



Electrostatics and heat conduction in high contrast composite materials

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Abstract

We present a robust integral equation method for the calculation of the electrostatic and thermal properties of systems made of piecewise homogeneous, high contrast materials. By high contrast, we mean that the electrical or thermal conductivity ratios are high.

Our approach involves a modification of the standard integral representation using, in electrostatic terms, the polarization charge as an unknown. It is related to the perturbation approach proposed by Tausch and White [J. Tausch, J. White, Capacitance extraction of 3-D conductor systems in dielectric media with high-permittivity ratios, *IEEE Trans. Microwave Theory Tech.*, 47 (1999) 18–26], but based on a simple form of projection rather than on the solution of auxiliary integral equations. Numerical implementation is straightforward in the multiple dielectric case.

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1. Introduction

A classical problem in electrostatics and heat conduction concerns the solution of the Poisson or Laplace equation in domains consisting of piecewise homogeneous materials. The governing equation can be written in the form

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$$-\nabla(\epsilon \nabla u) = f, \tag{1.1}$$

where ϵ is piecewise constant, subject to some appropriate boundary or radiation condition on u . We will refer to the function ϵ as the conductivity: regions with high values of ϵ are good conductors and regions with low values of ϵ are poor conductors.

Such problems are often referred to as “interface” problems because the differential equation can be reformulated as follows: find a continuous function u which satisfies the Poisson equation in each phase (where ϵ is constant), and whose flux $\epsilon \frac{\partial u}{\partial \nu}$ is continuous across each interface. Without loss of generality, we restrict our attention to the solution of (1.1) when the source distribution f is given by a small number of point sources and the dynamic range of ϵ is large.

In earlier work, such as [3,7,12,17], fast algorithms were developed for such problems based on combining a suitable boundary integral equation with the fast multipole method [2,6,8,9] and an iterative solver such as GMRES [20]. Other fast algorithms [1,11,18,25] and other iterative methods [4,21] could equally well be used. At low contrast, these schemes are essentially optimal; the CPU time required grows linearly with the number of points in the discretization of the boundaries and interfaces defining the geometry. Unfortunately, when the material contrast is high, the standard integral equation can become ill-conditioned. In this paper, we show that the nature of the ill-conditioning is easily understood and construct a new integral representation which is stable and robust. Our method builds on the work of Tausch et al. [22,23], who developed what we believe to be the first effective solution procedure for this class of problems. We have been able to replace the Tausch–White–Wang perturbation theory with a more direct approach, based on an elementary but systematic analysis of flux.

2. Classical potential theory

In describing the standard approach, we will find it convenient to make use of the language of scattering theory. For this, let us begin with the simplest problem, the determination of the electric field in an infinite medium D_0 of conductivity ϵ_0 in which is embedded an inclusion D_1 of conductivity ϵ_1 (Fig. 1).

We assume that the right-hand side f is given by

$$f(\mathbf{x}) = q_0 \delta(\mathbf{x} - \mathbf{x}_0) + q_1 \delta(\mathbf{x} - \mathbf{x}_1),$$

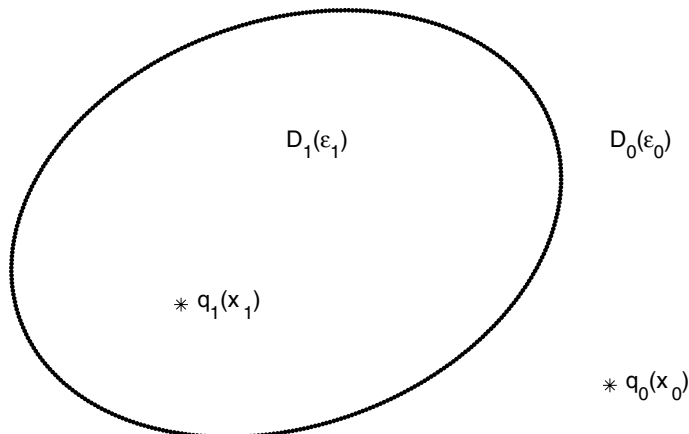


Fig. 1. An inclusion D_1 with conductivity ϵ_1 embedded in an infinite medium D_0 with conductivity ϵ_0 . \mathbf{x}_0 denotes a point in D_0 and \mathbf{x}_1 denotes a point in D_1 .

where $\mathbf{x}_1 \in D_1$ and $\mathbf{x}_0 \in D_0$. We define the driving field as the field in the infinite medium due to the point sources alone, based on the local conductivity. In other words, in two dimensions, we have

$$u^{\text{dr}} = \frac{q_0}{2\pi\epsilon_0} \log \frac{1}{\|\mathbf{x} - \mathbf{x}_0\|} + \frac{q_1}{2\pi\epsilon_1} \log \frac{1}{\|\mathbf{x} - \mathbf{x}_1\|}. \tag{2.1}$$

In three dimensions, we have

$$u^{\text{dr}} = \frac{q_0}{4\pi\epsilon_0} \frac{1}{\|\mathbf{x} - \mathbf{x}_0\|} + \frac{q_1}{4\pi\epsilon_1} \frac{1}{\|\mathbf{x} - \mathbf{x}_1\|}. \tag{2.2}$$

We define the scattered field u^{sc} by

$$u^{\text{sc}} = u - u^{\text{dr}},$$

where u is the *total potential* which satisfies (1.1). By construction, u^{dr} is continuous across the interface ∂D_1 and it is straightforward to see that u^{sc} must satisfy

$$\nabla^2 u^{\text{sc}} = 0 \quad \text{in } D_0, \tag{2.3}$$

$$\nabla^2 u^{\text{sc}} = 0 \quad \text{in } D_1, \tag{2.4}$$

$$[u^{\text{sc}}] = 0 \quad \text{on } \partial D_1, \tag{2.5}$$

$$\left[\epsilon \frac{\partial u^{\text{sc}}}{\partial \nu} \right] = - \left[\epsilon \frac{\partial u^{\text{dr}}}{\partial \nu} \right] \quad \text{on } \partial D_1. \tag{2.6}$$

Here, the expression $[f]$ denotes the jump in the quantity f across the interface.

