cos\theta - E_a r \cos\theta \\ u_e(r,\theta) &= E_a \lambda \frac{\cos\theta}{r} - E_a r \cos\theta, \end{aligned}$$

where $\lambda = (\sigma_d - \sigma_e)/(\sigma_d + \sigma_e)$.

Definition 1.2 The difference between the total potential and the applied potential will be referred to as the *induced potential* or the *induced response*:

$$u_{\text{induced}} = u - \Psi_a.$$

In the preceding example, the induced potential is given by $u_{\text{induced}} = E_a \lambda r \cos\theta$ for $r \leq 1$ and $u_{\text{induced}} = E_a \lambda \cos\theta / r$ for $r \geq 1$. Contour plots of the total and induced potentials are shown in Figure 1.

Remark 1.1 In this article, the applied potential will always be assumed to be $\Psi_a = -E_a x$.

1.2. Periodic arrays

A more difficult problem is that of determining the electrostatic field in a simple composite consisting of a periodic array of disks in a uniform background (Figure 2). Rayleigh (1892) describes a method for solving this problem based on multipole expansions. Recent extensions and refinements have been developed by several groups, including Perrins *et al.* (1979b), McPhedran *et al.* (1988), and Sangani and Yao (1988).

Consider the plane to be tiled by unit squares with conductivity σ_e, each containing a disk of radius R_0 and conductivity σ_d.

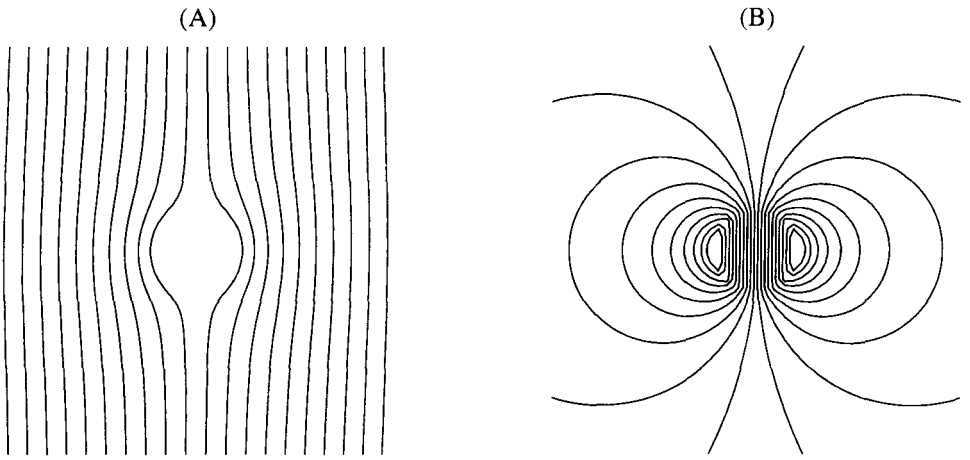

Fig. 1. The potential field in the vicinity of an inclusion in free space; the left-hand figure (A) is a contour plot of the total potential and the right-hand figure (B) is a contour plot of the induced potential. The x-axis is oriented in the horizontal direction.

Because of periodicity, it is sufficient to consider a single unit cell B centred at the origin and the governing equations

$$\begin{aligned} \nabla^2 u_e &= 0 \quad \text{in } B \setminus D, \\ \nabla^2 u_d &= 0 \quad \text{in } D, \\ u_e &= u_d \quad \text{on } \partial D, \qquad (1.4) \\ \sigma_e \frac{\partial u_e}{\partial \nu} &= \sigma_d \frac{\partial u_d}{\partial \nu} \quad \text{on } \partial D, \qquad (1.5) \end{aligned}$$

where u_d is the restriction of u to the disk D of radius R_0 and u_e is the restriction of u to $B \setminus D$. The boundary conditions on B are

$$u(x+1, y) - u(x, y) = -E_a \qquad (1.6)$$

$$u(x, y+1) - u(x, y) = 0. \qquad (1.7)$$

It is easy to see that outside the disk D, the potential can be represented as

$$u_e = A_0 + (A_1 r + B_1 r^{-1}) \cos\theta + (A_3 r^3 + B_3 r^{-3}) \cos 3\theta + \ldots \qquad (1.8)$$

and inside the disk D as

$$u_d = C_0 + C_1 r \cos\theta + C_3 r^3 \cos 3\theta + \ldots, \qquad (1.9)$$

where (r, θ) are the polar coordinates of a point with respect to the disk centre. (Note that we have had to introduce more unknown Fourier coeffi-

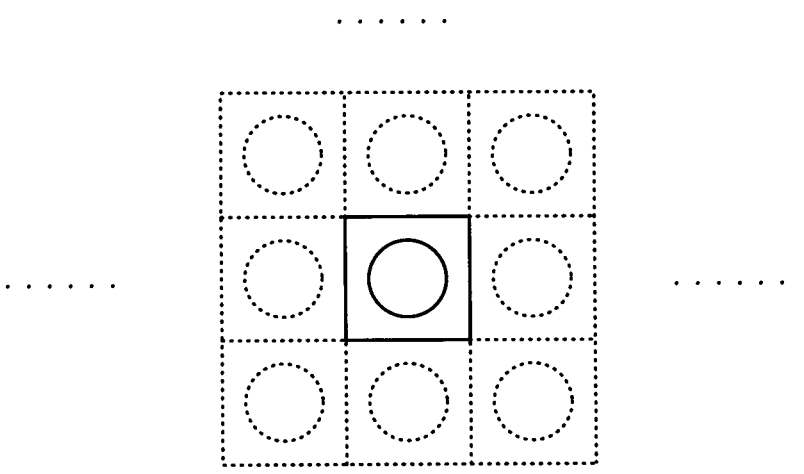

Fig. 2. A typical unit cell and its nearest neighbours in a periodic array of disks. Its length in the x-direction is α and its length in the y-direction is β. The disk is assumed to have radius R_0.

cients than in the earlier free-space example.) At the boundary of the disk, the potential must satisfy the interface conditions (1.4) and (1.5). Imposing these conditions on the above series, it is easy to derive a relation between the coefficients A_n and B_n, namely

$$B_n = -\lambda {R_0}^{2n} A_n \qquad \text{for } n \geq 1 \tag{1.10}$$

where, as before, $\lambda = (\sigma_d - \sigma_e)/(\sigma_d + \sigma_e)$. Letting A and B denote the vectors $(A_1, A_2, \cdots)$ and $(B_1, B_2, \cdots)$, respectively, and letting D be the infinite-dimensional diagonal matrix with entries $D_{nn} = -\lambda {R_0}^n$, the relations (1.10) can be written as

$$B = D\,A. \tag{1.11}$$

Since each square is subject to a constant potential drop $(-E_a)$, it is clear that the coefficient A_0 will depend on the particular location of the unit cell. It is also clear, however, that the coefficients $\{A_i\}$ and $\{B_i\}$ of the series expansions about the centre of each disk are translation invariant. In order to obtain the potential everywhere, it remains only to find another relation between the coefficient vectors A and B. For this, let (r, θ) be a point in $B \setminus D$ but close to the boundary of the disk. Then the part of the potential due to the applied field and to all disks other than D must be

$$A_0 + A_1 r \cos\theta + A_3 r^3 \cos 3\theta + \ldots. \tag{1.12}$$

If we now subtract Ψ_a, it is clear that the influence of all image disks is given by

$$\tilde{u} = E_0 r \cos\theta + A_0 + A_1 r \cos\theta + A_3 r^3 \cos 3\theta + \ldots \tag{1.13}$$

or, using complex notation,

$$\tilde{u} = \mathrm{Re}\,(A_0 + (E_0 + A_1)z + A_3 z^3 + \ldots), \tag{1.14}$$

where we identify the point $(r, \theta) \in \mathbb{R}^2$ with the complex number $z = re^{i\theta}$. Consider now a single distant disk centred at $w = m + in$. The influence it exerts at z, which we will denote by u_w, can be expressed in terms of a multipole expansion:

$$u_w = \mathrm{Re} \sum_{k=1}^{\infty} \frac{B_k}{(z-w)^k}. \tag{1.15}$$

Since the multipole coefficients B_k are the same for each image disk and $\tilde{u}$ is the field due to all image disks, we have

$$\tilde{u} = \mathrm{Re} \sum_{w \in \Lambda} \sum_{k=1}^{\infty} \frac{B_k}{(z-w)^k}, \tag{1.16}$$

where Λ denotes the set of lattice points (disk centres) excluding the origin,

$$\Lambda = \{(m,n) | m, n \in \mathbb{Z}, (m,n) \neq (0,0)\}.$$

Expanding each term as a Taylor series in z and using equation (1.13), the coefficients must satisfy the relations

$$A_n = \sum_{k=1}^{\infty} B_k \binom{n+k-1}{k-1} (-1)^k S_{n+k}, \quad n > 1 \tag{1.17}$$

$$A_1 + E_0 = \sum_{k=1}^{\infty} B_k\, k\, (-1)^k S_{k+1}, \tag{1.18}$$

where S_m denotes the lattice sum

$$S_m = \sum_{w \in \Lambda} \frac{1}{w^m}.$$

Letting P denote the matrix with entries

$$P_{nk} = \binom{n+k-1}{k-1} (-1)^k S_{n+k},$$

and letting $V^t = (E_0, 0, \cdots)$, the relations (1.17) and (1.18) can be rewritten as

$$P\, B = A - V. \tag{1.19}$$

Both (1.11) and (1.19) are infinite systems of equations. The error in truncating these systems depends on several factors, such as the distance between disks and the conductivity ratio σ_d/σ_e. Once truncated, however, it remains only to solve a finite-dimensional system for B

$$(P - D^{-1})B = V. \tag{1.20}$$

Rayleigh (1892) shows that the effective conductivity can be determined from the dipole moment B_1. This result is extended in a straightforward manner to arbitrary geometries and multiphase composites in Section 2.9.

