An integral equation method for electrostatics of anisotropic composites

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An interface integral equation is presented for the electrostatic problem in a composite where the components have anisotropic conductivity tensors. The electric potential is represented by a single-layer charge density on the component interfaces. In a simple numerical example involving anisotropic discs the charge density is expanded in a Fourier series. The integral equation is then solved to high accuracy with a modest computational effort.

1. Introduction

Interface integral-equation methods, based on Green's functions, have in some instances proven very successful for computing the effective response of *locally isotropic* composites. A locally isotropic composite is a material with physical properties described by piecewise constant isotropic tensors. See, for example, Greengard & Moura (1994) for an efficient algorithm and for a historic survey of integral-equation methods for electrostatics of composites. In brevity, interface integral-equation methods work well for composites since they incorporate analytic information about the solution via the Green's function, discretize the interfaces only, and lead to equations with low condition number which can be solved fast with the Fast Multipole Method (Greengard & Rokhlin 1987).

Many composites are not locally isotropic, but have physical properties described by piecewise constant anisotropic tensors. Such *locally anisotropic* composites, or polycrystals, are common in nature. They are also important in engineering. Designed magnetostrictives, piezoelectrics and piezooptics are some examples (Avelaneda & Olson 1992). Remarkably, there seem to be no fast and accurate computations done on locally anisotropic composites with interface integral-equation methods, nor with any other method. The reason for this may be the difficulty of finding a Green's function for the anisotropic electrostatic equation. For anisotropic electrostatics, the best numerical method as of today seems to be the finite element method accelerated with multigrid techniques (Bank 1994).

In this short paper we show that fast and accurate computations of effective properties of locally anisotropic composites with interface integral-equation methods are possible. We demonstrate this for conductivity in a square array of anisotropic discs where, due to symmetries, we claim accurate results with virtually no computational effort. In the limit of isotropy we show a connection between the Rayleigh multipole

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method for isotropic discs (Rayleigh 1892; Perrins *et al.* 1979) and a second-kind Fredholm integral-equation method. Finally, we argue that our interface integral-equation method will be competitive also for composites with general geometries.

2. Integral equation for anisotropic inclusions

In this section we will give the electrostatic equation for an anisotropic inclusion problem, chosen to be a square array of discs. Similar to previous work on isotropic electrostatics (Jaswon & Symm 1977; Hetherington & Thorpe 1992; Greengard & Moura 1994) we represent the electric potential $u(\mathbf{r})$ as a sum of an applied potential and an induced potential. The induced potential is represented by a single-layer charge density ρ on the inclusion interfaces. This representation allows us to rewrite the electrostatic equation for $u(\mathbf{r})$ as an interface integral equation for ρ , which is the fundamental equation of this paper.

Let discs with radius R be arranged in a square array, where the lattice points are separated by a unit distance and where one disc is centered at the origin. To begin with, let the discs have a conductivity tensor

$$\boldsymbol{\sigma}_d = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \quad (2.1)$$

so that the conductivity is σ_1 in the direction parallel to the x -axis and σ_2 in the direction parallel to the y -axis. Let the conductivity tensor of the medium surrounding the discs be

$$\boldsymbol{\sigma}_m = \begin{bmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{bmatrix} \quad (2.2)$$

The local conductivity $\boldsymbol{\sigma}$ of the composite will thus be either $\boldsymbol{\sigma}_d$ or $\boldsymbol{\sigma}_m$. Let a unit electric field $\mathbf{e}$ be applied in the direction of the x -axis. The purpose of this section is to find a solution $u(\mathbf{r})$ to the electrostatic equation

$$\nabla \cdot \boldsymbol{\sigma} \nabla u(\mathbf{r}) = 0, \quad (2.3)$$

subject to the constraint that the spatial average of ∇u is $\mathbf{e}$.

For subsequent use, let G be

$$G(\mathbf{r}, \boldsymbol{\sigma}) = -\frac{1}{4\pi} \ln [\mathbf{r} \cdot \boldsymbol{\sigma}^{-1} \mathbf{r}]. \quad (2.4)$$

This function satisfies

$$\nabla_{\mathbf{r}} \cdot \boldsymbol{\sigma}_d \nabla_{\mathbf{r}} G(\mathbf{r}, \boldsymbol{\sigma}_d) = -\sqrt{\sigma_1 \sigma_2} \delta(\mathbf{r}). \quad (2.5)$$