Following standard practice [7,13,14,24], we represent u^{sc} as a *single layer potential*

$$u^{\text{sc}}(\mathbf{x}) = \int_{\partial D_1} G(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}}, \tag{2.7}$$

where $G(\mathbf{x}, \mathbf{y}) = \frac{1}{2\pi} \log \frac{1}{\|\mathbf{x} - \mathbf{y}\|}$ in 2D, $G(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi} \frac{1}{\|\mathbf{x} - \mathbf{y}\|}$ in 3D, σ is an unknown ‘‘polarization’’ charge density defined on the interface, and $ds_{\mathbf{y}}$ indicates that the integral is a boundary integral. For the sake of simplicity, we will restrict our attention to the 2D case. Readers unfamiliar with integral equation methods should consult the references above or the more mathematical texts [10,16] for background material. One well-known theorem we require as follows.

Theorem 2.1 ([10,14,16]). *Let σ be a continuous function on ∂D_1 , let $\mathbf{y}' \in \partial D_1$ and let $\nu(\mathbf{y}')$ be the unit normal vector to ∂D_1 at \mathbf{y}' . Then the single-layer potential (2.7) is continuous across ∂D_1 and satisfies the following jump relations:*

$$\frac{\partial u^{\text{sc}}}{\partial \nu_-}(\mathbf{y}') \equiv \lim_{\substack{\mathbf{x} \rightarrow \mathbf{y}' \\ \mathbf{x} \in D_1}} \frac{\partial u^{\text{sc}}}{\partial \nu(\mathbf{y}')}(\mathbf{x}) = \frac{1}{2} \sigma(\mathbf{y}') + \int_{\partial D_1} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}}, \tag{2.8}$$

$$\frac{\partial u^{\text{sc}}}{\partial \nu_+}(\mathbf{y}') \equiv \lim_{\substack{\mathbf{x} \rightarrow \mathbf{y}' \\ \mathbf{x} \in D_0}} \frac{\partial u^{\text{sc}}}{\partial \nu(\mathbf{y}')}(\mathbf{x}) = -\frac{1}{2} \sigma(\mathbf{y}') + \int_{\partial D_1} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}}. \tag{2.9}$$

We will make use of the operator notation

$$\mathbf{K}_{D_1} \sigma(\mathbf{y}') = \int_{\partial D_1} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}}$$

to denote the normal derivative of the single-layer potential restricted to the interface. When the context is clear, we will abuse notation and drop the subscript from \mathbf{K} .

From the representation (2.7), it is clear that Eqs. (2.3) and (2.4) are automatically satisfied. Since the single-layer potential is continuous across the interface, (2.5) is also satisfied. Imposing the remaining condition (2.6) and using Theorem 2.1, we obtain a Fredholm integral equation of the second kind for σ :

$$\frac{1}{2}\sigma(\mathbf{y}') + \lambda \int_{\Gamma} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y})\sigma(\mathbf{y}) \, ds_{\mathbf{y}} = -\lambda \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}'), \tag{2.10}$$

where $\lambda = (\epsilon_1 - \epsilon_0)/(\epsilon_1 + \epsilon_0)$. In operator notation,

$$\frac{1}{2}\sigma + \lambda \mathbf{K}\sigma = -\lambda \frac{\partial u^{\text{dr}}}{\partial \nu}.$$

Remark 2.1. In \mathbb{R}^2 , $\frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y})$ has a removable singularity when $\mathbf{y}' = \mathbf{y}$. More precisely,

$$\lim_{\mathbf{y} \rightarrow \mathbf{y}'} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y}) = \frac{1}{2}\kappa(\mathbf{y}'),$$

where κ is the curvature of ∂D_1 . For infinitely differentiable curves, the kernel is infinitely differentiable. As a result, the trapezoidal rule using an equispaced discretization is “spectrally accurate.” That is, the error goes to zero faster than any finite power of $1/N$, where N points are used in the discretization of the boundary. In \mathbb{R}^3 , the kernel $\frac{\partial G}{\partial \nu_{\mathbf{x}}}(\mathbf{x}, \mathbf{y})$ has an integrable singularity and high-order schemes are significantly more involved.

Two more well-known results from potential theory follow.