1.3. Complex geometry

When the number of disks is large or the shapes of the inclusions are irregular, simple methods of the type described above are not available and other approaches need to be taken. A number of options have developed over the last century, including effective medium theory (Landauer, 1978; Bergman, 1978; Willis, 1981; Milton, 1985), variational methods (Hashin and Shtrikman, 1962; Beran, 1965; Prager, 1969; Phan-Tien and Milton, 1982; Torquato and Lado, 1988; Helsing, 1993), and asymptotic methods (Keller, 1987; McPhedran *et al.*, 1988; Bonnecaze and Brady, 1990).

The literature in each of these areas is vast and the references given above are by no means complete. Unfortunately, none of these approaches is suited to obtaining quantitatively precise evaluation of the field in complex geometries. For that purpose, one is obliged to consider direct solution of the governing partial differential equation.

Even within this category, there are several options including extensions of Rayleigh's method for systems of disks (Sangani and Yao, 1988), finite difference methods, finite element methods, and integral equation methods.

We will restrict our attention to the latter category since the problem we are interested in solving can be recast as a boundary integral equation. This reduces the dimensionality of the problem by one and greatly simplifies the discretization of the domain. Such methods are by no means new; integral equation techniques have been used to solve interface problems in electrostatics and magnetostatics for many years (Kellogg, 1953; Van Bladel, 1964; Jaswon and Symm, 1977; Lindholm, 1980; Brebbia *et al.*, 1983; Durand and Ungar, 1988; Hetherington and Thorpe, 1992; Nabors and White, 1992).

In the next section, we develop the mathematical apparatus of potential theory and construct second-kind Fredholm equations for interface problems by representing the solution as a single-layer potential. Numerical methods based on this formulation have been used previously for both smooth and polygonal inclusions (Jaswon and Symm, 1977; Hetherington and Thorpe, 1992). The dense linear systems which arise, however, will not be treated by standard factorization techniques which require $\mathcal{O}(N^3)$ operations where N is the number of points in the boundary discretization. Instead, the linear systems will be solved iteratively. This is by now standard in the integral equation community (see, for example, Atkinson (1976), Baker *et al.* (1982), Delves and Mohamed (1985), Rokhlin (1985), Nabors and White (1991)) and has been used for composite materials calculations as well (Gyure and Beale, 1992).

We have chosen to use the GMRES method of Saad and Schultz (1986), but a variety of other conjugate gradient type iterations are also acceptable. In addition, we will rely on the Fast Multipole Method (Rokhlin, 1985; Greengard and Rokhlin, 1987; Carrier *et al.*, 1988) to rapidly apply the integral operators at each step in the iterative process.* By combining these two schemes, the number of operations required is only $\mathcal{O}(N)$. Calculations with one hundred thousand boundary points, which have been viewed as intractable, require only minutes of CPU time on a workstation. Previous work which uses the Fast Multipole Method in this way includes that of Rokhlin (1985), Nabors and White (1991), and Greenbaum *et al.* (1992; 1993). A more thorough discussion of certain aspects of the present article and more extensive numerical experiments can be found in Moura (1993).

2. Potential theory

In this section, we review the basic properties of layer potentials involving a Green function for the Laplace equation. We then discuss two possible integral equation approaches to the solution of electrostatic problems in two phase composites. Both finite numbers of inclusions and periodic arrays will be treated. Our results will then be extended to multiphase systems.

2.1. Layer potentials

We will begin with some classical results from potential theory (Guenther and Lee, 1988; Jaswon and Symm, 1977; Kellogg, 1953; Mikhlin, 1957). Our treatment follows most closely that of Guenther and Lee (1988). We shall denote a two-dimensional domain by D and its boundary by S. S may consist of a number of disjoint components, but each is assumed to be a smooth curve with continuous curvature. If D is a bounded domain and $u, v \in C^2(D) \cap C^1_\nu(\overline{D})$, then Green identities state that

$$\int_D v\Delta u + \nabla v \nabla u = \int_S v\frac{\partial u}{\partial \nu}, \tag{2.1}$$

$$\int_D v\Delta u - u\Delta v = \int_S v\frac{\partial u}{\partial \nu} - u\frac{\partial v}{\partial \nu}, \tag{2.2}$$

$$\int_D \Delta u = \int_S \frac{\partial u}{\partial \nu}. \tag{2.3}$$

* Other fast algorithms could also be used (Anderson, 1986; Odlyzko and Schönhage, 1988; Hackbusch and Nowak, 1989; Van Dommelen and Rundensteiner, 1989; Brandt and Lubrecht, 1990).

Here ν denotes the unit outward normal vector and C^1_ν denotes the set of functions $u \in C^1(D) \cap C^0(\overline{D})$ such that

$$\frac{\partial u}{\partial \nu}(P) = \lim_{\substack{t \to 0 \\ t<0}} \nu(P) \cdot \nabla u(P + t\nu(P))$$

exists uniformly for all $P \in S$. For infinite regions, we require additional hypotheses on the functions involved. If we suppose, for example, that $u(P)$ is bounded at infinity and that $|\nabla u| = \mathcal{O}(1/|P|)$ as $|P| \to \infty$, then the Green identities hold.

One consequence of Green identities is that any function $u \in C^2(D) \cap C^1_\nu(\overline{D})$ can be expressed as the sum of three integrals.

Theorem 2.1 Every function $u \in C^2(D) \cap C^1_\nu(\overline{D})$ can be represented as

$$\begin{aligned} u(P) &= \int_S \frac{\partial G}{\partial \nu_Q}(P,Q) u(Q)\, ds_Q - \int_S G(P,Q) \frac{\partial u}{\partial \nu}(Q)\, ds_Q \\ &\quad + \int_D G(P,Q) \Delta u(Q)\, dQ, \end{aligned} \tag{2.4}$$

where $G(P,Q) = (1/2\pi) \log |P - Q|$ is the fundamental solution of the Laplacian and ν_Q denotes the normal direction at Q. If D is unbounded, the additional hypotheses that u be bounded and that $|\nabla u| = \mathcal{O}(1/|P|)$ as $|P| \to \infty$ are assumed to hold.

Proof. In Green's second identity let $v = G(P,Q)$. Take the domain to be $D \setminus K_\epsilon(P)$, where $K_\epsilon(P)$ is the disk of radius ϵ centred at P, and consider the limit $\epsilon \to 0$. □

The first integral in (2.4) is referred to as a double-layer potential (with density u), the second is referred to as a single-layer potential (with density $\partial u/\partial \nu$) and the third is referred to as a volume potential.

2.2. Jump relations

In order to develop integral equation methods for the problems of potential theory, we need to study the analytic properties of layer potentials. It is well known and straightforward to prove that the double-layer potential defined on a smooth curve S maps continuous functions into harmonic, infinitely differentiable functions in $\mathbb{R}^2 \setminus S$. The resulting functions, however, are not continuous in $\mathbb{R}^2$.

Theorem 2.2 Let D be a bounded domain with boundary S and suppose that the function μ is continuous on S. Then the double-layer potential

$$u(P) = \int_S \frac{\partial G}{\partial \nu_Q}(P,Q)\, \mu(Q)\, ds_Q$$

satisfies the jump relations at $P_0 \in S$

$$\lim_{\substack{P \to P_0 \\ P \in D}} u(P) = u(P_0) + \frac{1}{2}\mu(P_0) \tag{2.5}$$

$$\lim_{\substack{P \to P_0 \\ P \in \mathbb{R}^2 \setminus \overline{D}}} u(P) = u(P_0) - \frac{1}{2}\mu(P_0). \tag{2.6}$$

The single-layer potential maps continuous functions on S to continuous functions in $\mathbb{R}^2$. Although the result is infinitely differentiable and harmonic in $\mathbb{R}^2 \setminus S$, the normal derivative is discontinuous across S.

Theorem 2.3 Let D be a bounded domain with boundary S and suppose that the function ρ is continuous on S. Then the single-layer potential

$$u(P) = \int_S G(P, Q)\, \rho(Q)\, ds_Q$$

satisfies the following jump relations. Let $P_0 \in S$ and let ν_{P_0} be the unit normal vector to S at P_0. Then

$$\frac{\partial u}{\partial \nu_-} \equiv \lim_{\substack{P \to P_0 \\ P \in D}} \frac{\partial u}{\partial \nu_{P_0}}(P) = \int_S \frac{\partial G}{\partial \nu_{P_0}}(P_0, Q)\rho(Q)\, ds_Q - \frac{1}{2}\rho(P_0) \tag{2.7}$$

$$\frac{\partial u}{\partial \nu_+} \equiv \lim_{\substack{P \to P_0 \\ P \in \mathbb{R}^2 \setminus \overline{D}}} \frac{\partial u}{\partial \nu_{P_0}}(P) = \int_S \frac{\partial G}{\partial \nu_{P_0}}(P_0, Q)\rho(Q)\, ds_Q + \frac{1}{2}\rho(P_0). \tag{2.8}$$

We may relate, as a result of the previous theorem, the source density and the normal derivative of the potential.