Furthermore, let

$$j(\mathbf{r}) = \int_B \mathbf{n}_{\mathbf{r}} \cdot \boldsymbol{\sigma}_d \nabla_{\mathbf{r}} G(\mathbf{r} - \mathbf{r}', \boldsymbol{\sigma}_d) \rho(\mathbf{r}') dS' \quad \mathbf{r} \in B, \quad (2.6)$$

where B is the boundary of a bounded domain D and $\mathbf{n}_{\mathbf{r}}$ denotes the outward unit normal on B at $\mathbf{r}$. We now propose for $\mathbf{r}_0$ on B

$$\lim_{\substack{\mathbf{r} \rightarrow \mathbf{r}_0 \\ \mathbf{r} \in cD}} j(\mathbf{r}) = j(\mathbf{r}_0) - \frac{1}{2} \sqrt{\sigma_1 \sigma_2} \rho(\mathbf{r}_0) \quad (2.7)$$

and

$$\lim_{\substack{\mathbf{r} \rightarrow \mathbf{r}_0 \\ \mathbf{r} \in D}} j(\mathbf{r}) = j(\mathbf{r}_0) + \frac{1}{2} \sqrt{\sigma_1 \sigma_2} \rho(\mathbf{r}_0). \quad (2.8)$$

The proof for this closely follows the proof of the jump conditions for the normal derivative of an isotropic single-layer potential, see Guenther & Lee (1988). The key modification being a rescaling of the variables.

Now introduce six interface integral operators M_i^* and M_i acting on a charge density ρ placed on the interface B between the disc at the origin D and the surrounding medium: M_1^* gives the potential at $\mathbf{r}$ inside D that results from ρ at B . M_1 is the restriction of M_1^* to B . M_2^* gives the potential at $\mathbf{r}$ outside D that results from ρ at B and all its periodic images. M_2 is the restriction of M_2^* to B . M_3 and M_4 are normal components of the electric field associated with the potentials of M_1 and M_2 . This reads

$$M_1^* \rho = \int_B G(\mathbf{r} - \mathbf{r}', \sigma_d) \rho(\mathbf{r}') dS', \quad (2.9)$$

$$M_1 \rho = \int_B G(\mathbf{r} - \mathbf{r}', \sigma_d) \rho(\mathbf{r}') dS' \quad \mathbf{r} \in B, \quad (2.10)$$

$$M_2^* \rho = \int_{B^\infty} G(\mathbf{r} - \mathbf{r}', \sigma_m) \rho(\mathbf{r}') dS', \quad (2.11)$$

$$M_2 \rho = \int_{B^\infty} G(\mathbf{r} - \mathbf{r}', \sigma_m) \rho(\mathbf{r}') dS' \quad \mathbf{r} \in B, \quad (2.12)$$

$$M_3 \rho = \int_B \mathbf{n}_r \cdot \sigma_d \nabla_r G(\mathbf{r} - \mathbf{r}', \sigma_d) \rho(\mathbf{r}') dS' \quad \mathbf{r} \in B, \quad (2.13)$$

$$M_4 \rho = \int_{B^\infty} \mathbf{n}_r \cdot \sigma_m \nabla_r G(\mathbf{r} - \mathbf{r}', \sigma_m) \rho(\mathbf{r}') dS' \quad \mathbf{r} \in B, \quad (2.14)$$

In the above equations B^∞ denotes all disc interfaces in the plane.

Now we are ready to make an ansatz for the potential $u(\mathbf{r})$ in the composite. A most natural choice is

$$u(\mathbf{r}) = \begin{cases} u^-(\mathbf{r}) & \text{if } \mathbf{r} \in \bar{D} \\ u^+(\mathbf{r}) & \text{if } \mathbf{r} \in cD \end{cases} \quad (2.15)$$

where

$$\begin{aligned} u^-(\mathbf{r}) &= \mathbf{e} \cdot \mathbf{r} + M_1^* (M_1)^{-1} M_2 \rho, \\ u^+(\mathbf{r}) &= \mathbf{e} \cdot \mathbf{r} + M_2^* \rho. \end{aligned} \quad (2.16)$$

It is easy to check that this function $u(\mathbf{r})$ is continuous and that it solves (2.3) except for at the interfaces. For zero net charge ρ on B it also gives a spatial average of ∇u that is $\mathbf{e}$. Below, by demanding that ρ should be such that $u(\mathbf{r})$ solves (2.3) also at the interfaces, we arrive at an integral equation for ρ .

The normal current density just outside the interface B , $j_{\mathbf{r}}^+$, can be written as a sum of three parts

$$j_{\mathbf{r}}^+ = \mathbf{n}_r \cdot \sigma_m \mathbf{e} - \frac{1}{2} \sigma_3 \rho + M_4 \rho. \quad (2.17)$$

The first term comes from the applied field $\mathbf{e}$. The second term subtracts the jump in the normal current density of u^+ experienced when B is approached from outside. The third term is the normal current density at B as given by u^+ .