Theorem 2.2 ([15,16]). *If the homogeneous integral equation*

$$\frac{1}{2}\sigma(\mathbf{y}') + \lambda \int_{\Gamma} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y})\sigma(\mathbf{y}) \, ds_{\mathbf{y}} = 0 \tag{2.11}$$

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

Corollary 2.3. *As long as the ratio ϵ_1/ϵ_0 is bounded and lies away from the negative real axis, the integral equation (2.10) has a unique solution.*

Mathematically speaking, the story appears complete: one should simply be able to discretize Eq. (2.10) and solve it. At high contrast, however, a complicating phenomenon occurs. Fig. 2 shows the error in the numerical solution of the integral equation as a function of contrast ratio when D_1 is an ellipse in two dimensions with a point source $q_1 = 1$ at \mathbf{x}_1 as shown in Fig. 1. In these experiments, we use the trapezoidal rule (see Remark 2.1) with 200 points and Gaussian elimination to solve the 200×200 linear system. To study the stability of the scheme, we add random noise to the entries of the system matrix of relative magnitude 10^{-3} , 10^{-5} , 10^{-7} . In practice, such errors could stem from either noise in the data, errors in the geometry representation, or discretization error. Note that, for $\epsilon_1 \leq \epsilon_0$, the error is proportional to the noise. As $R = \epsilon_1/\epsilon_0 \rightarrow \infty$, however, there is a systematic loss of accuracy.

From an abstract viewpoint, the problem is that, in the limit $\epsilon_1/\epsilon_0 \rightarrow \infty$, the parameter $\lambda \rightarrow 1$ and the integral equation is not invertible. In fact, for $\lambda = 1$, the reader with some experience in potential theory may recognize the left-hand side of (2.10) as the integral operator corresponding to the interior Neumann problem, which is well-known to be rank-1 deficient. In the other direction, when $\epsilon_0/\epsilon_1 \rightarrow \infty$, the parameter $\lambda \rightarrow -1$ and the integral equation is nonsingular. Here, the experienced reader may recognize the left-hand side of (2.10) as the integral operator corresponding to the exterior Neumann problem, which is invertible.

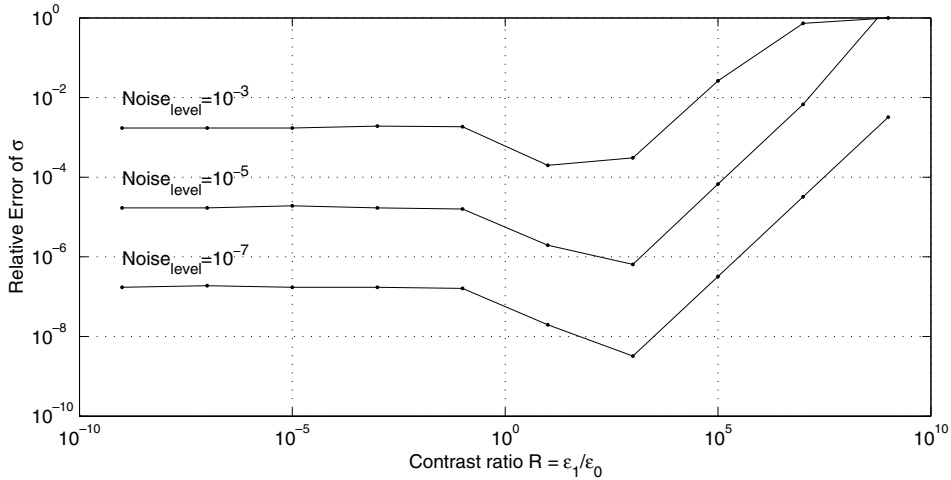


Fig. 2. Error in the solution of the integral equation (2.10) as a function of contrast ratio. If $R = \epsilon_1/\epsilon_0$, then $R \rightarrow \infty$ as the inclusion becomes highly conducting. If $R \rightarrow 0$ as the inclusion becomes poorly conducting.

Before proceeding with our detailed analysis of operators, let us carry out one more experiment. We “turn off” the source inside the high dielectric inclusion, i.e. we let $q_1 = 0$, $q_0 = 1$, and repeat the experiment of Fig. 2. Note that this only changes the right-hand side of the integral equation. The outcome is shown in Fig. 3 with no degradation of accuracy seen.

One obvious difference between this experiment and the first is that there is no net flux through the dielectric interface in the present case, while there was a net flux in the first. This turns out to be the crux of the problem.

3. Mathematical formulation

In this section, we describe a modification of the classical integral equation which removes the ill-conditioned behavior.

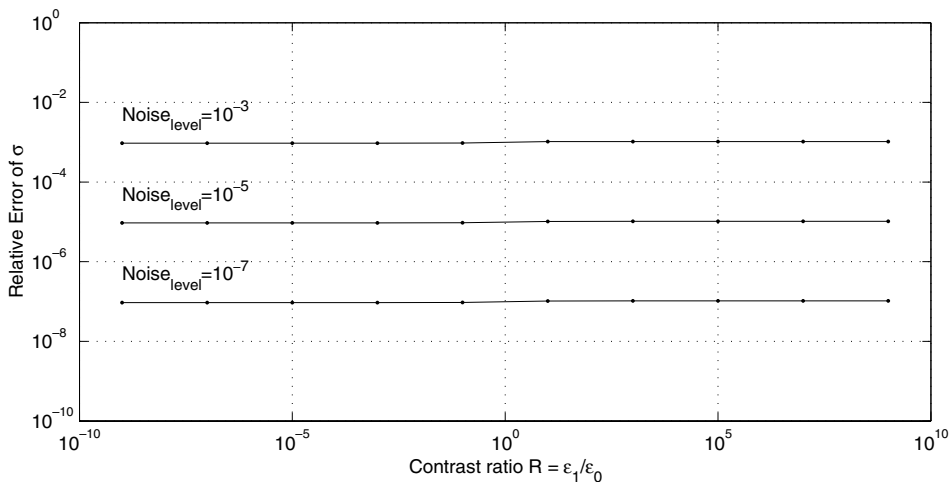


Fig. 3. Error in the solution of the integral equation (2.10) as a function of contrast ratio when $q_1 = 0$.