Corollary 2.1 Let $u(P) = \int_S G(P, Q)\, \rho(Q)\, ds_Q$. Then

$$\rho = \frac{\partial u}{\partial \nu_+} - \frac{\partial u}{\partial \nu_-}.$$

Remark 2.1 In $\mathbb{R}^2$, $(\partial G/\partial \nu_Q)(P, Q)$ has a removable singularity at $P = Q \in S$. In fact

$$\lim_{P \to Q} \frac{\partial G}{\partial \nu_Q}(P, Q) = \frac{1}{2}\kappa(Q),$$

where κ is the curvature of S. Thus, the smoothness of the kernel of the double-layer potential is limited only by the smoothness of S. For infinitely differentiable curves, the kernel is infinitely differentiable.

2.3. The Fredholm alternative

Before proceeding with our investigation of interface problems, we state the Fredholm alternative, which allows us to investigate the solvability of a large class of second-kind integral equations. The theorem and its proof are well known (Guenther and Lee, 1988; Mikhlin, 1957).

Theorem 2.4 Consider the Fredholm equation

$$\rho(P) - \lambda \int_a^b K(P,Q)\rho(Q)\,\mathrm{d}Q = f(P), \tag{2.9}$$

where $K(P,Q)$ is an L_2 kernel, so that K is a compact operator on $L_2[a,b]$. Then (2.9) has a unique solution if and only if the equation

$$\rho(P) - \lambda \int_a^b K(P,Q)\rho(Q)\,\mathrm{d}Q = 0 \tag{2.10}$$

has only the trivial solution $\rho(P) = 0$. Furthermore, the adjoint equation to (2.10), defined by

$$\psi(P) - \overline{\lambda} \int_a^b \overline{K(Q,P)}\psi(Q)\,\mathrm{d}Q = 0 \tag{2.11}$$

has the same number of linearly independent solutions as (2.10). Finally, if (2.11) has at least one non-trivial solution, then (2.9) will have a solution only if

$$(f,\psi) = \int_a^b f(P)\overline{\psi(P)}\,\mathrm{d}P = 0$$

for all ψ satisfying (2.11). In this case, such a solution will not be unique.

2.4. Two-phase materials

Suppose that in the plane $\mathbb{R}^2$ with uniform conductivity σ_e we have embedded a finite number of smooth bounded inclusions each with conductivity σ_d. Let Ω denote the region occupied by the inclusions, let $c\Omega = \mathbb{R}^2 \setminus \Omega$, and let Γ denote the interface $\partial\Omega$. We will determine the electrostatic field in the plane in terms of a total potential function u, whose restriction to Ω and $c\Omega$ will be denoted by u_d and u_e, respectively. This corresponds to solving

$$\Delta u_d = 0 \quad \text{in } \Omega, \tag{2.12}$$

$$\Delta u_e = 0 \quad \text{in } c\Omega, \tag{2.13}$$

$$u_e = u_d \quad \text{on } \Gamma, \tag{2.14}$$

$$\sigma_e \frac{\partial u_e}{\partial \nu} = \sigma_d \frac{\partial u_d}{\partial \nu} \quad \text{on } \Gamma, \tag{2.15}$$

with the far-field boundary condition

$$u_e(P) \to \Psi_a(P) \quad \text{as} \quad P \to \infty. \tag{2.16}$$

We now look for a solution of equations (2.12) to (2.16) in the form of a single-layer potential

$$u(P) = \Psi_a(P) + \int_\Gamma G(P,Q)\rho(Q)\,\mathrm{d}s_Q, \tag{2.17}$$

where P is an arbitrary point in the plane and ρ is an unknown source density. It is convenient to write the solution as a single-layer potential because the continuity condition (2.14) is automatically satisfied. Physically, ρ represents the charge distribution on the interface which develops in response to the applied field (Jaswon and Symm, 1977; Hetherington and Thorpe, 1992).

In order to determine ρ, observe that using the jump relations (2.7) and (2.8), the interface condition can be rewritten in the form

$$\sigma_d \left[\frac{\partial \Psi_a}{\partial \nu_P}(P) - \frac{1}{2}\rho(P) + \int_\Gamma \frac{\partial G}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q \right] = \sigma_e \left[\frac{\partial \Psi_a}{\partial \nu_P}(P) + \frac{1}{2}\rho(P) + \int_\Gamma \frac{\partial G}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q \right]. \tag{2.18}$$

Rearranging the previous equation we obtain the following second-kind Fredholm integral equation for ρ,

$$2\lambda \frac{\partial \Psi_a}{\partial \nu_P}(P) = \rho(P) - 2\lambda \int_\Gamma \frac{\partial G}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q, \tag{2.19}$$

where $\lambda = (\sigma_d - \sigma_e)/(\sigma_d + \sigma_e)$.

It remains to determine for what values of λ the preceding equation can be solved. For this, we invoke the Fredholm alternative and make use of the following result.

Theorem 2.5 If the homogeneous integral equation

$$\rho(P) - 2\lambda \int_\Gamma \frac{\partial G}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q = 0 \tag{2.20}$$

has a nontrivial solution, then $\lambda \in \mathbb{R}$ and lies on the rays $\lambda \geq 1$ or $\lambda < -1$.

Proof. See Kellogg (1953) or Mikhlin (1957). □

Corollary 2.2 As long as the ratio σ_d/σ_e is bounded and lies away from the negative real axis, the integral equation (2.19) has a unique solution.

2.5. Solution via the Green identity

Another, perhaps more common, integral formulation for the solution to the two-phase problem is based on Green's second identity (2.2). This is the approach taken, for example, by Van Bladel (1964) and Lindholm (1980). Letting $\phi_e = u - \Psi_a$ in $c\Omega$ and $\phi_d = u - \Psi_a$ in Ω and using Green's second identity, we have

$$u(P) = \int_\Gamma \frac{\partial G}{\partial \nu_Q}(P,Q)u(Q) - G(P,Q)\frac{\partial u}{\partial \nu}(Q)\,ds_Q, \quad P \in \Omega,$$

$$\Psi_a(P) = \int_\Gamma \frac{\partial G}{\partial \nu_Q}(P,Q)\Psi_a(Q) - G(P,Q)\frac{\partial \Psi_a}{\partial \nu}(Q)\,ds_Q, \quad P \in \Omega,$$

$$\phi_e(P) = \int_\Gamma G(P,Q)\frac{\partial \phi_e}{\partial \nu}(Q) - \frac{\partial G}{\partial \nu_Q}(P,Q)\phi_e(Q)\,ds_Q, \quad P \in c\Omega.$$

Taking the limit as P approaches a point on Γ, (2.5) and (2.6) yield

$$\frac{1}{2}u(P) = \int_\Gamma \frac{\partial G}{\partial \nu_Q}(P,Q)u(Q) - G(P,Q)\frac{\partial u}{\partial \nu}(Q)\,ds_Q, \tag{2.21}$$

$$\frac{1}{2}\Psi_a(P) = \int_\Gamma \frac{\partial G}{\partial \nu_Q}(P,Q)\Psi_a(Q) - G(P,Q)\frac{\partial \Psi_a}{\partial \nu}(Q)\,ds_Q, \tag{2.22}$$

$$\frac{1}{2}\phi_e(P) = \int_\Gamma G(P,Q)\frac{\partial \phi_e}{\partial \nu}(Q) - \frac{\partial G}{\partial \nu_Q}(P,Q)\phi_e(Q)\,ds_Q, \tag{2.23}$$

repectively. Subtracting (2.22) from (2.23), we obtain

$$\frac{1}{2}u(P) - \Psi_a(P) = \int_\Gamma G(P,Q)\frac{\partial u}{\partial \nu}(Q) - \frac{\partial G}{\partial \nu_Q}(P,Q)u(Q)\,ds_Q. \tag{2.24}$$

If we now multiply (2.21) by σ_d and (2.24) by σ_e, the flux interface condition and some algebra show that

$$u(P) - 2\lambda \int_\Gamma \frac{\partial G}{\partial \nu_Q}(P,Q)u(Q)\,ds_Q = (\lambda - 1)\,\Psi_a(P). \tag{2.25}$$

The integral operator obtained this way is the adjoint of the operator obtained in equation (2.19), so that the analysis of solvability is the same. We have chosen to use the single-layer potential approach because several quantities of interest are computed more easily from the surface charge distribution than from values of the potential function u itself on the boundary.