The normal current density just inside the interface B , $j_{\mathbf{r}}^-$, can also be written

as a sum of three parts

$$j_{\mathbf{r}}^- = \mathbf{n}_{\mathbf{r}} \cdot \boldsymbol{\sigma}_{\text{d}} \mathbf{e} + \frac{1}{2} \sqrt{\sigma_1 \sigma_2} (M_1)^{-1} M_2 \rho + M_3 (M_1)^{-1} M_2 \rho. \quad (2.18)$$

The first term comes from the applied field $\mathbf{e}$. The second term adds the jump in the normal current density of u^- in experienced when the interface is approached from inside. The third term is the normal current density at B as given by u^- . By equating $j_{\mathbf{r}}^+$ and $j_{\mathbf{r}}^-$ we arrive at an integral equation for ρ

$$\mathbf{n}_{\mathbf{r}} \cdot (\boldsymbol{\sigma}_{\text{m}} - \boldsymbol{\sigma}_{\text{d}}) \mathbf{e} = \left(\frac{1}{2} \sqrt{\sigma_1 \sigma_2} (M_1)^{-1} M_2 + \frac{1}{2} \sigma_3 + M_3 (M_1)^{-1} M_2 - M_4 \right) \rho. \quad (2.19)$$

Equation (2.19) is the fundamental integral equation of this paper upon which the numerics of the following sections is based. Unlike similar integral equations for isotropic electrostatics (Jaswon & Symm 1977; Hetherington & Thorpe 1992; Greengard & Moura 1994), equation (2.19) includes inversion of an integral operator, M_1 . This means solving a Fredholm integral equation of the first kind. In a recent book Atkinson (1994) remarks: ‘‘Some integral equations of the first kind are quite ill-conditioned, and that has led some people to avoid such equations in general. Boundary integral equations of the first kind, however, are generally quite well behaved and recently they have been an increasingly popular approach to solving various problems’’. As we shall see below, for the square array of discs inversion of the operator M_1 poses no problem whatsoever. Another nice feature with M_1 is that for polycrystals with many grains per unit cell, and upon discretization, it will have a block-diagonal structure. This greatly simplifies its inversion for large problems.

3. Integral operators on matrix form

In this section we expand the charge density ρ and the current density at the interface B in a Fourier base. This allows us to represent the integral operators M_i of the last section as matrices acting on Fourier coefficients. The integral equation becomes a system of linear equations for the Fourier coefficients of ρ .

Represent ρ as

$$\rho(\mathbf{r}) = \sum_{n=1}^N a_n \cos n\phi, \quad (3.1)$$

where ϕ is the angle between the x -axis and $\mathbf{r}$ and N is the number of terms in the base. Then

$$(M_1)_{mn} = \frac{R(1 + \lambda^m) \delta_{mn}}{2m}, \quad (3.2)$$

where

$$\lambda = \frac{\sqrt{\sigma_2} - \sqrt{\sigma_1}}{\sqrt{\sigma_2} + \sqrt{\sigma_1}}, \quad (3.3)$$

$$(M_2)_{mn} = \frac{R}{2m} (\delta_{mn} + U_{mn}), \quad (3.4)$$

where

$$U_{mn} = (-1)^n R^{m+n} \binom{m+n-1}{m-1} S_{m+n}, \quad (3.5)$$

and S_{n+m} are lattice sums introduced in the composite literature by Rayleigh (1892)

and accurately tabulated by Berman & Greengard (1994),

$$(M_3)_{mn} = -\frac{1}{2}\lambda^m \sqrt{\sigma_1 \sigma_2} \delta_{mn}, \quad (3.6)$$

and

$$(M_4)_{mn} = \frac{1}{2}\sigma_3 U_{mn}. \quad (3.7)$$

The integral equation (2.19) becomes the following system of linear equations:

$$2(\sigma_3 - \sigma_1)\delta_{1m} = \sum_{n=1}^N \left\{ \left(\sqrt{\sigma_1 \sigma_2} \frac{1 - \lambda^m}{1 + \lambda^m} + \sigma_3 \right) \delta_{mn} + U_{mn} \left(\sqrt{\sigma_1 \sigma_2} \frac{1 - \lambda^m}{1 + \lambda^m} - \sigma_3 \right) \right\} a_n. \quad (3.8)$$