3.1. A single inclusion

Let us consider again a domain of piecewise constant conductivity with one bounded inclusion D_1 where $\epsilon(\mathbf{x}) = \epsilon_1$ for $\mathbf{x} \in D_1$ and $\epsilon(\mathbf{x}) = \epsilon_0$ for $\mathbf{x} \in D_0 = \mathbb{R}^d \setminus \overline{D_1}$. The corresponding interface problem in the plane with P point sources $\mathbf{x}_p \notin \Gamma = \partial D_1$ is given by

$$-\nabla \cdot (\epsilon(\mathbf{x}) \nabla u(\mathbf{x})) = \sum_{p=1}^P q_p \delta(\mathbf{x} - \mathbf{x}_p). \tag{3.1}$$

This equation has a unique solution once a radiation condition is specified. We assume that $u(\mathbf{x}) \rightarrow u^{\text{dr}}(\mathbf{x})$ as $|\mathbf{x}| \rightarrow \infty$, where

$$\begin{aligned} u^{\text{dr}}(\mathbf{x}) &= \sum_{p=1}^P u_p^{\text{dr}}(\mathbf{x}), \\ u_p^{\text{dr}}(\mathbf{x}) &= \frac{q_p}{\epsilon_{ip}} G(\mathbf{x}, \mathbf{x}_p) \end{aligned} \tag{3.2}$$

for $\mathbf{x}_p \in D_{ip}$. The function $u_p^{\text{dr}}(\mathbf{x})$ can be thought of as a ‘‘particular solution’’ induced by the p th point source. As before, the solution can be written as the sum of the driving field and a scattered field $u(\mathbf{x}) = u^{\text{dr}}(\mathbf{x}) + u^{\text{sc}}(\mathbf{x})$, where

$$u^{\text{sc}}(\mathbf{x}) = \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}}.$$

From the continuity of flux condition, we obtain the integral equation

$$\left(\frac{1}{2} I + \lambda \mathbf{K} \right) \sigma = -\lambda \frac{\partial u^{\text{dr}}}{\partial \nu}. \tag{3.3}$$

Let us now consider the limiting case $\lambda = 1$. This is precisely the integral equation we would obtain if we were to solve the interior Neumann problem for the Laplace equation with right-hand side given by the Neumann data $g(\mathbf{y}')$ on the boundary Γ of domain D_1 :

$$\left(\frac{1}{2} I + \mathbf{K} \right) \sigma(\mathbf{y}') = g(\mathbf{y}'). \tag{3.4}$$

It is well-known that Eq. (3.4) is rank-1 deficient, and that the problem is not invertible unless

$$\int_{\Gamma} g(\mathbf{y}) \, ds_{\mathbf{y}} = 0. \tag{3.5}$$

In other words, the solvability condition is that the net flux through the boundary is zero. To carry through the standard Fredholm-type analysis, we define the null-space of the operator by

$$\mathcal{N}_1 = \{ \sigma \mid (\frac{1}{2} I + \mathbf{K}) \sigma = 0 \}. \tag{3.6}$$

We also denote by $\mathbf{1}$ the constant function that takes the value 1 along Γ . The integral equation (3.4) is well-conditioned as a map from say $L^2 \setminus \mathcal{N}_1 \rightarrow L^2 \setminus \mathbf{1}$. We will refer to the latter space as the space of functions with mean zero.

Returning now to the interface problem, suppose that λ is near 1 (the difficult case) and that $\sigma \in \mathcal{N}_1$. Then

$$\left(\frac{1}{2} I + \lambda \mathbf{K} \right) \sigma = \left(\frac{1}{2} I + \mathbf{K} \right) \sigma + (\lambda - 1) \mathbf{K} \sigma = (\lambda - 1) \mathbf{K} \sigma. \tag{3.7}$$

A straightforward calculation shows that

$$\left\| \left(\frac{1}{2}I + \lambda \mathbf{K} \right)^{-1} \right\| \geq \frac{1}{|\lambda - 1| \|\mathbf{K}\|}. \quad (3.8)$$

This is precisely why the integral operator $\frac{1}{2}I + \lambda \mathbf{K}$ is singular as λ approaches to 1 (or $\epsilon_1/\epsilon_0 \rightarrow \infty$).

On the other hand, suppose that the right-hand side satisfies the mean zero condition (3.5). Then we may write

$$\left(\frac{1}{2}I + \lambda \mathbf{K} \right)^{-1} = \left(\left[\frac{1}{2}I + \mathbf{K} \right] \left(I + \left[\frac{1}{2}I + \mathbf{K} \right]^{-1} (\lambda - 1) \mathbf{K} \right) \right)^{-1} \quad (3.9)$$

$$= \left(I + \left[\frac{1}{2}I + \mathbf{K} \right]^{-1} (\lambda - 1) \mathbf{K} \right)^{-1} \left[\frac{1}{2}I + \mathbf{K} \right]^{-1}. \quad (3.10)$$

The boundedness of $\left(\frac{1}{2}I + \lambda \mathbf{K} \right)^{-1}$ now follows from the fact that $\left(\frac{1}{2}I + \mathbf{K} \right)$ is a bounded operator as a map from $L^2(\Gamma) \setminus \mathcal{N}_1 \rightarrow L^2(\Gamma) \setminus \mathbf{1}$ and the fact that the first term on the right-hand side of (3.10) can be expanded in a Neumann series for $\lambda \approx 1$. The only technical aspect of the proof is to make sure that the operators $\left(\frac{1}{2}I + \mathbf{K} \right)^{-1}$ and \mathbf{K} map zero-mean functions to zero-mean functions. This is a well-known property of the single-layer potential [10,14,16].