2.6. Multiphase materials

Suppose now that a finite number of smooth bounded inclusions are embedded in a homogeneous background material with conductivity σ_e but that each inclusion is allowed a distinct conductivity. Ω_k will denote the region occupied by the kth inclusion with conductivity σ_k and its boundary will be denoted by Γ_k. Assuming there are M inclusions, the total interface is $\Gamma = \cup_{k=1}^M \Gamma_k$ and the total area occupied by the inclusions is $\Omega = \cup_{k=1}^M \Omega_k$. Let u denote the total potential, let u_k denote its restriction to the kth inclusion, and let u_e denote its restriction to the exterior domain $c\Omega$. Then

$$\Delta u_k = 0 \quad \text{in } \Omega_k,\ k = 1, \ldots, M, \tag{2.26}$$

$$\Delta u_e = 0 \quad \text{in } c\Omega, \tag{2.27}$$

$$u_e = u_k \quad \text{on } \Gamma_k,\ k = 1, \ldots, M, \tag{2.28}$$

$$\sigma_e \frac{\partial u_e}{\partial \nu} = \sigma_k \frac{\partial u_k}{\partial \nu} \quad \text{on } \Gamma_k,\ k = 1, \ldots, M \tag{2.29}$$

and

$$u_e(P) \to \Psi_a(P) \quad \text{as} \quad P \to \infty.$$

As for two-phase materials, we seek a solution in the form of a single-layer potential

$$u(P) = \Psi_a(P) + \int_\Gamma G(P,Q)\rho(Q)\,ds_Q. \tag{2.30}$$

If we impose the condition (2.29) at each interface and let

$$\lambda_k = (\sigma_k - \sigma_e)(\sigma_k + \sigma_e),$$

we obtain

$$2\lambda_k \frac{\partial \Psi_a}{\partial \nu_P}(P) = \rho(P) - 2\lambda_k \int_\Gamma \frac{\partial G}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q, \tag{2.31}$$

for $P \in \Gamma_k$, $k = 1, \ldots, M$. Since each of the λ_k may be distinct, this is actually a system of integral equations. Nevertheless, the Fredholm alternative can still be applied.

Theorem 2.6 Suppose λ_k is bounded for $k = 1, \ldots, M$ and that the homogeneous equation

$$\rho(P) - 2\lambda_k \int_\Gamma \frac{\partial G}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q = 0 \tag{2.32}$$

has a nontrivial solution. Then at least one of the ratios σ_k/σ_e has negative real part.

Proof. Let $u = u_R + iu_I$ denote the single-layer potential

$$u(P) = \int_\Gamma G(P,Q)\rho(Q)\,ds_Q$$

corresponding to a complex-valued nontrivial solution of (2.32). Then

$$\frac{2}{\sigma_i + \sigma_e}\left(\sigma_e \frac{\partial u}{\partial \nu}_+(P) - \sigma_k \frac{\partial u}{\partial \nu}_-(P)\right) = \rho(P) - 2\lambda_k \int_\Gamma \frac{\partial G}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q, \tag{2.33}$$

for $P \in \Gamma_k$, so that

$$\sigma_e \frac{\partial u}{\partial \nu}_+(P) - \sigma_k \frac{\partial u}{\partial \nu}_-(P) = 0. \tag{2.34}$$

To simplify notation, let us now define σ by

$$\sigma(P) = \sigma_k/\sigma_e$$

for $P \in \overline{\Omega_k}$, with $\sigma = \sigma_R + \subset \sigma_I$. Separating (2.34) into real and imaginary parts,

$$\frac{\partial u_R}{\partial \nu}_+ - \sigma_R \frac{\partial u_R}{\partial \nu}_- + \sigma_I \frac{\partial u_I}{\partial \nu}_- = 0, \tag{2.35}$$

$$\frac{\partial u_I}{\partial \nu}_+ - \sigma_R \frac{\partial u_I}{\partial \nu}_- - \sigma_I \frac{\partial u_R}{\partial \nu}_- = 0. \tag{2.36}$$

Multiplying equation (2.35) by u_R and (2.36) by u_I, adding them, and integrating along Γ yields

$$\int_\Gamma \left(u_R \frac{\partial u_R}{\partial \nu}_+ + u_I \frac{\partial u_I}{\partial \nu}_+ \right) - \int_\Gamma \sigma_R \left(u_R \frac{\partial u_R}{\partial \nu}_- + u_I \frac{\partial u_I}{\partial \nu}_- \right)$$
$$+ \int_\Gamma \sigma_I \left(u_R \frac{\partial u_I}{\partial \nu}_- - u_I \frac{\partial u_R}{\partial \nu}_- \right) = 0. \tag{2.37}$$

The third integral vanishes because of Green's second identity (2.2) and, from Green's first identity, we obtain

$$\iint_{c\Omega} (\nabla u_R)^2 + (\nabla u_I)^2 + \iint_\Omega \sigma_R((\nabla u_R)^2 + (\nabla u_I)^2) = 0.$$

Thus, if σ_R is nonnegative, u is identically zero and ρ is the trivial solution. □

Corollary 2.3 As long as all the ratios σ_k/σ_e are bounded and have nonnegative real part, the integral equation (2.31) has a unique solution.

2.7. Periodic structures

Consider a two-phase composite medium in the plane consisting of a periodic array of inclusions embedded in a uniform background with conductivity σ_e. Let Ω_k denote the kth inclusion with conductivity σ_d and boundary Γ_k, and suppose that a square unit cell denoted by B contains M such inclusions. Let $\Gamma = \cup_{k=1}^M \Gamma_k$ and let $\Omega = \cup_{k=1}^M \Omega_k$. We are interested in calculating the induced electrostatic potential (and eventually the effective conductivity of the material). The potential equation to be solved can be written as follows:

$$\Delta u_d = 0 \quad \text{in } B \setminus \Omega, \tag{2.38}$$
$$\Delta u_e = 0 \quad \text{in } c\Omega, \tag{2.39}$$
$$u_e = u_d \quad \text{on } \Gamma, \tag{2.40}$$
$$\sigma_e \frac{\partial u_e}{\partial \nu} = \sigma_d \frac{\partial u_d}{\partial \nu} \quad \text{on } \Gamma, \tag{2.41}$$

where u_d and u_e are the restrictions of the total potential to the inclusions and the background, respectively. We also require that $u - \Psi_a$ be doubly periodic, that is

$$u(x+1, y) - u(x, y) = -E_a, \tag{2.42}$$
$$u(x, y+1) - u(x, y) = 0. \tag{2.43}$$

We again look for a solution of equations (2.38) to (2.43) in the form of a single-layer potential

$$u(P) = \Psi_a(P) + \int_\Gamma K(P, Q)\rho(Q)\, ds_Q, \tag{2.44}$$

but now $K(P,Q)$ is the doubly periodic Green function rather than the fundamental solution. There are a number of questions which arise in the evaluation of such a Green function that we will not review here in detail (Rayleigh, 1892; Perrins *et al.*, 1979a; Greengard and Rokhlin, 1987). We simply observe that periodicity can be imposed by considering the entire lattice of charge sources in the plane. These sources are translates of the density ρ to all image cells (see Section 3.1).

It is clear from our construction that the function $u(P)$ defined in (2.44) satisfies the conditions (2.42), (2.43) and (2.40). It remains only to satisfy the flux interface condition. By using the jump relations (2.7) and (2.8), we obtain

$$2\lambda \frac{\partial \Psi_a}{\partial \nu_P}(P) = \rho(P) - 2\lambda \int_\Gamma \frac{\partial K}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q, \tag{2.45}$$

where $\lambda = (\sigma_d - \sigma_e)/(\sigma_d + \sigma_e)$. The analysis of solvability for this system is virtually identical to that of the two-phase composite in free space, so we simply state the result as

Theorem 2.7 If the homogeneous integral equation

$$\rho(P) - 2\lambda \int_\Gamma \frac{\partial K}{\partial \nu_P}(P,Q)\rho(Q)\,ds_Q = 0 \tag{2.46}$$

has a nontrivial solution, then $\lambda \in \mathbb{R}$ and lies on the rays $\lambda \geq 1$ or $\lambda < -1$.

2.8. Periodic multiphase composites

It is a straightforward matter to extend our integral equation approach to multiphase composites using the same single-layer potential representation as for the two-phase system. The integral equation is solvable if the real parts of all the conductivities are positive, as in Section 2.6.

2.9. Computing the effective conductivity

Once the integral equation (2.45), or its multiphase analogue, has been solved, one of the important functionals one can extract from the source density ρ is the effective conductivity. We assume that the periodic cell is a unit square with vertices A, B, C, and D, listed counterclockwise from the lower left hand corner. We denote the boundary of the square by L. The effective conductivity matrix

$$\sigma_{\text{eff}} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$$

relates the current density vector J and the applied field E via

$$J = \sigma_{\text{eff}} E. \tag{2.47}$$

If we suppose that $E = (1, 0)$, then clearly

$$\sigma_{11} = \int_B^C \frac{\partial u}{\partial \nu} \, \mathrm{d}s, \tag{2.48}$$

$$\sigma_{21} = \int_A^B \frac{\partial u}{\partial \nu} \, \mathrm{d}s. \tag{2.49}$$