The $(\sigma_{\text{eff}})_{11}$ component of the effective conductivity tensor is computed from (Green-gard & Moura 1994)

$$(\sigma_{\text{eff}})_{11} = \sigma_3(1 - \pi R^2 a_1) \quad (3.9)$$

In the limit $\sigma_1/\sigma_2 \rightarrow 0$ equation (3.8) becomes

$$2(\sigma_3 - \sigma_1)\delta_{1m} = \sum_{n=1}^N \{ (m\sigma_1 + \sigma_3) \delta_{mn} + (m\sigma_1 - \sigma_3) U_{mn} \} a_n. \quad (3.10)$$

In the limit $\sigma_1/\sigma_2 \rightarrow \infty$ (3.8) becomes

$$2(\sigma_3 - \sigma_1)\delta_{1m} = \sum_{n=1}^N \left\{ \left(\frac{\sigma_1}{m} + \sigma_3 \right) \delta_{mn} + \left(\frac{\sigma_1}{m} - \sigma_3 \right) U_{mn} \right\} a_n. \quad (3.11)$$

In order to check equation (3.8) numerically my colleague Klas Samuelsson made a computation for the anisotropic disc with area fraction $p = 0.78$ and $(\sigma_1, \sigma_2, \sigma_3) = (20, 2, 1)$ with the piecewise linear finite element multigrid (PLTMG) program (Bank 1994) and 10,000 discretization points. This gave $(\sigma_{\text{eff}})_{11} = 8.18$ after about one hour of computation on a workstation. Equation (3.8) with 75 non-zero terms, and solved with Crout's factorization method gave $\sigma_{\text{eff}} = 8.184366951820$ after 0.14 seconds on the workstation when lattice sums and binomial coefficients were precomputed. In table 1 we present numerical results for a more difficult geometry: $p = 0.785$ and $(\sigma_1, \sigma_2, \sigma_3) = (100, 0 - \infty, 1)$.

4. Rotated discs

If the principal axes of the conductivity tensor of the discs are not aligned with the coordinate axes, but rotated an angle α , the complexity of the formalism of the preceding sections has to be slightly increased. The local conductivity inside the discs becomes $Q^T \sigma_d Q$ where the rotation Q is

$$Q = \begin{bmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{bmatrix}. \quad (4.1)$$

If the charge density is represented on the form

$$\rho(\mathbf{r}) = \sum_{n=1}^N a_n \cos n\phi + b_n \sin n\phi, \quad (4.2)$$

the operator M_i of equations (2.9-2.14) can be represented by block matrices, where

Table 1. Components of the effective conductivity tensor, $(\sigma_{\text{eff}})_{11}$ and $(\sigma_{\text{eff}})_{22}$, for a square array of anisotropic discs at area fraction 0.785, as computed from (3.8-3.11). The discs have principal conductivities σ_1 and σ_2 . The eigenvector corresponding to σ_1 is parallel to the x -axis. The conductivity of the surrounding medium is σ_3 . The number of non-zero Fourier terms in the expansion of (2.19) varied from $N = 150$ to $N = 300$.

σ_1	σ_2	σ_3	$(\sigma_{\text{eff}})_{11}$	$(\sigma_{\text{eff}})_{22}$
100	0	1	20.03691345135	0.007266203015
100	1	1	20.76248916680	1.000000000000
100	10	1	24.3742132191	6.64675476754
100	100	1	33.759300400	33.759300400
100	1000	1	42.119574452	84.723834200
100	10000	1	45.013896931	123.28965566
100	∞	1	45.635755584	137.62346000

each block $(M_i)_{mn}$ acts on a coefficient pair (a_n, b_n) . The operator M_1 becomes a block diagonal matrix

$$(M_1)_{mn} = \frac{R(I + A_m)\delta_{mn}}{2m}, \quad (4.3)$$

where I is the 2×2 identity matrix and

$$A_m = \lambda^m \begin{bmatrix} \cos 2m\alpha & \sin 2m\alpha \\ \sin 2m\alpha & -\cos 2m\alpha \end{bmatrix}. \quad (4.4)$$