In summary, the integral equation $\left(\frac{1}{2}I + \lambda \mathbf{K} \right) \sigma = f$ is well-behaved and invertible so long as the right-hand side $f(t)$ has mean zero. Returning to our interface problem (3.3), this requires that

$$\int_{\Gamma} -\lambda \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, \text{d}s_{\mathbf{y}} = \lambda \sum_{x_p \in D_1} \frac{q_p}{\epsilon_1} = 0. \quad (3.11)$$

This is entirely consistent with our numerical observations in the previous section.

Since we cannot assume the net flux is zero across the interface, we next decompose the right-hand side into a constant and zero-mean part: $f(t) = \bar{f} : \mathbf{1}(t) + f^{\perp}(t)$. We also decompose the unknown density into a constant and zero-mean part: $\sigma(t) = \bar{\sigma} \mathbf{1}(t) + \sigma^{\perp}(t)$. The integral equation (3.3) can then be written as

$$\left(\frac{1}{2}I + \lambda \mathbf{K} \right) \sigma^{\perp} = - \left(\frac{1}{2}I + \lambda \mathbf{K} \right) \bar{\sigma} \mathbf{1} - \lambda \frac{\partial u^{\text{dr}}}{\partial \nu}. \quad (3.12)$$

In order for the right-hand side to have mean zero (be orthogonal to $\mathbf{1}$ on Γ), we must have

$$\left\langle \left(\frac{1}{2}I + \lambda \mathbf{K} \right) \bar{\sigma} \mathbf{1}, \mathbf{1} \right\rangle = \left\langle -\lambda \frac{\partial u^{\text{dr}}}{\partial \nu}, \mathbf{1} \right\rangle = -\lambda \int_{\Gamma} \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, \text{d}s_{\mathbf{y}}.$$

Simple algebra and the fact that $\mathbf{K}^* \mathbf{1} = (-\frac{1}{2}) \mathbf{1}$ [10,14,16] yields

$$\left\langle \left(\frac{1}{2}I + \lambda \mathbf{K} \right) \bar{\sigma} \mathbf{1}, \mathbf{1} \right\rangle = \frac{1}{2} (1 - \lambda) \int_{\Gamma} \bar{\sigma}(\mathbf{y}) \, \text{d}s_{\mathbf{y}} = -\lambda \int_{\Gamma} \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, \text{d}s_{\mathbf{y}}.$$

Thus, the integral equation (3.12) is well-behaved if we set the constant part of the single-layer density according to:

$$\int_{\Gamma} \bar{\sigma}(\mathbf{y}) \, \text{d}s_{\mathbf{y}} = \frac{-2\lambda}{1 - \lambda} \int_{\Gamma} \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, \text{d}s_{\mathbf{y}} = \left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon_1} \right) \sum_{x_p \in D_1} q_p. \quad (3.13)$$

It is possible to derive the same formula from a simple physical argument based on flux continuity. In short, the driving field is responsible for a flux difference defined by $(\epsilon_0 - \epsilon_1) \int_{\Gamma} \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, \text{d}s_{\mathbf{y}}$ across Γ . The constant part of the single layer density $\int_{\Gamma} \epsilon_0 \bar{\sigma}(\mathbf{y}) \, \text{d}s_{\mathbf{y}}$ is therefore chosen to compensate for this flux difference, yielding the result:

$$\int_{\Gamma} \bar{\sigma}(\mathbf{y}) \, ds_{\mathbf{y}} = -\left(\frac{\epsilon_0 - \epsilon_1}{\epsilon_0}\right) \int_{\Gamma} \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, ds_{\mathbf{y}} = \left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon_1}\right) \sum_{\mathbf{x}_p \in D_1} q_p. \tag{3.14}$$

3.2. Multiphase materials

Suppose now that a finite number of smooth bounded inclusions are embedded in a homogeneous background material with conductivity ϵ_0 but that each inclusion is allowed a distinct conductivity. D_k will denote the region occupied by the k th inclusion with conductivity ϵ_i and its boundary will be denoted by Γ_i . Assuming there are I inclusions, the total interface will be denoted by $\Gamma = \cup_{i=1}^I \Gamma_i$. We let u denote the total potential with P -point sources $\mathbf{x}_p \notin \Gamma$ as in the previous subsection. The solution can again be represented in terms of a single-layer potential

$$u(\mathbf{x}) = \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}} + \sum_{p=1}^P u_p^{\text{dr}}(\mathbf{x}), \tag{3.15}$$

where u_p^{dr} is defined in (3.2). Imposing the flux continuity condition $\epsilon_i \frac{\partial u}{\partial \nu_-} = \epsilon_0 \frac{\partial u}{\partial \nu_+}$ at every interface point $\mathbf{y}' \in \Gamma_i$, we obtain

$$\frac{1}{2} \sigma(\mathbf{y}') + \lambda_i \int_{\Gamma} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}} = -\lambda_i \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}'), \tag{3.16}$$

where $\lambda_i = \frac{\epsilon_i - \epsilon_0}{\epsilon_i + \epsilon_0}$. This is a system of integral equations, coupling the unknown charge densities on all interfaces Γ_i , $i = 1, \dots, I$.