Consider first the quantity σ_{11} and apply Green's second identity (2.2) in the region $B \setminus \Omega$ to the functions u and v where $v(x, y) = x$, $u(x, y)$ is the computed total potential, and Ω denotes the region occupied by the inclusions. Since u and v are harmonic functions in this domain, we have

$$\int_{\Gamma \cup L} v \frac{\partial u}{\partial \nu_*} - u \frac{\partial v}{\partial \nu_*} \, \mathrm{d}s = 0, \tag{2.50}$$

where ν_* denotes the unit inward normal to Γ. Green's third identity and a small amount of algebra show that

$$\int_\Gamma v \frac{\partial u}{\partial \nu_*} - u \frac{\partial v}{\partial \nu_*} \, \mathrm{d}s = \int_\Gamma v \left(\frac{\partial u_e}{\partial \nu} - \frac{\partial u_d}{\partial \nu} \right) \mathrm{d}s = \int_\Gamma x \rho \, \mathrm{d}s, \tag{2.51}$$

so that it remains to analyse the integral in (2.50) along L. A straightforward calculation yields

$$\int_L v \frac{\partial u}{\partial \nu_*} - u \frac{\partial v}{\partial \nu_*} \, \mathrm{d}s = \int_B^C \frac{\partial u}{\partial \nu} \, \mathrm{d}s - 1 \tag{2.52}$$

and, therefore,

$$\sigma_{11} = 1 + \int_\Gamma x \rho \, \mathrm{d}s. \tag{2.53}$$

Similarly,

$$\sigma_{21} = \int_\Gamma y \rho \, \mathrm{d}s. \tag{2.54}$$

Finally, the components σ_{12} and σ_{22} can be computed by applying a field in the y-direction. If $E = (0, 1)$, then

$$\sigma_{12} = \int_B^C \frac{\partial u}{\partial \nu} \, \mathrm{d}s = \int_\Gamma x \rho \, \mathrm{d}s, \tag{2.55}$$

$$\sigma_{22} = \int_C^D \frac{\partial u}{\partial \nu} \, \mathrm{d}s = 1 + \int_\Gamma y \rho \, \mathrm{d}s. \tag{2.56}$$

3. Fast solution of integral equations

Consider now the numerical solution of the two-phase interface problem in free space using the integral equation (2.19), which we write explicitly as

$$\rho(P) - \frac{\lambda}{\pi} \int_\Gamma \frac{\partial}{\partial \nu_P} \log |P - Q| \rho(Q) \, \mathrm{d}s Q = 2\lambda \frac{\partial \Psi_a}{\partial \nu_P}(P). \tag{3.1}$$

We select N_j points on the boundary Γ_j of the jth inclusion which are equispaced in arclength and define $h_j = |\Gamma_j|/N_j$, where $|\Gamma_j|$ denotes the length of boundary. The total number of discretization points is $N = \sum_{j=1}^{M} N_j$. Associated with each such point, denoted P_i^j, is an unknown charge density value ρ_i^j. Using the trapezoidal rule, we replace (3.1) by

$$\rho_i^j - \frac{\lambda}{\pi} \sum_{l=1}^{M} h_l \sum_{k=1}^{N_l} \frac{\partial}{\partial \nu_{P_i^j}} \log |P_i^j - P_k^l| \rho_k^l = -2\lambda \nu_i^j \cdot (1,0), \tag{3.2}$$

for $i = 1, \ldots, N_j$ and $j = 1, \ldots, M$. Care must be taken when $P_j^i = P_l^k$ to use the appropriate limit $\frac{1}{2}\kappa(P_l^k)$ in place of $(\partial/\partial \nu_{P_i^j}) \log |P_i^j - P_k^l|$, where κ denotes curvature. The trapezoidal rule is used for quadrature since it achieves superalgebraic convergence on smooth contours.

We solve linear systems like (3.2) iteratively, using the generalized minimum residual method GMRES (Saad and Schultz, 1986). The reason for choosing a conjugate gradient type iterative method is that the integral operator in (3.1) is compact and well approximated by a finite rank operator. The eigenvalues of $I + K$ are bounded and cluster at one. As a result, the linear system (3.2) has a bounded condition number and the number of iterations required is independent of N (for a fixed physical problem). The amount of work required to solve the linear system, therefore, scales like $J \cdot f(N)$ where J is the number of iterations and $f(N)$ is the amount of work required to compute matrix–vector products. Since K (or its discrete version) is dense, naive methods require $\mathcal{O}(J \cdot N^2)$ work. The Fast Multipole Method, however, allows the cost to be reduced to $\mathcal{O}(N)$, so that the cost of solving the linear system is $\mathcal{O}(J \cdot N)$.

3.1. The fast multipole method

The Fast Multipole Method (FMM) is a hierarchical scheme for the evaluation of Coulombic interactions in both two and three space dimensions (Rokhlin, 1985; Greengard and Rokhlin, 1987; Carrier *et al.*, 1988; Greengard, 1988; Greengard and Rokhlin, 1989). Like the schemes of Van Dommelen and Rundensteiner (1989), Odlyzko and Schönhage (1988), Appel (1985), Barnes and Hut (1986) and others, it is based on using multipole expansions and/or Taylor series to compute far field interactions. For a system of N sources (charges, dipoles, etc.), the FMM requires $\mathcal{O}(N)$ work to evaluate all pairwise interactions, with the constant depending on the desired precision. With minor modification, the FMM allows for the calculation of electrostatic interactions in a periodic array as well (Greengard and Rokhlin, 1987). We refer the reader to the articles listed above for a complete description of the method.

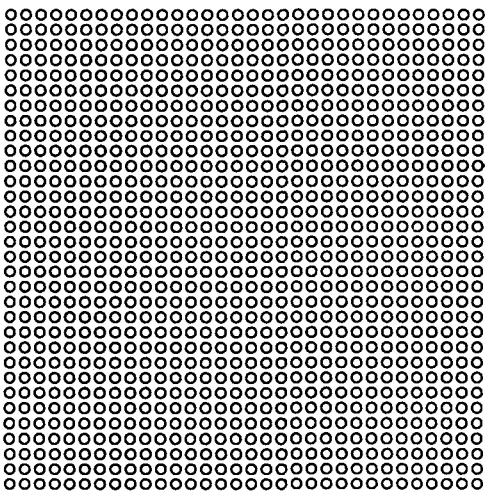

Fig. 3. A square array of 1,024 inclusions in the plane. This array is studied in free space and as a periodic system in Examples 1 and 2.

4. Numerical results

We have examined the behaviour of the integral equations (2.19), (2.31) and (2.45) over a wide range of geometries and conductivity ratios, and have selected three for the purpose of illustration. In each case, the GMRES method was used to reduce the Euclidean norm of the residual to below 10^{-6} and the FMM was used to compute matrix–vector products with a tolerance of 10^{-8}. All calculations were carried out on an IBM RS/6000 Model 580 in double precision. Evaluation of the potential off the boundary (once the integral equation was solved) was done using the FMM. Incorporation of Mayo's method (Mayo, 1984) would accelerate this part of the calculation and will be incorporated at a later date.

Example 1 The geometry in the first example consists of a square array of 1,024 disks in free space (Figure 3). The infinite medium is assumed to have conductivity one, while the inclusions have been assigned either a conductivity of 10^6 or a random number in the range $[10^{-7}, 10^2]$. Table 1 shows the type of problem being solved ($\sigma_i/\sigma_e = 10^6$ for the two-phase case and $\sigma_i/\sigma_e =$ 'Random' for the multiphase case), the number of boundary points used (N), the number of iterations required (Its), the time required for solving the integral equation (T) and the dipole moment

$$\mathbf{p} = \left(\int_\Gamma x\rho \, \mathrm{d}s, \int_\Gamma y\rho \, \mathrm{d}s \right)$$

induced in response to the applied field $E = (1, 0)$. Figure 4 shows contour plots of the total and induced potentials.

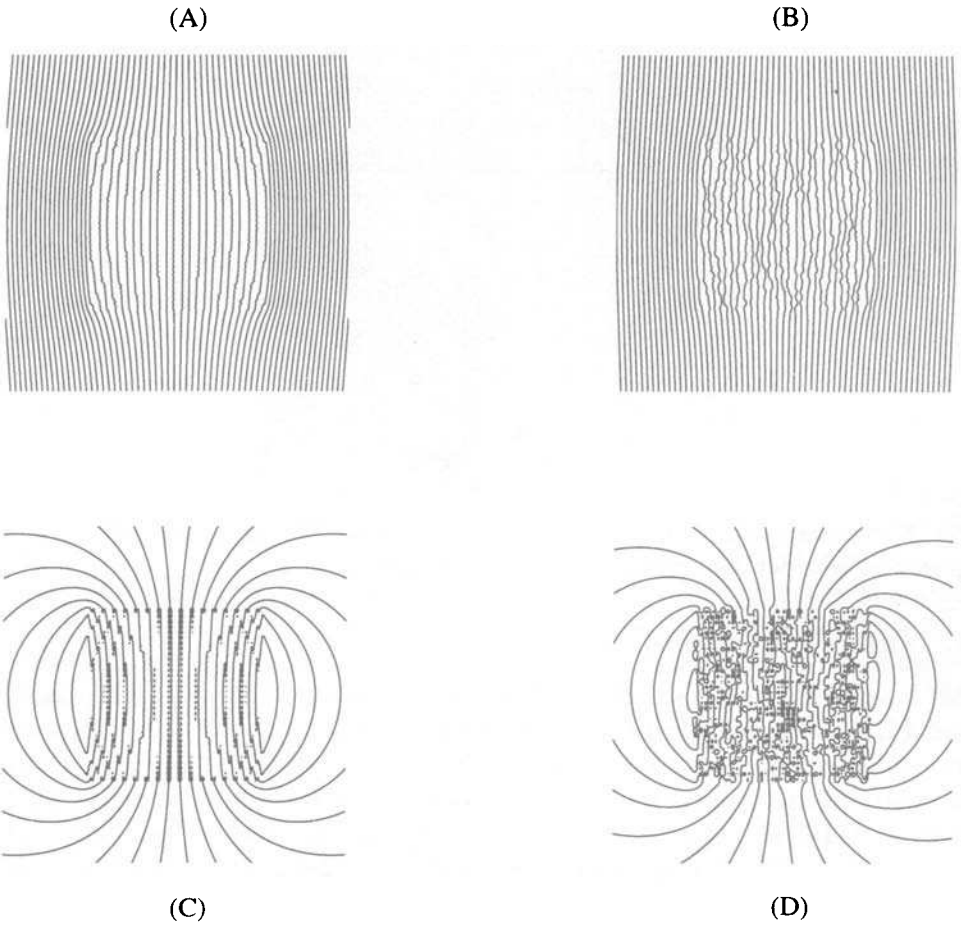

Fig. 4. Contour plots of the electrostatic potential for Example 1. (A) and (C) show the total and induced potential, respectively, for the two-phase case; (B) and (D) are the corresponding results for the (random) multiphase case.