The other matrices become

$$(M_2)_{mn} = \frac{RI\delta_{mn}}{2m} + \frac{RD_{mn}U_{mn}}{2m} \quad (4.5)$$

where

$$D_{mn} = \begin{bmatrix} 1 & 0 \\ 0 & 2\delta_{m1}\delta_{n1} - 1 \end{bmatrix}, \quad (4.6)$$

$$(M_3)_{mn} = -\frac{1}{2}\sqrt{\sigma_1\sigma_2}A_m\delta_{mn}, \quad (4.7)$$

and

$$(M_4)_{mn} = \frac{1}{2}\sigma_3 D_{mn}U_{mn}. \quad (4.8)$$

The integral equation of (2.19) becomes

$$\begin{aligned} & 2 \left(\sigma_3 - \sigma_1 \cos^2 \alpha - \sigma_2 \sin^2 \alpha, (\sigma_2 - \sigma_1) \sin \alpha \cos \alpha \right) \delta_{1m} \\ &= \sum_{n=1}^N \{ (\sqrt{\sigma_1\sigma_2}B_m + \sigma_3 I) \delta_{mn} + (\sqrt{\sigma_1\sigma_2}B_m - \sigma_3 I) D_{mn}U_{mn} \} (a_n, b_n), \end{aligned} \quad (4.9)$$

where

$$B_m = \frac{I - 2A_m + \lambda^{2m}I}{1 - \lambda^{2m}}. \quad (4.10)$$

Equation (3.9) still gives the $(\sigma_{\text{eff}})_{11}$ component of the effective conductivity tensor. The $(\sigma_{\text{eff}})_{21}$ component is given by

$$(\sigma_{\text{eff}})_{21} = -\sigma_3 \pi R^2 b_1. \quad (4.11)$$

Table 2. Eigenvalues of the effective conductivity tensor, $(\sigma_{\text{eff}})_1$ and $(\sigma_{\text{eff}})_2$, for a square array of anisotropic discs at area fraction 0.785. The discs have principal conductivities $\sigma_1 = 100$ and $\sigma_2 = 10$. The eigenvector corresponding to σ_1 forms an angle α with the x -axis. The conductivity of the surrounding medium is $\sigma_3 = 1$. The rotations α vary. Computations are done via (4.9).

α	$(\sigma_{\text{eff}})_1$	$(\sigma_{\text{eff}})_2$
0	24.3742132191	6.64675476754
$\pi/16$	22.9160683969	6.73735679214
$2\pi/16$	21.6892689386	6.82924599637
$3\pi/16$	22.9160683969	6.73735679214
$4\pi/16$	24.3742132191	6.64675476754
$5\pi/16$	22.9160683969	6.73735679214

In table 2 we present the eigenvalues of σ_{eff} for a geometry with $(\sigma_1, \sigma_2, \sigma_3) = (100, 10, 1)$ at various rotations α .

5. Discussion

We have found a single-layer representation for the electric potential in a composite with anisotropic inclusions. Roughly speaking, the idea is to let the charge density on one inclusion interact with interfaces of other inclusions via the fundamental solution to the Laplace equation. Only within individual inclusions the fundamental solution is translated into an anisotropic field. This representation was used to derive an integral equation (2.19) for the charge density.

For a numeric example we chose a simple geometry: an array of anisotropic discs. The integral equation was written as a small system of linear equations (3.8) by expanding the charge density in a Fourier base. It is interesting to note that in the limit of local isotropy, that is for $\sigma_1 = \sigma_2$, (3.8) reduces to the equations used by Perrins *et al.* (1979). These equations were derived with the recently much used Rayleigh Multipole Method which is applicable to locally isotropic suspensions of discs or spheres (Nicolovici *et al.* 1993; Helsing 1994; McPhedran & Movchan 1994; Chin *et al.* 1994). Our example thus shows that for electrostatics the Rayleigh Multipole Method can be viewed as a special case of an interface integral-equation method.

For a more general geometry we suggest, like Rokhlin (1984), the discretization of the integral equation (2.19) according to some n -point quadrature rule, that is a Nyström algorithm. The resulting system of linear equations is then solved with some iterative method where matrix vector multiplications are accelerated with the adaptive version of the Fast Multipole Method (Carrier *et al.* 1988). See Nachtigal *et al.* (1992) for a comparison of iterative methods for the solution of nonsymmetric systems of linear equations.

The integral equations for locally isotropic electrostatics used by previous authors (Van Bladel 1964; Jaswon & Symm 1977; Lindholm 1980; Hetherington & Thorpe 1992; Greengard & Moura 1994) are Fredholm equations of the second kind and involve an integral operator that is a double-layer potential or an adjoint of a double-layer potential. Such operators have smooth kernels for smooth interfaces. The integral equations can be discretized with the trapezoidal quadrature rule which then achieves superalgebraic convergence. Our integral equation is

more complicated since it involves the inversion of the operator M_1 of (2.9). This means solving a Fredholm integral equation of the first kind, where the kernel is the logarithm. To take care of this with high accuracy for general geometries some more sophisticated quadrature rule is needed. See Atkinson (1994) for a discussion of various numerical methods to solve this integral equation.

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