Theorem 3.1. [7] *Suppose that the homogeneous equation*

$$\frac{1}{2} \sigma(\mathbf{y}') + \lambda_i \int_{\Gamma} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}} = 0, \quad \mathbf{y}' \in \Gamma_i \tag{3.17}$$

has a nontrivial solution. Then at least one of the ratios λ_i lies on either the ray $\lambda \geq 1$ or the ray $\lambda < -1$.

Corollary 3.2. *As long as all the ratios ϵ_i/ϵ_0 are bounded and have nonnegative real part, the integral equation (3.16) has a unique solution.*

Let \mathbf{K}_{ij} denote the restriction of the operator \mathbf{K} from $L^2(\Gamma_j)$ to $L^2(\Gamma_i)$ defined by

$$(\mathbf{K}_{ij} \sigma_j)(\mathbf{y}') = \int_{\Gamma_j} \frac{\partial G}{\partial \nu(\mathbf{y}')}(\mathbf{y}', \mathbf{y}) \sigma(\mathbf{y}) \, ds_{\mathbf{y}} \quad \text{for } \mathbf{y}' \in \Gamma_i. \tag{3.18}$$

We leave it to the reader to verify that $(\mathbf{K}_{ij}^* \mathbf{1})(\mathbf{y}') = -\frac{1}{2} \delta_{ij}$ for $\mathbf{y}' \in \Gamma_i$ and that $\langle \mathbf{K}_{ij} \mathbf{1}, \mathbf{1} \rangle = 0$ if $i \neq j$.

Restricting our attention for the moment to the two inclusion problem in the limit $\lambda_1, \lambda_2 \rightarrow 1$, we have

$$\left(\frac{1}{2}I + \mathbf{K}\right)\sigma = \mathbf{f}, \quad \text{where } \mathbf{K} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix}, \quad \sigma = \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix}, \quad \text{and } \mathbf{f} = \begin{bmatrix} -\lambda_1 \frac{\partial u^{\text{dr}}}{\partial \nu} \\ -\lambda_2 \frac{\partial u^{\text{dr}}}{\partial \nu} \end{bmatrix}. \tag{3.19}$$

is orthogonal to the null space of $(\frac{1}{2}I + \mathbf{K})^*$. Since $(\frac{1}{2}I + \mathbf{K}^*) \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix} = (\frac{1}{2}I + \mathbf{K}^*) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$, the solvability condition is that the right-hand have mean zero on each interface:

$$\left\langle \mathbf{f}, \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix} \right\rangle = 0 \quad \text{and} \quad \left\langle \mathbf{f}, \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \right\rangle = 0. \tag{3.19}$$

This condition is satisfied a priori only when the total charge contained in either D_1 or D_2 is zero.

In order to make the right-hand side of the integral equation $(\frac{1}{2}I + \mathbf{K})\sigma = f$ orthogonal to both $\begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix}$ and $\begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}$, we follow the same recipe as above, and decompose σ on each interface into a constant part and a mean zero part: $\sigma_i = \bar{\sigma}_i + \sigma_i^\perp$. Then,

$$\left(\frac{1}{2}I + \mathbf{K}\right) \begin{bmatrix} \sigma_1^\perp \\ \sigma_2^\perp \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 - \bar{\sigma}_1 \mathbf{K}_{11} \mathbf{1} - \bar{\sigma}_2 \mathbf{K}_{12} \mathbf{1} \\ \mathbf{f}_2 - \bar{\sigma}_1 \mathbf{K}_{21} \mathbf{1} - \bar{\sigma}_2 \mathbf{K}_{22} \mathbf{1} \end{bmatrix}. \quad (3.20)$$

The solvability conditions (3.19) is satisfied if both

$$\langle \mathbf{f}_1 - \bar{\sigma}_1 \mathbf{K}_{11} \mathbf{1}, \mathbf{1} \rangle = 0 \quad \text{and} \quad \langle \mathbf{f}_2 - \bar{\sigma}_2 \mathbf{K}_{22} \mathbf{1}, \mathbf{1} \rangle = 0. \quad (3.21)$$

Therefore, we set $\bar{\sigma}_i$ as follows:

$$\int_{\Gamma_i} \bar{\sigma}_i(\mathbf{y}) \, ds_{\mathbf{y}} = \left(\frac{\epsilon_0 - \epsilon_i}{\epsilon_0}\right) \int_{\Gamma_i} \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, ds_{\mathbf{y}} = \left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon_i}\right) \sum_{x_p \in D_i} q_p. \quad (3.22)$$

By analogy with the single inclusion case, it is reasonable to expect that the integral equation (3.16) is well-behaved for λ_i close to 1 once we define the unknown functions to be σ_i^\perp , having enforced (3.22) for the constant part $\bar{\sigma}_i$. We do not have a proof in the general case and leave this as a conjecture.

3.3. Layered materials

Our analysis is easily extended to nested inclusions (layered materials) with non-intersecting boundaries. For this, we begin by assuming that the computational domain is given by Ω_0 with conductivity ϵ_0 . For every interface Γ_j within Ω_0 , we let Ω_j denote its interior and set the conductivity in Ω_j to be ϵ_j . If Ω_j itself contains additional interfaces, each of these (say Γ_k) defines a subregion (say Ω_k) and a distinct conductivity (say ϵ_k). This construction is carried out recursively until all interfaces have been accounted for. Examples with one or two level of nesting are shown in Figs. 4 and 5.