Example 2 We now consider the same collection of 1,024 disks as in Example 1, but extended periodically. The background matrix is assumed to have conductivity one, while the inclusions have again been assigned either a conductivity of 10^6 or a random number in the range $[10^{-7}, 10^2]$. Table 2 summarizes our results, while Figure 5 shows contour plots of the total and induced potentials. (Note that in the two-phase case, we are solving a problem 1,024 times larger than necessary.)

Example 3 While materials with disk-like inclusions constitute an important class of composites, other geometries are clearly of interest as well. We therefore consider a collection of eleven slender inclusions in free space (Figure 6). Each inclusion is an ellipse which has been slightly perturbed in

Table 1. *Performance of the numerical method in Example 1. For insufficiently resolved problems, GMRES was unable to achieve the desired residual in less than 100 iterations. The iteration counts in parentheses indicate the number of GMRES steps allowed in such cases.*

σ_i/σ_e	N	Its	T (s)	p
10^6	8,192	(7)	26.13	(−1.65231,0.0000000)
10^6	16,384	7	40.1	(−0.75483,0.0000000)
10^6	32,768	7	104.9	(−0.75484,0.0000000)
10^6	65,536	7	166.2	(−0.75484,0.0000000)
Random	8,192	(9)	32.1	(−0.396286,−0.000747)
Random	16,384	9	50.4	(−0.397286,−0.001183)
Random	32,768	9	131.5	(−0.397287,−0.001184)
Random	65,536	9	208.3	(−0.397287,−0.001184)

Table 2. *Performance of the numerical method in Example 2. For insufficiently resolved problems, GMRES was unable to achieve the desired residual in less than 100 iterations. The iteration counts in parentheses indicate the number of GMRES steps allowed in such cases.*

σ_i/σ_e	N	Its	T (s)	p
10^6	8,192	2	5.6	(−1.09217,0.0000000)
10^6	16,384	3	31.3	(−1.08005,0.0000000)
10^6	32,768	3	36.63	(−1.08005,0.0000000)
10^6	65,536	3	106.2	(−1.08005,0.0000000)
Random	8,192	(9)	23.1	(−0.475469,−0.001001)
Random	16,384	10	82.9	(−0.458208,−0.001211)
Random	32,768	9	88.0	(−0.458201,−0.001211)
Random	65,536	9	262.1	(−0.458201,−0.001211)

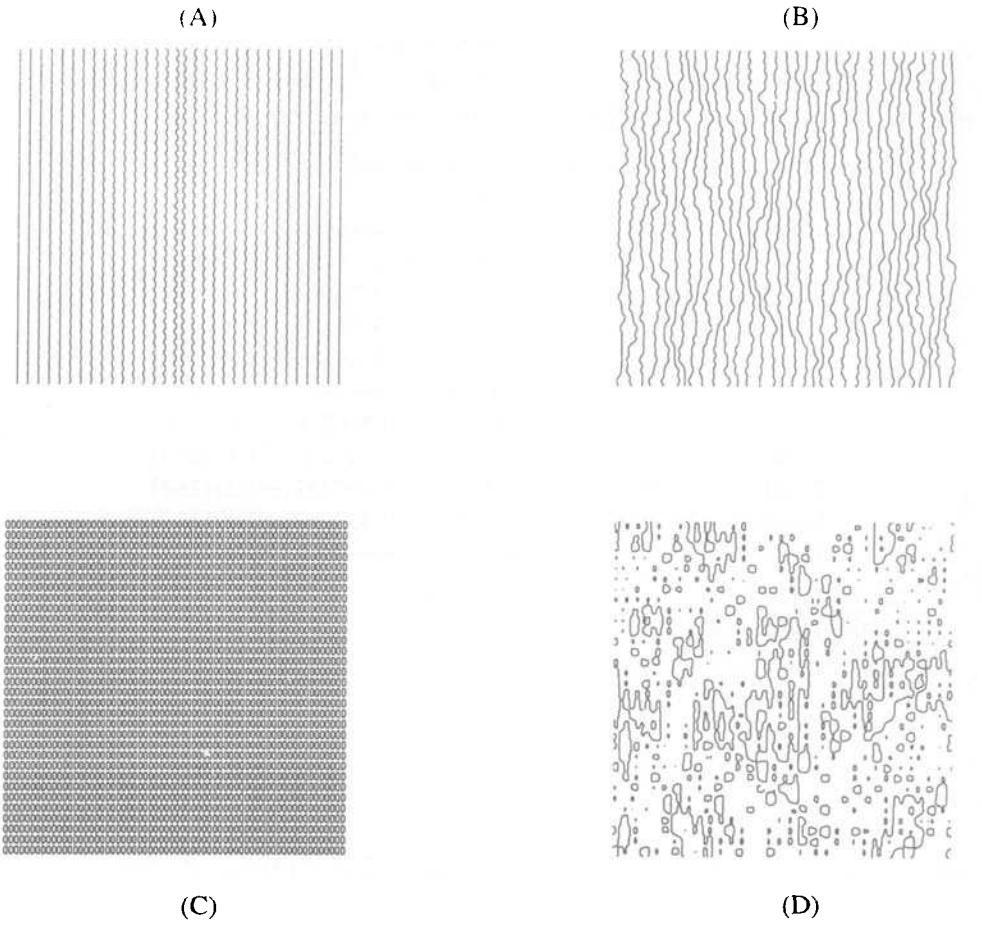

Fig. 5. Contour plots of the electrostatic potential for Example 2. (A) and (C) show the total and induced potential, respectively, for the two-phase case; (B) and (D) are the corresponding results for the (random) multiphase case.

order to make the geometry less regular. The background matrix is assumed to have conductivity one, while the inclusions have been assigned either a conductivity of 10^6 or 10^{-6}. Table 3 summarizes our results, while Figure 7 shows contour plots of the total and induced potentials.

Example 4 In this example, the slender inclusions of Example 3 are extended periodically. Table 4 summarizes our results, while Figure 8 shows contour plots of the total and induced potentials.

Example 5 The last geometry we consider is that of a fairly closely packed mixture of convex and nonconvex inclusions (Figure 9). In this free space calculation, the background matrix is assumed to have conductivity one,

Table 3. *Performance of the numerical method in Example 3. For insufficiently resolved problems, GMRES was unable to achieve the desired residual in less than 100 iterations. The iteration counts in parentheses indicate the number of GMRES steps allowed in such cases.*

σ_i/σ_e	N	Its	T (s)	**p**
10^6	1,100	(40)	15.5	(−0.688458,−0.387694)
10^6	2,200	(40)	25.7	(−0.874540,−0.251159)
10^6	4,400	40	45.2	(−0.874171,−0.251477)
10^6	8,800	40	87.6	(−0.874171,−0.251477)
10^{-6}	1,100	45	17.8	(0.860182,−0.252492)
10^{-6}	2,200	45	28.6	(0.855730,−0.251480)
10^{-6}	4,400	45	51.8	(0.855714,−0.251475)
10^{-6}	8,800	45	99.1	(−0.855714,−0.251475)

while the inclusions have been assigned either a conductivity of 10^6 or 10^{-6}. Table 5 summarizes our results, while Figure 10 shows contour plots of the total and induced potentials.

Example 6 In our last example, the inclusions of Example 5 are extended periodically. Table 6 summarizes our results, while Figure 11 shows contour plots of the total and induced potentials.

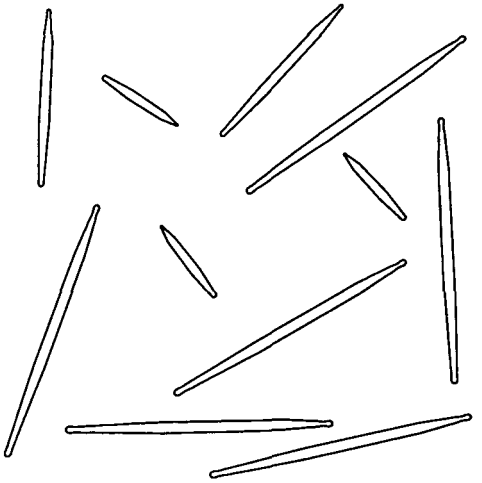

Fig. 6. Eleven slender inclusions in the plane. Each inclusion is a slightly perturbed ellipse. This geometry is studied in Examples 3 and 4.