The solution is again represented in the form (3.15), resulting in an integral equation of the form (3.16). On the i -th interface, we decompose the charge density σ_i as $\sigma_i = \bar{\sigma}_i + \sigma_i^\perp$. Considerations analogous to those above show that the right-hand side of the integral equation for σ_i^\perp on each interface has zero net flux if

$$\int_{\Gamma_i} \bar{\sigma}_i(\mathbf{y}) \, ds_{\mathbf{y}} = \left(\frac{1}{\epsilon_{i^+}} - \frac{1}{\epsilon_i}\right) \sum_{x_p \in \Omega_i} q_p, \quad (3.23)$$

where ϵ_{i^+} denotes the conductivity in the region to the exterior of Γ_i .

Remark 3.1. In many applications, one is given the integral equation (3.16), but the right-hand side on each interface is specified as raw data, rather than having the driving field in analytic form. In that case, the recipe (3.23) must be modified slightly and expressed in terms of the net fluxes $\int \frac{\partial u^{\text{dr}}}{\partial \nu} \, dt$ on each interface. This is straightforward to do, since the total charge in the interior of a simply connected domain D with interface ∂D_i is given by

$$Q = -\epsilon_i \int_{\partial D_i} \frac{\partial u^{\text{dr}}}{\partial \nu}(\mathbf{y}) \, ds_{\mathbf{y}}.$$

If a region Ω_i contains several such inclusions, the net charge in each must be computed. The total charge in Ω_i is then the sum of the individual subregion contributions plus the integral of the given interface data on $\partial \Omega_i$ itself. In the case of nested inclusions, this procedure is most easily carried out recursively, beginning with the innermost subregion (subregions).

3.4. Fast solution of integral equations

Consider now the numerical solution of the interface problem using the integral equation (3.16), which we write explicitly as

$$\frac{1}{2}\sigma(\mathbf{y}') + \frac{\lambda_j}{2\pi} \int_{\Gamma} \frac{\partial}{\partial v(\mathbf{y}')} \log \frac{1}{|\mathbf{y}' - \mathbf{y}|} \sigma(\mathbf{y}) \, ds_{\mathbf{y}} = -\lambda_j \frac{\partial u^{\text{dr}}}{\partial v}(\mathbf{y}') \tag{3.24}$$

for $\mathbf{y}' \in \Gamma_j$. We select N_j points on the boundary Γ_j , 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 \mathbf{y}'_i , is an unknown charge density value σ'_i . In the following, we let $v_{i,j}$ denote the normal at the point \mathbf{y}'_i . Using the trapezoid rule, we replace (3.24) by

$$\frac{1}{2}\sigma'_i - \frac{\lambda_j}{2\pi} \sum_{l=1}^M h_l \sum_{k=1}^{N_l} \frac{\partial}{\partial v_{i,j}} \log |\mathbf{y}'_i - \mathbf{y}'_k| \sigma'_k = -\lambda \frac{\partial u^{\text{dr}}}{\partial v}(\mathbf{y}'_i) \tag{3.25}$$

for $i = 1, \dots, N_j$ and $j = 1, \dots, M$. Care must be taken when $\mathbf{y}'_i = \mathbf{y}'_k$ to use the appropriate limit $\frac{1}{2}\kappa(\mathbf{y}'_i)$ in place of $\frac{\partial}{\partial v_{i,j}} \log |\mathbf{y}'_i - \mathbf{y}'_k|$, where κ denotes curvature. The trapezoidal rule is used for quadrature since it achieves superalgebraic convergence on smooth contours.

We solve the linear system (3.25) iteratively, using the generalized minimum residual method GMRES [4,20,21], since it achieves rapid convergence for well-conditioned linear systems. The amount of work required to solve the linear system, 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 \mathbf{K} (or its discrete version) is dense, naive methods require $O(J \cdot N^2)$ work. The Fast Multipole Method, however, allows the cost to be reduced to $O(N)$, so that the cost of solving the linear system is $O(J \cdot N)$. The algorithm has been described in great detail elsewhere (see, for example, [2,6,8,9,12,17,19]).

4. Numerical results

We will refer the integral equation method derived above as the *mean-zero* integral equation to contrast it with the classical approach. In this section, we illustrate the behavior of the method with two examples.

The code has been implemented in Fortran in slightly greater generality than discussed above. More precisely, we allow Neumann conditions to be imposed on the boundary of a collection of interior “holes” in addition to imposing continuity conditions at interfaces. This simply involves adding a single layer density on each Neumann boundary.

Example 1 (Convergence acceleration). In the first example (Fig. 4), we have five interfaces and let the driving field be that induced by two point sources (one contained in the multilayered inclusion on the left and one contained in the multi-layered inclusion on the right). 200 equispaced points are used in the discretization of each interface.

The central figure shows the rate of convergence of GMRES for the classical integral equation at low & high contrast. The right-hand figure shows the rate of convergence for the *mean-zero* integral equation.

Example 2 (Accuracy). In our second example (Fig. 5), we consider an interior Neumann problem with one hole on which Neumann conditions are imposed and five additional material interfaces. The driving field is again defined by two point sources, one in the upper right inclusion and one in the lower right inclusion.

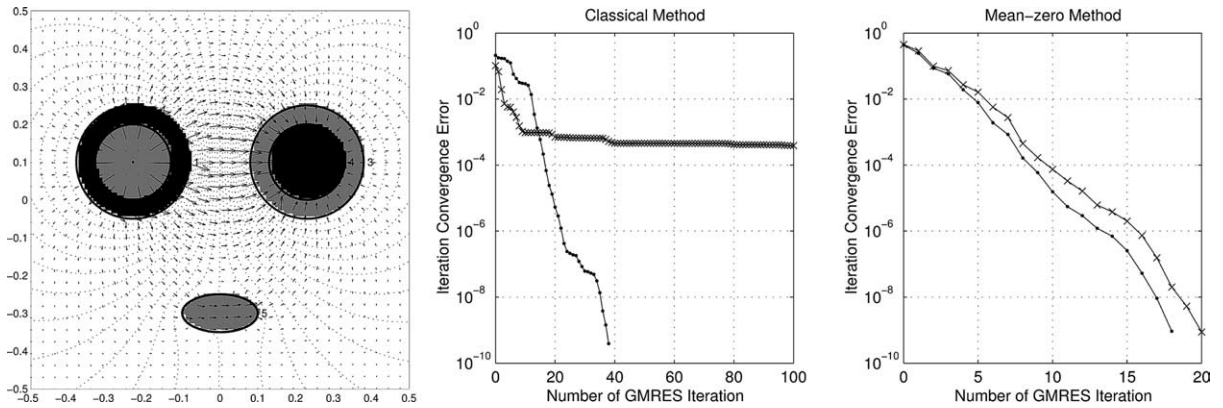


Fig. 4. Simple and multilayered inclusions in a background of conductivity one. In the “low contrast” case, (data marked by dots in right-hand figure), the conductivity in the black regions is set to 10^2 and in the grey regions to 10^1 . In the “high-contrast” case, (data marked by \times in right-hand figure), the conductivity in the black regions is set to 10^6 and in the grey regions to 10^3 . The center plot illustrates the performance of the classical integral equation at low and high contrast. The right-hand plot shows the performance of the *mean-zero* integral equation.

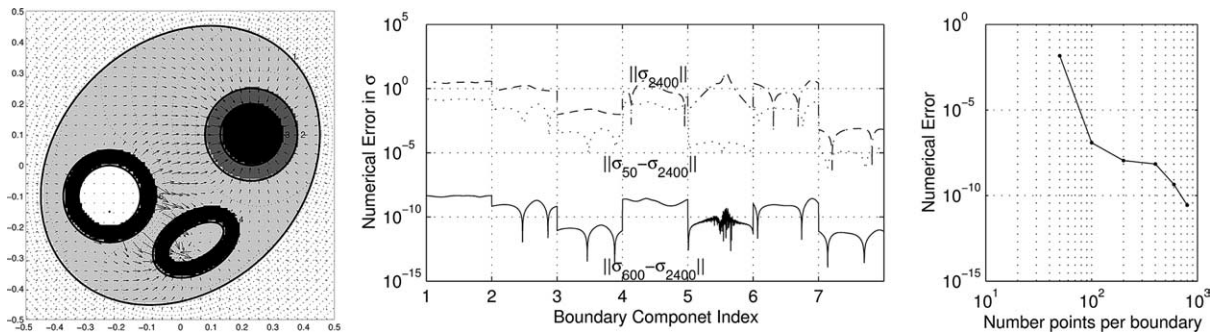


Fig. 5. For example 2, the conductivity in the light grey region is set to 1, in the dark grey region to 10^2 , and in the black region to 10^4 . The right-hand plot shows the errors in the computed density with 50 to 800 points per boundary/interface component. In the center plot, the x -axis denotes arclength on the total boundary/inteface and the y -axis the error as a function of arclength for the 50-pt and 600-pt discretizations. σ_{2400} was used as a reference solution (2400 pts per component).

As is clear from the figure on the right, the error in the computed solution decays rapidly with each mesh refinement, achieving better than ten digits of accuracy with only 800 points.

5. Conclusions

We have described a simple modification of the classical integral equation for the solution of electrostatics and heat conduction problems in piecewise homogeneous composite materials. While the classical equation becomes ill-conditioned at high contrast ratios, the new formulation (which we refer to as the *mean-zero* integral equation) maintains high precision and rapid convergence rates. For the sake of stability, it may be advantageous to explicitly add the constraint

$$\int_{\Gamma_i} \bar{\sigma}_i(\mathbf{y}) \, ds_{\mathbf{y}},$$

but we have not incorporated this extra equation into the solver.

The mean-zero equation is derived from three observations: (1) that the classical integral equation at infinite contrast is the same as that for an interior Neumann problem, (2) that projecting the right-hand side of the integral equation onto the range of the Neumann integral equation is the natural thing to do, and (3) that this projection can be carried out explicitly in terms of a constant density on each interface. We have only proven the boundedness of the inverse operator for a single inclusion, but suspect that a more involved analytic argument can be carried out in the general case. Experimental evidence (with many examples) supports this hypothesis.

We believe that the mean-zero equation will be of value in capacitance extraction and heat transfer calculations. Application of our approach to more complex geometries, such as cases where multiple subdomains meet at a single point, is straightforward but technically involved. Exterior Dirichlet problems, where a boundary/surface is coated with a high dielectric material can be handled using similar ideas. While the total charge on the Dirichlet surface is not known *a priori*, it can be attributed to an unknown constant as in [5] and incorporated into a mean-zero formulation. These extensions will be reported at a later date.

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