Table 4. *Performance of the numerical method in Example 4. For insufficiently resolved problems, GMRES was unable to achieve the desired residual in less than 100 iterations. The iteration counts in parentheses indicate the number of GMRES steps allowed in such cases.*

σ_i/σ_e	N	Its	T (s)	p
10^6	1,100	(48)	18.1	(−3.22233,−3.67602)
10^6	2,200	(48)	25.6	(−1.65745,−0.75526)
10^6	4,400	48	63.8	(−1.64403,−0.73715)
10^6	8,800	48	98.9	(−1.64399,−0.73723)
10^6	17,600	48	256.9	(−1.64399,−0.73723)
10^{-6}	1,100	51	19.8	(0.563947,−0.124834)
10^{-6}	2,200	48	25.3	(0.554749,−0.124215)
10^{-6}	4,400	48	63.3	(0.554611,−0.124189)
10^{-6}	8,800	48	99.4	(0.554611,−0.124189)
10^{-6}	17,600	48	258.0	(0.554611,−0.124189)

Table 5. *Performance of the numerical method in Example 5. For insufficiently resolved problems, GMRES was unable to achieve the desired residual in less than 100 iterations. The iteration counts in parentheses indicate the number of GMRES steps allowed in such cases.*

σ_i/σ_e	N	Its	T (s)	p
10^6	450	(29)	4.6	(−1.48303,−0.07427)
10^6	900	(29)	9.6	(−1.38406,−0.01940)
10^6	1,800	29	17.5	(−1.37925,−0.01722)
10^6	3,600	29	30.9	(−1.37925,−0.01723)
10^6	7,200	29	51.7	(−1.37925,−0.01723)
10^{-6}	450	34	5.4	(1.4857,−0.05119)
10^{-6}	900	31	10.5	(1.45736,−0.017431)
10^{-6}	1,800	31	18.3	(1.45698,−0.01723)
10^{-6}	3,600	31	32.8	(1.45698,−0.01723)
10^{-6}	7,200	31	55.6	(1.45698,−0.01723)

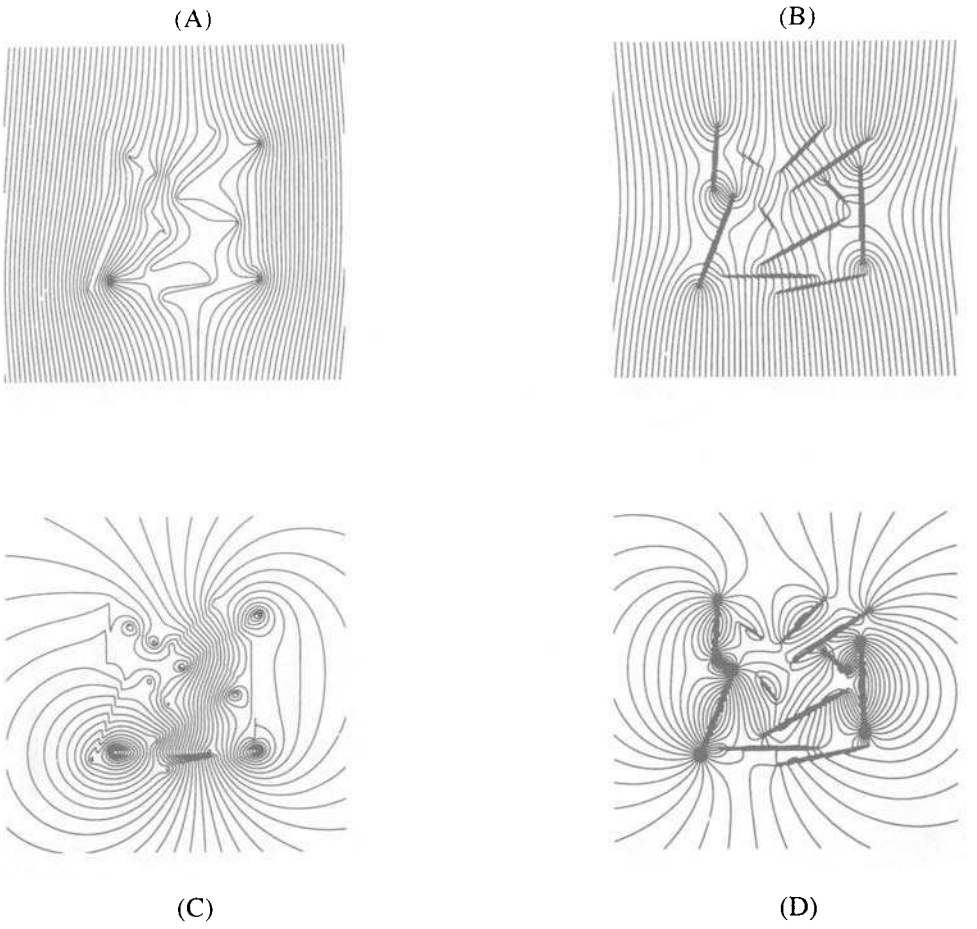

Fig. 7. Contour plots of the electrostatic potential for Example 3. (A) and (C) show the total and induced potential, respectively, for the case of highly conducting inclusions; (B) and (D) are the corresponding results for the case of poorly conducting inclusions.

Several observations can be made on the basis of the preceding examples.

1 For a fixed problem, the number of GMRES iterations required is constant, once sufficient resolution has been achieved.

2 The CPU time grows linearly with the number of discretization points.

3 The rate of convergence of the computed dipole moment is superalgebraic. (This rapid convergence can also be demonstrated for pointwise values of the charge density or other functionals of the solution.)

4 While the number of iterations required varies with the complexity of the geometry, it is remarkably insensitive to the conductivity ratio (in

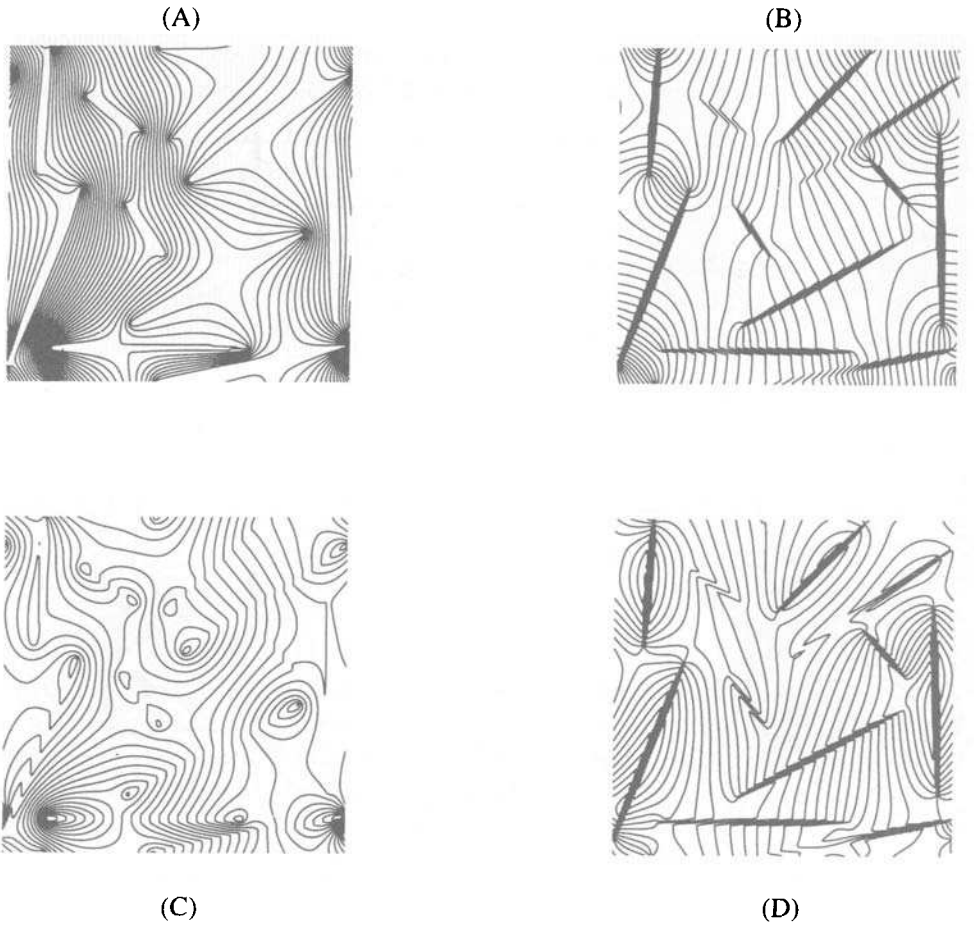

Fig. 8. Contour plots of the electrostatic potential for Example 4. (A) and (C) show the total and induced potential, respectively, for the case of highly conducting inclusions; (B) and (D) are the corresponding results for the case of poorly conducting inclusions.

marked contrast to the behavior of finite difference and finite element schemes).

As a final check on our calculations, we have computed the full effective conductivity tensor for the slender inclusion case (Example 4). With conductivity ratio 10^6,

$$\sigma_{\text{eff}}^1 = \begin{pmatrix} 4.93128 & 0.16328 \\ 0.16328 & 6.22091 \end{pmatrix},$$

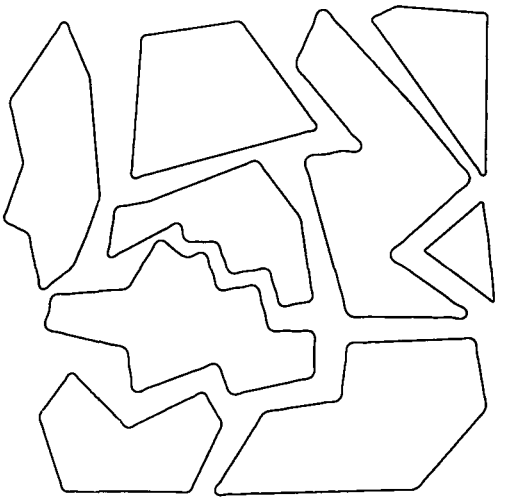

Fig. 9. A mixture of nine convex and nonconvex inclusions in the plane. This geometry is studied in Examples 5 and 6.

while with conductivity ratio 10^{-6},

$$\sigma_{\text{eff}}^2 = \begin{pmatrix} 0.160888 & 0.005327 \\ 0.005327 & 0.202963 \end{pmatrix}.$$

Table 6. *Performance of the numerical method in Example 6. For insufficiently resolved problems, GMRES was unable to achieve the desired residual in less than 100 iterations. The iteration counts in parentheses indicate the number of GMRES steps allowed in such cases.*

σ_i/σ_e	N	Its	T (s)	p
10^6	450	(30)	4.2	(−7.78783,2.2131022)
10^6	900	(30)	8.3	(−2.84366,0.74131)
10^6	1,800	30	14.9	(−3.93129,0.16328)
10^6	3,600	30	22.6	(−3.93128,0.16328)
10^6	7,200	30	49.6	(−3.93128,0.16328)
10^{-6}	450	30	4.1	(0.846530,−0.006531)
10^{-6}	900	29	7.8	(0.839114,0.005338)
10^{-6}	1,800	29	14.4	(0.839112,0.005327)
10^{-6}	3,600	29	22.8	(0.839112,0.005327)
10^{-6}	7,200	29	47.3	(0.839112,0.005327)

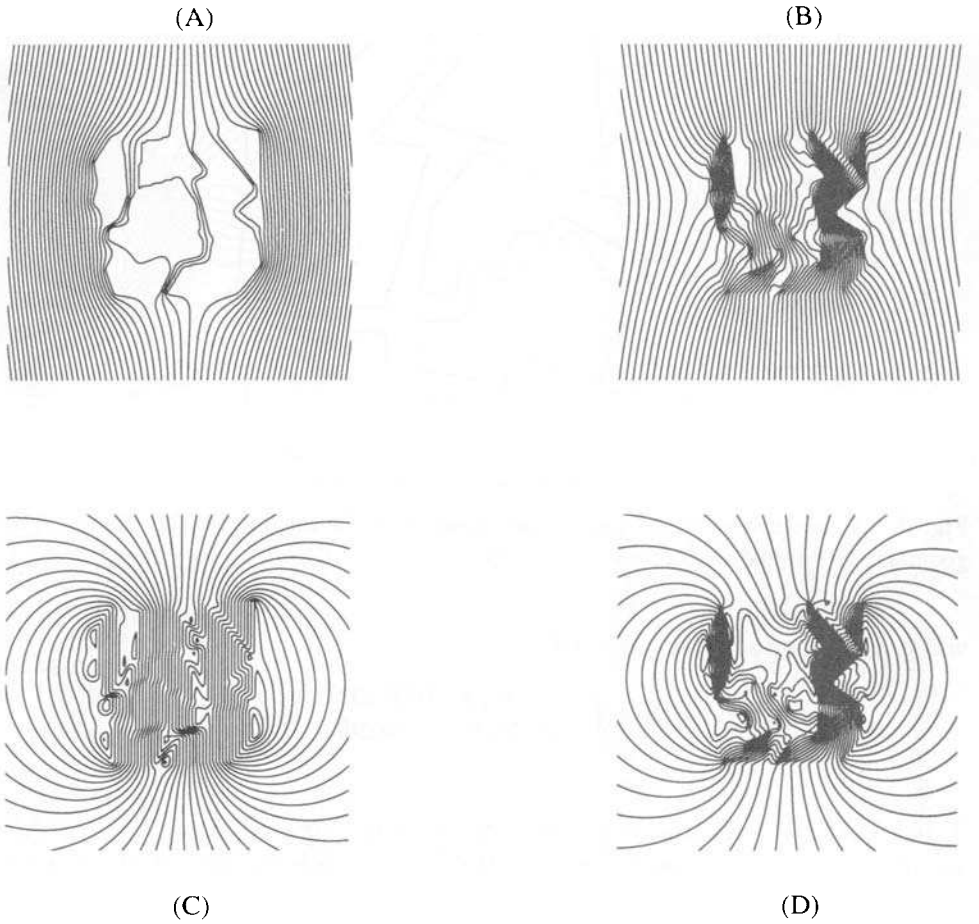

Fig. 10. Contour plots of the electrostatic potential for Example 5. (A) and (C) show the total and induced potential, respectively, for the case of highly conducting inclusions; (B) and (D) are the corresponding results for the case of poorly conducting inclusions.

These matrices satisfy the Keller–Dykhne–Mendelson relation (Keller, 1964; Dykhne, 1970; Mendelson, 1975)

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \left(\sigma^2_{\text{eff}}\right)^{-1} = \sigma^1_{\text{eff}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

to full accuracy.

5. Conclusions

We have presented an algorithm for the solution of the electrostatic field equations in composite media based on a fast multipole accelerated integral

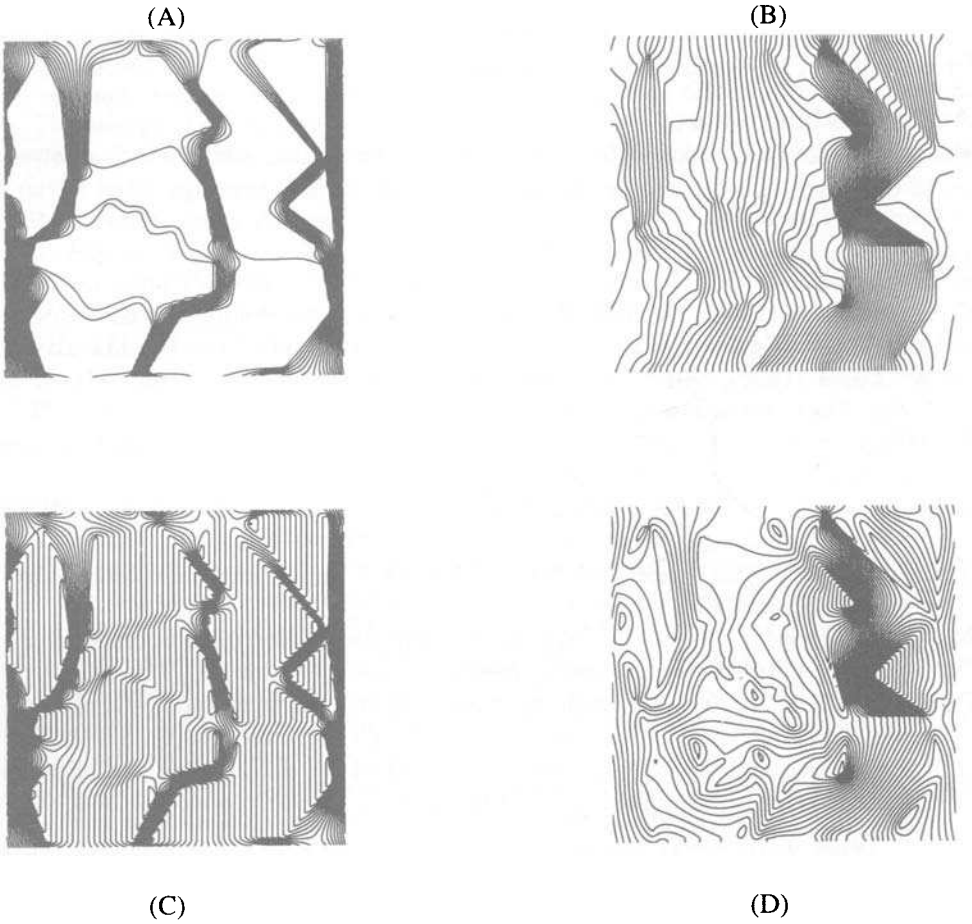

Fig. 11. Contour plots of the electrostatic potential for Example 6. (A) and (C) show the total and induced potential, respectively, for the case of highly conducting inclusions; (B) and (D) are the corresponding results for the case of poorly conducting inclusions.

equation solver. Large-scale problems, involving thousands of inclusions with perhaps one hundred thousand boundary points, can be solved in minutes using modest computational resources (such as a single workstation). Similar methods have been proposed for related problems by Rokhlin (1985), Nabors and White (1991), and Greenbaum *et al.* (1992, 1993). While we have only considered smooth inclusions, the method can be extended by modifying the quadrature to allow for the presence of corners (Hetherington and Thorpe, 1992). Extension to three dimensions is straightforward but requires incorporation of the three-dimensional FMM (Greengard and Rokhlin, 1988; 1989; Nabors and White, 1991). It is our hope that this

method will provide researchers in materials science with a new tool – the ability to compute effective properties of systems with complex microstructure by direct solution of the governing equation.

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